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Homogeneous generalized master equation retaining initial correlations

Victor F Los

Institute of Magnetism, National Academy of Sciences of Ukraine, 36-B Vernadsky Str., 03142 Kiev, Ukraine

E-mail: V.Los@ulrmc.org.ua

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Abstract
Using the projection operator technique, the exact homogeneous generalized master equation (HGME) for the relevant part of a distribution function (statistical operator) is derived. The exact (mass) operator governing the evolution of the relevant part of a distribution function and comprising arbitrary initial correlations is found. Neither the Bogolyubov principle of weakening of initial correlations with time nor any other approximation such as random phase approximation has been used to obtain the HGME. These approximations are usually used to derive the approximate homogeneous equation for the relevant part of a distribution function from the conventional exact generalized master equation (GME), which has a source containing the irrelevant part (initial correlations). The HGME does not have a source and contains only the linear, relative to the relevant part of a distribution function, terms of the GME modified by the dynamics of initial correlations. The obtained equation is valid on any timescale, for any initial moment of time and any initial correlations. In particular, it describes the short-time behaviour and allows for treating the influence of initial correlations consistently. As an example, we have considered a dilute gas of classical particles. By selecting the appropriate projection operator, we have derived the homogeneous equation for a one-particle distribution function retaining initial correlations in the linear approximation on the small density parameter and for the space homogeneous case. This equation allows for considering all stages of the time evolution. It converts into the conventional Boltzmann equation on the appropriate timescale if the contribution of all initial correlations vanishes on this timescale.

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1. Introduction

Deriving the kinetic equations from the microscopic dynamical equations of classical or quantum mechanics is one of the principal tasks of statistical physics. A kinetic equation in a common sense is a Markovian closed equation for a one-particle (or other relatively slowly changing) distribution function (or statistical operator) containing no many-particle (fast changing) distribution functions and describing an irreversible approach of the system under consideration to an equilibrium state. Generally, it is of interest to get an equation for a reduced distribution function (statistical operator), which is necessary and sufficient for calculating the average value of functions of the dynamical variables. A reduced distribution function (statistical operator) depends on a much smaller number of variables than the original distribution function, which depends on the total amount of variables necessary for the microscopic dynamical description of the entire system. The problem of getting an equation for a one-particle or reduced distribution function lies in an interaction of a particle or a subsystem under consideration with the rest of a whole system. In other words, the correlations in a many-body system is the main issue to deal with.

There are several ways of obtaining the kinetic equations. One can start with the Liouville–von-Neumann equation for a distribution function (statistical operator) of the entire system, and by integrating out all unnecessary variables get the chain of coupled first-order differential equations for many-particle distribution functions known as the BBGKY hierarchy. In order to obtain a kinetic equation for a one-particle distribution function from the BBGKY hierarchy, it is necessary to decouple the chain in some approximation using some small parameter: for example, a small interaction between particles or a density of the system. The most consistent approach to decoupling the BBGKY hierarchy was developed by Bogolyubov [1]. He suggested the principle of weakening of the initial correlations which implies that on a large enough timescale, $t - t_0 \gg t_{\text{cor}}$ (t_{cor} is the correlation time), the initial (existing at the initial time moment t_0) correlations damp. Assuming that the initial correlations vanish at $t - t_0 \gg t_{\text{cor}}$, it is possible to obtain from the BBGKY the Boltzmann equation in the first approximation in n and the corrections to it in the next approximations.

In another approach, leading to the so-called generalized master equation (GME) [2, 3], a distribution function or statistical operator is divided by means of a projection operator into the relevant and irrelevant parts. The relevant part, which is mainly of interest, is, as a rule, a vacuum (slowly changing) part of a distribution function (statistical operator), i.e. the part with no correlations. Trying to get the equation for the relevant part of a distribution function, one arrives at the GME, which is the exact integra-differential non-Markovian equation for the relevant part with a source containing the irrelevant part including all many-particle correlations at the initial moment t_0. To exclude many-particle correlations (a source), Bogolyubov's principle of weakening of initial correlations or the random phase approximation (RPA) may be employed, and it results in the approximate homogeneous linear equation for the relevant part of a distribution function (statistical operator). By means of an appropriate choice of a projection operator, an equation for the specific relevant part of a distribution function can be obtained from this equation. Expansion in some small parameter then results in a corresponding kinetic equation: for example, in the Pauli master equation. The same master equation technique can be applied for obtaining the equations for correlation functions.

One more approach worthy of mention is based on the Kadanoff–Baym equations for the two-time correlation functions. The original Kadanoff–Baym equations [4] do not contain initial correlations and follow from the exact equations for correlation functions under the assumption of Bogolyubov's principle of weakening of initial correlations.

All kinetic equations which follow from that principle are unable to describe the initial stage of the evolution, $t_0 \leqslant t \leqslant t_{\rm cor}$. Therefore, the influence of initial correlations, which can be important for, for example, the ultrafast relaxation processes, is not described by these equations. Moreover, the timescale $t \lesssim t_{\rm cor}$ may be of significant interest, because we expect that on this timescale the transition from the short-term 'non-kinetic' evolution of a multi-particle system to the long-term 'kinetic' behaviour occurs.

To overcome this shortcoming of kinetic equations, several approaches have been proposed. Grabert *et al* [5] used the path integral technique and obtained the exact solution for the reduced density matrix and equilibrium two-time correlation functions of the oscillator interacting with a heat bath for a large (but specific) class of initial states. In our papers [6] new equations of the evolution for the density matrix and equilibrium two-time correlation functions for a subsystem interacting with a reservoir were obtained. We made use of the exponential form of the Gibbs equilibrium distribution function, serving as the initial state, in order to obtain by means of the projection operator technique the exact homogeneous generalized master equations for the density matrix and correlations functions of a subsystem interacting with a heat bath. Craig [7] and Hall [8] used a generalized perturbation theory, which incorporates initial correlations, and derived the generalized Kadanoff–Baym equations. A more comprehensive approach has been proposed by Danielewicz [9] who developed a perturbation theory for a general initial state and derived generalized Kadanoff–Baym equations accounting for initial correlations. In [10], a generalization of the Kadanoff–Baym equations, which is not based on a perturbation theory and allows for including arbitrary initial correlations, has been presented.

In this paper, the exact homogeneous generalized master equation (HGME) for the relevant part of a distribution function (statistical operator) is derived. No approximation (like RPA) or principle (like Bogolyubov's principle of weakening of initial correlations) has been used in deriving this equation. Unlike the GME, it is homogeneous, i.e. has no source containing the irrelevant (comprising correlations) part of a distribution function. Instead, the arbitrary initial correlations and their dynamics are incorporated into the coefficients of the corresponding terms of the GME, linear relative to the relevant part of a distribution function. The HGME allows for description of all stages of the evolution of the relevant part of a distribution function including the consistent treatment of the influence of initial correlations on this process. In section 2, a derivation of the HGME for the relevant part of a distribution function (statistical operator) is presented. In section 3, by means of the appropriate choice of the projection operator, we derive from the HGME the equation for a one-particle distribution function in the linear approximation in the density of a dilute gas of the strongly interacting classical particles. For simplicity, the space homogeneous case is considered. This equation contains the additional terms related to a dynamics of initial correlations. In section 4 we demonstrate how and under which conditions the obtained equation for a one-particle distribution function converts into the conventional Boltzmann equation. General conclusions are presented in section 5.

