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Homogeneous Generalized Master Equations

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It is shown that the method proposed in V. F. Los [J. Phys. A: Math. Gen. **34**: 6389–6403 (2001)], which allows for turning the inhomogeneous time-convolution generalized master equation (TC-GME) into homogeneous (while retaining initial correlations) time-convolution generalized master equation (TC-HGME) for the relevant part of a distribution function, is fully applicable to the quantum case and to the time-convolutionless GME (TCL-GME). It is demonstrated by rederiving the TC-HGME and showing that it works in both the classical and quantum physics cases. The time-convolutionless HGME (TCL-HGME) retaining initial correlations, which is formally the same for both the classical and quantum physics, has also been derived. Both the TC-HGME and TCL-HGME are exact equations applicable on any timescale and allow for consecutive treating the initial correlations and collisions on the equal footing. A new equation for a momentum distribution function retaining initial correlations has been obtained in the linear in the density of quantum particles approximation. Connection of this equation to the quantum Boltzmann equation is discussed.

KEY WORDS: Generalized master equations; homogeneous generalized master equations; initial correlations; evolution equation; kinetic equation.

1. INTRODUCTION

Derivation of kinetic (irreversible) equations from the reversible microscopic dynamics of the many-particle systems remains one of the principal tasks of statistical physics. To achieve this goal, several assumptions are usually made. One of them is related to the initial state of a system: all derivations of the Boltzmann equations are mainly based on either factorizing initial conditions (random phase approximation (RPA) or "molecular chaos") corresponding to uncorrelated initial state or on Bogoliubov's

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principle of weakening of initial correlations.$^{(1)}$ The first is incorrect in principle (as it has been clearly pointed out by van Kampen$^{(2)}$) and the second allows for obtaining the kinetic equation only by jumping over the initial stage of the evolution, i.e. only for the timescale at which **all** initial correlations vanish. However, there may be correlations which do not damp, e.g. caused by the conservation laws, such as the collective plasma excitations; also, the initial quantum correlations, caused by the particles' statistics, do not damp with time. Thus, the latter approach to treating initial correlations results in the evolution equations which are not valid on all timescales and do not allow for consecutive considerations of all stages of the system of interest evolution, particularly, of the stage when a system switches from the initial short-term evolution (when initial correlations matter) to the long-term kinetic regime. This outlined problem is common for both main methods of deriving the kinetic equations: the BBGKY hierarchy$^{(1)}$ and the generalized master equation (GME).$^{(3–5)}$ In the second approach, the initial many-particle correlations lead to appearance of the (generally) non-negligible undesirable (irrelevant) inhomogeneous term in GME for the (relevant) part of interest of a distribution function (statistical operator).

A proper accounting for initial correlation is an important (and generally not easy) problem to deal with, which has already a history (some references may be found in my previous paper$^{(6)}$). The importance of initial correlations for an open quantum systems has also been discussed in the recently published book.$^{(7)}$

A progress achieved in the dynamics of the many-particle systems makes it possible, in principle, to study the entire evolution process of systems in statistical mechanics on any timescale and to determine the conditions under which a system evolves towards the equilibrium state. To do that, the dynamics of initial correlations should be included into consideration.

Recently, the method (based on the conventional projection operator technique) turning the conventional inhomogeneous generalized master equations (GMEs) into homogeneous form has been proposed in.$^{(6)}$ By introducing an additional identity for an irrelevant initial condition term, it has become possible to express this term through the relevant part of a distribution function. Thus, the irrelevant initial condition (inhomogeneous) term in time-convolution (i.e. non-Markovian) generalized master equation (TC-GME),$^{(3–5)}$ caused by the correlations at an initial (at $t = t_0$) state of the whole system, has been transferred to the memory kernel of TC-GME governing the relevant part of a distribution function. That resulted in time-convolution homogeneous generalized master equation (TC-HGME) for the relevant part of a distribution function for a many-particle system. An appropriate construction of the relevant part of a distribution function (using the projection operator technique) allows for obtaining from TC-HGME the equation for a reduced distribution function (e.g. for a one-particle distribution function or for a reduced probability distribution related to an open system interacting with an environment), which is necessary and sufficient for calculating the average values of the dynamical variables (appropriate quantities of interest to follow the time-evolution). The obtained TC-HGME is exact and, therefore, no information has been lost at its derivation. The influence of initial correlations on the time-evolution of the system of interest is treated by this equation on the equal footing with the correlations caused by subsequent collisions. It has been achieved through the modified memory kernel which includes additional terms related to initial correlations. No approximation like the Bogoliubov principle of weakening of initial correlations(1) or RPA is needed in order to exclude from TC-GME the undesirable inhomogeneous initial condition term and transferring it to the memory kernel.

