*METHODOLOGICAL NOTES*

# Irreversibility and the probabilistic treatment of the dynamics of classical particles

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## Contents

**Abstract.** It is shown that B B Kadomtsev's idea of small 'external noise' securing a time-irreversible evolution reduces the justification of statistical physics to a fundamentally new formulation which requires that the dynamics of a multiparticle system be treated by neglecting small acceleration particles. It turns out that this formulation not only leads naturally to irreversible evolution but also suggests a new way of constructing kinetic equations capable of correctly accounting for fluctuations. At the early, small-time, stage of evolution, the original correlations are forgotten and 'post-collisional' ones form. It is the final portion of the first stage and the formation of the 'post-collisional' correlations which can be described by a closed form kinetic equation. A relation between Kadomtsev's external noise idea and Bogolyubov's derivation of kinetic equations is established, leading to a new physical interpretation of the 'molecular chaos' hypothesis.

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## 1. Introduction

It is known from experiment that a closed macroscopic system approaches the state of thermodynamic equilibrium on a certain time scale called the relaxation time. Meantime, laws of both classical and quantum mechanics are time reversible. So the question of how the description of irreversible processes can be obtained from reversible dynamical equations has been broadly discussed in the physics literature [1]. We do not wish even try to comment on all the relevant points of view, but instead are going to focus on those approaches to the problem (although not totally sharing some of them) that somehow relate to the ideology of the present paper.

As shown in [1], in a rarefied gas only Bolzmann's hypothesis of 'molecular chaos' proves to be sufficient to explicitly introduce physical irreversibility: According to the $H$-theorem, Bolzmann's kinetic equation describes the irreversible relaxation of the gas to the thermal equilibrium state. When considering what exact physical phenomenon underlies the molecular chaos hypothesis, B B Kadomtsev [1] came to the conclusion that irreversibility of the dynamics of a gas consisting of classical particles and the possibility of its statistical treatment are due to a tiny interaction of the system with the irreversible surrounding. It is stated in [1] that the dynamic chaos by itself is insufficient for irreversibility to appear. According to B B Kadomtsev [1], "irreversibility is not

a direct consequence of chaos, although it can be indirectly related to chaos". Such a conclusion, deduced from qualitative considerations, is quite unexpected. In this connection we recall that arguments disfavoring the possibility of a consistent construction of statistical physics within the frame of the theory of 'external surrounding effects' are given in [2]. Paper [2], which was published significantly earlier than paper [1], states that the idea of introducing an external irreversible surrounding should be rejected and irreversible dynamics appears in dynamical systems through mixing.

The conclusion made in [1] that thermodynamic equilibrium can not be achieved without external noise is not only of theoretical interest. Indeed, according to [1], S A Majorov, A N Tkachev, and S I Yakovlev [3] showed, using the method of molecular dynamics for point-like charges in a closed volume with mirror walls, that a stationary state different from thermodynamic equilibrium is ultimately established. In particular, in this stationary state the process of recombination of a strongly overcooled plasma slows down very much.

However, it is well known that Bolzmann's equation can be obtained by 'cutting' the Bogolyubov–Born–Green–Kirkwood–Ivon (BBGKI) hierarchy with a small parameter, as was demonstrated by N N Bogolyubov [4]. In this approach, no external noise is required.

In the present paper we show that in fact there exists a tight connection between N N Bogolyubov's approach and B B Kadomtsev's ideas of the role of the external surrounding in producing time irreversible evolution, and suggest a new approach for deriving kinetic equations. As follows from below, the development of B B Kadomtsev's approach enables us to have a new look at the physical meaning of the 'molecular chaos' hypothesis and to point to a method for consistent description of fluctuations in the framework of the kinetic theory. In addition, in the framework of development of B B Kadomtsev's ideas, it is necessary to answer the question why an external noise leads to irreversible dynamics but the irreversible dynamics itself are independent of the external noise if it is sufficiently small.

## 2. Structure of the BBGKI hierarchy

We start with discussing some simple properties of the BBGKI hierarchy focusing on questions which will be related to the time irreversibility of the dynamics.

Consider a system of $N$ identical particles described by a Hamiltonian

$$H = \sum_{i=1}^{i=N} \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} U(\mathbf{r}_i - \mathbf{r}_j), \qquad (1)$$

where $U(\mathbf{r}_i - \mathbf{r}_j)$ and $m$ are the binary potential of inter-particle interaction and the mass of particles, respectively.

The dynamics of this system may be described by two equivalent means. It is possible to study trajectories of the system in the phase space or consider the evolution of functions determined in the phase space. The first approach corresponds to the treatment of dynamics by the Hamilton equations (the second Newton's law), the second one — by Liouville's equations. An arbitrary function $\rho(t, 1, \ldots, N)$, where $i = (\mathbf{p}_i, \mathbf{r}_i)$, determined in the $6N$-dimensional phase space of the system, evolves in time according to the Liouville equation

$$\frac{\partial \rho}{\partial t} = \widehat{\Lambda} \rho, \qquad (2)$$

where $\widehat{\Lambda}$ is the Liouville operator

$$\widehat{\Lambda} = \sum_{i=1}^{i=N} \left( \frac{\partial H}{\partial \mathbf{r}_i} \frac{\partial}{\partial \mathbf{p}_i} - \frac{\partial H}{\partial \mathbf{p}_i} \frac{\partial}{\partial \mathbf{r}_i} \right). \qquad (3)$$

Considering dynamical systems with a large number of particles, $N \to +\infty$, it proves convenient to transit from the function $\rho(t, 1, \ldots, N)$, which is symmetrical with respect to all groups of variables $1, 2, \ldots$, to s-particle distribution functions

$$F_s(t, 1, \ldots, s) = \int \frac{\mathrm{d}(s+1) \ldots \mathrm{d}i \ldots \mathrm{d}N}{(N-s)!}$$

$$\times \rho(t, 1, \ldots, i, \ldots, N), 1 \leqslant s \leqslant N, \qquad (4)$$

and all multi-particle distribution functions with $s \geqslant (N+1)$ we set zero by definition. Using $F_s$, Eqn (2) can be rewritten into a system of inter-coupled equations

$$\left( \frac{\partial}{\partial t} + \hat{l}_1 + \ldots + \hat{l}_s \right) F_s = \widehat{\Lambda}_s F_s + \int \sum_{1 \leqslant i \leqslant s} \widehat{\Lambda}(i, s+1)$$

$$\times F_{s+1}(t, 1, \ldots, i, \ldots, s, s+1) \, \mathrm{d}(s+1), \quad 1 \leqslant s \leqslant N, \, (5)$$

where

$$\hat{l}_i = \frac{\mathbf{p}_i}{m} \frac{\partial}{\partial \mathbf{r}_i},$$

$$\widehat{\Lambda}_s = \sum_{1 \leqslant i < j \leqslant s} \widehat{\Lambda}(i, j),$$

$$\widehat{\Lambda}(i, j) = \frac{\partial U(\mathbf{r}_i - \mathbf{r}_j)}{\partial \mathbf{r}_i} \frac{\partial}{\partial \mathbf{p}_i} + \frac{\partial U(\mathbf{r}_i - \mathbf{r}_j)}{\partial \mathbf{r}_j} \frac{\partial}{\partial \mathbf{p}_j}, \, i \neq j.$$

Now, making the thermodynamic limiting transition

$$N \to \infty, \ V \to \infty, \ \frac{N}{V} = \text{const}, \qquad (6)$$

where $V$ is the system volume and assuming all $F_s$ to have a finite limit, we arrive at the infinite system of intercoupled equations

$$\left( \frac{\partial}{\partial t} + \hat{l}_1 + \ldots + \hat{l}_s \right) F_s = \widehat{\Lambda}_s F_s + \int \sum_{1 \leqslant i \leqslant s} \widehat{\Lambda}(i, s+1)$$

$$\times F_{s+1}(t, 1, \ldots, i, \ldots, s, s+1) \, \mathrm{d}(s+1). \qquad (7)$$

The system of equations (7) differs from (5) only by an infinite number of equations. Some distinct features of Eqns (7) and the related system (5) should be mentioned. Firstly, Eqns (7) are time reversible. Secondly, all equations (7) are linear integro-differential equations. Indeed, if

$$\mathbf{\Gamma} = (F_1, F_2, \ldots, F_s, \ldots) \text{ и } \mathbf{\Gamma}' = (F'_1, F'_2, \ldots, F'_s, \ldots) \quad (8)$$

are two arbitrary solutions of system (7), then the set of functions

$$a\mathbf{\Gamma} + b\mathbf{\Gamma}' = (aF_1 + bF'_1, aF_2 + bF'_2, \ldots, aF_s + bF'_s, \ldots), \qquad (9)$$

where $a$ and $b$ are arbitrary numbers, are also a solution of system of equations (7).

At last, when deriving (7), no special restrictions were imposed on the symmetric function $\rho(t, 1, \ldots, N)$ besides the requirement that a limit $F_s$ exists at any $s$ when $N \to +\infty$. Non-negativeness and normalization of the function $\rho(t, 1, \ldots, N)$ have also not been assumed.

## 3. A physical sense of the simplest properties of the BBGKI hierarchy

The time irreversibility of the BBGKI hierarchy is a natural consequence of the time irreversibility of the Hamilton equations corresponding to (1). That quite arbitrary functions $\rho$ lead to (7) means that the evolution of arbitrary (symmetric) ensembles can be described by Eqn (7). Therefore the problem of the physical interpretation of particular solutions (7) appears. Indeed, from the point of view of physics, of most interest is the behavior of only those ensembles whose evolution enables one to study the dynamics (perhaps, 'rough') of separate points of the phase space. At the same time, we still have no criterion to separate 'physically interesting' ensembles and corresponding functions $(F_1, F_2, \ldots)$. These considerations can be illustrated by a simple example. Consider an ensemble defined as

$$\rho(t, 1, \ldots, N) = \exp\left(-\frac{H}{T_1}\right) + \exp\left(-\frac{H}{T_2}\right), \ T_1 \neq T_2,$$
(10)

where $T_1$ and $T_2$ should be interpreted as temperatures, and ensemble (10) should be thought of as a 'mixture' of systems with different temperatures. Clearly, it is physically meaningless to study ensemble (10). More proper examples related to a reasonable choice of the ensemble can be found, for example in [5, 6], where the relation of this question to the concept of quasi-averages [7] is pointed out.

The linearity of all equations (7) mentioned above, which follows from the linearity of Liouville's equation, has a clear physical meaning. Note that equations (7) describe not a single system, whose dynamics are defined by (1), but the whole ensemble of such systems with different initial conditions. The linearity of the BBGKI chain equations reflects the fact that a particle, which belongs to a given instance of a system with Hamiltonian (1), interacts only with the particles entering the same instance of the system, i.e. they do not interact with particles belonging to other systems from the ensemble under consideration. The latter becomes obvious when the integral in Eqn (4) is substituted by Riemann's sums. However, to avoid complications due to awkward notation, let us consider an ensemble containing only two points of the phase space with weights $\alpha$ and $1 - \alpha$, respectively. In this case we can write

$$F_1 = \alpha \sum_{i=1}^{i=N} \delta\big(\mathbf{r} - \mathbf{r}_i^{(1)}(t)\big)\delta\big(\mathbf{v} - \mathbf{v}_i^{(1)}(t)\big)$$

$$+ (1 - \alpha) \sum_{i=1}^{i=N} \delta\big(\mathbf{r} - \mathbf{r}_i^{(2)}(t)\big)\delta\big(\mathbf{v} - \mathbf{v}_i^{(2)}(t)\big),$$
(11)

$$F_2 = \alpha \sum_{i \neq j} \delta\big(\mathbf{r}_1 - \mathbf{r}_i^{(1)}(t)\big)\delta\big(\mathbf{v}_1 - \mathbf{v}_i^{(1)}(t)\big)\delta\big(\mathbf{r}_2 - \mathbf{r}_j^{(1)}(t)\big)$$

$$\times \delta\big(\mathbf{v}_2 - \mathbf{v}_j^{(1)}(t)\big) + (1 - \alpha) \sum_{i \neq j} \delta\big(\mathbf{r}_2 - \mathbf{r}_i^{(2)}(t)\big)$$

$$\times \delta\big(\mathbf{v}_2 - \mathbf{v}_i^{(2)}(t)\big)\delta\big(\mathbf{r}_1 - \mathbf{r}_j^{(2)}(t)\big)\delta\big(\mathbf{v}_1 - \mathbf{v}_j^{(2)}(t)\big)$$
(12)

etc., where in $\mathbf{r}_i^{(n)}(t)$ $(n = \overline{1, 2}, i = \overline{1, N})$ the superscript counts one of the two points of the phase space from this ensemble, and the subscript enumerates the particles. Substituting (11), (12) into Eqn (7) for the evolution of the one-particle distribution function, it is easy to ascertain that the linearity indeed admits the above interpretation. Eqns (11) and (12) imply that particles from a given representation (a point of the phase space) interact only with particles from this representation, i.e. from the same point in the 6N-dimensional phase space of the system.

## 4. Uncoupling the BBGKI hierarchy by N N Bogolyubov's method

To derive Bolzmann's kinetic equation, N N Bogolyubov suggested searching for solution (7) in the form [4]

$$F_2(t, 1, 2) = F_1(t, 1)F_1(t, 2) + G_2(t, 1, 2),$$

$$F_3(t, 1, 2, 3) = F_1(t, 1)F_1(t, 2)F_1(t, 3) + F_1(t, 1)G_2(t, 2, 3)$$

$$+ F_1(t, 2)G_2(t, 1, 3) + F_1(t, 3)G_2(t, 1, 2) + G_3(t, 1, 2, 3),$$
(13)

where the functions $G_2$, $G_3$, etc. are small in a certain sense. The 'smallness' of the correlation functions has a different sense in different problems. For example, for a rarefied gas with a short-action potential, the 'smallness' of the correlation functions assumes their small values at distances greatly exceeding the radius of action of the potential. In contrast, in the case of a gas with a weak interparticle interaction (much smaller than the temperature) the correlation functions are assumed really to be small everywhere.

