Kinetic Equations of Active Soft Matter

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Abstract

We consider a new approach to the description of the collective behavior of complex systems of mathematical biology based on the evolution equations for observables of such systems. This representation of the kinetic evolution seems, in fact, the direct mathematically fully consistent formulation modeling the collective behavior of biological systems since the traditional notion of the state in kinetic theory is more subtle and it is an implicit characteristic of the populations of living creatures.

Keywords: kinetic equation, marginal observables, scaling limit, active soft matter

1. Introduction

The rigorous derivation of kinetic equations for soft condensed matter remains an open problem so far. It should be noted wide applications of these evolution equations to the description of collective processes of various nature [1–14], in particular, the collective behavior of complex systems of mathematical biology [13–23]. We emphasize that the considerable advance in solving the problem of rigorous modeling of the kinetic evolution of systems with a large number of constituents (entities) of mathematical biology, in particular, systems of large number of cells, is recently observed [20–26] (and see references cited therein).

In modern research, the main approach to the problem of the rigorous derivation of kinetic equation consists in the construction of scaling limits of a solution of evolution equations which describe the evolution of states of a many-particle system, in particular, a perturbative solution of the corresponding BBGKY hierarchy [2–4].

In this chapter, we review a new approach to the description of the collective behavior of complex systems of mathematical biology [17, 18] within the framework of the evolution of observables. This representation of the kinetic evolution seems, in fact, the direct mathematically fully consistent formulation modeling kinetic evolution of biological systems since the notion of the state is more subtle and it is an implicit characteristic of populations of living creatures.
One of the advantages of the developed approach is the opportunity to construct kinetic
equations in scaling limits, involving initial correlations, in particular, that can characterize
the condensed states of soft matter. We note also that such approach is also related to the
problem of a rigorous derivation of the non-Markovian kinetic-type equations from underlying many-cell dynamics which make it possible to describe the memory effects of the kinetic
evolution of cells.

Using suggested approach, we establish a mean field asymptotic behavior of the hierarchy of
evolution equations for marginal observables of a large system of interacting stochastic pro-
cesses of collisional kinetic theory [24], modeling the microscopic evolution of active soft
condensed matter [14, 15]. The constructed scaling limit of a non-perturbative solution of this
hierarchy is governed by the set of recurrence evolution equations, namely, by the dual Vlasov
hierarchy for interacting stochastic processes.

Furthermore, we established that for initial states specified by means of a one-particle distri-
bution function and correlation functions the evolution of additive-type marginal observables
is equivalent to a solution of the Vlasov-type kinetic equation with initial correlations, and a
mean field asymptotic behavior of non-additive-type marginal observables is equivalent to the
sequence of explicitly defined correlation functions which describe the propagation of initial
correlations of active soft condensed matter.

2. On collisional dynamics of active soft condensed matter and the
evolution of marginal observables

The many-constituent systems of active soft condensed matter [14, 15] are dynamical systems
displaying a collective behavior which differs from the statistical behavior of usual gases [2, 4].
In the first place, their own distinctive features are connected with the fact that their constitu-
ents (entities or self-propelled particles) show the ability to retain various complexity features
[14–18]. To specify such nature of entities, we consider the dynamical system suggested in
papers [13, 24, 29] which is based on the Markov jump processes that must represent the
intrinsic properties of living creatures.

A description of many-constituent systems is formulated in terms of two sets of objects:
observables and states. The functional of the mean value of observables defines a duality
between observables and states and as a consequence there exist two approaches to the
description of the evolution of such systems, namely in terms of the evolution equations for
observables and for states. In this section, we adduce some preliminary facts about dynamics
of finitely many entities of various subpopulations described within the framework of non-
equilibrium grand canonical ensemble [2].

We consider a system of entities of various $M$ subpopulations introduced in paper [24] in case of
non-fixed, i.e., arbitrary, but finite average number of entities. Every $i$ th entity is characterized by:
$u_i = (j_i, u_i) \in J \times U$, where $j_i \in J \equiv (1, \ldots, M)$ is a number of its subpopulation, and $u_i \in U \subset \mathbb{R}^d$ is
its microscopic state [24]. The stochastic dynamics of entities of various subpopulations is
described by the semigroup $e^{t\Lambda} = \bigoplus_{n=0}^{\infty} e^{t\Lambda_n}$ of the Markov jump process defined on the space $C_\gamma$ of sequences $b = (b_0, b_1, \ldots, b_n, \ldots)$ of measurable bounded functions $b_n(u_1, \ldots, u_n)$ that are symmetric with respect to permutations of the arguments $u_1, \ldots, u_n$ and equipped with the norm:

$$\|b\|_{C_\gamma} = \max_{n \geq 0} \frac{\gamma^n}{n!} \|b_n\|_{C_n} = \max_{n \geq 0} \frac{\gamma^n}{n!} \max_{i_1, \ldots, i_n} |b_n(u_1, \ldots, u_n)|,$$

where $\gamma < 1$ is a parameter. The infinitesimal generator $\Lambda_n$ of collisional dynamics (the Liouville operator of $n$ entities) is defined on the subspace $C_n$ of the space $C_\gamma$ and it has the following structure [24]:

$$(\Lambda_n b_n)(u_1, \ldots, u_n) = \sum_{m=1}^{M} \epsilon^{m-1} \sum_{i_1 \neq \ldots \neq i_m} \left( \Lambda^{[m]}(i_1, \ldots, i_m) b_n \right)(u_1, \ldots, u_n) =$$

$$= \sum_{m=1}^{M} \epsilon^{m-1} \sum_{i_1 \neq \ldots \neq i_m} \left( \int_{\mathcal{J} \times \mathcal{U}} A^{[m]}(v; u_{i_1}, \ldots, u_{i_m}) \times b_n(u_1, \ldots, u_{i_1-1}, v, u_{i_1+1}, \ldots, u_n) d\nu - b_n(u_1, \ldots, u_n) \right),$$