The fact, that the effects of information on the system's initial state correlations may be accounted for through the changed memory kernel is quite important because this obtained exact kernel serves as a starting point for effective perturbation expansions. In connection with that, it is worth reminding that Bogoliubov's principle of weakening of initial correlations implies that on a large enough timescale, $|t-t_0| \gg t_{\mathrm{cor}}$ (t_{cor} is the correlation time caused by inter-particle interaction), **all** initial correlations damp and the time-dependence of multi-particle (irrelevant) distribution functions is completely defined by the time-dependence of a one-particle (relevant) distribution function(1) (the time hierarchy, $t_{\mathrm{rel}} \gg t_{\mathrm{cor}}$, however, is needed for such a procedure, where t_{rel} is the relaxation time for a one-particle distribution function). This supposed by Bogoliubov functional dependence of a multi-particle distribution function (Bogoliubov's anzats) leads to an approximate (valid only on the pointed above large timescale) conversion of the inhomogeneous (including two-particle correlations) equation for a one-particle distribution function of the BBGKY hierarchy into a homogeneous one. Subsequent perturbation expansion of this equation (e.g. in the small density powers) allows for avoiding the so-called 'secular terms', essential at $|t-t_0| \backsim t_{\mathrm{rel}}$, and which make the direct perturbation expansion of the distribution functions in the BBGKY hierarchy ineffective at $|t-t_0| \backsim t_{\mathrm{rel}}$ (the latter is valid only at $|t-t_0| \ll t_{\mathrm{rel}}$ and, therefore, cannot be applied to studying the kinetic stage of the time-evolution characterized by the timescale t_{rel}). Thus, employing the mentioned approach, Bogoliubov was successful in deriving the kinetic (Markovian) equation for a one-particle distribution function, particularly the Boltzmann equation, which describes the time-evolution with the characteristic time t_{rel} but is unable to account for the initial stage of the evolution, $t_0 \leqslant t \leqslant t_{\mathrm{cor}}$.

Bogoliubov's principle of weakening of initial correlations or RPA have also been used to get rid of an irrelevant part (a source) containing all multi-particle correlations at the initial moment t_0 in the GMEs and to obtain the approximate homogeneous equations for the relevant part of a distribution function (see, e.g. ref. 8).

It is also worth noting, that in order to get rid of some singled out initial moment t_0 and to obtain a definite solution, the limiting procedure $t_0 \to -\infty$ is used in Bogoliubov's approach, which serves as a boundary (factorizing initial) condition and introduces an irreversibility into the Liouville equation.(1,8)

On the contrary, the exact kernel of TC-HGME, obtained in ref. 6 describes the influence of all correlations on the evolution process at all times including the initial stage, $t_0 \leqslant t \leqslant t_{\mathrm{cor}}$, when initial correlations may matter. For example, to properly describe the effects of interaction of the condensed matter systems with ultra-short (femtosecond) laser pulses with duration which may match t_{cor}, this initial stage of evolution can not be ignored. On the other hand, the correlation time t_{cor} often is of the order of the timescale t_{mem} on which the memory kernel of TC-GME decays. Thus, if one studies the non-Markovian (memory) effects, which are important on the timescale t_{mem}, the initial correlations damping on the timescale $t_{\mathrm{cor}} \backsim t_{\mathrm{mem}}$ may be essential. Also, as was already mentioned, the obtained exact expression for the TC-HGME memory kernel allows for effective perturbation expansions, e.g. with respect to the density of a system, the inter-particle interaction or the subsystem-reservoir coupling (for an open system), and the mentioned problem with the 'secular terms' does not appear on all timescales. Therefore, it may be stated that the method suggested in ref. 6 allows for consecutive and effective perturbational consideration of the evolution of a system of interest without use of various rather artificial approaches (anzatses) to decoupling the BBGKY hierarchy or avoiding the undesirable inhomogeneous terms in GMEs.