Bogolyubov's approach is consistent from the mathematical point of view, although its applicability is restricted by the finite order in the small parameter due to the increase to infinity of contributions from four-particle collisions [8] (see [9] for more detail). However its physical content requires certain comments. Note first of all that Eqn (13) is an implicit definition of the ensemble of systems we are going to study with the help of equations (7). Since Bogolyubov's approach assumes that

$$\int G_2 \, \mathrm{d}1 \, \mathrm{d}2 = 0,$$
(14)

then according to (13), (14)

$$\int F_2(t, 1, 2) \, \mathrm{d}1 \, \mathrm{d}2 = \int F_1(t, 1) \, \mathrm{d}1 \int F_1(t, 2) \, \mathrm{d}2,$$
(15)

which with account of (4) leads to the equality $(N \to +\infty)$

$$\int \rho(t, 1, \ldots, N) \, \mathrm{d}1 \ldots \mathrm{d}N = \left(1 - \frac{1}{N}\right)N!,$$
(16)

i.e. a certain normalization of the ensemble under study is required, which allows the probability theory terms to be used. It is also necessary to note that the use of non-linear factorization (13) implies a principle assumption, from the physical point of view. Namely, it is assumed that the dynamics of the system permit the construction of such an ensemble, in which the actual interaction of a particle from

any fixed system of the ensemble, with particles from the same system can be approximated to a good accuracy by the ensemble-averaged interaction with particles from different systems of the ensemble. In other words, factorization (13) 'introduces' an interaction between different particles from different systems of the ensemble. This can be directly checked by representing Eqn (13) in the form of the production of Riemann's sums which approximate $F_1$ according to Eqn (4). Yet the point above is illustrated by the example of a 'two-point' ensemble considered earlier. Indeed, in this particular case, the use of the first of equations (13) would mean the following approximation of function $F_2$:

$$F_2 = \alpha^2 \sum \delta(\mathbf{r}_1 - \mathbf{r}_i^{(1)}(t))\delta(\mathbf{v}_1 - \mathbf{v}_i^{(1)}(t))\delta(\mathbf{r}_2 - \mathbf{r}_j^{(1)}(t))$$
$$\times \delta(\mathbf{v}_2 - \mathbf{v}_j^{(1)}(t)) + (1 - \alpha)^2 \sum \delta(\mathbf{r}_1 - \mathbf{r}_i^{(2)}(t))\delta(\mathbf{v}_1 - \mathbf{v}_i^{(2)}(t))$$
$$\times \delta(\mathbf{r}_2 - \mathbf{r}_j^{(2)}(t))\delta(\mathbf{v}_2 - \mathbf{v}_j^{(2)}(t)) + \alpha(1 - \alpha) \sum (\delta(\mathbf{r}_1 - \mathbf{r}_i^{(1)}(t))$$
$$\times \delta(\mathbf{v}_1 - \mathbf{v}_i^{(1)}(t))\delta(\mathbf{r}_2 - \mathbf{r}_j^{(2)}(t))\delta(\mathbf{v}_2 - \mathbf{v}_j^{(2)}(t)) + \delta(\mathbf{r}_1 - \mathbf{r}_i^{(2)}(t))$$
$$\times \delta(\mathbf{v}_1 - \mathbf{v}_i^{(2)}(t))\delta(\mathbf{r}_2 - \mathbf{r}_j^{(1)}(t))\delta(\mathbf{v}_2 - \mathbf{v}_j^{(1)}(t))). \quad (17)$$

It is important to note that because of the third term in (17), which is proportional to $\alpha(1 - \alpha)$, and analogous terms in more complex ensembles, approach (13) 'incorporates' the interaction between particles from different representatives of the ensemble. Indeed, in Eqn (17) in comparison with Eqn (12), a new term has appeared which is proportional to $\alpha(1 - \alpha)$. This term contains the product of $\delta$-functions including particles from different representatives of the ensemble (with different superscripts).

Now it becomes clear why it is possible to obtain time irreversible kinetic equations using approach (13). Indeed, Eqn (13) 'introduces' the interaction between different representatives of the ensemble, i.e. each system of the ensemble becomes incomplete and the appearance of irreversible evolution under such conditions for an infinite number of systems in the ensemble seems to be very natural.

Of course, the irreversibility appears during calculations at such an order of small parameter, in which the difference between different points of the phase space becomes noticeable (a plasma may provide an example: Vlasov's equation, i.e. the first order in the reverse number of particles within the Debye sphere, is reversible, while Vlasov's equation with Landau's collision integral, i.e. with account of the second order in small parameter, is no longer reversible). Notice that this explains Bolzmann's hypothesis of 'molecular' chaos: a particle simply 'collides' (with the corresponding weight) with particles from different ensemble representatives, so the particles are statistically independent before the collision.

Running somewhat ahead, we wish to make one more important note. From the above point of view the justification of the principle of 'molecular' chaos means at least the determination of such properties of a dynamical system and its treatment in such an approximation, when the change of the actual interparticle interaction inside one ensemble representative by the interaction of its particles with those from the ensemble-'averaged' representative is valid. The precise meaning of the latter considerations becomes clear from the subsequent discussion.

## 5. N N Bogolyubov's method and B B Kadomtsev's idea of external surrounding effects

Let us consider in more detail the tight connection between N N Bogolyubov's method of deriving Bolzmann-type kinetic equations and the ideas suggested by B B Kadomtsev [1] on the necessity of introducing an interaction with 'external' noise (with an external irreversible surrounding) for irreversible dynamics to appear in the system.

We have seen earlier that approach (13) corresponds to the introduction of an interaction with particles from different representatives of the ensemble under study, i.e. each ensemble representative becomes incomplete and the interaction with other representatives of the ensemble plays the role of the interaction with the external surrounding. Note that the continuity of the distribution function requires the ensembles to contain an infinite number (more precisely, a continuum) of representatives. A non-trivial result of N N Bogolyubov's approach is the proof that at some time intervals, for some states of system (1) (the initial conditions) with small parameters (see [4, 8] for more detail), the interaction of particles introduced by Eqn (13) with a far from low external noise (see, e.g., the third and first two sums in Eqn (17)) well approximates, in some sense, the 'rough' dynamics of the system.

At the same time, such a treatment of irreversibility appears not to be fully satisfactory for a number of reasons. First of all, the change of the actual interparticle interaction inside each particular ensemble representative by the interaction with particles of the 'averaged' ensemble representative means in fact that fluctuations are neglected, which was first noted by M A Leontovich [10]. The first attempt to get rid of this shortcoming of the Bolzmann equation was undertaken in the well-known paper by B B Kadomtsev "On fluctuations in gas" [11] (see also [13]). However, the method used in this paper and a huge number of studies, initiated by this paper, on fluctuations in kinetic equations, enable only the case of small fluctuations to be considered, i.e. the case where the notion of a 'fluctuationless' state perturbed by small fluctuations is admissible.

Thus Bogolyubov's method is applicable to construct kinetic equations only for such media and only in states where fluctuations are negligibly small. To avoid misunderstanding we specially emphasize that fluctuations of the 'averaged' ensemble representative can be described, i.e. the theory must be made precise such that to take into account that for different specific problems the ensembles should be constructed differently or, in other terms, the fluctuations of the 'averaged' ensemble representative must be treated differently. Here it is easy to see that such a method can not in principle fully describe fluctuations. Note that in Bogolyubov's approach irreversibility finally appears due to the possibility of approximating the actual interparticle interaction by a fictive interaction emerging due to non-linear factorization (13). Unfortunately, such a mechanism of appearance of irreversibility does not shed light on physical processes in the system with Hamiltonian (1), which lead to irreversible dynamics. And at last, from our point of view, the method itself of reducing the multiparticle problem to the interaction of particles with particles of the 'mean' representative is very artificial. Due to this fact Bogolyubov's method of uncoupling allows us to obtain kinetic equations for sufficiently a narrow class of systems (in fact, using Bogolyu-

bov's method it is impossible to get kinetic equations even for systems with arbitrary power-law potential for interparticle interaction).

Below we show a novel method for studying irreversible dynamics, but first another approach to the BBGKI hierarchy should be addressed.

## 6. Singular distribution functions and the BBGKI hierarchy

Let us turn to a somewhat different treatment of the BBGKI hierarchy based on the formalism of singular distribution functions [11 – 13].

Using a one-particle distribution function [11 – 13]

$$\phi_1(t,1) = \sum_{i=1}^{i=N} \delta(\mathbf{r}_1 - \mathbf{r}_i(t))\delta(\mathbf{v}_1 - \mathbf{v}_i(t)) \tag{18}$$

we construct singular $s$-particle distribution functions

$$\phi_s(t,1,\ldots,s) = \phi_1(t,1)\ldots\phi_1(t,i)\ldots\phi_1(t,s). \tag{19}$$

According to Newton's 2nd law we find equations describing the evolution of singular distribution functions $\phi_1(t,1),\ldots,\phi_s(t,1,\ldots,s)$

$$\left(\frac{\partial}{\partial t} + \hat{l}_1\right)\phi_1(t,1) = C_1(t,1), \tag{20}$$

$$\left(\frac{\partial}{\partial t} + \hat{l}_1 + \ldots + \hat{l}_s\right)\phi_s(t,1,\ldots,s) = C_s(t,1,\ldots,s), \tag{21}$$

where

$$\hat{l}_i = \mathbf{v}_i\frac{\partial}{\partial \mathbf{r}_i},$$

$$C_s(t,1,\ldots,s) = \frac{1}{m}\sum_{i=1}^{i=s}\int\frac{\partial U(\mathbf{r}_i - \mathbf{r}_{(s+1)})}{\partial \mathbf{r}_i}$$

$$\times \phi_{s+1}(t,1,\ldots,s,s+1)\,\mathrm{d}(s+1).$$

Equations (20), (21) deserve some comments. Equations (21) for $\phi_s$, $s \geqslant 2$ are valid for all different $\mathbf{r}_1,\ldots,\mathbf{r}_s$, and when taking the integrals entering $C_s$, $s \geqslant 1$, an infinitesimal neighborhood of point $\partial U(\mathbf{r}_i - \mathbf{r}_{(s+1)})/\partial \mathbf{r}_i$ should be excluded from the integral containing $\mathbf{r}_i$ to exclude 'self-interaction' of a particle at this point.

Now we try to transit from singular distribution functions $\phi_s$, $s \geqslant 1$ to a description of the dynamics by smoothed distribution functions using averaging equations (20), (21) over the ensemble. It would be desirable to use the freedom in the ensemble choice to obtain as simple as possible equations after averaging, i.e. to choose the ensemble in such a way that the equalities

$$\langle\phi_s(t,1,\ldots,s)\rangle = \langle\phi_1(t,1)\rangle\ldots\langle\phi_1(t,i)\rangle\ldots\langle\phi_1(t,s)\rangle. \tag{22}$$

be fulfilled. Unfortunately, this is impossible. Now we turn to definition of function $\phi_3(t,1,2,3)$ at $\mathbf{r}_1 \neq \mathbf{r}_2$:

$$\langle\phi_3(t,1,2,3)\rangle = \big(\delta(\mathbf{r}_1 - \mathbf{r}_3)\delta(\mathbf{v}_1 - \mathbf{v}_3) + \delta(\mathbf{r}_2 - \mathbf{r}_3)$$

$$\times \delta(\mathbf{v}_2 - \mathbf{v}_3)\big)F_2(t,1,2) + F_3(t,1,2,3), \tag{23}$$

where $F_2$ and $F_3$ are smooth distribution functions defined by Eqn (4). Eqn (23) implies that no ensemble can be chosen such that Eqn (22) is satisfied. The required choice is prohibited by $\delta$-function factors entering in some terms in Eqn (24). Note that these terms appeared due to ensemble averaging of strongly singular expressions like

$$\delta(\mathbf{r}_1 - \mathbf{r}_i(t))\delta(\mathbf{v}_1 - \mathbf{v}_i(t))\delta(\mathbf{r}_3 - \mathbf{r}_i(t))\delta(\mathbf{v}_3 - \mathbf{v}_i(t)), \tag{24}$$

containing the square of $\delta$-functions. Thus the impossibility of satisfying Eqn (22) has no relation to particle interactions and is simply formal consequence of the definition of $s$-particle distribution functions.

Let us study the physical sense of the latter somewhat formal considerations. First of all, we note the averaging over the ensemble of equations (20), (21) leads to the BBGKI hierarchy if the strongly singular contribution to $\langle\phi_s\rangle$ is correctly taken into account:

$$\langle\phi_s(t,1,\ldots,s)\rangle = \left(\sum_{1 \leqslant i \leqslant s-1}\delta(\mathbf{r}_i - \mathbf{r}_s)\delta(\mathbf{v}_i - \mathbf{v}_s)\right)$$

$$\times F_{s-1}(t,1,\ldots,s-1) + F_s(t,1,\ldots,s),$$

$$\text{where}\quad \mathbf{r}_i \neq \mathbf{r}_j,\ 1 \leqslant i < j \leqslant (s-1). \tag{25}$$

Here strongly singular terms in $\phi_s$, $s \geqslant 3$ lead to terms $\widehat{\Lambda}_{s-1}F_{s-1}$ in the r.h.s. of Eqn (7), and less singular ones give rise to integral terms in Eqn (7) which contain $F_s$. The attempt to choose the ensemble such that equalities (22) be satisfied is equivalent, from the mathematical point of view, to solving Eqn (7) by variable separation method, which the terms $\widehat{\Lambda}_{s-1}F_{s-1}$, arisen, of course, from strongly singular terms in $\phi_s$, prevent to.