where $\epsilon > 0$ is a scaling parameter [28], the functions $a^{[m]}(u_{i_1}, \ldots, u_{i_m}), m \geq 1$, characterize the interaction between entities, in particular, in case of $m = 1$ it is the interaction of entities with an external environment. These functions are measurable positive bounded functions on $(\mathcal{J} \times \mathcal{U})^n$ such that: $0 \leq a^{[m]}(u_{i_1}, \ldots, u_{i_m}) \leq a^{[m]}_{\text{max}}$, where $a^{[m]}_{\text{max}}$ is some constant. The functions $A^{[m]}(v; u_{i_1}, \ldots, u_{i_m}), m \geq 1$, are measurable positive integrable functions which describe the probability of the interaction with entities in the states $u_{i_1}, \ldots, u_{i_m}$ (in case of $m = 1$ it is the interaction with an external environment). The functions $A^{[m]}(v; u_{i_1}, \ldots, u_{i_m}), m \geq 1$, satisfy the conditions:

$$\int_{\mathcal{J} \times \mathcal{U}} A^{[m]}(v; u_{i_1}, \ldots, u_{i_m}) d\nu = 1, m \geq 1.$$  

We refer to paper [24], where examples of the functions $a^{[m]}$ and $A^{[m]}$ are given in the context of biological systems.

In case of $M = 1$ generator (1) has the form $\sum_{i=1}^{n} A^{[1]}(i_1)$ and it describes the free stochastic evolution of entities, i.e., the evolution of self-propelled particles. The case of $M = m \geq 2$ corresponds to a system with the $m$-body interaction of entities in the sense accepted in kinetic theory [30]. The $m$-body interaction of entities is the distinctive property of biological systems in comparison with many-particle systems, for example, gases of atoms with a pair-interaction potential.

On the space $C_n$ the one-parameter mapping $e^{t\Lambda_n}$ is a bounded $*$-weak continuous semigroup of operators.

The observables of a system of a non-fixed number of entities of various subpopulations are the sequences $O = (O_0, O_1(u_1), \ldots, O_n(u_1, \ldots, u_n), \ldots)$ of functions $O_n(u_1, \ldots, u_n)$ defined on $(\mathcal{J} \times \mathcal{U})^n$ and $O_0$ is a real number. The evolution of observables is described by the sequences $O(t) = (O_0, O_1(t, u_1), \ldots, O_n(t, u_1, \ldots, u_n), \ldots)$ of the functions

$$O_n(t) = e^{t\Lambda_n} O_n^0, n \geq 1,$$
that is, they are the corresponding solution of the Cauchy problem of the Liouville equations (or the Kolmogorov forward equation) with corresponding initial data $O^0_0$:

$$\frac{\partial}{\partial t} O_n(t) = \Lambda_n O_n(t),$$

$$O_n(t)|_{t=0} = O^0_n, \quad n \geq 1,$$

or in case of $n$ noninteracting entities (self-propelled particles) these equations have the form.

$$\frac{\partial}{\partial t} O_n(t, u_1, \ldots, u_n) = \sum_{i=1}^n a^{[1]}(u_i) \left( \int_{J \times U} A^{[1]}(\nu; u_i) O_n(t, u_1, \ldots, u_{i-1}, \nu, u_{i+1}, \ldots, u_n) d\nu. \right)$$

$$-O_n(t, u_1, \ldots, u_n), \quad n \geq 1.$$

The average values of observables (mean values of observables) are determined by the following positive continuous linear functional defined on the space $C_γ$:

$$\langle O \rangle(t) = (I, D(0))^{-1}(O(t), D(0)) = (I, D(0))^{-1} \sum_{n=0}^\infty \frac{1}{n!} \int_{(J \times U)^n} du_1 \ldots du_n \ O_n(t) \ D^0_n,$$  \(2\)

where $D(0) = (1, D_1^0, \ldots, D_n^0, \ldots)$ is a sequence of nonnegative functions $D_n^0$ defined on $(J \times U)^n$ that describes the states of a system of a non-fixed number of entities of various subpopulations at initial time and $(I, D(0)) = \sum_{n=0}^\infty \frac{1}{n!} \int_{(J \times U)^n} du_1 \ldots du_n \ D^0_n$ is a normalizing factor (the grand canonical partition function).

Let $L^1_\alpha = \bigoplus_{n=0}^\infty \alpha^n L^1_n$ be the space of sequences $f=(f_0, f_1, \ldots, f_n, \ldots)$ of the integrable functions $f_n(u_1, \ldots, u_n)$ defined on $(J \times U)^n$, that are symmetric with respect to permutations of the arguments $u_1, \ldots, u_n$, and equipped with the norm:

$$\|f\|_{L^1_\alpha} = \sum_{n=0}^\infty \alpha^n \|f_n\|_{L^1_n} = \sum_{n=0}^\infty \alpha^n \sum_{j_1 \in J} \ldots \sum_{j_n \in J} \int_{(J \times U)^n} du_1 \ldots du_n |f_n(u_1, \ldots, u_n)|,$$

where $\alpha > 1$ is a parameter. Then for $D(0) \in L^1_\alpha$ and $O(t) \in C_\gamma$, average value functional (2) exists and it determines a duality between observables and states.

As a consequence of the validity for functional (2) of the following equality:

$$(I, D(0))^{-1}(O(t), D(0)) = (I, D(0))^{-1}(e^{t\Lambda} O(0) D(0)) =$$

$$(I, e^{t\Lambda} D(0))^{-1}(O(0) e^{t\Lambda} D(0)) \equiv (I, D(t))^{-1}(O(0), D(t)),$$

where $e^{t\Lambda} = \bigoplus_{n=0}^\infty e^{t\Lambda_n}$ is the adjoint semigroup of operators with respect to the semigroup $e^{t\Lambda} = \bigoplus_{n=0}^\infty e^{t\Lambda_n}$, it is possible to describe the evolution within the framework of the evolution of states. Indeed, the evolution of all possible states, i.e. the sequence $D(t) = (D_1(t, u_1), \ldots, D_n(t, u_1, \ldots, u_n), \ldots) \in L^1$ of the distribution functions $D_n(t), n \geq 1$, is determined by the formula:
where the functions $A^{[m]}$ and $a^{[m]}$ are defined as above in (1). The function $D_n(t)$ is a solution of the Cauchy problem of the dual Liouville equation (or the Kolmogorov backward equation).