2. Homogeneous generalized master equation

Let us consider the Liouville–von-Neumann equation for a distribution function (statistical operator) $F(t)$ of N interacting particles

$$\frac{\partial}{\partial t}F(t) = LF(t) \tag{1}$$

where $F(t)$ is a symmetric function of N variables $x_i = (\boldsymbol{x}_i, \boldsymbol{p}_i)$ $(i = 1, \ldots, N)$ representing the coordinates and momenta of the particles in the case of classical mechanics or the statistical operator $\rho(t)$ in the case of quantum mechanics, L is the Liouville operator acting on $F(t)$ as

$$LF(t) = \{H, F(t)\}_{\mathrm{P}} = \sum_{i=1}^{N} \left\{ \frac{\partial H}{\partial \boldsymbol{x}_i} \frac{\partial F(t)}{\partial \boldsymbol{p}_i} - \frac{\partial H}{\partial \boldsymbol{p}_i} \frac{\partial F(t)}{\partial \boldsymbol{x}_i} \right\} \tag{2}$$

in the case of classical mechanics ($\{H, F(t)\}_{\mathrm{P}}$ is the Poisson bracket), while L is the operator acting on $\rho(t)$ as

$$L\rho(t) = \frac{1}{\mathrm{i}\hbar}[H, \rho(t)] \tag{3}$$

in the case of quantum mechanics ($[H, \rho(t)]$ is a commutator), and H is the Hamilton function (Hamiltonian) for the system under consideration.

A distribution function F and a statistical operator $\rho(t)$ satisfy the normalization conditions

$$\int \mathrm{d}x_1 \cdots \int \mathrm{d}x_N F(x_1, \ldots, x_N, t) = 1 \qquad \mathrm{Tr}\,\rho(t) = 1 \tag{4}$$

where the integration over the dynamical states x_i of each particle is performed over a whole phase space volume Ω_V. The phase space of each particle corresponds to an arbitrary momentum $\boldsymbol{p}_i$ and coordinate $\boldsymbol{x}_i$ limited by a system volume V.

It is convenient to break a distribution function (in what follows the same is applicable to a statistical operator) into the relevant $f_{\mathrm{r}}(t)$ and irrelevant $f_{\mathrm{i}}(t)$ parts by means of a projection operator P ($P^2 = P$)

$$\begin{aligned} &F(t) = f_{\mathrm{r}}(t) + f_{\mathrm{i}}(t) \\ &f_{\mathrm{r}}(t) = PF(t) \qquad f_{\mathrm{i}}(t) = QF(t) \end{aligned} \tag{5}$$

where $Q = 1 - P$ is a complementary to the P projection operator ($Q^2 = Q$). A projection operator is selected from the physical point of view for each problem under consideration, as we will see below.

Applying the projection operators P and Q to equation (1), it is easy to obtain the equations for f_{r} and f_{i}, defined by (5),

$$\frac{\partial}{\partial t} f_{\mathrm{r}}(t) = PL[f_{\mathrm{r}}(t) + f_{\mathrm{i}}(t)] \tag{6}$$

$$\frac{\partial}{\partial t} f_{\mathrm{i}}(t) = QL[f_{\mathrm{r}}(t) + f_{\mathrm{i}}(t)]. \tag{7}$$

A formal solution to equation (7) is

$$f_{\mathrm{i}}(t) = \int_{t_0}^{t} \exp[QL(t - t_1)]QLf_{\mathrm{r}}(t_1)\,\mathrm{d}t_1 + \exp[QL(t - t_0)]f_{\mathrm{i}}(t_0) \tag{8}$$

where t_0 is the initial moment of time when the initial condition for the Liouville–von-Neumann equation (1) should be set. Inserting this solution into (6), we obtain the exact GME for the relevant part of a distribution function [2, 3]

$$\frac{\partial}{\partial t} f_{\mathrm{r}}(t) = PLf_{\mathrm{r}}(t) + \int_{t_0}^{t} PL\exp[QL(t - t_1)]QLf_{\mathrm{r}}(t_1)\,\mathrm{d}t_1 + PL\exp[QL(t - t_0)]f_{\mathrm{i}}(t_0). \tag{9}$$

The conventional GME (9) contains the irrelevant part of a distribution function at the initial moment t_0, $f_{\mathrm{i}}(t_0) = QF(t_0)$. Because the relevant part of a distribution function (statistical operator) is commonly associated with the part which contains no correlations (or with other relatively slowly changing part of a distribution function), the irrelevant part comprises all correlations. Thus, equation (9) is the linear inhomogeneous integra-differential equation for the relevant part of a distribution function (statistical operator) with the source containing all initial multi-particle correlations. Therefore, we have not reached a complete reduced description of a multi-particle system in terms of relevant (reduced) distribution function.

In order to get from (9) a kinetic equation in a common sense, which includes only the relevant part of a distribution function, one needs to handle somehow the irrelevant part of a distribution function $f_{\mathrm{i}}(t_0)$. To avoid dealing with the source in (9) describing initial correlations, one may choose the initial condition in such a way that it contains no correlations, i.e. $f_{\mathrm{i}}(t_0) = 0$, which corresponds to the RPA. But this condition does not look very natural. Moreover, it arbitrarily singles out some moment t_0 when a distribution function $F(t)$ is replaced by its relevant part. To get rid of the latter, the limiting procedure $t_0 \to -\infty$ is often used, which serves as a boundary condition and introduces an irreversibility into the Liouville equation [1, 11].

The most physically consistent approach to getting rid of initial correlations was proposed by Bogolyubov [1] and is based on the suggestion that all initial correlations vanish beyond some time interval exceeding the correlation time t_{cor}, $t - t_0 \gg t_{\mathrm{cor}}$. A correlation time t_{cor} for a system of N interacting particles is of the order of $r_0/\bar{v}$, where r_0 is a radius of an inter-particle interaction and $\bar{v}$ is mean particle velocity.

Thus, according to the principle of weakening of initial correlations, for a large enough time exceeding the correlation time t_{cor} the irrelevant part of the initial value of a distribution function $f_{\mathrm{i}}(t_0)$ can be neglected, and (9) becomes the homogeneous equation for the relevant part of a distribution function. This homogeneous equation is approximate, valid only on a large enough timescale $t - t_0 \gg t_{\mathrm{cor}}$ and is still non-Markovian, i.e. it is not a kinetic equation in a conventional sense. But if, for example, the relaxation time t_{rel} for the relevant part $f_{\mathrm{r}}(t)$ is much larger than t_{cor}, $t_{\mathrm{rel}} \gg t_{\mathrm{cor}}$, equation (9) can be reduced to the Markovian kinetic equation for the relevant part of a distribution function using a perturbation theory on the small parameter $t_{\mathrm{cor}}/t_{\mathrm{rel}} \ll 1$. Moreover, at $t - t_0 \gg t_{\mathrm{cor}}$ the upper limit of integration in (9) can be extended to infinity, and this equation becomes time irreversible. Therefore, the time hierarchy $t_{\mathrm{rel}} \gg t_{\mathrm{cor}}$ may be essential for obtaining the conventional kinetic equation.