The appearance of the terms $\widehat{\Lambda}_{s-1}F_{s-1}$ along with integrals for $s > 2$ in the r.h.s. of Eqn (7) has a simple dynamical sense: the functions $F_s$, $s > 2$ are determined such that the integral term in Eqn (7), which they enter, does not take into account the force action from the particle at the point $\mathbf{r}_i$, $1 \leqslant i \leqslant s-1$, which leads ultimately to the appearance of the terms $\mathbf{r}_j$, $i \neq j$ in equation (7) for the function $F_{s-1}$. This can be checked by noticing that according to Eqn (4)

$$F_s(t,1,\ldots,s) = \left\langle \sum_{i_1 \neq \ldots \neq i_s}\prod_{j=1}^{j=s}\delta(\mathbf{r}_j - \mathbf{r}_{i_j}(t))\delta(\mathbf{v}_j - \mathbf{v}_{i_j}(t))\right\rangle. \tag{26}$$

Note that function $F_2$ does not have this 'shortcoming', which is common for functions $F_s$ at $s > 2$.

Thus, the emergence of terms in the BBGKI equations that impede uncoupling is due to the definition of the functions $F_s$ and has nothing to do with the interaction between particles [see Eqns (24), (25)]. Therefore, the procedure of obtaining kinetic equations can be simplified by transiting to a description of relaxation processes using other functions.

However it should be borne in mind that these terms $\widehat{\Lambda}_{s-1}F_{s-1}$ have a dynamical sense as well: they take into account those interparticle interactions that are not accounted for by integral terms in Eqn (7), which is due to the very definition of $s$-particle distribution functions for $s > 2$.

## 7. A novel method of derivation of kinetic equations

Let us explain the basic ideas underlying our approach to derive the kinetic equations. Note first of all that in the method of kinetic equation derivation described above an attempt was made to describe the interaction between particles coming from given distribution functions. As the zero approximation to solve the BBGKI hierarchy, a gas of non-interacting particles was taken, which was used as a basis for representation of the solution in the form of Eqn (13). Thus for some problems we have managed not only to describe the ensemble of systems whose evolution is driven by kinetic equation, but to construct irreversible Bolzmann type equations. At the same time, it is necessary to recognize that time irreversible evolution is related just to interparticle interaction, i.e. from this point of view the use of non-interacting particle gas as a zero approximation seems to be not quite logical. In this connection papers [5, 6] suggested solving in some sense the inverse problem in comparison with what is usually considered when constructing Bolzmann's kinetic equations. Assuming the spatial distribution of 'forces' acting on the particles specified, papers [5, 6] suggest looking for distribution functions that provide some configuration of the 'force' vectors. Such an approach requires introducing the 'extended' distribution functions (see the last paragraph of the preceding section). These are functions that depend, in addition, on particle accelerations. We recall that M Born and A Vlasov first noted the possibility of using the distribution functions but did not use this formalism.

Note that introducing an additional variable, the acceleration, carries us from a $6N$-dimensional phase space into $9N$-dimensional 'extended' phase space in which, as we show below, it is much easier to describe the interaction between particles. In other words, we first 'plunge' into the 'extended' phase space and then 'come' back but only after the system's particles have substantially interacted with each other.

After these introductory remarks we are in a position to derive the kinetic equations for the 'extended' distribution functions.

## 8. Equations for singular 'extended' distribution functions

In the subsequent paragraphs we shall mainly use the method suggested in paper [6] to derive a new class of kinetic equations.

By performing additional differentiation of equations of motion following from Eqn (1) we obtain the system of differential equations

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \quad \frac{d\mathbf{v}_i}{dt} = \mathbf{a}_i, \quad i = \overline{1, N},$$

$$\frac{d\mathbf{a}_i}{dt} = -\frac{1}{m}\sum_{j \neq i}\left(\mathbf{v}_i - \mathbf{v}_j, \frac{\partial}{\partial \mathbf{r}_i}\right)\frac{\partial U(\mathbf{r}_i - \mathbf{r}_j)}{\partial \mathbf{r}_i}, \quad (27)$$

where $\mathbf{a}_i$ is the acceleration of the $i$-th particle.

The system of equations (27) is of higher order than the equations of motions, i.e. it has solutions that do not correspond to any real particle motions. Below we shall show a way to exclude 'non-physical' solutions and hereafter we shall mean only 'physical' solutions of Eqns (27).

In full analogy with Eqns (18), (19) we introduce singular 'extended' distribution functions

$$\Phi_1(t, 1) = \sum_{i=1}^{i=N}\delta(\mathbf{r}_1 - \mathbf{r}_i(t))\delta(\mathbf{v}_1 - \mathbf{v}_i(t))\delta(\mathbf{a}_1 - \mathbf{a}_i(t)), \quad (28)$$

$$\Phi_s(t, 1, \ldots, s) = \Phi_1(t, 1) \ldots \Phi_1(t, s), \quad (29)$$

where $i = (\mathbf{r}_i, \mathbf{v}_i, \mathbf{a}_i)$.

It is easy to check that according to Eqn (27) the functions $\Phi_s$, $s \geqslant 1$ satisfy to equations

$$\left(\frac{\partial}{\partial t} + \widehat{L}_1\right)\Phi_1(t, 1) = C_1^*(t, 1), \quad (30)$$

$$\left(\frac{\partial}{\partial t} + \widehat{L}_1 + \ldots + \widehat{L}_s\right)\Phi_s(t, 1, \ldots, s) = C_s^*(t, 1, \ldots, s), \quad (31)$$

where

$$\widehat{L}_i = \mathbf{v}_i\frac{\partial}{\partial \mathbf{r}_i} + \mathbf{a}_i\frac{\partial}{\partial \mathbf{v}_i},$$

$$C_s^*(t, 1, \ldots, s) = \sum_{i=1}^{i=s}\int \widehat{Q}(i, s+1)$$
$$\times \Phi_{s+1}(t, 1, \ldots, s, s+1)\, d(s+1),$$

$$\widehat{Q}(i, j) = \frac{1}{m}\left[\left(\mathbf{v}_i - \mathbf{v}_j, \frac{\partial}{\partial \mathbf{r}_i}\right)\frac{\partial U(\mathbf{r}_i - \mathbf{r}_j)}{\partial \mathbf{r}_i}, \frac{\partial}{\partial \mathbf{a}_i}\right], \quad i \neq j,$$

and the equation for $\Phi_s$ is valid at $\mathbf{r}_i \neq \mathbf{r}_j$, $1 \leqslant i < j \leqslant s$, and in the integral containing $\widehat{Q}(i, s+1)$, the infinitesimally small neighborhood of point $\mathbf{r}_i$ is omitted.

The appearance of the additional argument in the distribution functions enables the kinetic equations to be constructed by a method that is totally different from Bogolyubov's. Then in the formalism of the theory, constructions that have no analogs in the standard BBGKI hierarchy emerge.

## 9. Method of asymptotic integration

Let us check that in the limit of large time scales $t$, irreversible dynamics appear in the exact equations (30), (31).

Assuming the r.h.s. of Eqn (30) is known, we solve the linear inhomogeneous equation for $\Phi_1$

$$\Phi_1(t, 1) = \exp(-t\widehat{L}_1)\Phi_1(t = 0, 1)$$
$$+ \int_0^t \exp(-\tau\widehat{L}_1)\int \widehat{Q}(1, 2')\Phi_2(t - \tau, 1, 2')\, d2'\, d\tau, \quad (32)$$

where $\Phi_1(t = 0, 1)$ is the 'extended' one-particle distribution function at the time $t = 0$.

Note that the emerged operator $\exp(-t\widehat{L}_1)$ is principally different from that of the free evolution playing an important role in the BBGKI hierarchy. Indeed, it is easy to see that

$$\lim_{t \to \infty}\exp(-t\widehat{L}_1)\Phi_1(t = 0, 1) = 0. \quad (33)$$

Consider equation (33) in more detail. Consider an arbitrary function $g(1) = g(\mathbf{r}_1, \mathbf{v}_1, \mathbf{a}_1)$ satisfying the condition

$$\lim_{\mathbf{v}_1 \to \infty}g(1) = 0.$$

Then by definition of the operator $\exp(-t\widehat{L}_1)$

$$\lim_{t\to\infty} \exp(-t\widehat{L}_1)g(1)$$
$$= \lim_{t\to\infty} g\left(\mathbf{r}_1 - \mathbf{v}_1 t + \frac{\mathbf{a}_1 t^2}{2}, \mathbf{v}_1 - \mathbf{a}_1 t, \mathbf{a}_1\right) = 0, \qquad (34)$$

since for $\mathbf{a}_1 \neq 0$, the operator $\exp(-t\widehat{L}_1)$ increases the speed unboundedly at $t \to \infty$. This is a principal feature of operator $\exp(-t\widehat{L}_1)$ that makes it distinct from the free evolution one. Note that at this stage it is already clear that particles with zero and close to zero value of acceleration play a special role in the system dynamics. Below we consider the role of these particles in more detail and now we only mention that approaching the limit in Eqn (34) is nonuniform due to these particles.

Therefore in the limit of large positive $t$ (during the evolution 'ahead' in time)

$$\Phi_1(t, 1) = \int_0^{+\infty} \exp(-\tau\widehat{L}_1) \int \widehat{Q}(1, 2')$$
$$\times \Phi_2(t - \tau, 1, 2')\, \mathrm{d}2'\, \mathrm{d}\tau, \quad t \gg \tau^* = \frac{v_{\mathrm{ch}}}{a_{\mathrm{ch}}}, \qquad (35)$$

and in the limit of large negative time (during evolution 'back' in time)

$$\Phi_1(t, 1) = \int_0^{-\infty} \exp(-\tau\widehat{L}_1) \int \widehat{Q}(1, 2')$$
$$\times \Phi_2(t - \tau, 1, 2')\, \mathrm{d}2'\, \mathrm{d}\tau, \quad t \ll -\tau^* = \frac{v_{\mathrm{ch}}}{a_{\mathrm{ch}}}, \qquad (36)$$

where $v_{\mathrm{ch}}$ and $a_{\mathrm{ch}}$ are the characteristic velocity and acceleration of a particle, respectively. Note that integrals over $\tau$ in Eqns (35), (36) converge nonuniformly. The nonuniform convergence of these integrals comes, for instance, from nonuniform convergence to the limit in Eqn (34) for small accelerations.

Now we use equations (35), (36) to obtain evolutionary equations for the singular distribution functions in the limit of large time scales. These expressions allows one to make such transformations of evolutionary equations (28) that are not algebraic identities and are valid only due to considering solutions of Eqns (30), (31) on large time scales.

Later we shall use the formalism of generalized functions, so some features that make them distinct from standard continuous functions must be taken into account. First of all, in the generalized function formalism, the products of functions are undetermined when carriers of the factors overlap. In the application to our problem this means that power-law functions of the singular distribution functions under consideration are 'poorly' determined. Indeed, it is easy to see that the product of functions $\delta(x + y)$ and $\delta(x - y)$, $y > 0$ is a correctly determined expression

$$\delta(x + y)\delta(x - y) = 0, \quad y > 0,$$

and $\delta^2(x)$ is an undetermined value. This example also demonstrates the difficulty connected with the limiting transitions in expressions containing generalized functions

$$\lim_{y\to 0} \delta(x + y)\delta(x - y) \neq \delta^2(x).$$

The last note is important for us since any integral, including that entering in Eqns (35), (36), relates to a limiting transition.

Considering all said above, it is necessary to watch attentively the correctness of computations when using expressions (35), (36), since our purpose is to transform $C_s^*$, entering Eqn (31), using these concepts for $\Phi_1$. Difficulties arise when the value of the group of variables $(s + 1)$, over which the integration in Eqn (31) is performed, coincides with that of the group of variables $i$, $1 \leqslant i \leqslant s$. So it is necessary to consider separately the contribution to integral $C_s^*$ (31) from the points $(s + 1) = i$, $i = \overline{1, s}$ and from the rest of the region of the integration $(s + 1) \neq i$, $i = \overline{1, s}$. For this we rewrite $C_s^*$ entering Eqn (31) in the form

$$C_2^* = \widehat{Q}^*(1, 2)\Phi_2(t, 1, 2) + \Phi_1(t, 1)\int \widehat{Q}(2, 2')$$
$$\times \Phi_2(t, 2, 2')\, \mathrm{d}2' + \Phi_1(t, 2)\int \widehat{Q}(1, 2')\Phi_2(t, 1, 2')\, \mathrm{d}2',$$
$$C_s^* = \sum_{1\leqslant i < j \leqslant s} \widehat{Q}^*(i, j)\Phi_s(t, 1, \ldots, i, \ldots, j, \ldots, s)$$
$$+ \sum_{1\leqslant i \leqslant s} \Phi_1(t, 1)\ldots \Phi_1(t, i - 1)\Phi_1(t, i + 1)\ldots \Phi_1(t, s)$$
$$\times \int \widehat{Q}(i, s + 1)\Phi_2(t, i, (s + 1))\, \mathrm{d}(s + 1), \quad s \geqslant 3,$$
$$(37)$$

$$\widehat{Q}^*(i, j) = \frac{1}{m}\left[\left(\mathbf{v}_i - \mathbf{v}_j, \frac{\partial}{\partial \mathbf{r}_i}\right)\frac{\partial U(\mathbf{r}_i - \mathbf{r}_j)}{\partial \mathbf{r}_i}, \frac{\partial}{\partial \mathbf{a}_i} - \frac{\partial}{\partial \mathbf{a}_j}\right], \quad i \neq j,$$

where infinitely small neighborhoods of points $\mathrm{d}(s + 1)$ are excluded from integrals over $i$, $i = \overline{1, s}$.

