ФІЗИКА МАТЕРІАЛІВ

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ON PROPAGATION OF INITIAL CORRELATIONS IN ACTIVE SOFT MATTER

For collisional dynamics modeling the collective behavior of complex systems of mathema-tical biology, the process of propagation of initial correlations is described. The developed approach is based on the construction of a mean field limit for a solution of the Cauchy problem of the nonlinear BBGKY hierarchy for marginal correlation functions.

Key words: kinetic equation, correlation function, scaling limit, active soft matter.

1. Introduction

As well known a main consistent approach to the problem of the derivation of kinetic equations from underlying large particle dynamics was formulated by M.M. Bogolyubov [1] (see also [2]). The rigorous derivation of kinetic equations for many-particle systems in condensed states is an open problem so far [3, 4].

In modern researches, the main approach to the problem of the rigorous derivation of kinetic equations consists in the construction of scaling asymptotics of a solution of evolution equations which describe the evolution of states of large particle systems, for example, a mean field limit of a solution of the BBGKY (Bogolyubov−Born−Green−Kirkwood−Yvon) hierarchy constructed by methods of the perturbation theory [3, 4].

It should be noted modern wide applications of kinetic equations to the description of collective processes of various nature, in particular, the collective behavior of complex systems of biology. We emphasize that the considerable advance in modeling of the kinetic evolution of systems of mathematical biology with a large number of constituents (entities), for example, systems of large number of cells, is recently observed [5−11] (see also references cited therein).

In this paper we consider the problem of a rigorous description of the evolution of states within the framework of marginal correlation functions governed by the nonlinear BBGKY hierarchy for a large system of interacting stochastic processes of collisional kinetic theory [12], modeling the microscopic evolution of active soft condensed matter [6, 7]. The developed approach to the derivation of kinetic equations is based on the construction of a mean field limit of a nonperturbative solution of the Cauchy problem of the nonlinear BBGKY hierarchy. One of the advantages of a such approach is the opportunity to describe the processes of propagation of initial correlations in scaling limits, in particular, that can characterize the condensed states of soft matter.

2. On collisional dynamics of active soft condensed matter

The many-constituent systems of active soft condensed matter [6, 7] are dynamical systems displaying a collective behavior which differs from the statistical behavior of usual many-particle systems [4]. To specify such nature of constituents (entities) we consider dynamical system suggested in papers [5, 12] which is based on the Markov jump processes that must represent the intrinsic properties of living creatures (self-propelled particles).

We consider a system of entities of various M subpopulations introduced in paper [12] in case of non-fixed, i.e. arbitrary, but finite average number of entities. Every i-th entity is characterized by: $\boldsymbol{u}_i = (j_i, u_i) \in \mathcal{J} \times \mathcal{U}$, where $j_i \in \mathcal{J} \equiv (1,\ldots,M)$ is a number of its subpopulation, and values $u_i \in \mathcal{U} \subset \mathbb{R}^d$ is its microscopic characteristics.

The stochastic dynamics of n entities of various subpopulations is described by the semi-group $e^{t\Lambda_n^*}$ of the Markov jump processes defined on the space L_n^1 of the integrable functions $f_n(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n)$ defined on $(\mathcal{J} \times \mathcal{U})^n$, that are symmetric with respect to permutations of the arguments $\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n$, and equipped with the norm:

$$\| f_n \|_{L_n^1} = \sum\nolimits_{j_1 \in \mathcal{J}} \ldots \sum\nolimits_{j_n \in \mathcal{J}} \int_{\mathcal{U}^n} du_1 \ldots du_n \left| f_n(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n) \right|.$$