This general scheme and TC-HGME were tested in ref. 6 by applying them to the case of a dilute gas of classical particles that resulted in a new homogeneous equation for a one-particle distribution function retaining initial correlations obtained in the linear approximation on the small density parameter and for the space homogeneous case. This equation describes the dilute classical gas evolution at all times and converts into the conventional Boltzmann equation on the appropriate timescale if all initial correlations vanish on this timescale.

In this paper we apply the method proposed in ref. 6 to the time-convolutionless (time-local) generalized master equation (TCL-GME)(9, 10) with the inhomogeneous term containing initial correlations and show how to convert it into exact time-convolutionless homogeneous generalized master equation (TCL-HGME). This equation describes the evolution of a many-body system by means of the modified (by initial correlations) time-local operator acting on the relevant part of a particles' distribution function (statistical operator). The time-local equations provide a convenient tool for studying the non-Markovian (showing retardation) effects (see, e.g. ref. 7).

The important question is whether the method developed in ref. 6 is applicable to the quantum physics case. The quantum case is more complicated, particularly, because of quantum correlations which are present even in the absence of interaction between particles and do not damp with time. The problem of the existence of some invert operators may also arise. It will be shown in this paper that the obtained in ref. 6 TC-HGME (and TCL-HGME obtained in this paper) may be as well applied to the quantum systems. The quantum HGMEs have exactly the same structures as the classical HGMEs, but the meaning of symbols are different in the classical and quantum physics cases. To test our approach in terms of concrete application in the quantum physics realm, we apply the time-convolution quantum HGME to the case of space homogeneous gas of quantum particles and derive a new homogeneous quantum equation retaining initial correlations for the one-particle density matrix (momentum distribution function) in the linear approximation in the gas density. This equation describes the evolution process at all times and includes both the quantum initial correlations and initial correlations caused by interaction between particles. Then we show how and under which conditions this equation converts into the quantum Boltzmann kinetic equation.

The paper is organized as follows. We start with re-derivation of TC-HGME in order to emphasize the main steps leading to this equation and the formal similarity of the classical and quantum physics cases, and then to derive the time-convolutionless HGME. Then, after a brief outlining of the application of TC-HGME to a gas of classical particles considered in, ref. 6 we turn to the quantum case, which can be formally presented in exactly the same way as the classical physics case but in terms of appropriate operators. It allows us to generalize the method of the paper(6) on the quantum physics case and thus to treat the TC-HGME and TCL-HGME as the homogeneous generalized master equations retaining initial correlations for the relevant part of a density operator. Then the TC-HGME is applied to the space homogeneous gas of quantum particles.

2. TIME-CONVOLUTION HOMOGENEOUS GENERALIZED MASTER EQUATION

Let us start from the very beginning with the Liouville–von-Neumann equation for a distribution function (statistical operator) $F_N(t)$ of N ($N \gg 1$) particles

$$\frac{\partial}{\partial t} F_N(t) = LF_N(t). \tag{1}$$

Here, $F_N(t)$ is a symmetric function of N variables $x_i = (\mathbf{r}_i, \mathbf{p}_i)$ ($i = 1, \ldots, N$) representing the coordinates and momenta of the particles (classical physics) or a statistical operator (quantum mechanics), which satisfy the normalization conditions

$$\int dx_1 \ldots \int dx_N F_N(x_1, \ldots x_N, t) = 1, \quad Tr F_N = 1, \tag{2}$$

L is the Liouville operator acting on $F_N(t)$ in the case of classical physics as

$$LF_N(t) = \{H, F_N(t)\}_P = \sum_{i=1}^{N} \left\{ \frac{\partial H}{\partial \mathbf{r}_i} \frac{\partial F_N(t)}{\partial \mathbf{p}_i} - \frac{\partial H}{\partial \mathbf{p}_i} \frac{\partial F_N(t)}{\partial \mathbf{r}_i} \right\}, \tag{3}$$

where $\{H, F_N(t)\}_P$ is the Poisson bracket and H is the Hamilton function for the system under consideration, while in the quantum physics case L is the superoperator acting on a statistical operator as

$$LF_N(t) = \frac{1}{i\hbar} [H, F_N(t)], \tag{4}$$

where $[,]$ is a commutator and H is the Hamiltonian (for simplicity we consider the case of a closed isolated system when H does not depend on time t).