On the space $L^1_n$ the one-parameter mapping $\text{et}\Lambda^*$ is a bounded strong continuous semigroup of operators [26].

For the description of microscopic behavior of many-entity systems we also introduce the hierarchies of evolution equations for marginal observables and marginal distribution functions known as the dual BBGKY hierarchy and the BBGKY hierarchy, respectively [26]. These hierarchies are constructed as the evolution equations for one more method of the description of observables and states of finitely many entities.

An equivalent approach to the description of observables and states of many-entity systems is given in terms of marginal observables $B(t) = (B_0(t), B_1(t, \mathbf{u}_1), \ldots, B_s(t, \mathbf{u}_1, \ldots, \mathbf{u}_s), \ldots)$ and marginal distribution functions $F(0) = \left(1, f_{1,0,\epsilon}(\mathbf{u}_1), \ldots, f_{s,0,\epsilon}(\mathbf{u}_1, \ldots, \mathbf{u}_s), \ldots\right) \in L^1_n$.

Considering formula (2), marginal observables and marginal distribution functions are introduced according to the equality:

\[ \langle O \rangle(t) = (I, D(0))^{-1} (O(t), D(0)) = (B(t), F(0)), \]

where $(I, D(0))$ is a normalizing factor defined as above. If $F(0) \in L^1_n$ and $B(0) \in C_{\gamma \alpha}$ then at $t \in \mathbb{R}$ the functional $(B(t), F(0))$ exists under the condition that: $\gamma > \alpha^{-1}$.

Thus, the relationship of marginal distribution functions $F(0) = \left(1, f_{1,0,\epsilon}, \ldots, f_{s,0,\epsilon}, \ldots\right)$ and the distribution functions $D(0) = \left(1, D^0_1, \ldots, D^0_n, \ldots\right)$ is determined by the formula:

\[ F_{s,0,\epsilon}(\mathbf{u}_1, \ldots, \mathbf{u}_s) = (I, D(0))^{-1} \sum_{n=0}^{\infty} \frac{1}{n!} \int_{(\mathcal{J} \times \mathcal{U})^n} d\mathbf{u}_{s+1} \ldots d\mathbf{u}_{s+n} D^0_{s+n}(\mathbf{u}_1, \ldots, \mathbf{u}_{s+n}), \quad s \geq 1, \]

and, respectively, the marginal observables are determined in terms of observables as follows:

\[ B_s(t, \mathbf{u}_1, \ldots, \mathbf{u}_s) = \sum_{n=0}^{s} \frac{(-1)^n}{n!} \sum_{j_1 \neq \ldots \neq j_n=1}^s O_{s-n}(t, (\mathbf{u}_1, \ldots, \mathbf{u}_j) (\mathbf{u}_{j+1}, \ldots, \mathbf{u}_s)), \quad s \geq 1. \]
Two equivalent approaches to the description of the evolution of many interacting entities are the consequence of the validity of the following equality for the functional of mean values of marginal observables:

$$(B(t), F(0)) = (B(0), F(t)),$$

where $B(0) = (1, B_1^{0,1}, \ldots, B_s^{0,s}, \ldots)$ is a sequence of marginal observables at initial moment.

We remark that the evolution of many-entity systems is usually described within the framework of the evolution of states by the sequence $F(t) = (1, F_1(t, u_1), \ldots, F_s(t, u_1, \ldots, u_s), \ldots)$ of marginal distribution functions $F_s(t, u_1, \ldots, u_s)$ governed by the BBGKY hierarchy for interacting entities [13, 24].

The evolution of a non-fixed number of interacting entities of various subpopulations within the framework of marginal observables (4) is described by the Cauchy problem of the dual BBGKY hierarchy [25]:

$$\frac{d}{dt} B(t) = \Lambda + \sum_{n=1}^{\infty} \frac{1}{n!} \left[ \ldots [\Lambda, a^+] \ldots, a^+] \right] B(t) ,$$

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

where on $C_T$ the operator $a^+$ (an analog of the creation operator) is defined as follows

$$(a^+ b)(u_1, \ldots, u_s) \doteq \sum_{j=1}^{s} b_{k-1}(u_1, \ldots, u_{j-1}, u_{j+1}, \ldots, u_s),$$

the operator $\Lambda = \bigoplus_{n=0}^{\infty} \Lambda_n$ is defined by (1), and the symbol $[\cdot, \cdot]$ denotes the commutator of operators.

In the componentwise form, the abstract hierarchy (5) has the form:

$$\frac{\partial}{\partial t} B_s(t, u_1, \ldots, u_s) = \Lambda_s B_s(t, u_1, \ldots, u_s) + \sum_{n=1}^{s} \frac{1}{n!} \sum_{k=n+1}^{s} \frac{1}{(k-n)!} \times$$

$$\times \sum_{j_1 \neq \ldots \neq j_k}^{s} \mathcal{L}^{k-1} \Lambda^{|k|}(j_1, \ldots, j_k) \sum_{i_1 \neq \ldots \neq i_k} B_{s-n}(t, (u_1, \ldots, u_s) \setminus (u_{i_1}, \ldots, u_{i_k})),$$

$$B_s(t, u_1, \ldots, u_s) \big|_{t=0} = B_s^{0,s}(u_1, \ldots, u_s), \quad s \geq 1,$$

where the operators $\Lambda_s$ and $\Lambda^{|k|}$ are defined by formulas (1) and the functions $B_s^{0,s}, s \geq 1,$ are scaled initial data.

A solution $B(t) = (B_0, B_1(t, u_1), \ldots, B_s(t, u_1, \ldots, u_s), \ldots)$ of the Cauchy problem of recurrence evolution Eqs (7), (8) is given by the following expansions [26]:
The sets of indexes are denoted by $Y \equiv (1, \ldots, s), Z \equiv (j_1, \ldots, j_n) \subset Y$, the set $\{Y \setminus Z\}$ consists from one element $Y \setminus Z = (1, \ldots, j_1 - 1, j_1 + 1, \ldots, j_n - 1, j_n + 1, \ldots, s)$ and the mapping $\theta(\cdot)$ is the declusterization operator defined as follows: $\theta((Y \setminus Z), Z) = Y$.