To avoid confusion, we specially emphasize that Eqn (37) is an identity for the singular distribution functions. In addition, we note that $C_s^*$ can be expressed through singular functions $\Phi_1, \ldots, \Phi_s$ not only according to Eqn (37), but also by many other means. Below it becomes clear where one or another factorization is more convenient, and now let us use Eqn (37) for a while simply as a formal identity.

Note that representation (37) permits us to change $\Phi_1$ by an integral from $\Phi_2$ according to Eqns (35), (36). Thus we have arrived at a system of kinetic equations describing the evolution of the singular distribution functions $\Phi_s$, $s \geqslant 2$ at times $t \geqslant \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$ (evolution 'ahead' in time):

$$\left(\frac{\partial}{\partial t} + \widehat{L}_1 + \ldots + \widehat{L}_s\right)\Phi_s = C_s^+(t, 1, \ldots, s), \quad s \geqslant 2, \quad (38)$$

where

$$C_s^+ = \sum_{1\leqslant i < j \leqslant s} \widehat{Q}^*(i, j)\Phi_s(t, 1, \ldots, i, \ldots, j, \ldots, s)$$
$$+ \sum_{1\leqslant i \leqslant s} \Phi_1(t, 1)\ldots \Phi_1(t, i - 1)\Phi_1(t, i + 1)\ldots \Phi_1(t, s)$$
$$\times \int \widehat{Q}(i, s + 1)\Phi_2(t, i, (s + 1))\, \mathrm{d}(s + 1), \quad s \geqslant 3,$$
$$C_2^+ = \widehat{Q}^*(1, 2)\Phi_2(t, 1, 2) + \Phi_1(t, 1)\int \widehat{Q}(2, 2')$$
$$\times \Phi_2(t, 2, 2')\, \mathrm{d}2' + \Phi_1(t, 2)\int \widehat{Q}(1, 2')\Phi_2(t, 1, 2')\, \mathrm{d}2',$$
$$\Phi_1(t, i) = \int_0^{+\infty} \exp(-\tau\widehat{L}_i) \int \widehat{Q}(i, 2'')\Phi_2(t - \tau, i, 2'')\, \mathrm{d}2''\, \mathrm{d}\tau,$$

as well as at a system of equations determining evolution of singular distribution functions at large negative times

$t \ll -\tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$ (evolution 'back' in time):

$$\left(\frac{\partial}{\partial t} + \widehat{L}_1 + \ldots + \widehat{L}_s\right)\Phi_s = C_s^-(t, 1, \ldots, s), \quad s \geqslant 2, \quad (39)$$

where

$$C_2^- = \widehat{Q}^*(1, 2)\Phi_2(t, 1, 2) + \Phi_1(t, 1)\int \widehat{Q}(2, 2')$$

$$\times \Phi_2(t, 2, 2') \, \mathrm{d}2' + \Phi_1(t, 2)\int \widehat{Q}(1, 2')\Phi_2(t, 1, 2') \, \mathrm{d}2',$$

$$C_s^- = \sum_{1 \leqslant i < j \leqslant s} \widehat{Q}^*(i, j)\Phi_s(t, 1, \ldots, i, \ldots, j, \ldots, s)$$

$$+ \sum_{1 \leqslant i \leqslant s} \Phi_1(t, 1)\ldots\Phi_1(t, i-1)\Phi_1(t, i+1)\ldots\Phi_1(t, s)$$

$$\times \int \widehat{Q}(i, s+1)\Phi_2(t, i, (s+1)) \, \mathrm{d}(s+1), \quad s \geqslant 3,$$

$$\Phi_1(t, i) = \int_0^{-\infty} \exp(-\tau\widehat{L}_i)\int \widehat{Q}(i, 2'')\Phi_2(t-\tau, i, 2'') \, \mathrm{d}2'' \, \mathrm{d}\tau.$$

Of course, equations (35), (36) can be solved for arbitrary $t$. Here it is necessary to understand that this means identifying the initial time moment with $t = -\infty$ for equations (35), and with $t = +\infty$ for equations (36).

We stress that equations (35) and (36) results from asymptotic (for large positive and negative time) integration of exact equations of motion.

## 10. On the relation between one-particle and two-particle distribution functions

In the standard BBGKI hierarchy no ways are known to derive the one-particle distribution function at a time $t$ at a point $\mathbf{r}$ of space from the two-particle distribution function determined at a time close to $t$ in a neighborhood of the point $\mathbf{r}$. The only common relation between $F_1$ and $F_2$ known from the standard BBGKI chain reduces to the equality

$$F_1(t, \mathbf{r}, \mathbf{r}) = \frac{1}{N}\int F_2(t, \mathbf{r}, \mathbf{v}, \mathbf{r}', \mathbf{v}') \, \mathrm{d}\mathbf{v}' \, \mathrm{d}\mathbf{r}', \quad (40)$$

which comes directly from Eqn (4). Expression (40) is extremely awkward: the main contribution to Eqn (4) is due to $\mathbf{r}'$ that differs significantly from $\mathbf{r}$.

From the physical point of view, the two-particle distribution function contains more information on the system dynamics in comparison with the one-particle distribution function, so it seems natural if the one-particle distribution function is expressed through the two-particle one by an 'almost' local operator. Such an operator for the 'extended' distribution functions is given by Eqn (35). This expression is valid only over sufficiently large time scales $t \geqslant \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$, which appears reasonable from physical considerations: particles 'forget' their original states and correlations over the time $\tau^*$ due to interactions, and the formation of 'post-collision' correlations, which arise during the interactions, causes the one- and two-particle distribution functions to be related.

The initial correlations in any dynamical system are more or less arbitrary, while the 'post-collision' ones are determined by the interaction. So the formation of the 'post-collision' correlations should necessarily lead to irreversible dynamics. In the next section we consider this problem in more detail, and now make two important notes.

Firstly, expression (35) is linear both in function $\Phi_1$ and function $\Phi_2$. So the transition in Eqn (32) to smooth distribution functions (probabilistic treatment) $f_1, f_2$, which appears after ensemble averaging of $\Phi_1, \Phi_2$, respectively, can be performed straightforwardly and yields, due to the linear relation between $\Phi_1$ and $\Phi_2$,

$$f_1(t, 1) = \int_0^{+\infty} \exp(-\tau\widehat{L}_1)\int \widehat{Q}(1, 2)f_2(t-\tau, 1, 2) \, \mathrm{d}2 \, \mathrm{d}\tau. \quad (41)$$

Secondly, when deriving Eqns (35) and (41), we never used the smallness of the interparticle interaction, i.e. these expressions are valid for any value of the potential $U(\mathbf{r}_1 - \mathbf{r}_2)$ in Eqn (1). Moreover, the transition to the limit $U \to 0$ in Eqn (35) and (41) is a complicated task: these equations are valid only at $t \geqslant \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$, and at $U \to 0$ time $\tau^* \to +\infty$, but here the potential $U$ enters linearly into operator $\widehat{Q}$. However, in the present paper we shall not specially study the case of small interactions and restrict ourselves to the note made.

We specially pay attention to the principal difference between expression (40) and (41). In Eqn (40), the main contribution to the integral is due to $\mathbf{r}'$, which is significantly different from $\mathbf{r}$. In Eqn (41), the integration is formally performed over arbitrarily large $\mathbf{r}_2$, however because of the presence of a kernel, a region localized in a small neighborhood around point $\mathbf{r}_1$ mainly contributes to the integral. The size of the region mainly contributing to integral (41) is determined by the interparticle interaction in the system. Such a relation between one- and two-particle distribution functions is quite natural. Indeed, the one-particle distribution function is formed due to particles that 'arrived' at a given point in space from other points, but particles cannot 'arrive' at this point from very remote points without having been scattered by other particles. Thus, to determine the one-particle distribution function, it is sufficient to know the two-particle distribution function in a neighborhood with a size of the order of the scale of scattering of particles by force fields. The formalism of extended distribution functions allows us to take these points into account, which removes all difficulties connected with the divergent contribution from four- and higher-order collisions that appears using the conventional approach [9].

## 11. Time irreversibility

Let us make sure that Eqn (38) that appears due to relation (35) between one- and two-particle distribution functions describes irreversible dynamics establishing in dynamical system (1) on large time scales $t \geqslant \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$.

Consider the functions $\Phi_s$, $s \geqslant 2$ satisfying (38) and function $\Phi_1$ determined by Eqn (35) from function $\Phi_2$. We denote this set of functions by $\Phi_s^+$, $s \geqslant 1$. For functions that relate in a similar way to equations (36) and (39) we introduce the notation $\Phi_s^-$, $s \geqslant 1$. We shall use this notation below without special comments. Now introduce the operator of time inversion $\widehat{T}$, i.e. each of the functions $\Phi_s^+$ and $\Phi_s^-$ corresponds to new functions $\widehat{T}\Phi_s^+$ and $\widehat{T}\Phi_s^-$ determined by the relationships

$$(\widehat{T}\Phi_s^+)(t, 1, \ldots, s) = \Phi_s^+(-t, \widehat{T}1, \ldots, \widehat{T}s), \quad (42)$$

$$(\widehat{T}\Phi_s^-)(t, 1, \ldots, s) = \Phi_s^-(-t, \widehat{T}1, \ldots, \widehat{T}s), \quad (43)$$

where $\widehat{T}i = (\mathbf{r}_i, -\mathbf{v}_i, \mathbf{a}_i)$.

Note that such defined functions $\widehat{T}\Phi_s^+$, $s \geqslant 2$ are solutions of equations (39) and functions $\widehat{T}\Phi_1^+$ and $\widehat{T}\Phi_2^+$ are related by Eqn (35). Therefore, the time inversion operator transforms solutions of one set of kinetic equations to those of another set. Thus time irreversibility means that solutions of the kinetic equations describing evolution 'ahead' in time can not generally be transformed by Eqns (42) into solutions of the same kinetic equations. At the same time the equivalence of two time directions in classical mechanics also take place: solutions of system of equations (38) during time inversion transit into the solutions to Eqns (39), and vice versa.

If consider Eqn (30) as a linear inhomogeneous equation relative to $\Phi_1$, then expressions (39), (36) do not describe the general shape of the solution. The general solution represents the sum of a particular solution of equation (30) itself and an arbitrary solution of the corresponding linear homogeneous equation. Equalities (35), (36) appeared from the assumption that the solution of the homogeneous equation [the first term in Eqn (32)] rapidly decreases with increasing $|t|$. Physically this means that $v_{\mathrm{ch}}$ and $a_{\mathrm{ch}}$ can be introduced into the system. This puts some constraints on both the physical system described by Eqn (1) and its states which can be described in a similar way. Indeed, if the Hamiltonian (1) admits an equilibrium state for a given energy, i.e. equations

$$\frac{\partial H}{\partial \mathbf{p}_i} = \frac{\partial H}{\partial \mathbf{r}_i} = 0, \quad i = \overline{1, N}, \tag{44}$$

have solutions, the motion corresponding to the equilibrium state (all particles have zero velocities and zero accelerations) can not be described by Eqns (35) and (36). There are other 'pathological' motions that can not admit the transition from Eqn (35) to Eqn (36). However, for a wide class of systems Eqns (38) and (39) enable irreversible dynamics to be introduced for 'general position' motions, which is of principal importance since it permits the notion of relaxation to be introduced [2].

Let us consider in more detail the physical and mathematical reasons for which the asymptotic integration leads to irreversible dynamics. From the mathematical point of view, irreversibility appears due to the limiting transition, which led to Eqns (35), (36), being nonuniform. This can be easily checked using, for example, Eqn (33); for small $\mathbf{a}_1$ the function

$$\exp(-t\widehat{L}_1)\Phi_1(t = 0, 1)$$

is not small even for very large $t$, i.e. in the space $(\mathbf{r}_1, \mathbf{v}_1, \mathbf{a}_1)$ there are regions in which equalities (35) and (36) are invalid for arbitrarily large $|t|$, but these regions themselves shrink with increasing $|t|$. Physically, such regions relate to particles which are not substantially affected by other particles or their action is compensated, which corresponds to small $\mathbf{a}_1$.

The emerging irreversibility has a clear physical meaning. Because of the limiting transitions performed, particles 'weakly coupled' with other particles of the system were excluded. Note that the exclusion of these particles was realized by a very non-trivial means. First, the effect of low-acceleration particles on other particles of the system was correctly taken into account. (Some 'other' particles of the system can be strongly affected by the low-acceleration particles. For instance, consider three particles at the center and ends of a segment of sufficiently short length; in this case the particle located at the center has zero acceleration, but

significantly affects the particles located at its ends). After that these 'weakly coupled' particles were as if excluded from the system by the limiting transition. In some sense, the 'weakly coupled' particles during such a transition play the role of an external surrounding with respect to other particles. It is easy to see that in this case Kadomtsev's idea on the role of the external noise also remains 'almost' true: there is a source of 'noise' ('external surrounding') in this problem, but it is inside the system itself. At the same time, the irreversibility introduced can be and even must be interpreted in the framework of Kadomtsev's hypothesis.