On the other hand, the initial stage of the evolution $t_0 \leqslant t \leqslant t_{\mathrm{cor}}$ is very interesting and essential for understanding the irreversibility problem. We can expect that on the timescale $t \lesssim t_{\mathrm{cor}}$ a multi-particle system begins 'forgetting' the starting (initial) conditions for its evolution and passes from 'non-kinetic' reversible stage into 'kinetic' irreversible stage of the evolution if the specific conditions are met. A progress achieved in the classical mechanics makes it possible, in principle, to study the entire evolution process on any timescale and to determine the conditions under which a system evolves towards the equilibrium state. The behaviour of a system distribution function depends on the properties of a system dynamics. If, for example, there is a mixing ergodic flow in a phase space caused by the local (stochastic) instability of the system's dynamics, then the initial correlations vanish exponentially with the characteristic time t_{cor}. Therefore, in principle, we may try to consider the entire evolution process with the help of the exact GME (9) and not using the approximations like Bogolyubov's principle of weakening of initial correlations or RPA. To do that, we should include into consideration the dynamics of initial correlations.

Thus, in order not to jump over the initial stage of the evolution $t_0 \leqslant t \leqslant t_{\mathrm{cor}}$, one could try to find a solution to equation (9) according to general rules of integration of inhomogeneous integral equations. But equation (9) is very complicated and includes the multi-particle ($N \gg 1$) distribution function $f_{\mathrm{i}}(t_0)$ depending on a much larger number of variables than the relevant distribution function f_{r}. The operators governing the time evolution of f_{r} and f_{i} are also very complicated. One way to simplify the GME (9) is to expand in series on some small parameter: for example, a density of the system or a small inter-particle interaction parameter. However, the expansion of a source in equation (9) or in the solution to this equation may appear not to be effective and may lead to the convergency problem. Moreover, the integration of equation (9) may result in the so-called 'secular terms' [1] essential at $t \sim t_{\mathrm{cor}}$ (they may come from the term of a solution containing a source). These problems may necessitate the summation of infinite series of terms. As is well known, the mentioned problems do not appear if one deals with a homogeneous equation. The series expansion of a coefficient (mass operator) at the unknown function in a homogeneous equation is much more effective and corresponds, in general, to the summation of infinite series of terms in an inhomogeneous equation. Thus, as a rule, to deal with a homogeneous equation is easier than with an inhomogeneous one.

Having all that in mind, we may consider the following problem. Is it possible to find an exact HGME describing the time evolution of the relevant part of a distribution function (statistical operator)? In other words, one may wish to have the linear equation of the type

$$\frac{\partial}{\partial t} f_{\mathrm{r}}(t) = (\pounds * f_{\mathrm{r}})_{t,t_0} \tag{10}$$

i.e. to define a linear (generally integral and time-dependent) operator £ acting on the relevant part f_{r} and governing its time evolution. It would be surprising if we could find such an operator in explicit form for any relevant part of a distribution function (any projection operator P) and any initial correlations as an exact consequence of the Liouville–von-Neumann equation (1). It is clear that if equation (10) is exact, an operator £ should comprise in some way the initial correlations. If we manage to get such an equation, it will provide a substantial mathematical advantage and a new consistent approach to dealing with initial correlations. Incorporating the initial correlations into the linear in $f_{\mathrm{r}}(t)$ terms is equivalent to reorganizing the structure of the GME (9) in such a way that the initial correlations are exactly included into the operator £, which is a kind of 'mass' operator acting on $f_{\mathrm{r}}(t)$. It is well known that a formal introduction of a 'mass' operator allows one to close (see, for example, [4]) the equation for the relevant part of a distribution function (for example, a one-particle distribution function) by reorganizing and summing the infinite series of expansion of the corresponding quantities, which provides a more powerful approach in terms of the perturbation theory.

We now will show that the exact HGME (10) for the relevant part of a distribution function (statistical operator) does exist and can be obtained on the arbitrary timescale, i.e. not using the principle of weakening of initial correlations. The proposed procedure allows transfer of the irrelevant part of a distribution function (initial correlations) from the source of equation (9) into the additional terms of the operator acting on the relevant part of a distribution function (statistical operator). As a result, we obtain the exact HGME. The structure of the obtained HGME shows explicitly how the initial correlations influence the flow, collision and other terms of the conventional GME. How this approach works we will see later. Particularly, in order to get a kinetic equation from the obtained HGME, some small parameter related to the time hierarchy may be needed.

In order to obtain a homogeneous equation for the relevant part of a distribution function, we will use the additional equation connecting the irrelevant part at an initial moment of time $f_{\mathrm{i}}(t_0) = QF(t_0)$ (entering the source of the master equation (9)) with a distribution function at time t, $F(t) = f_{\mathrm{r}}(t) + f_{\mathrm{i}}(t)$. It is easy to see that

$$f_{\mathrm{i}}(t_0) = C_0 \exp[-L(t-t_0)][f_{\mathrm{r}}(t) + f_{\mathrm{i}}(t)] \tag{11}$$

where the (operator) function C_0 defines a parameter related to the irrelevant part of a distribution function at $t = t_0$

$$C_0 = [QF(t_0)]F^{-1}(t_0) = f_{\mathrm{i}}(t_0)[f_{\mathrm{r}}(t_0) + f_{\mathrm{i}}(t_0)]^{-1}. \tag{12}$$

It is essential to note that C_0 (12) is always less than unity.

Now, we have two equations, (8) and (11), connecting $f_{\mathrm{i}}(t)$ with $f_{\mathrm{i}}(t_0)$. Finding $f_{\mathrm{i}}(t_0)$ from these equations and inserting it into (9), we obtain the following equation for the relevant part of a distribution function:

$$\frac{\partial}{\partial t} f_{\mathrm{r}}(t) = PLR(t) f_{\mathrm{r}}(t) + \int_{t_0}^{t} PLR(t) \exp[QL(t-t_1)] QL f_{\mathrm{r}}(t_1)\,\mathrm{d}t_1 \tag{13}$$

where the function $R(t)$ is defined as

$$\begin{aligned} R(t) &= 1 + \mathrm{e}^{QL(t-t_0)} \frac{1}{1 - C_0 \mathrm{e}^{-L(t-t_0)} \mathrm{e}^{QL(t-t_0)}} C_0 \mathrm{e}^{-L(t-t_0)} \\ &= \frac{1}{1 - C_0(t-t_0)} \\ C_0(t-t_0) &= \mathrm{e}^{QL(t-t_0)} C_0 \mathrm{e}^{-L(t-t_0)}. \end{aligned} \tag{14}$$

Equation (13) is the main result of this section. It is the equation of equation (10) type with the operator £ easily defined by (13) and (14). Thus, the exact operator governing the time evolution of the relevant part of a distribution function does exist ($|C_0(t-t_0)| < 1$) in the explicit and closed form for arbitrary initial correlations and depends on their evolution in time. If initial correlations dampen with time, then the operator £ becomes independent of them.