The simplest examples of expansions for marginal observables (9) have the following form:

$$B_1(t, u_1) = A_1(t, 1)B_{1,0}^0(u_1),$$

$$B_2(t, u_1, u_2) = A_1(t, \{1, 2\})B_{2,0}^0(u_1, u_2) + A_2(t, 1, 2)(B_{1,0}^0(u_1) + B_{1,0}^0(u_2)),$$

and, respectively:

$$A_1(t, \{1, 2\}) = e^{\lambda_2(1,2)},$$

$$A_2(t, 1, 2) = e^{\lambda_2(1,2)} - e^{\lambda_2(1)}e^{\lambda_2(2)}.$$

For initial data $B(0) = (B_0, B_{1,0}^0, \ldots, B_{s,0}^0, \ldots) \in C_Y$ the sequence $B(t)$ of marginal observables given by expansions (9) is a classical solution of the Cauchy problem of the dual BBGKY hierarchy for interacting entities (7), (8).

We note that a one-component sequence of marginal observables corresponds to observables of certain structure, namely the marginal observable $B_1^{(1)}(0) = (0, b_1^1 (u_1), 0, \ldots)$ corresponds to the additive-type observable, and a one-component sequence of marginal observables $B^{(k)}(0) = (0, \ldots, 0, b_k^k (u_1, \ldots, u_k), 0, \ldots)$ corresponds to the $k$-ary-type observable [25]. If in capacity of initial data (8) we consider the additive-type marginal observables, then the structure of solution expansion (9) is simplified and attains the form

$$B_1^{(1)}(t, u_1, \ldots, u_s) = A_1(s, 1, \ldots, s) \sum_{j=1}^{s} b^1_j(u_j), \quad s \geq 1.$$  

In the case of $k$-ary-type marginal observables solution expansion (9) has the form
3. A mean field asymptotic behavior of the marginal observables and the kinetic evolution of states

To consider mesoscopic properties of a large system of interacting entities we develop an approach to the description of the kinetic evolution within the framework of the evolution equations for marginal observables. For this purpose we construct the mean field asymptotics [9] of a solution of the Cauchy problem of the dual BBGKY hierarchy for interacting entities, modeling of many-constituent systems of active soft condensed matter [26, 27].

We restrict ourself by the case of \( M = 2 \) subpopulations to simplify the cumbersome formulas and consider the mean field scaling limit of non-perturbative solution (9) of the Cauchy problem of the dual BBGKY hierarchy for interacting entities (7), (8).

Let for initial data \( b^{0, \epsilon}_s \in \mathcal{C}_s \) there exists the limit function \( b^0_s \in \mathcal{C}_s \)

\[
\lim_{\epsilon \to 0} \left( \epsilon^{-\frac{1}{2}} b^{0, \epsilon}_s - b^0_s \right) = 0, \quad s \geq 1,
\]

then for arbitrary finite time interval there exists a mean field limit of solution (9) of the Cauchy problem of the dual BBGKY hierarchy for interacting entities (7), (8) in the sense of the \( \ast \)-weak convergence of the space \( \mathcal{C}_s \)

\[
\lim_{\epsilon \to 0} \left( \epsilon^{-\frac{1}{2}} B_s(t) - b_s(t) \right) = 0, \quad s \geq 1,
\]

where the limit sequence \( b(t) = (b_0, b_1(t), \ldots, b_s(t), \ldots) \) of marginal observables is determined by the following expansions:

\[
b_{s}(t, u_1, \ldots, u_s) = \sum_{n=0}^{s-1} \int_{0}^{t_{n+1}} \cdots \int_{0}^{t_{n-1}} dt_{1} \cdots dt_{n} \epsilon^{(t_{n+1} - t_{n})} \sum_{k_1 = 1}^{s} \Lambda^{[1]}(k_1) \sum_{i_1 \neq j_1}^{s} \Lambda^{[2]}(i_1, j_1) e^{-\sum_{k_1 \neq j_1}^{s} \Lambda^{[1]}(j_1)} \cdots \sum_{k_s \neq (j_1, \ldots, j_{s-1})}^{s} \Lambda^{[1]}(k_s) \sum_{i_s \neq (j_1, \ldots, j_{s-1})}^{s} \Lambda^{[2]}(i_s, j_s) e^{-\sum_{i_s \neq (j_1, \ldots, j_{s-1})}^{s} \Lambda^{[1]}(j_s)} b^{0}_{s-n}((u_1, \ldots, u_s) \setminus (u_{j_1}, \ldots, u_{j_{s-1}})), \quad s \geq 1.
\]
In particular, the limit marginal observable $b_1(t)$ of the additive-type marginal observable (11) is determined as a special case of expansions (13):

$$
\begin{align*}
  b_1^{(1)}(t, \mathbf{u}_1, \ldots, \mathbf{u}_s) &= \int_0^t dt_1 \ldots \int_0^{t-s} dt_{s-1} e^{(t-t_1) \sum_{k_1=1} s \Lambda_1^1(k_1) \sum_{i_1, j_1} \Lambda_2^2(i_1, j_1) e^{(t_1-t_{i_1-1})} \sum_{l_1} \Lambda_1^1(l_{i_1-1}) e^{(l_{i_1-1}-l_{i_1-1})} \sum_{l_{i_1-1}} \Lambda_1^1(l_{i_1-1})} \\
  &\times e^{t_1 \sum_{l_{i_1}=1} \Lambda_1^1(l_{i_1})} e^{t_{i_1} \sum_{l_{i_1, j_1}} \Lambda_2^2(i_{i_1-1}, j_{i_1-1}) e^{t_{i_1} \sum_{l_{i_1, j_1}} \Lambda_1^1(l_{i_1-1})} e^{t_{i_1} \sum_{l_{i_1, j_1}} \Lambda_2^2(i_{i_1-1}, j_{i_1-1})} \times b_1((\mathbf{u}_1, \ldots, \mathbf{u}_s) \setminus (\mathbf{u}_{i_1}, \ldots, \mathbf{u}_{i_1-1})), \quad s \geq 1,
\end{align*}
$$