Note that low-acceleration particles [for the time $t$ low-acceleration particles include those with acceleration smaller than $v_{\mathrm{ch}}/t$, i.e. the larger $t$, the smaller acceleration, since it is these particles that cause the nonuniformity in Eqn, (34)] are very sensitive to even minute external effects. To avoid confusion, we specially emphasize that at different moments of time different particles have a low acceleration, but in the 9-dimensional (three coordinates, three components of velocity, and three components of acceleration) 'extended' phase space of a single particle there are some regions in which arbitrarily small external noise becomes significant, but these regions themselves are small due to the external noise smallness. From this point of view, the method of obtaining irreversible dynamics suggested in this work exactly corresponds to Kadomtsev's idea: any small external and, generally speaking, uncontrolled effect is significant for a small number of 'weakly coupled' particles. Neglecting these particles leads to irreversible dynamics, which is independent of the external effect itself if it is smaller than the interparticle interaction. Thus, this is the external noise that leads to irreversible dynamics, but the irreversible dynamics are independent of the small external noise. Note that this is the consideration of Eqns (35), (36) from the point of view of interaction with 'external' noise that enables the physical content of the nonuniform limiting transition (34) leading to Eqns (35), (36) to become clear.

It is interesting to compare the considered mechanism of irreversible dynamics formation with the properties of the integrating dynamical system (1). Consider, for example, a system of particles with the Hamiltonian (1), in which the interparticle interaction potential $U(\mathbf{r}_1 - \mathbf{r}_2)$ is unable to make it bound, i.e. on large time scales the system 'disintegrates' into separate free particles. An example of such a system is provided by a gas with a short-acting repulsive intermolecular interaction potential. If the system contains $N$ particles, it has $3N$ first integrals in the involution [14]. Projections of particle momentum onto the coordinate frame axes can be taken as such integrals as $t \to +\infty$, i.e. after the disintegration has finished. For a kinetic consideration of such a system it must be significantly changed: introducing the 'walls' described by an external potential should hamper the disintegration $V(\mathbf{r})$. During this procedure equations (30) and (31) preserve their shapes but the definition of the operators $\widehat{L}_i$ alters. Now $\widehat{L}_i$ are determined as

$$\widehat{L}_i = \mathbf{v}_i \frac{\partial}{\partial \mathbf{r}_i} + \left( \mathbf{a}_i - \frac{1}{m} \frac{\partial V(\mathbf{r}_i)}{\partial \mathbf{r}_i} \right) \frac{\partial}{\partial \mathbf{v}_i}. \tag{45}$$

For the operator $\widehat{L}_1$, determined by Eqn (45), relationship (33) is no longer valid since operator $\exp(-t\widehat{L}_1)$ increases or decreases the velocity alternately after collision with the wall. At the same time, assuming infinite size of the system, i.e. $N = +\infty$, we can again use Eqn (33). Thus in the dynamical

systems considered, the asymptotic integration leading to Eqns (35) and (36), automatically assumes the system to have an infinite number of particles, which solves the problem of integration at any finite $N$. Indeed, infinity in $N$ implies infinite time of disintegration, so it proves impossible to construct $3N$ first integrals by the means considered above.

## 12. Introducing smooth distribution functions

Equations (38) and expression (35), which resulted from the asymptotic integration of exact equations (3) and (31), describe the irreversible dynamics using singular distribution functions. However, from the practical point of view it is much more convenient to deal not with generalized but with genuine (continuous) distribution functions. To describe the dynamics by continuous distribution functions, we average Eqns (35), (38) over the ensemble. The transition to a description by continuous distribution functions can be thought of as the transition to a probabilistic treatment of irreversible dynamics, which already emerged in Eqns (35), (38) as a property of the equations of motion over long time intervals.

After these preliminary comments we can pass to a consecutive construction of the probabilistic treatment of classical particle dynamics. First of all we note that in the description of irreversible processes in the dynamical systems that we use, ensemble averaging plays a quite different role compared to that in the BBGKI hierarchy. As shown above, irreversibility in the hierarchy of the 'extended' distribution functions naturally appears without introducing an ensemble of systems provided that only the external noise is taken into account. The hierarchy

$$\langle \Phi_1(t,1) \rangle = f_1(t,1),  \tag{46}$$

$$\langle \Phi_{s+1}(t, 1 \ldots, s, (s+1)) \rangle$$
$$= \left( \sum_{1 \leqslant i \leqslant s} \delta(\mathbf{r}_i - \mathbf{r}_{s+1}) \delta(\mathbf{v}_i - \mathbf{v}_{s+1}) \delta(\mathbf{a}_i - \mathbf{a}_{s+1}) \right)$$
$$\times f_s(t, 1, \ldots, s) + f_{s+1}(t, 1, \ldots, s, (s+1)),$$
$$s > 1, \quad \mathbf{r}_i \neq \mathbf{r}_{s+1}, \quad i = \overline{1, s}, \tag{47}$$

where $f_s$ are smooth 'extended' $s$-particle distribution functions satisfying the equations

$$\left( \frac{\partial}{\partial t} + \widehat{L}_1 \right) f_1(t,1) = \int \widehat{Q}(1,2) f_2(t,1,2) \, \mathrm{d}2,$$
$$\left( \frac{\partial}{\partial t} + \widehat{L}_1 + \ldots + \widehat{L}_s \right) f_s = \widehat{Q}_s f_s + \int \sum_{1 \leqslant i \leqslant s} \widehat{Q}(i, (s+1))$$
$$\times f_{s+1}(t, 1, \ldots, s, (s+1)) \, \mathrm{d}(s+1), \quad s \geqslant 2, \tag{48}$$

and

$$\widehat{Q}_s = \sum_{1 \leqslant i < j \leqslant s} \widehat{Q}^*(i,j).$$

Equations (48) are fully similar to those of the BBGKI hierarchy (7).

Now we use Eqn (35) to obtain a description of the system dynamics in the limit of large time scales $t \gg \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$, which is different from Eqns (48). We introduce the functions

$$f^{(k)}(t_1, 1', 1''; \ldots; t_k, k', k'')$$
$$= \langle \Phi_2^+(t_1, 1', 1'') \ldots \Phi_2^+(t_k, k', k'') \rangle_{\mathrm{r}}, \tag{49}$$

where the subscript $r$ means that regularized averaging is considered, i.e. if two arguments of function $f^{(k)}$ coincide with each other, this means that the product of binary correlation functions with different arguments was averaged, after which the limiting transition was performed. The function $f^{(k)}$ enables functions $f_k$ and $f_{k+1}$ to be represented as integrals on large time scales $t \gg \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$:

$$f_k(t, 1, \ldots, k) = \int_0^{+\infty} \mathrm{d}\tau_1 \ldots \int_0^{+\infty} \mathrm{d}\tau_k \exp\left( -\sum_{i=1}^{k} \tau_i \widehat{L}_i \right)$$
$$\times \int \mathrm{d}1' \ldots \mathrm{d}k' \left( \prod_{i=1}^{i=k} \widehat{Q}(i, i') \right)$$
$$\times f^{(k)}(t - \tau_1, 1, 1'; \ldots; t - \tau_j, j, j'; \ldots; t - \tau_k, k, k'), \tag{50}$$

$$f_{k+1}(t, 1, \ldots, k, k') = \int_0^{+\infty} \mathrm{d}\tau_1 \ldots \int_0^{+\infty} \mathrm{d}\tau_{k-1}$$
$$\times \exp\left( -\sum_{i=1}^{k-1} \tau_i \widehat{L}_i \right) \int \mathrm{d}1' \ldots \mathrm{d}(k-1)' \left( \prod_{i=1}^{i=(k-1)} \widehat{Q}(i, i') \right)$$
$$\times f^{(k)}(t - \tau_1, 1, 1'; \ldots; t - \tau_j, j, j'; \ldots; t - \tau_{k-1}, (k-1),$$
$$(k-1)'; t, k, k'), \tag{51}$$

which follows from Eqn (35).

Thus the integral representations (50), (51) imply that at $t \gg \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$ functions $f_s$ and $f_{s+1}$ are connected by the equations

$$\left( \frac{\partial}{\partial t} + \widehat{L}_1 \right) f_1(t,1) = \int \widehat{Q}(1,2) f_2(t,1,2) \, \mathrm{d}2,$$
$$\left( \frac{\partial}{\partial t} + \widehat{L}_1 + \ldots + \widehat{L}_s \right) f_s(t, 1, \ldots, s)$$
$$= \int \sum_{i=1}^{i=s} \widehat{Q}(i, (s+1)) f_{s+1}(t, 1, \ldots, s, s+1) \, \mathrm{d}(s+1), \quad s > 1. \tag{52}$$

Note that the system of equations (52) is notably different from equations (48), which functions $f_s$ and $f_{s+1}$ satisfy at an arbitrary moment of time. Equations (52) do not contain terms $\widehat{Q}_s f_s$ analogous to the terms $\widehat{\Lambda}_s F_s$ in the BBGKI chain, which cause problems of correct uncoupling of the BBGKI hierarchy. The system of equations of the asymptotic evolution (52) describing relaxation at $t \gg \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$ and containing only integral terms in the r.h.s. is much simpler than the system of equations (48), which allows relaxation treatment at any time, so the relation between these two systems of equations is in order.

## 13. Two stages of evolution of the 'extended' distribution functions and a weak form of the $H$-theorem

Note that the terms $\widehat{Q}_s f_s$, $s \geqslant 2$ in general have no small parameter that allows considering them small compared to the integral terms in the r.h.s. of Eqn (48). At the same time, equations (52) differ from (48) in that they do not contain

$\widehat{Q}_s f_s$, $s \geqslant 2$ in the r.h.s. and describe the evolution correctly only for large time intervals. This leads to the conclusion of qualitatively different dynamics of the system for $t < \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$ and $t \gg \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$. Over the time $t \sim \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$, the initial distribution functions $f_s(t = 0, 1, \ldots, s)$, $s \geqslant 2$ evolve to the functions $f_s(t, 1, \ldots, s)$ that provide smallness of expressions $\widehat{Q}_s f_s(t, 1, \ldots, s) = 0$, $s \geqslant 2$. More precisely, the equalities

$$\lim_{t \to +\infty} \widehat{Q}_s f_s(t, 1, \ldots, s) = 0, \quad s \geqslant 2. \tag{53}$$

must hold. There is some analogy here with the collision integral vanishing in the Boltzmann's type kinetic equations in the process of thermal equilibrium establishing. In the situation under consideration the fulfillment of Eqn (53) is due to 'forgetting' the initial correlations.

Equation (53) for $s = 2$ is of special interest. Note that all equalities considered above remain valid when substituting the operators $\widehat{Q}(i, j)$ by the operators $\widehat{Q}^*(i, j)$. However, on the one hand, Eqn (53) holds, and on the other hand after this substitution, expression $\widehat{Q}_2 f_2$ (by definition, $\widehat{Q}_2 = \widehat{Q}^*$) enters into Eqn (41), but the one-particle distribution function is not zero. From the mathematical point of view we meet here the well-known phenomenon of nonuniform convergence. However in view of the importance of the question we wish to discuss it in more detail. Note that despite the validity of Eqn (34), the integral

$$\int \widehat{Q}^*(1, 1') \exp(-t\widehat{L}_{1'}) g(1') \, \mathrm{d}\mathbf{v}_{1'}$$

should not necessarily tend to zero or become small. Conversely, due to a non-linear in $\mathbf{v}_{1'}$ term in $\widehat{Q}^*(1, 1')$ and differentiation with respect to $\mathbf{a}_{1'}$ that lead to a term $t^2$ emerging, this integral may even tend to infinity at large $t$. Coming back to expression (41), it is easy to see that after this substitution a finite contribution to this integral arises due to the neighborhood of the point $\mathbf{a}_{1'} = 0$. These expressions are very difficult to operate with. However, the form of kinetic equations we use, which has a direct physical sense but is somewhat more awkward due to the difference between operators $\widehat{Q}(i, j)$ and $\widehat{Q}^*(i, j)$, has no such difficulties.

At $t \geqslant \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$ evolution is described by equations (52), with $f_s$, $s \geqslant 2$ all the time very accurately satisfying Eqn (53). Consequently, the disappearance of the term $\widehat{Q}_s f_s$, $s \geqslant 2$ in the r.h.s. of Eqn (48) when studying evolution over large time scales, i.e. when transiting to Eqns (52), is justified by the large value of $t/\tau^*$. Such a different role of integral and out-of-integral terms in the r.h.s. of Eqn (48) becomes natural if we notice that these two different types of terms appear in principally different ways [see comments preceding Eqn (37)].

Thus one more treatment of irreversible relaxation in dynamical systems arises. Any set of initial multi-particle distribution functions evolves 'towards' functions which approximately satisfy Eqn (53). The latter statement should be considered as a weak form of the $H$-theorem, which is however valid in systems with arbitrary value of interaction.

Note that in finite-size systems the transition to the second stage of evolution can be absent in the absence of external noise and under suitable boundary conditions. This can be checked using considerations similar to those used in the section devoted to time irreversibility. We can not enter into more detail in the present paper, but note that in this way a natural interpretation of the results of numerical modeling presented in [3] can be suggested.

It should be stressed that the appearance of two qualitatively different stages of evolution is obtained using the 'extended' distribution function formalism. Below this issue will be addressed on the basis of the treatment of kinetics by standard distribution functions.

We recall that Bogolyubov's method supposes that all multi-particle distribution functions become functionals of a one-particle distribution function beginning from some time moment. This assumption naturally leads to different stages in the evolution of distribution functions. The first stage lasts until this time moment, the second stage starts after this time. In some papers the second stage is subdivided into two substages, kinetic and hydrodynamic [15]. Such an 'axiomatic' approach leads to some difficulties, the most well-known being the so-called 'non-adiabaticity' of slow modes. If in the system there are modes with large characteristic times, they have no time to follow the evolution of one-particle distribution functions and require a special consideration. For example, hydrodynamic modes show this feature. A lot of papers address this issue. In our approach presented in this paper we have proved (not supposed!) that starting from some time moment, a one-particle distribution function (and below we shall see that higher-order distribution functions as well) is expressed through a two-particle distribution function. In this approach, no 'non-adiabaticity' problem for slow modes appears, but the kinetic equations obtained turn out to be much more complicated.