The infinitesimal generator Λ_n^* of this semigroup (the generator of the Kolmogorov backward equation for states of n entities) is defined on the space L_n^1 and it has the following structure [12]:

$$(\Lambda_n^* f_n)(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n) = \sum_{m=1}^{M} \varepsilon^{m-1} \sum_{i_1 \neq \ldots \neq i_m = 1}^{n} \left(\Lambda^{*[m]}(i_1,\ldots,i_m) f_n \right)\left(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n \right) \doteq$$

$$\sum_{m=1}^{M} \varepsilon^{m-1} \sum_{i_1 \neq \ldots \neq i_m = 1}^{n} \int\limits_{\mathcal{J} \times \mathcal{U}} A^{[m]}(\boldsymbol{u}_{i_1}; \boldsymbol{v}, \boldsymbol{u}_{i_2},\ldots,\boldsymbol{u}_{i_m}) a^{[m]}(\boldsymbol{v}, \boldsymbol{u}_{i_2},\ldots,\boldsymbol{u}_{i_m}) \tag{1}$$

$$f_n(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_{i_1-1}, \boldsymbol{v}, \boldsymbol{u}_{i_1+1},\ldots,\boldsymbol{u}_n) d\boldsymbol{v} - a^{[m]}(\boldsymbol{u}_{i_1},\ldots,\boldsymbol{u}_{i_m}) f_n(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n)),$$

where $\varepsilon > 0$ is a scaling parameter [13], the functions $a^{[m]}(\boldsymbol{u}_{i_1},\ldots,\boldsymbol{u}_{i_m})$, $m \geq 1$, 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: $0 \leq a^{[m]}(\boldsymbol{u}_{i_1},\ldots,\boldsymbol{u}_{i_m}) \leq a_*^{[m]}$, where $a_*^{[m]}$ is some constant. The functions $A^{[m]}(\boldsymbol{v}; \boldsymbol{u}_{i_1},\ldots,\boldsymbol{u}_{i_m})$, $m \geq 1$, are measurable positive integrable functions which describe the probability of the transition of the i_1 entity in the microscopic state u_{i_1} to the state v as a result of the interaction with entities in the states $u_{i_2},\ldots,u_{i_m}$ (in case of $m = 1$ it is the interaction with an external environment). The functions $A^{[m]}(\boldsymbol{v}; \boldsymbol{u}_{i_1},\ldots,\boldsymbol{u}_{i_m})$, $m \geq 1$, satisfy the conditions: $\int_{\mathcal{J} \times \mathcal{U}} A^{[m]}(\boldsymbol{v}; \boldsymbol{u}_{i_1},\ldots,\boldsymbol{u}_{i_m}) d\boldsymbol{v} = 1$, $m \geq 1$. We refer to paper [12], 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 $\sum\nolimits_{i_1=1}^{n} \Lambda_n^{[1]}(i_1)$ 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 [4]. 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 L_n^1 the one-parameter mapping $e^{t\Lambda_n^*}$ is a bounded strong continuous semigroup of operators.

Further we restrict ourself by the case of $M=2$ subpopulations to simplify the cumbersome formulas.

3. Dynamics of correlations

The evolution of all possible states of a system of non-fixed number of the Markov jump processes within the framework of dynamics of correlations [14], [15] is described by means of the sequence $g(t)=(1,g_1(t,\boldsymbol{u}_1),\ldots,g_n(t,\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n),\ldots)$ of correlation functions governed by the following Liouville hierarchy (hierarchy of the Kolmogorov backward equations) [15], [16]:

$$\frac{\partial}{\partial t}g_n(t,\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n)=(\Lambda_n^* g_n(t))(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n)+ \tag{2}$$
$$+\varepsilon\sum_{\mathrm{P}:\,(1,\ldots,n)=X_1\bigcup X_2}\;\sum_{i_1\in X_1}\sum_{i_2\in X_2}\Lambda^{*[2]}\left(i_1,i_2\right)g_{|X_1|}\left(t,\boldsymbol{U}_1\right)g_{|X_2|}\left(t,\boldsymbol{U}_2\right),\;\; n\geq 1,$$

where $\sum_{\mathrm{P}:\,(1,\ldots,n)=X_1\bigcup X_2}$ is the sum over all possible partitions P of the set of indexes $(1,\ldots,n)$ into two nonempty mutually disjoint subsets X_1,X_2 and the arguments $\mathbf{U}_i$ of the function $g_{|X_i|}$ correspond to indexes from the set X_i.