The HGME (13) is different from the GME (9) in several important respects. It is the exact homogeneous equation for the relevant part of a distribution function while retaining the initial correlations. The initial correlations enter the HGME (13) through the function $R(t)$ (14). This function represents a sum of the infinite series of expansion in the properly defined time-dependent parameter $C_0(t-t_0)$ which emerges in equation (13) and describes the influence of initial correlations in time. Presence of the function $R(t) \neq 1$ in equation (13) has led to modification of the first term in the right-hand side of the GME (9) as well as the second (collision) term. This modification reflects the influence of initial correlations on the corresponding processes (flow and relaxation) with time. It does not seem easy to get directly from conventional GME (9) such a picture of the influence of initial correlations and their dynamics on the evolution of the relevant part of a distribution function (it is evident from (14) that the infinite series should be summed). The HGME also allows for treating the correlations arising from collisions and initial correlations on the equal footing by expanding the operator £ in series on some small parameter.

The same result is valid for the relevant part of a statistical operator $\rho_{\mathrm{r}}(t)$ if we use in (13) and (14) the rule (3) of action of L on an arbitrary operator instead of rule (2), as follows from the Liouville–von-Neumann equation (1).

Let us now try to get from (13) the equation for some specific system.

3. Equation for a one-particle distribution function with initial correlations

In this section we consider a gas of N ($N \gg 1$) interacting identical classical particles. It is supposed that the Hamiltonian of the system can be split into two parts

$$\begin{aligned} H &= H^0 + H' \\ H^0 &= \sum_{i=1}^{N} H_i^0 \qquad H_i^0 = \frac{\boldsymbol{p}_i^2}{2m} \\ H' &= \sum_{i<j=1}^{N} V_{ij} \qquad V_{ij} = V(|\boldsymbol{x}_i - \boldsymbol{x}_j|). \end{aligned} \tag{15}$$

Here, H^0 describes an ideal gas of noninteracting particles having the momenta $\boldsymbol{p}_i$ and mass m, and the Hamiltonian of interaction between particles H' is supposed to be a sum of potentials V_{ij} dependent only on the difference of coordinates of two particles. We will not suppose here that the interaction is weak and will take that all usual necessary requirements to the properties of forces by which particles interact with each other are met. Particularly, we suppose that the bound states are not formed (an interaction is repulsive).

To obtain the equation of evolution in this case, we will presume that the density of particles n is small enough and will use a perturbation theory with respect to the small parameter

$$\gamma = r_0^3 n \ll 1 \tag{16}$$

where r_0 is the effective radius of an inter-particle interaction. This small parameter guarantees that collisions between particles are well separated events and defines the time hierarchy, because $t_{\text{cor}}/t_{\text{rel}} \sim \gamma \ll 1$.

First of all, we have to define the projection operator P selecting the relevant part $f_{\text{r}}(t)$ of the N-particle distribution function $F(t)$. It is easy to see that the required projection operator is

$$P = \left[\prod_{i=2}^{N} f_1(x_i)\right] \frac{1}{V^{N-1}} \int \mathrm{d}x_2 \cdots \int \mathrm{d}x_N. \tag{17}$$

Here, $f_1(x_i)$ is an one-particle distribution function

$$f_1(x_i, t) = V \int \mathrm{d}x_1 \cdots \int \mathrm{d}x_{i-1} \int \mathrm{d}x_{i+1} \cdots \int \mathrm{d}x_N F(x_{1,\ldots,}x_N, t) \tag{18}$$

taken at the initial time moment, $f_1(x_i) = f_1(x_i, t_0)$. In (18) a symmetry of distribution function relative to a permutation of space-phase coordinates is taken into account.

In general, the s-particle distribution function is defined as

$$f_s(x_1, \ldots, x_s, t) = V^s \int \mathrm{d}x_{s+1} \cdots \int \mathrm{d}x_N F(x_1, \ldots, x_N, t). \tag{19}$$

From conditions (4) we have the normalization conditions for the reduced distribution functions f_s

$$\int \mathrm{d}x_1 \cdots \int \mathrm{d}x_s f_s(x_1, \ldots, x_s, t) = V^s. \tag{20}$$

Applying the projection operator (17) to the distribution function $F(t)$, we get the following relevant part f_{r}:

$$f_{\text{r}} = \frac{1}{V^N}\left[\prod_{i=2}^{N} f_1(x_i)\right] f_1(x_1, t). \tag{21}$$

We suppressed in (21) the arguments of the $f_{\text{r}}(x_{1,} \ldots, x_N, t)$ for brevity.

The irrelevant part comprising initial correlations, $f_{\text{i}}(0) = (1 - P)F(0) = F(0) - f_{\text{r}}(0)$, which is of interest for us, can be presented in terms of multi-particle correlation functions (hereinafter we put $t_0 = 0$, because equation (13) is valid for any initial moment of time t_0). They are introduced for the reduced distribution functions (19) (see, for example, [3]). Taking into account (21), and that in accordance with (19) a distribution function $F(x_1, \ldots, x_N, 0) = V^{-N} f_N(x_1, \ldots, x_N, 0)$, we have

$$V^N f_{\text{i}}(0) = \sum_{i<j=1}^{N} g_2(x_i, x_j) \prod_{k=1(k\neq i,j)}^{N-2} f_1(x_k) + \sum_{i<j<k=1}^{N} g_3(x_i, x_j, x_k) \prod_{l=1(l\neq i,j,k)}^{N-3} f_1(x_l) + \cdots. \tag{22}$$

Here, $g_2(x_1, x_2)$ and $g_3(x_1, x_2, x_3)$ are a two-particle and a three-particle correlation functions.

In order to find out the rules governing the action of the Liouvillian L and the functions of the Liouvillian (which enter equation (13)) on the relevant distribution function (21), note that, in accordance with the form of the Hamiltonian (15), the Liouvillian L can be presented as

$$\begin{aligned}
&L = L^0 + L' \\
&L^0 = \sum_{i=1}^{N} L_i^0 \qquad L_i^0 = -\boldsymbol{v}_i \cdot \boldsymbol{\nabla}_i \quad \boldsymbol{v}_i = \frac{\boldsymbol{p}_i}{m} \quad \boldsymbol{\nabla}_i = \frac{\partial}{\partial \boldsymbol{x}_i} \\
&L' = \sum_{i<j=1}^{N} L'_{ij} \qquad L'_{ij} = (\boldsymbol{\nabla}_i V_{ij}) \cdot \left(\frac{\partial}{\partial \boldsymbol{p}_i} - \frac{\partial}{\partial \boldsymbol{p}_j} \right).
\end{aligned} \tag{23}$$

We will suppose, as usual, that all functions $\Phi(x_1, \ldots, x_N)$, defined on the phase space, and their derivatives vanish at the boundaries of the configurational space and at $\boldsymbol{p}_i = \pm\infty$. These properties of distribution functions and the explicit form of the Liouville operators (23) lead to the following relations:

$$\begin{aligned}
&\int \mathrm{d}x_i L_i^0 \Phi(x_i, \ldots, x_N, t) = 0 \\
&\int \mathrm{d}x_i \int \mathrm{d}x_j L'_{ij} \Phi(x_1, \ldots, x_N, t) = 0.
\end{aligned} \tag{24}$$

These equations also follow, in general, from the Liouville–von-Neumann equation (1) and conditions (4).