The formal solution to equation (1) is

$$F_N(t) = e^{L(t-t_0)} F_N(t_0), \tag{5}$$

where $F_N(t_0)$ is a distribution function (statistical operator) at an initial moment of time, t_0, when the initial condition for the Liouville–von-Neumann Eq. (1) should be set.

Employing the projection operator technique$^{(3–5)}$ and applying the projection operators $P=P^2$ and $Q=Q^2=1-P$ to Eq. (1), it is easy to obtain the equations for the relevant $f_r(t)=PF_N(t)$ and irrelevant $f_i(t)=QF_N(t)$ parts of $F_N(t)$

$$\frac{\partial}{\partial t}f_r(t) = PL[f_r(t)+f_i(t)], \tag{6}$$

$$\frac{\partial}{\partial t}f_i(t) = QL[f_r(t)+f_i(t)]. \tag{7}$$

A formal solution to Eq. (7) has the form

$$f_i(t)=\int_{t_0}^{t} \exp[QL(t-t_1)]QLf_r(t_1)dt_1+\exp[QL(t-t_0)]f_i(t_0). \tag{8}$$

Inserting this solution into (6), we obtain the conventional exact time-convolution generalized master equation (TC-GME) known as the Nakajima–Zwanzig equation for the relevant part of the distribution function (statistical operator)

$$\begin{aligned}\frac{\partial}{\partial t}f_r(t) = PLf_r(t)+\int_{t_0}^{t} PL\exp[QL(t-t_1)]QLf_r(t_1)dt_1\\ +PL\exp[QL(t-t_0)]f_i(t_0).\end{aligned} \tag{9}$$

It is important to stress that $f_r(t)$ and $f_i(t_0)$ are the basic quantities we are dealing with in Eq. (9). All functions of dynamical variables, the average values of which we can calculate with the help of $f_r(t)$ by multiplying Eq. (9) with the corresponding functions (operators) from the right and calculating an average value (a trace), are dependent only on the variables which are not projected off by P (P integrates off all excessive variables in $F_N(t)$). Therefore, if we represent $f_r(t)$ and $f_i(t_0)$ in (9) as $f_r(t)=PF_N(t)$ and $f_i(t_0)=QF_N(t_0)$, correspondingly, then the projection operators P and Q in these expressions act only on $F_N(t)$ but not on the functions (if any) to the right of them. This is the essence of the reduced description method, when, in order to calculate the average values of the functions dependent on a much smaller number of variables than the whole distribution function $F_N(t)$, we actually need only the reduced (relevant) distribution function (density matrix) $f_r(t)$.

Serving as a basis for many applications, Eq. (9), nevertheless, contains the undesirable and in general non-negligible inhomogeneous term (the last term in the right hand side of (9)), which depends (through $f_i(t_0)$)

on the same large number of variables as the distribution function $F_N(t_0)$ at the initial moment does. Therefore, Eq. (9) does not provide for a complete reduced description of a multi-particle system in terms of relevant (reduced) distribution function. Applying Bogoliubov's principle of weakening of initial correlations (allowing to eliminate the influence of $f_i(t_0)$ on the large enough timescale, $t-t_0 \gg t_{\mathrm{cor}}$) or using a factorizing initial condition (RPA),when $f_i(t_0)=QF_N(t_0)=0$, one may achieve the above-mentioned goal and obtain the homogeneous GME for $f_r(t)$, i.e. Eq. (9) with no initial condition term. However, in such a way obtained homogeneous GME is either approximate one and valid only on a large enough timescale (when **all** initial correlations vanish) or applicable only for a rather artificial (actually unreal, as pointed in ref. 2) initial conditions (no correlations at an initial moment of time). Also, it is important to note, that in order to get rid of dealing with a singled out moment of time t_0, when a distribution function $F_N(t)$ is replaced by its relevant part, Bogoliubov$^{(1)}$ used the limiting procedure $t_0 \to -\infty$, and thus introduced a special boundary (factorizing) conditions at $t_0 \to -\infty$ leading to an irreversibility of the relaxation process.