For initial states $g(0)=(g_0,g_1^{0,\varepsilon},\ldots,g_n^{0,\varepsilon},\ldots)$ from the space $L^1=\oplus_{n=0}^{\infty}L_n^1$ a nonperturbative solution of the Cauchy problem of hierarchy (2) is represented as follows:

$$g(t,\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n)=\mathcal{G}(t;1,\ldots,n\mid g(0)),\quad n\geq 1, \tag{3}$$

where on the space L^1 the nonlinear one-parameter mapping $\mathcal{G}(t\mid\bullet)$ is defined by the expansion [15]

$$\mathcal{G}(t;1,\ldots,n\mid f)\doteq\sum_{\mathrm{P}:\,(1,\ldots,n)=\bigcup_j X_j}\mathfrak{A}_{|\mathrm{P}|}\left(t,\{X_1\},\ldots,\{X_{|\mathrm{P}|}\}\right)\prod_{X_j\subset\mathrm{P}}f_{|X_j|}\left(\mathbf{U}_j\right),\;\; n\geq 1, \tag{4}$$

in which the generating operator is the $|\mathrm{P}|\,th$-order cumulant of groups of operators $e^{t\Lambda_n^*}$, $n\geq 1$,

$$\mathfrak{A}_{|\mathrm{P}|}(t,\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})\doteq\sum_{\mathrm{P}':\,(\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})=\bigcup_k Z_k}\left(-1\right)^{|\mathrm{P}'|-1}\left(|\,\mathrm{P}'\,|-1\right)!\prod_{Z_k\subset\mathrm{P}'}e^{t\Lambda^*_{|\theta(Z_k)|}}, \tag{5}$$

the symbol $\sum_{\mathrm{P}:\,(1,\ldots,n)=\bigcup_j X_j}$ means the sum over all possible partitions P of the set $(1,\ldots,n)$ into $|\mathrm{P}|$ nonempty mutually disjoint subsets X_j, the set $(\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})$ consists from elements of which are subsets $X_j\subset(1,\ldots,s)$ and the declusterization mapping θ is defined by the equality: $\theta(\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})\doteq(1,\ldots,n)$.

The evolution of states of large particle systems can be also described within the framework of marginal (s-particle) correlation functions governed by the fundamental evolution equations known as the nonlinear BBGKY hierarchy [16, 17]. We note that macroscopic characteristics of fluctuations of mean values of observables are determined by means of marginal correlation functions [1].

The marginal correlation functions are defined within the framework of solution (3) of the Cauchy problem of hierarchy (2) by the following series expansions:

$$G_s(t,\boldsymbol{u}_1,\ldots,\boldsymbol{u}_s)\doteq\sum_{n=0}^{\infty}\frac{1}{n!}\int_{(\mathcal{J}\times\mathcal{U})^n}d\boldsymbol{u}_{s+1}\ldots d\boldsymbol{u}_{s+n}\,\mathcal{G}(t;1,\ldots,s+n\mid g(0)),\quad s\geq 1. \tag{6}$$

According to the estimate:

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

where $c \equiv e^3 \max(1, \max_{\mathrm{P}:(1,\ldots,s)=\bigcup_i X_i} \| f_{|X_i|} \|_{L^1_{|X_i|}})$, series (6) exists and the following estimate holds: $\|G_s(t)\|_{L^1_s} \leq s!(2e^2)^s \mathrm{c}^s \sum_{n=0}^{\infty} (2e^2)^n \mathrm{c}^n$.

Then, according to definition (6), the evolution of all possible states of a system of non-fixed number of stochastic processes defined above can be described by means of the sequence $G(t) = (1, G_1(t), G_2(t), \ldots, G_s(t), \ldots) \in L^1 = \oplus_{n=0}^{\infty} L^1_n$ of marginal correlation functions governed by the Cauchy problem of the nonlinear BBGKY hierarchy: [16], [17]:

$$\begin{aligned} \frac{\partial}{\partial t} G_s(t, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_s) &= (\Lambda^*_s G_s(t))(\boldsymbol{u}_1, \ldots, \boldsymbol{u}_s) + \\ +\varepsilon \sum_{\mathrm{P}:(1,\ldots,s)=X_1 \bigcup X_2} \sum_{i_1 \in X_1} \sum_{i_2 \in X_2} & \Lambda^{*[2]}(i_1, i_2) G_{|X_1|}(t, \mathbf{U}_1) G_{|X_2|}(t, \mathbf{U}_2) + \\ +\varepsilon \int_{\mathcal{J}\times\mathcal{U}} d\boldsymbol{u}_{s+1} \sum_{i=1}^{s} & \Lambda^{*[2]}(i, s+1)\big(G_{s+1}(t, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_{s+1}) + \\ + \sum_{\substack{\mathrm{P}:(1,\ldots,s+1)=X_1 \bigcup X_2, \\ i \in X_1;\, s+1 \in X_2}} & G_{|X_1|}(t, \mathbf{U}_1) G_{|X_2|}(t, \mathbf{U}_2)\big), \end{aligned} \tag{7}$$

$$G_s(t)\mid_{t=0} = G^{0,\varepsilon}_s, \quad s \geq 1, \tag{8}$$

where $\varepsilon > 0$ is a scaling parameter and we use accepted in hierarchy (2) notations.

A nonperturbative solution of the Cauchy problem (7), (8) is represented by a sequence of marginal correlation functions:

$$G_s(t, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_s) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{(\mathcal{J}\times\mathcal{U})^n} d\boldsymbol{u}_{s+1} \ldots d\boldsymbol{u}_{s+n}\, \mathfrak{A}_{1+n}(t; \{1, \ldots, s\}, s+1, \ldots, s+n \mid G(0)), \quad s \geq 1, \tag{9}$$

where we denote by $G(0) = (1, G^{0,\varepsilon}_1, \ldots, G^{0,\varepsilon}_s, \ldots)$ a sequence of initial marginal correlation functions. The generating operator $\mathfrak{A}_{1+n}(t \mid \bullet)$ of series expansion (9) is the $(1+n)th$-order cumulant of groups of nonlinear operators (4) of the Liouville hierarchy (2)

$$\mathfrak{A}_{1+n}(t; \{1, \ldots, s\}, s+1, \ldots, s+n \mid G(0)) \doteq \tag{10}$$

$$\sum_{\mathrm{P}:(\{1,\ldots,s\},s+1,\ldots,s+n)=\bigcup_k X_k} (-1)^{|\mathrm{P}|-1}(|\mathrm{P}|-1)! \mathcal{G}\big(t; \theta(X_1) \mid \ldots \mathcal{G}\big(t; \theta(X_{|\mathrm{P}|}) \mid G(0)\big)\ldots\big),$$

where the composition of mappings (4) of corresponding noninteracting groups of interacting stochastic processes is denoted by $\mathcal{G}(t; \theta(X_1) \mid \ldots \mathcal{G}(t; \theta(X_{|\mathrm{P}|}) \mid G(0))\ldots)$ [17].

Series expansion (9) exists under the condition that: $\max_{n \geq 1} \left\| G^{0,\varepsilon}_n \right\|_{L^1_n} < (2e^3)^{-1}$. If $G^{0,\varepsilon}_n \in L^1_{0,n} \subset L^1_n$, it is a strong solution and for arbitrary initial data $G^{0,\varepsilon}_n \in L^1_n$ it is a weak solution of the Cauchy problem (7), (8).

The sequence of marginal correlation functions (9) describes the processes of the creation and the propagation of correlations in a large system of interacting stochastic processes, modeling the microscopic evolution of active soft condensed matter.

5. A mean field asymptotic behavior of marginal correlation functions

We describe the processes of the creation and the propagation of correlations in a mean field limit, namely, we establish the mean field asymptotic behavior [18] of constructed marginal correlation functions (9) in case of the initial state specified by the one-particle marginal correlation function with correlations

$$G^{(cc)}=\left(1,G_1^{0,\varepsilon}(\boldsymbol{u}_1),g_2^{\varepsilon}(\boldsymbol{u}_1,\boldsymbol{u}_2)\prod_{i=1}^{2}G_1^{0,\varepsilon}(\boldsymbol{u}_i),\ldots,g_n^{\varepsilon}(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n)\prod_{i=1}^{n}G_1^{0,\varepsilon}(\boldsymbol{u}_i),\ldots\right),\qquad(11)$$

where functions $g_n^{\varepsilon}(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n)\equiv g_n^{\varepsilon}$, $n\geq 2$, are specified the initial correlations. We note that a such assumption about initial states is intrinsic for the kinetic description of many-particle systems [4], on the other hand, initial states (11) are typical for soft condensed matter.