## 14. Uncoupling the system of equations of the asymptotic evolution

The asymptotic evolution equations (52), as well as the BBGKI hierarchy, represent an infinite set of coupled linear integro-differential equations relating $s$- and $(s + 1)$-particle distribution function for arbitrary natural number $s$. First we use a not very rigorous but visual means of uncoupling kinetic equations (48) and (52), which allows us to understand the physical sense of the uncoupling, and then we point to a more formal approach. One can try to find solutions to Eqn (52) in the form

$$f_s(t, 1, \ldots, s) = \prod_{i=1}^{i=s} f_1(t, i), \tag{54}$$

but such distribution functions are in no way subject to relations (53). Of course, in some dynamical systems having small parameters, the treatment of dynamics with the use of Vlasov's equations, which result from Eqns (54), can be well justified. However, in the general case another approach is required to uncouple kinetic equations (48) and (52). To this end, we use a small parameter that appears in the system dynamics at large time scales due to large value of $t/\tau^*$ and provides the transition from Eqn (48) to (52).

In the Appendix we consider in more detail the way of uncoupling the equations for the extended distribution functions. However, it seems relevant here to discuss the main differences of this method of uncoupling from those based on the idea of 'molecular chaos', i.e. on the representation of higher-order distribution functions through a one-particle distribution like Eqn (12) and (13). The 'molecular chaos' hypothesis assumes the possibility at *any* time moment of considering atoms non-correlated before collisions. It is this physical assumption that is equivalent to factorizations (12) and (13) and the like for higher-order distribution functions. Here the non-trivial part of the hypothesis is just

that it is valid at any time moment. In other words, it is necessary to prove the validity of such an approach over large time scales when interparticle interactions are present. The justification of the possibility of such a consideration represents the main (but not the only) problem when constructing kinetic equations. Attention should be paid to the 'molecular chaos' hypothesis being not allowed by the choice of 'general position' initial conditions. This hypothesis is a significant dynamical assumption and requires a sufficiently deep study of multi- particle system dynamics.

Now we wish to address this point from a somewhat different point of view. Notice that in the BBGKI hierarchy this is the non-integral terms in the r.h.s. of Eqn (5) that can violate the 'molecular chaos' hypothesis while the integral terms in the r.h.s. of Eqn (5) do not lead to any difficulty when justifying this hypothesis. The transition to the extended distribution function changes the situation in a principal way. Indeed, in equations for the extended distribution functions (48) there are non-integral terms that are fully analogous to terms in the BBGKI hierarchy, which create difficulties in justifying the 'molecular chaos' hypothesis. However, it is a purely formal similarity. The point is that on large time scales these terms in the equations for the extended distribution functions vanish according to the weak form of the *H*-theorem [see Eqn (53)]:

$$\lim_{t \to +\infty} \widehat{Q}_s f_s(t, 1, \ldots, s) = 0, \quad s \geqslant 2 \,.$$

Thus, introducing the extended distribution functions radically changes the problem of uncoupling the infinite chain of coupled equations describing multi-particle system dynamics. It turns out that the use of the extended distribution functions enables us to effectively eliminate the terms preventing the uncoupling in the large evolution time scale limit. Considering this we arrive at a closed kinetic equation for the two-particle distribution function

$$\left( \frac{\partial}{\partial t} + \widehat{L}_1 + \widehat{L}_2 \right) f_2(t, 1, 2) = \widehat{Q}^*(1, 2) f_2(t, 1, 2)$$
$$+ D(t, 1, 2) + D(t, 2, 1) \,, \quad (55)$$

and also at the equations allowing higher-order extended distributions to be calculated through the two-particle distribution function

$$\left( \frac{\partial}{\partial t} + \widehat{L}_1 + \ldots + \widehat{L}_s \right) f_s = \widehat{Q}_s f_s$$

$$+ \sum_{1 \leqslant i \leqslant s} f_{s-1}(t, 1, \ldots, i-1, i+1, \ldots, s)$$

$$\times \int \widehat{Q}\big(i, (s+1)\big) f_2(t, i, (s+1)) \, \mathrm{d}(s+1) \,, \quad s \geqslant 3 \,, \quad (56)$$

Expressions (55) and (56) answer Ulenbeck's question on the possibility of expressing all distributions through the two-particle one [15]. Indeed, relation (41) enables the one-particle distribution to be expressed through the two-particle one, Eqn (55) is a closed equation for the evolution of the two-particle distribution, and equations (56) provide us with the possibility to express the higher-order distributions via the two-particle one. To avoid misunderstanding we point out that the special role of the two-particle distribution function is caused by only systems with two-particle interaction potential being considered in the present paper.

## 15. Physical sense of the 'extended' distribution function formalism

Let us discuss the physical reasons for the possibility of finding a closed kinetic equation for the extended distribution functions.

Note that any extended distribution function contains the 'information' which can be obtained only knowing all the infinite chain of ordinary distribution functions (indeed, even a one-particle distribution function enables $\langle \mathbf{a} \rangle^{2n}$ to be computed for any $n$, although to calculate this average $(2n+1)$-particle standard distribution function $F_{2n+1}$ should be specified).

In real systems with an infinite number of particles even the entire infinite chain of multi-particle distribution functions does not totally describe the dynamics. We specially emphasize that such a situation takes place only for $N = +\infty$. Note that to compute the value of $\langle |\mathbf{a}|^r \rangle$ where $r$ is a non-integer number in an $N$-particle system the function $F_N$ should be used.

Thus the information on the non-integer moments of the acceleration is lost in systems with an infinite number of particles when treating them by standard distribution functions. The latter seems strange if we note that in the equations of motion the transition to the limit $N \to +\infty$ occurs comparatively easily, and the function $\rho$ becomes a function determined over infinite space, i.e. $\rho$ becomes a very 'unpleasant' object from the point of view of mathematics.

At the same time, the information on the non-integer moments of accelerations is contained in the extended distribution functions. However, even the entire infinite chain of distribution functions does not contain all the information on the classical system dynamics. Considering non-integer moments of, e.g., derivatives of the acceleration can check it. The incompleteness of treatment of dynamics by functions $f_s$, $s \geqslant 1$ makes the time irreversible character of relations (41) natural. The presence of additional information in $f_2$ compared to that contained in the whole infinite chain of standard multi-particle distribution functions permits us to understand why closed kinetic equations can be found comparatively easily for $f_2$.

## 16. Additional constraints on the 'extended' distribution functions

Kinetic equations for the 'extended' distribution functions are obtained from equations (27), which follow from the equations of motion. However, the order of the system of equations (27) is $9N$, i.e. exceeds that of the equations of motion, which is $6N$. Therefore, solutions of system of differential equations (27) depend on $9N$ independent constants, while those of the true differential equations of motion depend only on $6N$ arbitrary constants ($3N$ coordinates and the same number of velocities at the initial moment of time). Thus it is necessary to exclude from consideration the solutions of Eqn (27) that do not correspond to any real motions of physical particles. For this, it is enough to take into account that the particle acceleration at the initial time is determined by Newton's second law. The 'non-physical' solutions also exist for kinetic equations (48), (52) and they can be rejected by imposing similar constraints on the extended distribution functions. For example, the one-particle distribution function must be additionally subjected to the condition

$$\mathbf{a}_1 \Phi_1(t, 1) = -\frac{1}{m} \int \frac{\partial U(\mathbf{r}_1 - \mathbf{r}_2)}{\partial \mathbf{r}_1} \Phi_2(t, 1, 2) \, \mathrm{d}2 \,, \tag{57}$$

which according to Eqn (35) reduces at $t \geqslant \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$ to

$$\mathbf{a}_1 \int_0^{+\infty} \exp(-\tau \widehat{L}_1) \int \widehat{Q}(1, 2) \Phi_2(t - \tau, 1, 2) \, \mathrm{d}2 \, \mathrm{d}\tau$$
$$= -\frac{1}{m} \int \frac{\partial U(\mathbf{r}_1 - \mathbf{r}_2)}{\partial \mathbf{r}_1} \Phi_2(t, 1, 2) \, \mathrm{d}2 \,. \tag{58}$$

Note that if Eqn (57) is initially satisfied, it holds in future as well. Thus relation (58) should be considered as a bound on the initial conditions.

We recall that expression (35) itself is valid only for 'physical' and solutions close to them (27). Indeed, the transition from Eqn (32) to (35) is possible only provided that $v_{\mathrm{ch}}$ increases in time more slowly than $a_{\mathrm{ch}}t$, which is violated for the solutions (27) that strongly differ from those having a physical sense. If consider only 'strictly' physical solutions for an isolated system, $v_{\mathrm{ch}}$ does not depend on time at all. Thus expression (35) is necessarily valid for physical solutions and closed to them.

## 17. Transition to Boltzmann's equation

Let us ascertain that equations (55) and (56) allows the transition to Boltzmann's equation. First of all, note that Boltzmann's equation does not allows the correct description of fluctuations and takes into account only binary collisions [10]. However, many specific features of particle motion are explicitly accounted for in Boltzmann's equation (it is sufficiently to note that Boltzmann's equation explicitly contains not the interparticle interaction potentials but the binary collision cross-sections). Thus the problem of the transition from Eqn (55) and (56) to Boltzmann's equation is separated into two stages. First, it is necessary to specify which approximation in equations (55) and (56) Boltzmann's equation corresponds to, and second, in this approximation it is necessary to make a transition to the parameters that enter Boltzmann's equation. The first stage has a principal meaning and the second stage is of a purely technical character.

First of all, we point to the approximation in which the transition from equations (55) and (56) to Boltzmann's can be performed. To this aim we shall find the solutions in the form

$$f_n(1, 1, \ldots, n) = F_n(t, 1^-, \ldots, n^-) F_n^{(\delta)}(t, 1^{(\delta)}, \ldots, n^{(\delta)}) \,, \tag{59}$$

where $f_n$ is the extended $n$-particle distribution function, $F_n$ is the ordinary $n$-particle distribution function, $F_n^{(\delta)}$ is a new function subjected to the condition

$$\int F_n^{(\delta)}(t, 1^{(\delta)}, \ldots, n^{(\delta)}) \, \mathrm{d}\mathbf{a}_n = F_{(n-1)}^{(\delta)}(t, 1^{(\delta)}, \ldots, (n-1)^{(\delta)}) \,,$$

$i = (\mathbf{r}_i, \mathbf{v}_i, \mathbf{a}_i)$, $i^- = (\mathbf{r}_i, \mathbf{v}_i)$ and $i^{(\delta)} = (\mathbf{r}_i, \mathbf{a}_i)$. Note that neglecting fluctuations, solutions of the form (59) must exist in equations (55) and (56) at least for local thermodynamic equilibrium. Indeed, due to the local thermodynamic equilibrium, velocities are separated from accelerations according to the Gibbs distribution for classical particle systems, and due to neglecting fluctuations one can state that this 'separation' occurs at any time, not on average in time.

Now substitute expressions for $f_n$ given by Eqn (59) into equations (5) and (56). Integrating the resulting equations

over accelerations with account of the additional constraints that appear in analogy with (57), yields equations of the standard BBGKI hierarchy for the functions $F_n(t, 1^-, \ldots, n^-)$, and integrating over velocities enables us to arrive at equations for the functions $F_n^{(\delta)}(t, 1^{(\delta)}, \ldots, n^{(\delta)})$. Note that the equations for the functions $F_n^{(\delta)}(t, 1^{(\delta)}, \ldots, n^{(\delta)})$ depend on integrals contained in the integrands $F_n(t, 1^-, \ldots, n^-)$ and the equations for $F_n(t, 1^-, \ldots, n^-)$, which coincide with the standard BBGKI hierarchy, are independent of the functions $F_n^{(\delta)}(t, 1^{(\delta)}, \ldots, n^{(\delta)})$. Thus any justified means of uncoupling the standard BBGKI hierarchy near the thermal equilibrium state neglecting fluctuations enables the determination of both functions $F_n^{(\delta)}(t, 1^{(\delta)}, \ldots, n^{(\delta)})$ and $F_n(t, 1^-, \ldots, n^-)$, i.e. allows the corresponding solutions of Eqn (55) and (56) to be found. Consequently, in this particular class of solutions (59), equations (55) and (56) indeed transit to Boltzmann's equation. In other words, the closed form kinetic equation (55), being more general compared to Boltzmann's kinetic equation, enables the applicability region of the latter equation to be specified from the point of view of the degree of non-equilibrium of the medium, which can still be described by Boltzmann type kinetic equations.

## 18. Time irreversibility and the probabilistic treatment of dynamics

Let us turn once again to the relation between time irreversibility and the probabilistic treatment of dynamics. The method discussed in this paper allowed us to introduce irreversible evolution as a property of dynamics on large time scales. The transition to the probabilistic treatment of irreversible dynamics of a multi-particle system required a sufficiently detailed description of the event space. The lack of any information on the event space is a significant shortcoming of the approach to deriving Boltzmann's equation using the molecular chaos idea; this shortcoming was noted by M A Leontovich [10].