for example,

$$
\begin{align*}
  b_1^{(1)}(t, \mathbf{u}_1) &= e^{t \Lambda_1^1(1)} b_1^0(\mathbf{u}_1), \\
  b_2^{(1)}(t, \mathbf{u}_1, \mathbf{u}_2) &= \int_0^t dt_1 \prod_{i=1}^2 e^{(t-t_1) \Lambda_1^1(i)} \Lambda_2^2(1, 2) \sum_{j=1}^2 e^{t_1 \Lambda_1^1(j)} b_1^0(\mathbf{u}_i).
\end{align*}
$$

The proof of this statement is based on the corresponding formulas for cumulants of asymptotically perturbed semigroups of operators (10).

If $b^0 \in \mathcal{C}_\gamma$, then the sequence $b(t) = (b_0, b_1(t), \ldots, b_s(t), \ldots)$ of limit marginal observables (13) is generalized global in time solution of the Cauchy problem of the dual Vlasov hierarchy:

$$
\begin{align*}
  \frac{\partial}{\partial t} b_s(t) &= \sum_{j=1}^s \Lambda_1^1(j) b_j(t) + \sum_{j_1, j_2=1}^s \Lambda_2^2(j_1, j_2) b_{j_1-1}(t, \mathbf{u}_1, \ldots, \mathbf{u}_{j_1-1}, \mathbf{u}_{j_1+1}, \ldots, \mathbf{u}_s), \quad s \geq 1, \\
  b_s(t, \mathbf{u}_1, \ldots, \mathbf{u}_s)_{|t=0} = b_s^0(\mathbf{u}_1, \ldots, \mathbf{u}_s), \quad s \geq 1,
\end{align*}
$$

where in recurrence evolution Eq. (14) the operators $\Lambda_1^1(j)$ and $\Lambda_2^2(j_1, j_2)$ are determined by Formula (1).

Further we consider initial states specified by a one-particle marginal distribution function in the presence of correlations, namely

$$
\begin{align*}
  f^{(c)} = \left(1, f_1^0(\mathbf{u}_1), g_2(\mathbf{u}_1, \mathbf{u}_2) \prod_{i=1}^2 f_i^0(\mathbf{u}_i), \ldots, g_s(\mathbf{u}_1, \ldots, \mathbf{u}_s) \prod_{i=1}^s f_i^0(\mathbf{u}_i), \ldots\right),
\end{align*}
$$

where the bounded functions $g_s \equiv g_s(\mathbf{u}_1, \ldots, \mathbf{u}_s), s \geq 2$, are specified initial correlations. Such assumption about initial states is intrinsic for the kinetic description of complex systems in condensed states.

If $b(t) \in \mathcal{C}_\gamma$ and $f_1^0 \in L^1(\mathcal{J} \times \mathcal{U})$, then under the condition that $\|f_1^0\|_{L^1(\mathcal{J} \times \mathcal{U})} < \gamma$, there exists a mean field scaling limit of the mean value functional of marginal observables and it is determined by the following series expansion:
\[
\left( b(t), f^0 \right) = \sum_{s=0}^{\infty} \frac{1}{s!} \int_{(\mathcal{J} \times \mathcal{U})^s} du_1 \ldots du_s \ b_s(t, u_1, \ldots, u_s) \mathbf{g}(u_1, \ldots, u_s) \prod_{i=1}^{s} f^0_1(u_i).
\]

Then for the mean-value functionals of the limit initial additive-type marginal observables, i.e. of the sequences \( b^{(1)}(0) = (0, b^0_1(u_1), 0, \ldots) \) [25], the following representation is true:

\[
\left( b^{(1)}(t), f^0 \right) = \sum_{s=0}^{\infty} \frac{1}{s!} \int_{(\mathcal{J} \times \mathcal{U})^s} du_1 \ldots du_s \ b^{(1)}_s(t, u_1, \ldots, u_s) \mathbf{g}(u_1, \ldots, u_s) \prod_{i=1}^{s} f^0_1(u_i)
\]

\[
= \int_{(\mathcal{J} \times \mathcal{U})^s} du_1 \ b^0_1(u_1) f_1(t, u_1).
\]

In equality (17) the function \( b^{(1)}(t) \) is given by a special case of expansion (13), namely

\[
\begin{align*}
&b^{(1)}_s(t, u_1, \ldots, u_s) = \int_0^t dt_1 \ldots \int_0^{t_{s-2}} dt_{s-1} e^{i(t_{s-1}) \sum_{k_{s-1}=1}^s \Lambda^{[1]}(k_{s-1})} \sum_{i_1 \neq j_1=1}^s \Lambda^{[2]}(i_1, j_1) e^{i(t_{i_1} - t_{j_1})} \sum_{k_{i_1, j_1} \neq (j_1, \ldots, j_{s-2})}^{(t_{i_1} - t_{j_1})} \Lambda^{[1]}(k_{i_1, j_1}) \sum_{i_{s-1} \neq j_{s-1} = 1}^s \Lambda^{[2]}(i_{s-1}, j_{s-1}) \sum_{i_{s-1} \neq j_{s-1} = 1}^s \Lambda^{[1]}(i_{s-1}) \sum_{i_{s-1} \neq j_{s-1} = 1}^s \Lambda^{[1]}(j_{s-1}) \sum_{i_{s-1} \neq j_{s-1} = 1}^s \Lambda^{[1]}(j_{s-1}) \prod_{l=1}^{l_{s-1}} e^{i(t_{l_{s-1}} - t_{j_{s-1}}) \Lambda^{[1]}(l_{s-1})} b^0_1((u_1, \ldots, u_s) \setminus (u_{j_1}, \ldots, u_{j_{s-1}})), \quad s \geq 1,
\end{align*}
\]