We assume the existence of a mean field limit of initial one-particle marginal correlation function in the following sense

$$\lim_{\varepsilon\to 0}\left\|\varepsilon G_1^{0,\varepsilon}-g_1^0\right\|_{L_1^1}=0,\qquad(12)$$

and for initial correlations, respectively,

$$\lim_{\varepsilon\to 0}\left\|g_n^{\varepsilon}-g_n\right\|_{L_n^1}=0,\ \ n\geq 2.\qquad(13)$$

Hence a mean field limit of initial state (11) is specified by the sequence of the limit marginal correlation functions

$$g^{(cc)}=\left(1,g_1^0(\boldsymbol{u}_1),g_2(\boldsymbol{u}_1,\boldsymbol{u}_2)\prod_{i=1}^{2}g_1^0(\boldsymbol{u}_i),\ldots,g_n(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n)\prod_{i=1}^{n}g_1^0(\boldsymbol{u}_i),\ldots\right).\qquad(14)$$

Under conditions (12), (13) on initial state (11) there exists a mean field limit of marginal correlation functions (9) in the following sense:

$$\lim_{\varepsilon\to 0}\left\|\varepsilon^s G_s(t)-g_s(t)\right\|_{L_s^1}=0,\ \ s\geq 1,$$

where for $s\geq 2$ the limit marginal (s-particle) correlation function $g_s(t)$ is determined by the formula

$$g_s(t,\boldsymbol{u}_1,\ldots,\boldsymbol{u}_s)=\prod_{i_1=1}^{s}e^{t\Lambda^{*[1]}(i_1)}\sum_{\mathrm{P}:(1,\ldots,s)=\bigcup_i X_i}\ \prod_{X_i\subset\mathrm{P}}g_{|X_i|}(\mathrm{U}_i)\prod_{i_2=1}^{s}e^{-t\Lambda^{*[1]}(i_2)}\prod_{j=1}^{s}g_1(t,\boldsymbol{u}_j),\qquad(15)$$

and, respectively, the limit one-particle correlation function $g_1(t)$ is represented by the following series expansion:

$$\begin{aligned}g_1(t,\boldsymbol{u}_1)=\sum_{n=0}^{\infty}\int_0^t dt_1\ldots\int_0^{t_{n-1}}dt_n\int_{(\mathcal{J}\times\mathcal{U})^n}d\boldsymbol{u}_2\ldots d\boldsymbol{u}_{n+1}\,e^{(t-t_1)\Lambda^{*[1]}(1)}\times\\ \times\Lambda^{*[2]}(1,2)\prod_{j_1=1}^{2}e^{(t_1-t_2)\Lambda^{*[1]}(j_1)}\ldots\prod_{j_{n-1}=1}^{n}e^{(t_{n-1}-t_n)\Lambda^{*[1]}(j_{n-1})}\times\\ \times\sum_{i_n=1}^{n}\Lambda^{*[2]}(i_n,n+)\prod_{j_n=1}^{n+1}e^{t_n\Lambda^{*[1]}(j_n)}\sum_{\mathrm{P}:(1,\ldots,n+1)=\bigcup_i X_i}\ \prod_{X_i\subset\mathrm{P}}g_{|X_i|}(\mathrm{U}_i)\prod_{i=1}^{n+1}g_1^0(\boldsymbol{u}_i),\end{aligned}\qquad(16)$$

where it is used notations accepted above.