Let us consider the first term in the right-hand side of equation (13). Applying operators (23) to the relevant distribution function (21) and taking into account (24), we have

$$\begin{aligned}
&PL^0 f_{\mathrm{r}} = \frac{1}{V^N} \left[\prod_{i=2}^{N} f_1(x_i) \right] L_1^0 f_1(x_1, t) \\
&PL' f_{\mathrm{r}} = \frac{1}{V^N} \left[\prod_{i=2}^{N} f_1(x_i) \right] n \int \mathrm{d}x_2 L'_{12} f_1(x_2) f_1(x_1, t).
\end{aligned} \tag{25}$$

To calculate the additional term

$$C(t) = P(L^0 + L') \mathrm{e}^{Q(L^0+L')t} \frac{1}{1 - C_0 \mathrm{e}^{-(L^0+L')t} \mathrm{e}^{Q(L^0+L')t}} C_0 \mathrm{e}^{-(L^0+L')t} f_{\mathrm{r}}(t) \tag{26}$$

arising due to initial correlations, we will use the following relations:

$$\mathrm{e}^{(A+B)t} = \mathrm{e}^{At} + \int_0^t \mathrm{d}\theta \, \mathrm{e}^{A(t-\theta)} B \mathrm{e}^{(A+B)\theta} \tag{27}$$

$$\begin{aligned}
\mathrm{e}^{L^0 t} \Phi(x_1, \ldots, x_N, t) &= \left[\prod_{i=1}^{N} \mathrm{e}^{L_i^0 t} \right] \Phi(x_1, \ldots, x_N, t) \\
&= \Phi(\boldsymbol{x}_1 - \boldsymbol{v}_1 t, \boldsymbol{p}_1, \ldots, \boldsymbol{x}_N - \boldsymbol{v}_N t, \boldsymbol{p}_N, t)
\end{aligned} \tag{28}$$

where A and B are the arbitrary operators. Equation (28) follows from the definition (23) of the Liouvillian L^0 of the free-propagating particles. Note, also, that the parameter of initial correlations $C_0 = f_{\mathrm{i}}(0)/[f_{\mathrm{r}}(0) + f_{\mathrm{i}}(0)]$ can be expanded into the power series in $f_{\mathrm{i}}(0)/f_{\mathrm{r}}(0)$. Using (21) and (22), we have

$$\frac{f_{\mathrm{i}}(0)}{f_{\mathrm{r}}(0)} = \sum_{i<j=1}^{N} \frac{g_2(x_i, x_j)}{f_1(x_i) f_1(x_j)} + \sum_{i<j<k} \frac{g_3(x_i, x_j, x_k)}{f_1(x_i) f_1(x_j) f_1(x_k)} + \cdots. \tag{29}$$

Making use of (27) and expanding (26) in PL^0, L', QL' and $f_{\mathrm{i}}(0)/f_{\mathrm{r}}(0)$, it is easy to see that (26) can be presented as a sum of products of operators PL^0, L', PL', $\exp(L^0\theta)$, one-particle distribution functions and correlations functions (29). Applying the projection operator (17) to such products and accounting for (21), (23), (24), (28) and (29), we find that (26) can be presented as a series expansion in the density parameter γ (16).

In what follows, we restrict ourselves to the linear approximation in the density parameter γ (16). Also, in order to simplify formulae, a space homogeneous case will be considered. In this case a one-particle distribution function does not depend on a particle coordinate, $f_1(x_j,t) = f_1(\boldsymbol{p}_j,t)$ ($\int f(\boldsymbol{p},t)\,\mathrm{d}\boldsymbol{p} = 1$), and the multi-particle correlation functions depend only on the differences of coordinates: for example, $g_2(x_i,x_j) = g_2(\boldsymbol{x}_i - \boldsymbol{x}_j, \boldsymbol{p}_i, \boldsymbol{p}_j)$. A space homogeneity allows us to cancel all terms with PL^0(such as the first equation (25)), because, according to (23) and (24), all these terms contain a derivative with respect to a variable $\boldsymbol{x}_1$, which is not under the integration. The second equation of (25) also vanishes in a space homogeneous case, because we consider a potential V_{ij} (15) dependent on the particles' coordinates difference. Taking also into account that the terms containing PL' result in expressions proportional at least to the first power of n, we can replace operators $Q = 1 - P$ in (26) by unity and simplify it to

$$C(t) = PL'\mathrm{e}^{(L^0+L')t}\frac{1}{1-C_0}C_0\mathrm{e}^{-(L^0+L')t}f_{\mathrm{r}}(t). \tag{30}$$

Expanding formally $\frac{1}{1-C_0}$ and C_0 in the power series in $f_{\mathrm{i}}/f_{\mathrm{r}}$, restricting ourselves to the first order in n and then converting the series, we obtain the following expression for the contribution of initial correlations (26):

$$C(t) = V^{-N}\left[\prod_{i=2}^{N} f_1(\boldsymbol{p}_i)\right] n\int \mathrm{d}x_2 L'_{12}\mathrm{e}^{(L^0_{12}+L'_{12})t}\frac{g_2(x_1,x_2)}{f_1(\boldsymbol{p}_1)f_1(\boldsymbol{p}_2)}\mathrm{e}^{-(L^0_{12}+L'_{12})t}f_1(\boldsymbol{p}_2)f_1(\boldsymbol{p}_1,t) \tag{31}$$

where $L^0_{12} = L^0_1 + L^0_2$, $f_1(\boldsymbol{p}_i) = f_1(\boldsymbol{p}_i, 0)$. The parameter of initial correlations $C_0(x_1,\ldots,x_N)$ in (30) under the accepted linear approximation in n (binary collisions) reduces to the parameter $C_0^{12}(x_1,x_2)$, which contains only a two-particle correlation function $g_2(x_1,x_2) = g_2(\boldsymbol{x}_1 - \boldsymbol{x}_2, \boldsymbol{p}_1, \boldsymbol{p}_2)$:

$$\frac{1}{1-C_0^{12}(x_1,x_2)}C_0^{12}(x_1,x_2) = \frac{g_2(x_1,x_2)}{f_1(\boldsymbol{p}_1)f_1(\boldsymbol{p}_2)}. \tag{32}$$

Deriving (31), we have also taken into account that each additional integration over $x_3,\ldots$ adds an additional power of n and, therefore, in the linear approximation in n all formulae can contain no more than one integration over the phase space.