and the limit one-particle distribution function \( f_1(t) \) is represented by the series expansion:

\[
\begin{align*}
f_1(t, u_1) &= \sum_{n=0}^{\infty} \int_0^t dt_1 \ldots \int_0^{t_{n-1}} dt_n \int_{(\mathcal{J} \times \mathcal{U})^n} du_2 \ldots du_{n+1} e^{(t_{n+1}) \Lambda^{[1]}(1)} \times \Lambda^{[2]}(1, 2) \prod_{j=1}^2 e^{i(t_{j} - t_{j+1}) \Lambda^{[0]}(j)} \prod_{j=1}^n e^{(t_{j+1} - t_1) \Lambda^{[1]}(j_{n-j})} \times \sum_{i_{n+1}=1}^{\Lambda^{[2]}(i_{n+1}, n+1)} \prod_{j=1}^{n+1} e^{i(t_{j} - t_{j+1}) \Lambda^{[0]}(j_{n-j})} \mathbf{g}(u_1, \ldots, u_{n+1}) \prod_{i=1}^{n+1} f^0_1(u_i),
\end{align*}
\]

where the operators \( \Lambda^{[i]}(i) \), \( i = 1, 2 \), are adjoint operators (3) to the operators \( \Lambda^{[i]}(i) \), \( i = 1, 2 \) defined by formula (1), and on the space \( L^1 \) defined as follows:

\[
\begin{align*}
\Lambda^{[1]}(i) f_n(u_1, \ldots, u_n) &= \int_{\mathcal{J} \times \mathcal{U}} \Lambda^{[1]}(i; v) a^{[1]}(v) \times f_n(u_1, \ldots, u_{i-1}, v, u_{i+1}, \ldots, u_n) dv - a^{[1]}(u_i) f_n(u_1, \ldots, u_n),
\end{align*}
\]

\[
\begin{align*}
\Lambda^{[2]}(i, j) f_n(u_1, \ldots, u_n) &= \int_{\mathcal{J} \times \mathcal{U}} \Lambda^{[2]}(i; v, u_j) a^{[2]}(v, u_j) \times f_n(u_1, \ldots, u_{i-1}, v, u_{i+1}, \ldots, u_n) dv - a^{[2]}(u_i, u_j) f_n(u_1, \ldots, u_n),
\end{align*}
\]

where the functions \( a^{[m]}, m = 1, 2 \), are defined above in formula (1).
For initial data \( f_0^1 \in L^1(J \times U) \) limit marginal distribution function (18) is the Vlasov-type kinetic equation with initial correlations:

\[
\frac{\partial}{\partial t} f_1(t, u_1) = \Lambda^{[1]}(1) f_1(t, u_1) + \int_{J \times U} \left[ \mathcal{A}_2 \psi^{[2]}(1, 2) \right] g_2(u_1, u_2) f_1(t, u_1) f_1(t, u_2),
\]

(19)

where the function \( g_2(u_1, u_2) \) is initial correlation function specified initial state (16).

For mean value functionals of the limit initial \( k \)-ary marginal observables, i.e. of the sequences \( b^{[k]}(0) = (0, \ldots, 0, b_1^0(u_1, \ldots, u_k), 0, \ldots) \), the following representation is true:

\[
\left( b^{[k]}(t), f^{(c)} \right) = \frac{1}{s!} \int_{(J \times U)^s} d u_1 \ldots d u_s \ b^{[k]}(t, u_1, \ldots, u_k) g^{(c)}(u_1, \ldots, u_s) \prod_{i=1}^s f_i^0(u_i) =
\]

\[
= \frac{1}{k!} \int_{(J \times U)^k} d u_1 \ldots d u_k \ b^{[k]}(u_1, \ldots, u_k) \times \prod_{i=1}^k e^{i \lambda u_i t} g^{[k]}(u_1, \ldots, u_k) \prod_{i=1}^k e^{-i \lambda u_i t} f_i(t, u_i), \quad k \geq 2,
\]

(21)

where the limit one-particle marginal distribution function \( f_1(t, u_1) \) is determined by series expansion (18) and the functions \( g[(u_1, \ldots, u_n), k \geq 2, \) are initial correlation functions specified initial state (16).

Hence in case of \( k \)-ary marginal observables the evolution governed by the dual Vlasov hierarchy (14) is equivalent to a property of the propagation of initial correlations (21) for the \( k \)-particle marginal distribution function or in other words mean field scaling dynamics does not create correlations.

In case of initial states of statistically independent entities specified by a one-particle marginal distribution function, namely \( f^{(c)} \equiv (1, f_1^0(u_1), \ldots, \prod_{i=1}^s \prod_{j=1}^u f_i^0(u_i), \ldots) \), the kinetic evolution of \( k \)-ary marginal observables governed by the dual Vlasov hierarchy means the property of the propagation of initial chaos for the \( k \)-particle marginal distribution function within the framework of the evolution of states [4], i.e. a sequence of the limit distribution functions has the form \( f(t) \equiv (1, f_1(t, u_1), \ldots, \prod_{i=1}^s \prod_{j=1}^u f_i(t, u_j), \ldots) \), where the one-particle distribution function \( f_1(t) \) is governed by the Vlasov kinetic Eq. [26]

\[
\frac{\partial}{\partial t} f_1(t, u_1) = \Lambda^{[1]}(1) f_1(t, u_1) + \int_{J \times U} \left[ \mathcal{A}_2 \psi^{[2]}(1, 2) \right] f_1(t, u_1) f_1(t, u_2).
\]

We note that, according to equality (21), in the mean field limit the marginal correlation functions defined as cluster expansions of marginal distribution functions [30, 33, 34] namely,

\[
f_s(t, u_1, \ldots, u_s) = \sum_{P \cup \{u_1, \ldots, u_s\} = \bigcup_{i=1}^s U_i} \prod_{i \in P} g_{|U_i|}(t, U_i), \quad s \geq 1,
\]
has the following explicit form [27]:

\[ g_1(t, u_1) = f_1(t, u_1), \]

\[ g_s(t, u_1, \ldots, u_s) = \prod_{i=1}^{s} e^{i \Lambda^y(i_1)} \tilde{g}_s(u_1, \ldots, u_s) \prod_{i=1}^{s} e^{-i \Lambda^y(i_2)} \prod_{j=1}^{s} f_1(t, u_j), \quad s \geq 2, \]

where for initial correlation functions (16) it is used the following notations:

\[ \tilde{g}_s(u_1, \ldots, u_s) = \sum_{P: (u_1, \ldots, u_s) = \bigcup_i U_i} \prod_{i \in P} g(U_i), \]

the symbol \( \sum_{P} \) means the sum over possible partitions \( P \) of the set of arguments \( (u_1, \ldots, u_s) \) on \( |P| \) non-empty subsets \( U_i \) and the one-particle marginal distribution function \( f_1(t) \) is a solution of the Cauchy problem of the Vlasov-type kinetic equation with initial correlations (19), (20).