The operator $g_1(t)$ represented by series (16) is a solution of the Cauchy problem of the Vlasov-type kinetic equation with initial correlations:

$$\frac{\partial}{\partial t}g_1(t,\boldsymbol{u}_1)=\Lambda^{*[1]}(1)g_1(t,\boldsymbol{u}_1)+\qquad(17)$$

$$+\int_{\mathcal{J}\times\mathcal{U}}d\boldsymbol{u}_2\Lambda^{*[2]}(1,2)\prod_{i_1=1}^{2}e^{t\Lambda^{*[1]}(i_1)}\left(1+g_2(\boldsymbol{u}_1,\boldsymbol{u}_2)\right)\prod_{i_2=1}^{2}e^{-t\Lambda^{*[1]}(i_2)}g_1(t,\boldsymbol{u}_1)g_1(t,\boldsymbol{u}_2),$$

$$g_1(t,\boldsymbol{u}_1)|_{t=0}=g_1^0(\boldsymbol{u}_1),\qquad(18)$$

where the operators $\Lambda^{*[1]}(1)$ and $\Lambda^{*[2]}(1,2)$ are defined according to formula (1). We point out that derived kinetic equation for a many-constituent system modeling collective behavior of active soft condensed matter (17) is the non-Markovian evolution equation.

We remark that in case of initial states of statistically independent interacting stochastic processes specified by a one-particle marginal distribution function the kinetic evolution is governed by the Vlasov kinetic equation and equality (15) means the property of the propagation of initial chaos [18].

The proof of stated results is based on the corresponding formulas for cumulants of asymptotically perturbed semigroups of operators (5).

Indeed, if $f_s \in L^1_s$, then for arbitrary finite time interval for the strongly continuous semigroup $e^{t\Lambda^*_s}$ the following equality is valid:

$$\lim_{\varepsilon\to 0}\Big\| e^{t\Lambda^*_n} f_s - \prod_{j=1}^{s} e^{t\Lambda^{*[1]}(j)} f_s \Big\|_{L^1_s} = 0.$$

As a result of this equality for the $(s+n)th$-order cumulants of semigroups of operators (5) the following equalities are true:

$$\lim_{\varepsilon\to 0}\Big\| \frac{1}{\varepsilon^n}\, \mathfrak{A}_{s+n}(t,1,\ldots,s+n) f_{s+n} \Big\|_{L^1_s} = 0, \ \ s \ge 2.$$

In consequence of the validity of this equalities the representation of the limit one-particle correlation function $g_1(t)$ by series expansion (16) is also obtained directly in view that series expansion (9) in the case of initial data (11) takes the form

$$G_1(t,\boldsymbol{u}_1) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{(\mathcal{J}\times\mathcal{U})^n} d\boldsymbol{u}_2 \ldots d\boldsymbol{u}_{n+1}\, \mathfrak{A}_{1+n}(t,1,\ldots,n+1) \sum_{\mathrm{P}:(1,\ldots,n+1)=\bigcup_i X_i} \prod_{X_i\subset \mathrm{P}} g^{\varepsilon}_{|X_i|}(\mathbf{U}_i) \prod_{i=1}^{n+1} G_1^{0,\varepsilon}(\boldsymbol{u}_i),$$

where it is used notations accepted above.

We note that the sequence of limit marginal correlation functions (16) and (15) is a solution of the nonlinear Vlasov hierarchy which describe the evolution of marginal correlation functions in a mean field limit for arbitrary initial states [16, 18].

6. Conclusion

For a large system of interacting stochastic processes of collisional kinetic theory [12], modeling the microscopic evolution of active soft condensed matter, a mean field scaling asymptotics of nonperturbative solution (9) of the Cauchy problem of the nonlinear BBGKY hierarchy (7),(8) for marginal correlation functions was constructed.

The marginal correlation functions give an equivalent approach to the description of the evolution of states of large particle systems in comparison with marginal density functions governed by the BBGKY hierarchy [4]. The macroscopic characteristics of fluctuations of observables are directly determined by marginal correlation functions (9) on the microscopic level [1, 16].

In case of initial states specified by correlation functions (14), which can characterize the analogs of condensed states of many-particle systems of statistical mechanics for interacting entities of complex biological systems, a mean field asymptotic behavior of the processes of the creation and the propagation of correlations were described (15). It was established that mean field dynamics does not create new correlations except of those that generating by initial correlations. It was also proved the property known as a propagation of initial chaos, which underlies in mathematical derivation of effective evolution equations of complex systems [4, 18].