Consider now the second (collision) term of the HGME (13). Initial correlations also contribute to this term through the second term of function $R(t) = 1 + [R(t) - 1]$ (14). We will start with the conventional collision term of the GME taking $R(t) = 1$. To simplify this term, note that the following relations hold in general:

$$\begin{aligned} &PL^0\mathrm{e}^{L^0t}Q = 0 \\ &\mathrm{e}^{QL^0t}Q = \mathrm{e}^{L^0t}Q. \end{aligned} \tag{33}$$

The second equation (33) follows from the first one, which in its turn follows from (17), (20), (23), (24), (27) and (28). The term in the considered collision integral, which is proportional to $QL^0f_{\mathrm{r}}(t)$, gives zero contribution in the case of space homogeneity. Thus, the kinetic term under consideration acquires the form

$$K(t) = \int_0^t \mathrm{d}t_1 PL'\mathrm{e}^{(L^0+QL')t_1}QL'f_{\mathrm{r}}(t-t_1). \tag{34}$$

Using the procedure described above, we have the collision term (34) in the accepted linear approximation on the density parameter γ as the following:

$$K(t) = V^{-N}\left[\prod_{i=2}^{N} f_1(\boldsymbol{p}_i)\right] n \int_0^t \mathrm{d}t_1 \int \mathrm{d}x_2 L'_{12} \mathrm{e}^{(L^0_{12}+L'_{12})t_1} L'_{12} f_1(\boldsymbol{p}_2) f_1(\boldsymbol{p}_1, t-t_1). \qquad (35)$$

In the same way we can consider the contribution of initial correlations to the collision integral. Accounting for the second term of $R(t)$ (14) in the kinetic term of equation (13) leads to modification of the collision integral (35). In the linear approximation on γ we have for the kinetic term of equation (13) instead of (35)

$$\tilde{K}(t) = V^{-N} \prod_{i=2}^{N} f_1(\boldsymbol{p}_i) n \int_0^t \mathrm{d}t_1 \int \mathrm{d}x_2 L'_{12} R_{12}(t) \mathrm{e}^{(L^0_{12}+L'_{12})t_1} L'_{12} f_1(\boldsymbol{p}_2) f_1(\boldsymbol{p}_1, t-t_1) \qquad (36)$$

$$R_{12}(t) = 1 + \mathrm{e}^{(L^0_{12}+L'_{12})t} \frac{g_2(x_1, x_2)}{f_1(\boldsymbol{p}_1) f_1(\boldsymbol{p}_2)} \mathrm{e}^{-(L^0_{12}+L'_{12})t}. \qquad (37)$$

Now collecting all obtained formulae (31), (36) and (37) and accounting for the definition of the relevant distribution function (21), we get from the HGME (13) the following equation for a one-particle momentum distribution function:

$$\begin{aligned}\frac{\partial}{\partial t} f_1(\boldsymbol{p}_1, t) = n &\int \mathrm{d}x_2 L'_{12} \left[R_{12}(t) - 1\right] f_1(\boldsymbol{p}_2) f_1(\boldsymbol{p}_1, t) \\ &+ n \int \mathrm{d}x_2 \int_0^t \mathrm{d}t_1 L'_{12} R_{12}(t) \mathrm{e}^{(L^0_{12}+L'_{12})t_1} L'_{12} f_1(\boldsymbol{p}_2) f_1(\boldsymbol{p}_1, t-t_1)\end{aligned} \qquad (38)$$

where $R_{12}(t)$ is defined by (37).

Equation (38) is the main result of this section. We have obtained the closed homogeneous integra-differential equation for a one-particle distribution function retaining initial correlations not using the Bogolyubov principle of weakening of initial correlations or any other hypothesis. It is not clear how to get such an equation directly from the GME (9). Equation (38) is exact in the linear approximation in n and accounts for initial correlations in this approximation exactly. The first term in the right-hand side of this equation is defined by initial correlations. Initial correlations also modify the collision integral (the second term in the right-hand side). This contains, in addition to the term related to an interaction between particles (described by Liouvillian L'_{12}), also initial correlations described by the parameter C^0_{12} (32). Evolution in time of initial correlations as well as of the collision term is defined by the exact two-particle propagator $G_{12}(t) = \exp[(L^0_{12} + L'_{12})t]$, which, as follows from (27), satisfies the integral equation

$$G_{12}(t) = G^0_{12}(t) + \int_0^t \mathrm{d}t_1 G^0_{12}(t-t_1) L'_{12} G_{12}(t_1) \qquad (39)$$

where $G^0_{12}(t) = \exp(L^0_{12}t)$ is the propagator for non-interacting particles. In the case of a weak inter-particle interaction, we can iterate the integral equation (39) in L'_{12} and obtain equation (38) in the desired approximation on the small interaction parameter (note that a correlation function $g_2(x_1, x_2)$ also depends on an interaction between particles).

The obtained homogeneous integra-differential equation (38) differs from that which could be found from the conventional GME (9) using the projection operator (17) and the principle of weakening of initial correlations or RPA. In the latter case we would have equation (38) in which the time-dependent factor $R_{12}(t)$ comprising the dynamics of initial correlations would be replaced by unity. Moreover, such an equation would be valid only at $t \gg t_{\mathrm{cor}}$, whereas equation (38) is valid at any time.

It should be noted that there may be large-scale correlations associated with, for example, the quantities that are conserved. These correlations may only vanish on the timescale of the order of the relaxation time t_{rel} of a distribution function $f_1(\boldsymbol{p}_i, t)$. If at $t \gg t_{\mathrm{cor}}$ ($t_{\mathrm{cor}} \ll t_{\mathrm{rel}}$) the function $R(t)$ is replaced by unity, this would signify that *all* initial correlations vanish on this timescale, i.e. the large-scale correlations do not matter.

4. Connection to the Boltzmann equation

The closed equation (38) for a one-particle distribution function is not a kinetic equation in the conventional sense. It does not describe generally an irreversible evolution with time. It is easily seen that equation (38) is time reversible if the parameter of initial correlations (32) remains unchanged when all the particle velocities are reversed (see below). Thus, a time-asymmetric behaviour may be secured by the special choice of an initial condition. If we suppose that $C_0^{12}(\boldsymbol{x}_1 - \boldsymbol{x}_2, \boldsymbol{p}_1, \boldsymbol{p}_2) = C_0^{12}(\boldsymbol{x}_1 - \boldsymbol{x}_2, -\boldsymbol{p}_1, -\boldsymbol{p}_2)$, i.e. $g_2(\boldsymbol{x}_1 - \boldsymbol{x}_2, \boldsymbol{p}_1, \boldsymbol{p}_2) = g_2(\boldsymbol{x}_1 - \boldsymbol{x}_2, -\boldsymbol{p}_1, -\boldsymbol{p}_2)$ and $f_1(\boldsymbol{p}_i) = f_1(-\boldsymbol{p}_i)$, then equation (38) is invariant under the transformation $t \to -t$, because such a transformation results in changing the sign of all Liouvillians L_i^0 and L'_{ij}. Such reversibility is understandable in the very early stage of the system's evolution, when $t \lesssim t_{\mathrm{cor}}$ and memory of the initial state has not been lost. At timescale $t \gg t_{\mathrm{cor}}$ the situation may change.