Time irreversibility has only been shown as a property of the operator $\widehat{T}$ to transform solutions of one system of equations into solutions of another system of equations. The transition to smooth distribution functions has permitted us to formulate the weak form of the $H$-theorem, i.e. to find a class of functions 'toward which' initial multi-particle distribution functions evolve. At the same time, we have not managed to construct Lyapunov's functional for the irreversible equations obtained. In fact, it is hard to expect some value increasing in time at each point of space to be associated with equation (55). Indeed, since equation (55) correctly describes fluctuations, it admits evolution in different directions, both toward an equilibrium (a stationary state) and away from it. To avoid confusion, we point out once again that equations of Boltzman's type admitting the $H$-theorem can not correctly take into account fluctuations [10]. This follows at least from the fact that when deriving these kinetic equations the true interparticle interactions are substituted by an interaction with particles of an 'averaged' ensemble representative.

## 19. Conclusions

The problems emerging when relating kinetic theory and mechanics reduce to two main difficulties of quite different nature. Firstly, these are difficulties due to using probabilistic

concepts and the relaxation notion in classical mechanics; secondly, the difficulties related to the necessity of determining class of dynamical system to which kinetic theory results can be applied [2]. To solve these problems, different approaches are suggested, which are based, as a rule, on sufficiently complex properties of dynamical systems. They appeal to the notions of dynamical chaos, phase space mixing, ergodicity, etc. In comparison with these fairly complex theories, which often use deep results of dynamical system theory, B B Kadomtsev's ideas relying upon clear physical concepts seem somewhat naive at the first glance. So even more unexpected is the fact that the elaboration of these ideas provides us with an answer to the questions which have not been answered for a long time using other approaches.

First of all, we note that Kadomtsev's ideas, which require 'external noise', enable a clear description of the reasons for irreversibility to appear in statistical mechanics. Indeed, in a system with a large number of particles there are particles that interact with other particles of the system more weakly than with the external noise. This implies that the acceleration caused by the interaction with the external noise is greater than the acceleration due to interaction with other particles.

The number of such particles is small because of the smallness of interaction with the external surroundings, and their acceleration is mainly determined by the uncontrolled value of the external noise. So from the physical point of view it would be desirable to construct a description (let it be approximate) of the dynamics of the system that neglects these particles because of their small number relative to the total number of particles in the system.

The problem is that at different instants of time different particles fall into the class of low-acceleration particles. To handle this technical difficulty, it is convenient to introduce particle acceleration as a new 'independent' variable and consider the problem in the 'extended' phase space thus formed.

In the present paper we have shown that neglecting these 'weakly coupled' particles in fact leads to irreversible dynamics, which turn out universal, i.e. independent of the specific external noise. From the mathematical point of view the problem of description of the dynamics of a multi-particle system neglecting low-acceleration particles was considered. Such a setting of the problem is new in kinetic theory and its interpretation relies upon Kadomtsev's ideas on the external noise role in establishing irreversible dynamics.

Let us discuss in more detail the principal role of low-acceleration particles. Notice that the external noise affects, of course, both the small number of low-acceleration particles and other particles of the system. Thus a multi-particle system consists of a large number of particles (almost all particles of the system) for which the external noise is only a small perturbation, and of a small number of particles (small because of the small value of the external noise) whose acceleration, oppositely, is determined mostly by the external noise.

So the question arises as to what is more significant for dynamics of the system on large time scales, the external noise effect on a small number of particles which is comparable with the interparticle interaction, or the small (compared to the interparticle interaction) influence of the external noise on other particles of the system.

In the framework of the formalism discussed in this paper, neglecting the relatively small number of particles with a low acceleration due to interaction with other particles of the

system in comparison with the acceleration due to the external noise, leads to the selection of a certain type of solution for distribution functions (see Section 11). After that the external noise effect on other particles can be accounted for by a perturbation theory constructed for these solutions. Interestingly, the possibility of phase 'breaks' due to system interaction with the external irreversible surrounding and of the selection of a certain type of solutions, was recognized earlier in quantum mechanics.

In paper [1] Kadomtsev wrote: "Now assume that the gas under consideration weakly interacts with an irreversible external surrounding. The first and main effect of such an interaction is the violation of the precise phase relations between converging and diverging waves. A so-called phase break occurs. A corresponding effect can be called the 'collapse' of the wave function".

Kadomtsev believed that the 'first and main' effect of the interaction with the external irreversible surrounding is that the induced phase 'break' (the violation of exact phase relations) differently affects the 'converging' and 'diverging' waves. In fact, Kadomtsev's argumentation is very sophisticated, and statements pulled out of the context can be erroneously understood. Nevertheless, we cite one of the main results of his analysis. With account of interaction with the irreversible external surrounding, only some solutions of the Schrödinger equation describing multi-particle problem dynamics have physical sense.

Consider this point in more detail. Note that the Schrödinger equation is a first-order equation in time, so specifying the initial conditions determines absolutely the subsequent evolution of the system. However, the account of a small external noise, i.e. some action on the system, makes it open. On large time scale only such solutions of the Schrödinger equation that are stable in some sense with respect to this noise 'survive'. Other solutions are 'attracted' to them, which does not violate any dynamical principle, since the account of the external noise makes the system open and dissipative.

This is the possibility of the gradual transformation of some solutions to the Schrödinger equation into other ones under the action of the external noise, i.e. the 'attraction' of unstable with respect to the external noise solutions to 'stable' ones, that leads to a specific principle of 'selection' of solutions and introduces irreversibility into quantum mechanical problems [1].

Here the possibility of irreversibility emerging by the same mechanism (due to the selection of solutions of the required type) in classical mechanics remained completely unnoticed. Probably, such a situation emerged due to the linearity of the Schrödinger equation and 'wave' analogs being apparently quite natural, while equations of motion in classical mechanics are non-linear. However, Liouville's equation, the BBGKI chain equations or equations for the 'extended' distribution functions are also linear equations, which makes it not surprising that irreversibility appears in a similar way.

Using Kadomtsev's understanding of the problem of statistical mechanics foundation we managed to show that irreversible evolution appears in the 'extended' distribution function formalism as a natural property of the dynamics of a system of classical particles on large time scales. The probabilistic treatment of dynamics in this time interval is only a convenient formal tool that allows us to avoid using generalized function formalism. The larger the time scales ($t \gg \tau^*$), the more justified the use of this treatment seems. A

kinetic equation is obtained that describes evolution of the 'extended' two-particle distribution function and provides us with an analytical description of irreversible dynamics of the system of classical particles. Thus dynamical consideration makes it possible to justify the 'molecular chaos' hypothesis and to find a form for it that can be used not only for gases.

In this paper we have ascertained that the development of B B Kadomtsev's ideas on the nature of irreversibility leads to a novel setting of the problem of foundation of statistical physics, and have also already permitted us to solve some problems, which can not be solved by other methods. Unfortunately, in spite of a physical clarity and the possibility of a formal description, Kadomtsev's ideas have not yet been widely recognized and generally accepted. Undoubtedly, they are of a great interest and possibly represent the most adequate approach to solve this problem.

## 20. Appendix

Note first of all that the BBGKI hierarchy, as well as the systems of equations (48), (52), can be treated by different means. They can be considered as being evolutionary equations for multi-particle distribution functions. However, a different point of view is possible. Since the equation for an $s$-particle distribution function contains an $(s+1)$-particle distribution function, it can be considered as an integro-differential equation that allows the determination of $(s+1)$-particle distribution function using function $f_s$, $s \geqslant 1$. Notice that the latter point of view is possible only for a system with an infinite number of particles $N = +\infty$. In a system containing a finite number of particles $N$ the equation for an $N$-particle distribution function, which coincides with Liouville's equation, does not allow such an interpretation. In addition, the second interpretation of coupled infinite chains appeals to the problem of solvability of the corresponding linear integro-differential equations.

Bogolyubov's method of uncoupling uses both these interpretations of the BBGKI hierarchy. To calculate the function $G_2$ determined according to Eqn (13), it is sufficient to require that the equation for the two-particle distribution function, which is considered as an integro-differential equation relative to the function $G_3$, has a solution $G_3 \ll G_2$. The function $G_2$ found in this way permits us to determine $F_2$ according to Eqn (13) and to obtain, as was shown by Bogolyubov, Boltzmann's kinetic equation and its analogs for other media.

To apply Eqns (48) or (52) to the final part of the first and second stages of the evolution by the 'extended' distribution functions, we subject the three-particle distribution function to the integro-differential equation

$$\int \widehat{Q}(1,3) f_3(t,1,2,3)\, \mathrm{d}3 + \int \widehat{Q}(2,3) f_3(t,1,2,3)\, \mathrm{d}3$$
$$= f_1(t,1) \int \widehat{Q}(2,3) f_2(t,2,3)\, \mathrm{d}3 + f_1(t,2)$$
$$\times \int \widehat{Q}(1,3) f_2(t,1,3)\, \mathrm{d}3 . \qquad (A.1)$$

In other terms, we write down evolutionary equations for $f_1$ and $f_2$ in the form

$$\left(\frac{\partial}{\partial t} + \widehat{L}_1\right) f_1(t,1) = \int \widehat{Q}(1,2) f_2(t,1,2)\, \mathrm{d}2 , \qquad (A.2)$$

$$\left(\frac{\partial}{\partial t} + \widehat{L}_1 + \widehat{L}_2\right) f_2(t,1,2)$$
$$= f_1(t,1) \int \widehat{Q}(2,3) f_2(t,2,3)\, \mathrm{d}3 + f_1(t,2)$$
$$\times \int \widehat{Q}(1,3) f_2(t,1,3)\, \mathrm{d}3 . \qquad (A.3)$$

Equation (A.1) will be used as the integro-differential equation to determine $f_3$ and Eqn (48) for $s \geqslant 3$ will be considered as integro-differential equations for the functions $f_{s+1}$, $s \geqslant 3$:

$$\left(\frac{\partial}{\partial t} + \widehat{L}_1 + \ldots + \widehat{L}_s\right) f_s(t,1,\ldots,s)$$
$$= \int \sum_{i=1}^{i=s} \widehat{Q}(i,(s+1)) f_{s+1}(t,1,\ldots,s,s+1)\, \mathrm{d}(s+1), \quad s \geqslant 3 .$$
$$(A.4)$$

First of all, we note that in a system with an infinite number of particles $N = +\infty$ equations (A.1)–(A.4) do not contradict the integral relation between functions $f_s$ and $f_{s+1}$, $s \geqslant 1$

$$\int f_{s+1}(t,1,\ldots,s,(s+1))\, \mathrm{d}(s+1) = N f_s(t,1,\ldots,s) . \quad (A.5)$$

Thus the question of the existence of an ensemble with dynamical properties described by Eqns (A.1)–(A.4) reduces to the problem of the solvability of the corresponding integro-differential equations that determine $f_s$, $s \geqslant 3$. Unfortunately, with the literal understanding, equation (A.1) has no solutions. Considering, for example, a system of particles with infinitely strong repulsion at zero distance can easily check it. In this case $f_3 = 0$ at $\mathbf{r}_1 = \mathbf{r}_2$ and the l.h.s. vanishes at $\mathbf{r}_1 = \mathbf{r}_2$, whereas the r.h.s. of Eqn (A.1) takes a non-zero value. However, for our purposes it is sufficient if there is a solution to Eqn (A.1) in the small parameter limit providing the transition from Eqn (48) to Eqn (52). Simple physical considerations allow us to ascertain that a solution of Eqn (A.1) thus understood really exists.

Instead of a system of particles described by the Hamiltonian (1), let us consider a related new system of particles with the potential of interparticle interactions $g^2 U$, mass $gm$, and concentration $n/g$, where $g \to +0$. Note that as $g \to +0$ the evolution of multiparticle distribution functions is described by just the system of equations (52). Thus the second stage of the evolution of extended distribution functions means that inside this time interval the system of particles can be treated in a 'continuous' limit, and the larger the value of $t/\tau^*$, the more accurate such a description is. Consequently, the study of distribution functions of the actual problem can be substituted by the study of the distribution function of the 'continuous' model. For a fixed characteristic velocity of particles with mass $gm$, the 'temperature' is $gT$ and the energy of binary interaction of particles of the 'continuous' model is determined by the value $g^2 U$ as $g \to 0$. In the considered 'continuous' model the effective temperature $gT$ is much exceeds the binary interaction energy $g^2 U$. This enables the studied infinite chain of equations for the extended distribution function to be uncoupled. Thus in the 'continuous' model an ensemble must exist for which the following relations hold

$$\int \widehat{Q}(1,3) f_3(t,1,2,3) \, d3 = f_1(t,2) \int \widehat{Q}(1,3) f_2(t,1,3) \, d3 \, , \tag{A.6}$$

$$\int \widehat{Q}(2,3) f_3(t,1,2,3) \, d3 = f_1(t,1) \int \widehat{Q}(2,3) f_2(t,2,3) \, d3 \, . \tag{A.7}$$

Equalities (A.6), (A.7) and the relation of the 'continuous' model with evolution of a real system of particles on large time scales provide the solvability of Eqns (A.1), (A.4) in the above sense. In other words, the existence of an ensemble that satisfies to Eqns (A.6), (A.7) for the 'continuous' model provides solvability of integro-differential equations (A.1) and (A.4) in the limit of large $t/\tau^*$. We stress once again that functions $f_1$ and $f_2$ evolve in such a way that the region of 27-dimensional space (1, 2, 3) where solutions of the integro-differential equations (A.6), (A.7) exist shrinks with increasing $t/\tau^*$. Therefore, in the limit of large ratio $t/\tau^*$ the transition from Eqn (48) to (A.1)–(A.4) is fully justified. By solving Eqn (A.2) with respect to $f_1$ at $t \geqslant \tau^* = v_{ch}/a_{ch}$, which leads to Eqn (41), and by substituting the obtained expression for $f_1$ into Eqn (A.3), we get a kinetic equation for the function $f_s$, $s \geqslant 2$ (see explications below),

$$\left( \frac{\partial}{\partial t} + \widehat{L}_1 + \widehat{L}_2 \right) f_2(t,1,2) = \widehat{Q}^*(1,2) f_2(t,1,2)$$
$$+ D(t,1,2) + D(t,2,1), \quad (\Pi.8)$$

$$\left( \frac{\partial}{\partial t} + \widehat{L}_1 + \ldots + \widehat{L}_s \right) f_s = \widehat{Q}_s f_s$$
$$+ \sum_{1 \leqslant i \leqslant s} f_{s-1}(t, 1, \ldots, i-1, i+1, \ldots, s)$$
$$\times \int \widehat{Q}\big(i, (s+1)\big) f_2\big(t, i, (s+1)\big) \, d(s+1), \quad s \geqslant 3 \, ,$$

$$D(t,1,2) = \int_0^{+\infty} \exp(-\tau \widehat{L}_1) \int \widehat{Q}(1,1') f_2(t-\tau,1,1') \, d1' \, d\tau$$
$$\times \int \widehat{Q}(2,2') f_2(t,2,2') \, d2' \, .$$

Note that Eqn (A.8) is a non-linear kinetic equation relative to function $f_2$ and equations for higher- order distribution functions are linear integro-differential equations.