Thus, an equivalent approach to the description of the kinetic evolution of large number of interacting constituents in terms of the Vlasov-type kinetic equation with correlations (19) is given by the dual Vlasov hierarchy (14) for the additive-type marginal observables.

4. The non-Markovian generalized kinetic equation with initial correlations

Furthermore, the relationships between the evolution of observables of a large number of interacting constituents of active soft condensed matter and the kinetic evolution of its states described in terms of a one-particle marginal distribution function are discussed.

Since many-particle systems in condensed states are characterized by correlations we consider initial states specified by a one-particle marginal distribution function and correlation functions, namely

\[ F^{(e)} = \left( 1, F_1^{(0)}(u_1), g_2^{(e)}(u_1, u_2) \prod_{i=1}^{2} F_1^{(0)}(u_i), \ldots, g_s^{(e)}(u_1, \ldots, u_s) \prod_{i=1}^{s} F_1^{(0)}(u_i), \ldots \right). \]

If the initial state is completely specified by a one-particle distribution function and a sequence of correlation functions (23), then, using a non-perturbative solution of the dual BBGKY hierarchy (9), in [31, 32] it was proved that all possible states at the arbitrary moment of time can be described within the framework of a one-particle distribution function governed by the non-Markovian generalized kinetic equation with initial correlations, i.e. without any approximations like in scaling limits as above.

Indeed, for initial states (23) for mean value functional (4) the equality holds

\[ \left( B(t), F^{(e)} \right) = (B(0), F(t|F_1(t))), \]

(24)
where\( F(t|F_1(t)) = (1,F_1(t),F_2(t|F_1(t)),\ldots,F_s(t|F_1(t)),\ldots) \) is a sequence of marginal functionals of the state with respect to a one-particle marginal distribution function:

\[
F_1(t,\mathbf{u}_1) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{(\mathcal{S} \times \mathcal{U})^n} \mathbf{d}\mathbf{u}_2 \ldots \mathbf{d}\mathbf{u}_{n+1} \mathfrak{A}_{1+n}^t(t,1,\ldots,n+1) \mathcal{G}_{n+1}^{e}(\mathbf{u}_1,\ldots,\mathbf{u}_{n+1}) \prod_{i=1}^{n+1} F_i^0(e^\mathbf{u}_i). \tag{25}
\]

The generating operator \( \mathfrak{A}_{1+n}^t(t) \) of series (25) is the \((1+n)\)-order cumulant of the semigroups of operators \( \{e^{e^t\mathfrak{A}_{1+n}}\}_{t \geq 0} \).

The marginal functionals of the state is defined by the series expansions:

\[
F_s(t,\mathbf{u}_1,\ldots,\mathbf{u}_s|F_1(t)) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{(\mathcal{S} \times \mathcal{U})^n} \mathbf{d}\mathbf{u}_{s+1} \ldots \mathbf{d}\mathbf{u}_{s+n} \mathfrak{W}_{1+n}^t(t,\{Y\},X\backslash Y) \prod_{i=1}^{s+n} F_i(t,\mathbf{u}_i), \tag{26}
\]

where the following notations used: \( Y = (1,\ldots,s) \), \( X \backslash Y = (s+1,\ldots,s+n) \) and the generating operators \( \mathfrak{W}_{1+n}(t), n \geq 0 \), are defined by the expansions [31]:

\[
\mathfrak{W}_{1+n}(t,\{Y\},X\backslash Y) = \sum_{k=0}^{n} (-1)^k \sum_{m_1=1}^{n} \ldots \sum_{m_k=1}^{n-m_1-\ldots-m_{k-1}} \frac{n!}{(n-m_1-\ldots-m_k)!} \times \mathfrak{A}_{1+n-m_1-\ldots-m_k}(t,\{Y\},s+1,\ldots,s+n-m_1-\ldots-m_k) \prod_{j=1}^{k} m_j \sum_{k'_{m_1-\ldots-m_k}=0}^{k} \prod_{i=1}^{k} \left( \frac{1}{k'_{n-m_1-\ldots-m_j+i-1-j} - k'_{n-m_1-\ldots-m_j+i}} \right) \times \mathfrak{A}_{1+k'_{m_1-\ldots-m_j+i-1-j}} \mathfrak{A}_{1+k'_{m_1-\ldots-m_j+i}} + \ldots \right),
\]

where \( k'_i \equiv m_{jp} - m_{jp-1} - 1 \equiv 0 \) and the evolution operators \( \mathfrak{A}_n(t), n \geq 1 \), are cumulants of the semigroups of scattering operators \( \left\{e^{e^t\mathfrak{A}_{1+n}} \mathcal{G}_{s}^{e} \prod_{i=1}^{k} e^{-tA^{+\alpha\beta}(i)}\right\}_{t \geq 0}, k \geq 1 \). We adduce some examples of evolution operators (27):

\[
\mathfrak{W}_1(t,\{Y\}) = \mathfrak{A}_1(t,\{Y\}) = e^{e^t\mathfrak{A}_1} \mathcal{G}_{s}^{e} \prod_{i=1}^{k} e^{-tA^{+\alpha\beta}(i)},
\]

\[
\mathfrak{W}_2(t,\{Y\},s+1) = \mathfrak{A}_2(t,\{Y\},s+1) - \mathfrak{A}_1(t,\{Y\}) \sum_{i=1}^{s} \mathfrak{A}_2(t,i,s+1).
\]

If \( \|F_1(t)\|_{L^1(\mathcal{S} \times \mathcal{U})} < e^{-(3s+2)} \), then for arbitrary \( t \in \mathbb{R} \) series expansion (26) converges in the norm of the space \( L^1 \) [30].
The proof of equality (24) is based on the application of cluster expansions to generating operators (10) of expansions (9) which are dual to the kinetic cluster expansions introduced in paper [35]. Then the adjoint series expansion can be expressed in terms of one-particle distribution function (25) in the form of the functional from the right-hand side of equality (24).