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

We remark also that in papers [19, 20] it was developed two other approaches to the description of the process of the propagation of initial correlations in a mean field limit. In paper [19] the process of the propagation of initial chaos was established within the framework of the evolution of marginal observables (in [21] this result was generalized on case of initial states with correlations) and in paper [20] the property of the propagation of initial correlations was proved within the framework of the description of the evolution by means of a one-particle (marginal) density function governed by the generalized kinetic equation.

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Анотація. ***В. І. Герасименко. Про розповсюдження початкових кореляцій в активних м'яких речовинах.*** *Для системи багатьох стохастичних марковських стрибкоподібних процесів, якою моделюється колективна поведінка складних систем математиної біології, описано процес поширення початкових кореляцій. Розвинутий підхід ґрунтується на побудові скейлінгової границі середнього поля для послідовності маргінальних кореляційних функцій, яка є непертурбативним розв'язком задачі Коші для ієрархії нелінійних рівнянь ББҐКІ (Боголюбов — Борн − Ґрін — Кірквуд − Івон). Доведення отриманих результатів ґрунтується на відповідних граничних теоремах для кумулянтів асимптотично збурених груп нелінійних операторів, якими описується динаміка кореляцій скінченої кількості марковських стрибкоподібних процесів та на використанні явного вигляду твірних операторів розкладів в ряд для маргінальних кореляційних функцій.*

У випадку початкових станів, якими характерезуються конденсовані стани активних м'яких речовин, а саме, які описуються одночастинковою функцією розподілу та кореляційними функціями, в скейлінговій границі середнього поля встановлено явний вигляд граничних маргинальних функцій розподілу. В зазначеному наближенні еволюція стану системи описується за допомогою граничної одночастинкової функції розподілу, яка є розв'язком задачі Коші для немарковського кінетичного рівняння Власова з початковими кореляціями. Для граничних маргинальних функцій розподілу також встановлено властивість, відому як властивість поширення початкового хаосу. Розвинутий підхід пов'язаний з проблемою строгого виведення з динаміки складних систем кінетичних рівнянь немарковського типу, які дають можливість описувати ефекти пом'яті колективної поведінки активних м'яких конденсованих речовин.

Ключові слова: ієрархія нелінійних рівнянь ББҐКІ, кінетичне рівняння, кореляційна функція, скейлінгова границя, активна м'яка речовина.

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SEVERE PLASTIC DEFORMATION BY KOBO METHOD – ESTIMATIONS AND MODEL

A new phenomenological model for the description and simulation of Severe Plastic Deformation (SPD) is developed based on the inverse dependence of the material's viscosity on the concentration of point defects (the higher the concentration, the less the viscosity). In this case, the local concentration of point defects is determined by (1) the intensity of deformation, (2) the annihilation of interstitial defects and vacancies, (3) the absorption of defects at dislocations, (4) diffusive redistribution of defects. The solution of the corresponding system of nonlinear differential equations for the field of defect concentrations and the differential equation for the velocity field at a given rate of deformation at the boundary of the sample provides a non-equilibrium phase transition - a jump in viscosity and a jump in the concentration of defects at a certain distance from the surface. In this case, the width of the zone of reduced viscosity and increased defect concentration is proportional to the surface velocity of the deformation. It is in this zone that it makes sense to consider the material as a viscous medium.

Keywords: severe plastic deformation, interstitial defects, vacancies, diffusion, viscosity, creep, nonlinear differential equations.

1. Introduction

An important example of nano-trend in science and technology during last decades is a production of nano-grained metals by Severe Plastic Deformation (SPD) [1, 2]. The most popular methods of SPD are ECAP (equi-channel angular pressing) and HPT (high-pressure torsion). Less than 20 years ago Korbel and Bochniak from AGH (Cracow) suggested their own method (KoBo) for extrusion of metals and alloys [3-5]. This method has something in common with HPT, but torsion is oscillating: the external surface is subjected to periodic rotations with a frequency of a few Hertz (say, 5 Hz) and amplitude of a few (6-8) degrees.