We specially note that the terms $\widehat{Q}_s^* f_s$, $s \geqslant 2$ are kept in Eqn (A.8) and its analogs for higher-order distribution functions. If only the second stage of evolution is to be described, such terms must be omitted. However, the description of the final stage of evolution requires these terms to be conserved as well. Notice that kinetic equation (A.8) is simultaneously the definition of the ensemble these kinetic equations describe. Indeed, the uncoupling used is justified in the limit of an infinitely large time, i.e. when Eqn (53) is satisfied. From this point of view, these kinetic equations describe such an ensemble in which the terms $\widehat{Q}_s^* f_s$, $s \geqslant 2$, vanishing on finite time scales, yield corrections to functions $f_s$, $s \geqslant 2$ in accordance with the equations under consideration. Note that the kinetic equations obtained do not contradict relation (A.5).

The method described in the main text of the paper represents another approach to justifying the uncoupling of equations for the extended distribution functions. Note that expressions (A.6) and (A.7) are valid *a priori* for such ensembles in which distribution functions are close to a set of $\delta$-functions, in other words, in ensembles which are composed from a narrow neighborhood of some point of the phase space. This can always be achieved for the initial moment of time. Let us choose the neighborhood to be sufficiently narrow that by the time the non-integral terms in the chain of equations become small enough according to Eqn (53), equations (A.6) and (A.7) are again satisfied with a good accuracy. However, then equations (A.6) and (A.7) will be held in future as well, which allows us to perform uncoupling according to the scheme discussed above.

Note that in the approach used the 'interaction' between particles of different ensemble representatives appeared from using only equations of motion, after obtaining the irreversible dynamics [see Eqns (41), (52)]. However, the irreversibility in (A.8) can also be interpreted in the language of the 'intersystem' interaction introduced by Eqn (A.1). Thus it is shown that the irreversibility that results from only the dynamics of a system of classical particles in the limit of large times, can be interpreted as an 'interaction' between particles of different representatives of the ensemble, i.e., as explained above, in agreement with the 'molecular' chaos hypothesis. Therefore, the approach used permits us to justify the 'molecular' chaos hypothesis and to formulate it correctly Eqn (A.1) when the interparticle interaction is not small.

The physical reason for the possibility of effective use of factorization (A.1) is that the integro-differential equation (A.1) has no solutions for $\mathbf{r}_1$ close to $\mathbf{r}_2$. However, for $U(r) \to \infty$, when $r \to 0$, a tiny fraction of particles approach each other so closely. The impossibility of constructing a solution due to the smallness of the number of particles is not a significant obstacle.

Notice that Eqn (A.8) can be arrived at by a different way. According to Eqn (35), function $f_3$ for $t \geqslant \tau^* = v_{ch}/a_{ch}$ can be written as

$$f_3(t,1,2,3) = \int_0^{+\infty} \exp(-\tau \widehat{L}_1) \int \widehat{Q}(1,1')$$
$$\times \big\langle \Phi_2(t-\tau,1,1') \Phi_2(t,2,3) \big\rangle \, d1' \, d\tau \, . \tag{A.9}$$

Assuming that the substitution

$$\big\langle \Phi_2(t-\tau,1,1') \Phi_2(t,2,3) \big\rangle$$
$$= \big\langle \Phi_2(t-\tau,1,1') \big\rangle \big\langle \Phi_2(t,2,3) \big\rangle, \tag{A.10}$$

is permitted in the integrand of expression (A.9), we again arrive at equation (A.8). However, factorization (A.10) is invalid in the general case, which follows at least from the fact that at $\tau = 0$ the l.h.s. of expression (A.10) is symmetric relative to any permutation of the groups of variables $1, 1', 2, 3$, and the r.h.s. is not. However, in some problems with a small parameter, such values of $\tau$ mostly contribute to the integral (A9), in which the quantities $\Phi_2(t-\tau,1,1')$ and $\Phi_2(t,2,3)$ can be considered independent, which allows us to justify Eqn (A.10).

Note that if function $f_2$ slowly changes over the time $\tau^* = v_{ch}/a_{ch}$, functions $D(t,1,2)$ and $D(t,2,1)$ allow an appreciable simplification. By computing the integral over $\tau$ that determines these functions, we can neglect the time dependence of the two-particle distribution function, i.e.

write

$$\left(\frac{\partial}{\partial t} + \widehat{L}_1 + \widehat{L}_2\right)f_2(t,1,2) = \widehat{Q}^*(1,2)f_2(t,1,2)$$

$$+ D(t,1,2) + D(t,2,1)\,, \quad (A.11)$$

where

$$D(t,1,2) = \int_0^{+\infty} \exp(-\tau\widehat{L}_1)\int\widehat{Q}(1,1')f_2(t,1,1')\,\mathrm{d}1'\,\mathrm{d}\tau$$

$$\times \int\widehat{Q}(2,2')f_2(t,2,2')\,\mathrm{d}2'\,.$$

Thus, in the case considered, the evolution of the two-particle distribution function is fully determined by its value at the same moment of time.

Additional conditions, which should be imposed on the 'extended' distribution functions to select physically reasonable solutions (see the main text), can be used to transit to the description of the dynamics by the standard distribution functions. To obtain the standard $s$-particle distribution function from the 'extended' $s$-particle distribution function, the latter should be integrated over all accelerations. Considering the above, we integrate the equation for the $s$-particle distribution function from the system of equations (48) over all accelerations which are present in the function $f_s$, which yields

$$\frac{\partial}{\partial t}\int f_s(t,1,\dots,s)\,\mathrm{d}\mathbf{a}_1\dots\mathrm{d}\mathbf{a}_s$$

$$+ \int\widehat{L}_1 f_s(t,1,\dots,s)\,\mathrm{d}\mathbf{a}_1\dots\mathrm{d}\mathbf{a}_s + \dots$$

$$+ \int\widehat{L}_s f_s(t,1,\dots,s)\,\mathrm{d}\mathbf{a}_1\dots\mathrm{d}\mathbf{a}_s = 0\,, \quad s \geqslant 1\,. \quad (A.12)$$

In view of the fact that for all distribution functions analogs to expression (53)

$$\mathbf{a}_i f_s(t,1,\dots,i,\dots,s) = -\frac{1}{m}\sum_{j=1,j\neq i}^{j=s}\frac{\partial U(\mathbf{r}_i - \mathbf{r}_j)}{\partial \mathbf{r}_i}$$

$$\times f_s(t,1,\dots,i,\dots,j,\dots,s) - \frac{1}{m}\int\frac{\partial U(\mathbf{r}_i - \mathbf{r}_{s+1})}{\partial \mathbf{r}_i}$$

$$\times f_{s+1}\big(t,1,\dots,i,\dots,s,(s+1)\big)\,\mathrm{d}(s+1)\,, \quad (\Pi.13)$$

are fulfilled, the expression

$$\int\mathbf{a}_i f_s(t,1,\dots,i,\dots,s)\,\mathrm{d}\mathbf{a}_1\dots\mathrm{d}\mathbf{a}_s\,,$$

which enters Eqn (A.12), can be rewritten with account of Eqn (A.13), after which equations (A.12) exactly transform into the BBGKI chain of equations. Note that integrating the asymptotic evolution equations (52) over all accelerations, we again get equation (A.12), and the use of Eqn (A.13) again leads to the BBGKI hierarchy. Thus the description of relaxation processes by the standard distribution functions is too rough to note two principally different stages of the evolution, which we considered above in detail. It is due to this fact that, without making use of equations for the 'extended' distribution functions, the 'hidden' small para-

meter relating to a large value of $t/\tau^*$ and leading to the transition from Eqn (48) to (52) remains unnoticed, which enables the disruption of the infinite chain of equations using Eqn (A.1) and the transition to Eqn (55). However, if the uncoupling is possible, it can be performed without using the 'extended' distribution functions.

Indeed, as follows from the considerations that led us to Eqn (A.6), (A.7), these relations somewhat stronger than Eqns (A.6), (A.7) are satisfied:

$$f_1(t,1)\int\left[\left(\mathbf{v}_2 - \mathbf{v}_3,\frac{\partial}{\partial\mathbf{r}_2}\right)\frac{\partial U(\mathbf{r}_2 - \mathbf{r}_3)}{\partial\mathbf{r}_2}\right]f_2(t,2,3)\,\mathrm{d}3$$

$$= \int\left[\left(\mathbf{v}_2 - \mathbf{v}_3,\frac{\partial}{\partial\mathbf{r}_2}\right)\frac{\partial U(\mathbf{r}_2 - \mathbf{r}_3)}{\partial\mathbf{r}_2}\right]f_3(t,1,2,3)\,\mathrm{d}3\,, \quad (A.14)$$

$$f_1(t,2)\int\left[\left(\mathbf{v}_1 - \mathbf{v}_3,\frac{\partial}{\partial\mathbf{r}_1}\right)\frac{\partial U(\mathbf{r}_1 - \mathbf{r}_3)}{\partial\mathbf{r}_1}\right]f_2(t,1,3)\,\mathrm{d}3$$

$$= \int\left[\left(\mathbf{v}_1 - \mathbf{v}_3,\frac{\partial}{\partial\mathbf{r}_1}\right)\frac{\partial U(\mathbf{r}_1 - \mathbf{r}_3)}{\partial\mathbf{r}_1}\right]f_3(t,1,2,3)\,\mathrm{d}3\,. \quad (A.15)$$

Let us integrate Eqns (A.14), (A.15) over the accelerations $\mathbf{a}_1$, $\mathbf{a}_2$ to transit in these expressions from the 'extended' to the standard distribution functions

$$F_1(t,1)\int\left[\left(\mathbf{v}_2 - \mathbf{v}_3,\frac{\partial}{\partial\mathbf{r}_2}\right)\frac{\partial U(\mathbf{r}_2 - \mathbf{r}_3)}{\partial\mathbf{r}_2}\right]F_2(t,2,3)\,\mathrm{d}3$$

$$= \int\left[\left(\mathbf{v}_2 - \mathbf{v}_3,\frac{\partial}{\partial\mathbf{r}_2}\right)\frac{\partial U(\mathbf{r}_2 - \mathbf{r}_3)}{\partial\mathbf{r}_2}\right]F_3(t,1,2,3)\,\mathrm{d}3\,, \quad (A.16)$$

$$F_1(t,2)\int\left[\left(\mathbf{v}_1 - \mathbf{v}_3,\frac{\partial}{\partial\mathbf{r}_1}\right)\frac{\partial U(\mathbf{r}_1 - \mathbf{r}_3)}{\partial\mathbf{r}_1}\right]F_2(t,1,3)\,\mathrm{d}3$$

$$= \int\left[\left(\mathbf{v}_1 - \mathbf{v}_3,\frac{\partial}{\partial\mathbf{r}_1}\right)\frac{\partial U(\mathbf{r}_1 - \mathbf{r}_3)}{\partial\mathbf{r}_1}\right]F_3(t,1,2,3)\,\mathrm{d}3\,. \quad (A.17)$$

Thus equations (A.16), (A.17) should be considered as integral equations for the determination of function $F_3(t,1,2,3)$, and the evolution of functions $F_1(t,1)$ and $F_2(t,1,2)$ is described by the first two equations of the BBGKI hierarchy:

$$\left(\frac{\partial}{\partial t} + \widehat{l}_1\right)F_1 = \widehat{A}(1,2)F_2(t,1,2)\,\mathrm{d}2\,, \quad (A.18)$$

$$\left(\frac{\partial}{\partial t} + \hat{l}_1 + \hat{l}_2\right)F_2 = \widehat{A}_2 F_2 + \int\sum_{1\leqslant i\leqslant 2}\widehat{A}(i,3)F_3(t,1,2,3)\,\mathrm{d}3\,.$$

$$(A.19)$$

The system of equations (A.16)–(A.19) is an analog of the kinetic equation (A.18), however for irreversibility to be introduced and a closed form equation for $F_2$ to be obtained, it is necessary to explicitly find a solution to the integral equations (A.16), (A.17) and to study the character of solutions (A.18), (A.19) at $t \geqslant \tau^* = v_{\mathrm{ch}}/a_{\mathrm{ch}}$. Now the advantages of the 'extended' distribution functions become clear. Firstly, for this formalism no explicit solutions to equations (A.6), (A.7) have been necessary, and secondly, the one-particle distribution function has easily been expressed through the 'extended' two-particle distribution function, which easily permitted us to obtain time irreversible dynamics.

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