We emphasize that marginal functionals of the state (26) characterize the processes of the creation of correlations generated by dynamics of many-constituent systems of active soft condensed matter and the propagation of initial correlations.

For small initial data $F_0^0, \varepsilon_1 \in L^1(J \times \mathcal{U}) [31]$, series expansion (25) is a global in time solution of the Cauchy problem of the generalized kinetic equation with initial correlations:

$$\frac{\partial}{\partial t} F_1(t, u_1) = \Lambda^{[1]}(t) F_1(t, u_1) + \sum_{k=1}^{M-1} \frac{\varepsilon_k}{k!} \int_{(J \times \mathcal{U})^k} du_2 \ldots du_{k+1} \sum_{j_1 \neq \ldots \neq j_{k+1} \in (1, \ldots, k+1)} \Lambda^{[k+1]}(j_1, \ldots, j_{k+1}) F_{k+1}(t, u_1, \ldots, u_{k+1}|F_1(t)), \quad (28)$$

$$F_1(t, u_1)_{|t=0} = F_0^0, \varepsilon_1(u_1). \quad (29)$$

For initial data $F_0^0, \varepsilon_1 \in L^1(J \times \mathcal{U})$ it is a strong (classical) solution and for an arbitrary initial data it is a weak (generalized) solution.

In particular case $M=2$ of two subpopulations kinetic Eq. (28) has the following explicit form:

$$\frac{\partial}{\partial t} F_1(t, u_1) = \int_{J \times \mathcal{U}} A^{[1]}(u_1; v) a^{[1]}(v) F_1(t, v) dv - a^{[1]}(u_1) F_1(t, u_1) +$$

$$\int_{J \times \mathcal{U}} du_2 \left( \int_{J \times \mathcal{U}} A^{[2]}(u_1; v, u_2) a^{[2]}(v, u_2) F_2(t, v, u_2|F_1(t)) dv - a^{[2]}(u_1, u_2) F_2(t, u_1, u_2|F_1(t)) \right),$$

where the functions $A^{[k]}$ and $a^{[k]}$ are defined above.

We note that for initial states (23) specified by a one-particle (marginal) distribution function, the evolution of states described within the framework of a one-particle (marginal) distribution function governed by the generalized kinetic equation with initial correlations (28) is dual to the dual BBGKY hierarchy for additive-type marginal observables with respect to bilinear form (2), and it is completely equivalent to the description of states in terms of marginal distribution functions governed by the BBGKY hierarchy of interacting entities.

Thus, the evolution of many-constituent systems of active soft condensed matter described in terms of marginal observables in case of initial states (23) can be also described within the framework of a one-particle (marginal) distribution function governed by the non-Markovian generalized kinetic equation with initial correlations (28).

We remark, considering that a mean field limit of initial state (23) is described by sequence (16), a mean field asymptotics of a solution of the non-Markovian generalized kinetic equation with
5. Conclusion

We considered an approach to the description of kinetic evolution of large number of interacting constituents (entities) of active soft condensed matter within the framework of the evolution of marginal observables of these systems. Such representation of the kinetic evolution seems, in fact, the direct mathematically fully consistent formulation modeling the collective behavior of biological systems since the notion of state is more subtle and implicit characteristic of living creatures.

A mean field scaling asymptotics of non-perturbative solution (9) of the dual BBGKY hierarchy (7) for marginal observables was constructed. The constructed scaling limit of a non-perturbative solution (9) is governed by the set of recurrence evolution equations (14), namely, by the dual Vlasov hierarchy for interacting stochastic processes modeling large particle systems of active soft condensed matter.

We established that the limit additive-type marginal observables governed by the dual Vlasov hierarchy (14) gives an equivalent approach to the description of the kinetic evolution of many entities in terms of a one-particle distribution function governed by the Vlasov kinetic equation with initial correlations (19). Moreover, the kinetic evolution of non-additive-type marginal observables governed by the dual Vlasov hierarchy means the property of the propagation of initial correlations (22) within the framework of the evolution of states.

One of the advantages of suggested approach in comparison with the conventional approach of the kinetic theory [2, 3, 4] is the possibility to construct kinetic equations in various scaling limits in the presence of initial correlations which can characterize the analogs of condensed states of many-particle systems of statistical mechanics for interacting entities of complex biological systems.

We note that the developed approach is also related to the problem of a rigorous derivation of the non-Markovian kinetic-type equations from underlying many-entity dynamics which make it possible to describe the memory effects of collective dynamics of complex systems modeling active soft condensed matter.

In case of initial states completely specified by a one-particle distribution function and correlations (23), using a non-perturbative solution of the dual BBGKY hierarchy (9), it was proved that all possible states at the arbitrary moment of time can be described within the framework of a one-particle distribution function governed by the non-Markovian generalized kinetic equation with initial correlations (28), i.e. without any approximations. A mean field asymptotics of a solution of kinetic equation with initial correlations (28) is governed by the Vlasov-type kinetic equations.
equation with initial correlations (19) derived above from the dual Vlasov hierarchy (14) for limit marginal observables.

Moreover, in the case under consideration the processes of the creation of correlations generated by dynamics of large particle systems of active soft condensed matter and the propagation of initial correlations are described by the constructed marginal functionals of the state (26) governed by the non-Markovian generalized kinetic equation with initial correlations (28).

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