It can be seen from (38) that, in order to enter the kinetic (irreversible) stage of the evolution, the reversible terms connected with initial correlations should vanish on some timescale. Moreover, irreversibility of collision integral may be realized if it is possible to extend the integral over t_1 to infinity. Thus, we have to consider the behaviour of initial correlations and the integral over t_1 in equation (38) in time.

It should be noted that the irreversible evolution may go ‘forwards’ or ‘backwards’. The question as to which of these evolutions should be chosen cannot be answered on the basis of the present consideration of the time-reversible Liouville equation only, and we will consider the evolution in the future ($t > 0$).

In the accepted approximation of the binary collisions, the initial correlations are described by a correlation function $g_2(x_1, x_2)$ depending on coordinates and momenta of only two particles. The time evolution of this binary correlation function is governed by the two-particle propagator (39). In the zero approximation on the interaction L'_{12}, the action of the propagator $G_{12}(t) = G_{12}^0(t)$ on a correlation function $g_2(x_1, x_2)$ (and on all functions of coordinates) results in shifting the coordinates $\boldsymbol{x}_1$and $\boldsymbol{x}_2$ with time according to (28)

$$G_{12}^0(t) g_2(x_1, x_2) = g_2(\boldsymbol{r} - \boldsymbol{g}t, \boldsymbol{p}_1, \boldsymbol{p}_2) \tag{40}$$

where $\boldsymbol{r} = \boldsymbol{x}_1 - \boldsymbol{x}_2$ is the relative distance between particles 1 and 2 and $\boldsymbol{g} = \boldsymbol{v}_1 - \boldsymbol{v}_2$ is the relative velocity. Therefore, in this case a binary correlation function changes with time according to a change of a distance between particles $|\boldsymbol{v}_1 - \boldsymbol{v}_2|t$, which is linear in time. In general, an evolution of a two-particle correlation function $g_2(x_1, x_2)$ under the action of the exact two-particle propagator $G_{12}(t)$ may be found from the well known solution to the two-body problem.

It is very important to know how a correlation function behaves as time passes. If there is a big fraction of a ‘parallel motion’, and a distance between particles (or, more generally, a distance between points in a phase space) does not change significantly, a correlation function does not vanish, i.e. the initial correlations do not disentangle with time. This may be so even in the case of the ergodic flow in a phase space. If a distance between particles grows with time and the radius of correlation between particles $r_{\mathrm{cor}} \backsim r_0$ is limited, a correlation function $g_2(x_1, x_2)$ will fade with time. But for existence of a limited relaxation time, i.e. a finite time for vanishing a correlation function, it should diminish with time exponentially. As is well known, such an exponential disentangling of correlations with time may be secured by a mixing ergodic flow in a phase space. A mixing ergodic flow is closely connected with the property of dynamical systems known as the local (stochastic) instability (see, for example, [12]). If we assume that the dynamics of the system of classical particles under consideration possesses the property of mixing flow (and this is the case), then the initial correlations will weaken with time and disappear after a short correlation time $t_{\rm cor}$. In this case, at $t \gg t_{\rm cor}$, we can neglect the contribution of initial correlations to equation (38) and replace $R_{12}(t)$ by unity.

This cannot be done if there are the correlations associated with the large-scale fluctuations such as the collective excitations: for example, the plasma oscillations. A relaxation time for such fluctuations can be of the order of a kinetic relaxation time $t_{\rm rel} \gg t_{\rm cor}$ and, therefore, they are essential in the kinetic and other large-timescale regimes. The conventional kinetic equations do not take into account such large-scale correlations and do not describe the fluctuations of the distribution functions. A kinetic theory of fluctuations can be found in, for example, [13].

Initial correlations enter equation (38) in combination with other functions, particularly with an inter-particle interaction L'_{12}. Dependence of an initial correlation function $g_2(x_1, x_2)$ and a potential of an inter-particle interaction $V_{ij} = V(|\boldsymbol{x}_i - \boldsymbol{x}_j|)$ on distance between particles is essential for the behaviour of integrals over $\boldsymbol{x}_2$ in (38) with time. Let us consider an example, when this dependence is defined as

$$\begin{aligned} g_2(x_1, x_2) &= g_0 \exp\left(-\frac{r^2}{r_{\rm cor}^2}\right)\phi(\boldsymbol{p}_1, \boldsymbol{p}_2) \\ V(r) &= V_0 \exp\left(-\frac{r^2}{r_0^2}\right) \end{aligned} \tag{41}$$

where g_0 and V_0 are the constant parameters and $\phi(\boldsymbol{p}_1, \boldsymbol{p}_2)$ is a properly normalized function of particles' momenta. We will estimate the time dependence of terms in equation (38), defined by initial correlations, in the case of weak inter-particle interaction, when the time evolution is governed by the 'free' propagator $G_{12}^0(t)$. The correlation function (41) under the action of $G_{12}^0(t)$ transforms according to (40) as

$$G_{12}^0(t) g_2(x_1, x_2) = g_2(\boldsymbol{r} - \boldsymbol{g}t, \boldsymbol{p}_1, \boldsymbol{p}_2) = g_0 \exp\left(-\frac{|\boldsymbol{r} - \boldsymbol{g}t|^2}{r_{\rm cor}^2}\right)\phi(\boldsymbol{p}_1, \boldsymbol{p}_2). \tag{42}$$

The function (42) goes to zero at $t \to \infty$ and any fixed distance $\boldsymbol{r}$ and velocity $\boldsymbol{g}$.

Using (41) and (42), the first right-hand side term of equation (38) may be presented as

$$n \int \mathrm{d}\boldsymbol{p}_2 \int \mathrm{d}\boldsymbol{r} \left[\frac{\partial}{\partial \boldsymbol{r}} V_0 \exp\left(-\frac{r^2}{r_0^2}\right)\right] \left(\frac{\partial}{\partial \boldsymbol{p}_1} - \frac{\partial}{\partial \boldsymbol{p}_2}\right) \frac{g_2(\boldsymbol{r} - \boldsymbol{g}t, \boldsymbol{p}_1, \boldsymbol{p}_2)}{f_1(\boldsymbol{p}_1) f_1(\boldsymbol{p}_2)} f_1(\boldsymbol{p}_2) f_1(\boldsymbol{p}_1, t) \tag{43}$$

where $g_2(\boldsymbol{r} - \boldsymbol{g}t, \boldsymbol{p}_1, \boldsymbol{p}_2)$ is defined by (42).

It is easy to see that the integral (43) over $\boldsymbol{r}$ is not equal to zero only if $t < t_{\rm cor}$, where $t_{\rm cor} \backsim r_{\rm cor}/\bar{v} \sim r_0/\bar{v}$ and $\bar{v}$ is a typical mean particle velocity. At $t \gg t_{\rm cor}$ the integral (43) practically vanishes because of the finite range r_0 of an inter-particle interaction. Of course, such a behaviour is possible if a contribution of the 'parallel motion' with small g to (43) is negligible. The term related to initial correlations and contributing to the second right-hand side term of equation (38) (collision integral) displays the same behaviour with time. Thus, in the considered example, the terms with initial correlations in equation (38) vanish at $t \gg t_{\rm cor}$.

If the effective interaction between particles vanishes at a distance between particles $r \gg r_{\rm cor}$, then at $t_1 \gg t_{\rm cor}$ the action of $G_{12}^0(t_1)$ on the interaction Liouvillian L'_{12} (23) under the integral over t_1 in (38) results in increasing the distance between particles beyond the radius of inter-particle interaction $r_0 \backsim r_{\rm cor}$ and, therefore, in vanishing the integrand. As follows from equation (38), the initial moment $t = 0$ refers to the time just before the collision. Given that the time between collisions, t_{rel}, which defines the time of an essential change of a one-particle distribution function $f_1(\boldsymbol{p}_i, t)$, exceeds considerably t_{cor} due to the condition (16), $f_1(\boldsymbol{p}_1, t - t_1)$ does not practically change within the interval $0 \leqslant t_1 \leqslant t_{\mathrm{cor}}$. Thus, $f_1(\boldsymbol{p}_1, t - t_1)$ under the integral in (38) may be substituted by $f_1(\boldsymbol{p}_1, t)$ with the accuracy of $t_{\mathrm{cor}}/t_{\mathrm{rel}} \backsim \gamma \ll 1$. Moreover, at $t \gg t_{\mathrm{cor}}$ the upper limit of integral over t_1 can be extended to infinity. After such a transformation the collision integral becomes Markovian and irreversible.

Therefore, the transition from the microscopic timescale $0 \leqslant t \leqslant t_{\mathrm{cor}}$ to the macroscopic one $t \gg t_{\mathrm{cor}}$ is essential for obtaining an irreversible Markovian kinetic equation. On the macroscopic timescale the reversible-in-time terms of equation (38) caused by initial correlations may vanish (if the particles' dynamics possesses the necessary properties) and the collision term acquires the needed form. Extension of the upper limit of the integral in equation (38) to infinity ($t \to \infty$) and the existence of this limit may assume some coarse-graining (smoothing) procedure. The coarse-graining time interval Δt, which may be interpreted as the 'observation time' (see, for example, [13]), should be, naturally, much larger than t_{cor} and much less than the relaxation time t_{rel}

$$t_{\mathrm{cor}} \ll \Delta t \ll t_{\mathrm{rel}}. \tag{44}$$

The inequality $\Delta t \ll t_{\mathrm{rel}}$ guarantees that the kinetic stage of the evolution is not blurred by the coarse-graining (smoothing) procedure on the timescale, defined by (44), and the kinetic equation obtained on the considered macroscopic timescale describes the relaxation of the system with the characteristic time t_{rel}.

As follows from equation (38), change in time of the relevant part of a distribution function is defined by the operator which is proportional to n. Then, in the adopted linear approximation in the small parameter (16), we may replace the function $f_1(\boldsymbol{p}_2) = f_1(\boldsymbol{p}_2, 0)$ in equation (38) with $f_1(\boldsymbol{p}_2, t)$ (for more details see below).

Summing up, we can rewrite equation (38) on the considered macroscopic timescale (44) as follows:

$$\frac{\partial}{\partial t} f_1(\boldsymbol{p}_1, t) = n \int \mathrm{d}x_2 \int_0^\infty \mathrm{d}t_1 L'_{12} G_{12}(t) L'_{12} f_1(\boldsymbol{p}_1, t) f_1(\boldsymbol{p}_2, t). \tag{45}$$

This equation is already Markovian and time irreversible. Using the two-particle scattering theory, it may be shown that equation (45) is equivalent to the conventional Boltzmann equation (see, for example, [3]). In the case of a classical gas with a weak inter-particle interaction the exact two-particle propagator $G_{12}(t)$ in (45) may be replaced by the 'free' propagator $G^0_{12}(t)$ according to (39). In this case (45) is equivalent to the Landau equation (see [3]).

We have obtained the Boltzmann equation (45), which is nonlinear as it should be, using the linear theory of projection operators. Actually, equation (38), which has been used for deriving the Boltzmann equation (45), is linear with respect to a distribution function $f_1(\boldsymbol{p}_1, t)$ but contains a one-particle distribution function $f_1(\boldsymbol{p}_2)$ at the initial moment $t = 0$ preceding the collisions. The collision integral is proportional to the density of particles and this means that $f_1(\boldsymbol{p}_i, t)$ does not change in the zero approximation in n (at $n = 0$). More precisely, $f_1(\boldsymbol{p}_i, t) = f_1(\boldsymbol{p}_i) + (\partial f_1/\partial t)_0 t + \cdots$, where the derivative may be estimated as $\partial f_1/\partial t \sim f_1/t_{\mathrm{rel}} \sim n f_1$. Thus, in the linear approximation in n under consideration there is no difference in equation (38) (with the accuracy of $\gamma \sim t_{\mathrm{cor}}/t_{\mathrm{rel}} \ll 1$) between $f_1(\boldsymbol{p}_2)$ and $f_1(\boldsymbol{p}_2, t)$ and that makes this equation nonlinear. Actually, this nonlinearity follows from the adopted form of the relevant part of a distribution function (21).

The described procedure of obtaining the time-irreversible equation (45) from equation (38) clearly indicates that irreversibility emerges on the macroscopic timescale (44) as a result of the loss with time of the information about both the initial correlations and correlations that emerge due to collisions.

5. Conclusion

We have derived the exact HGME (13) for the relevant part of a distribution function (statistical operator). In the derivation of this equation we have not used any approximation or principle like the Bogolyubov principle of weakening of initial correlations or RPA. This equation has several advantages as compared to the GME. The HGME contains the right parameter of initial correlations depending on time in the 'mass' operator acting on the relevant part of a distribution function. The obtained equation is valid on any timescale, particularly at the initial stage of evolution $t_0 \leqslant t \leqslant t_{\mathrm{cor}}$, which may be important for studying the irreversibility problem and the ultrafast relaxation processes. The HGME enables consideration of the entire evolution process of the relevant part of a distribution function and the influence of initial correlations on this process, because equation (13) can switch in principle, for example, from the initial (reversible) regime into the kinetic (irreversible) one, automatically. This equation allows for treating the initial correlations consistently and on an equal footing with the collision integral by expanding the 'mass' operator into the series on the appropriate small parameter.

By appropriate selection of the projection operator, one can rewrite equation (13) for the system under consideration. We have considered a dilute gas of classical particles with an arbitrary repulsive inter-particle interaction and obtained in the linear approximation on the small density parameter (16) the closed equation (38) for a one-particle distribution function retaining initial correlations. In this approximation the evolution equation for a one-particle distribution function contains only binary collisions and a two-particle correlation function in the parameter accounting for initial correlations. We have shown that on the macroscopic timescale (44) this equation becomes equivalent to the Boltzmann equation (45) if a system's dynamics in the phase space has such properties that the contribution of initial correlations vanishes on this timescale.

All stages of evolution described by equation (38) may be numerically modelled for some specific interaction between particles, specific initial correlation function $g_2(x_1, x_2)$ and initial values $f_1(\boldsymbol{p}_i)$ $(i = 1, 2)$.

Application of the developed approach to the quantum mechanical systems will be considered in future publications.

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