To treat the inhomogeneous initial correlations term in the right hand side of Eq. (9) by transferring it to the operator (kernel) acting on the relevant part $f_r(t)$, we suggested in ref. 6 to present the initial (irrelevant) value $f_i(t_0)=QF_N(t_0)$ as a following exact identity

$$\begin{aligned} f_i(t_0) &= [QF_N(t_0)]F_N^{-1}(t_0)e^{-L(t-t_0)}(P+Q)e^{L(t-t_0)}F_N(t_0) \\ &= C_0 \exp[-L(t-t_0)][f_r(t)+f_i(t)]. \end{aligned} \tag{10}$$

Here, we assumed that the inverse operator $F_N^{-1}(t_0) = [f_r(t_0)+f_i(t_0)]^{-1}$ exists (see below), used that $P+Q=1$ and that the backward propagator of the system is $\exp[-L(t-t_0)]$ (as it follows from (5)). In (10) the initial correlation parameter C_0 is introduced

$$\begin{aligned} C_0 &= [QF_N(t_0)]F_N{}^{-1}(t_0) = f_i(t_0)[f_r(t_0)+f_i(t_0)]^{-1} \\ &= f_i(t_0)f_r^{-1}(t_0)[1+f_i(t_0)f_r^{-1}(t_0)]^{-1} \\ &= (1-C_0)f_i(t_0)f_r^{-1}(t_0), \end{aligned} \tag{11}$$

where the projection operator Q acts only on $F_N(t_0)$, which is reflected in comprising $QF_N(t_0)$ into the parenthesis.

Thus, the additional identity (10) has been obtained by multiplying the irrelevant part by unity $F_N^{-1}(t_0)F_N(t_0)$ (which implies the existence of $F_N^{-1}(t_0)$) and inserting the unities $\exp[-L(t-t_0)]\exp[L(t-t_0)]=1$ and

$P+Q=1$. Therefore, neither divergency (caused by possible vanishing of $F_N(t_0)$) nor indetermination of the 0/0 type (behaviours of the numerator and denominator in $F_N(t_0)/F_N(t_0)=1$ are similar) may happen. This holds over all further (identical) manipulations (see below). As it is seen from (11), the correlation parameter is a series in $f_i(t_0)f_r^{-1}(t_0)$ and, therefore, one may only need a formal existence of the function (operator) $f_r^{-1}(t_0)$ (see also (51)), which is invert to the relevant distribution function (statistical operator) chosen with the help of the appropriate projection operator P (generally, it may provide some restriction on the class of appropriate projectors). The relevant part, which is mainly of interest, is, as a rule, a vacuum (relatively slowly changing) part of a distribution function (statistical operator), i.e. the part with no correlations (e.g. a one-particle distribution function). The discussed issue of the existence of an invert distribution function does not pose any problem in a system of classical particles (see ref. 6). In the quantum physics case considered below, the example of construction of the appropriate invert operator $f_r^{-1}(t_0)$ will be given (see (54) and (57)). It seems plausible that the invert relevant part of a distribution function (statistical operator) defined in a pointed above sense (uncorrelated part) may always be constructed.

As a result of introducing the additional identity (10), we have two Eqs. (8) and (10), connecting $f_i(t)$ with $f_i(t_0)$. Finding $f_i(t_0)$ from these equations and inserting it into (9), we obtain the following exact equation for the relevant part of a distribution function (statistical operator):

$$\frac{\partial}{\partial t}f_r(t)=PLR(t-t_0)f_r(t)+\int_{t_0}^{t}PLR(t-t_0)\exp[QL(t-t_1)]QLf_r(t_1)dt_1, \tag{12}$$

where function $R(t-t_0)$ is defined as

$$\begin{aligned} R(t-t_0) &= 1+C(t-t_0)=\frac{1}{1-C_0(t-t_0)}, \\ C(t-t_0) &= e^{QL(t-t_0)}\frac{1}{1-C_0e^{-L(t-t_0)}e^{QL(t-t_0)}}C_0e^{-L(t-t_0)}, \\ C_0(t-t_0) &= e^{QL(t-t_0)}C_0e^{-L(t-t_0)}. \end{aligned} \tag{13}$$

We have rederived the TC-HGME (12), obtained in ref. 6, in order to underline again the main steps leading to this equation and some important features of it. This equation holds in both the classical and quantum physics cases if the proper redefinition of the symbols is done and all (super)operators exist (we will address the latter problem below). We have not removed any information while deriving Eq. (12), and, therefore, it is exact integra-differential equations which accounts for initial correlations and their dynamics through the modification of the (super)operator (memory kernel) in GME (9) acting on the relevant part of a distribution function (statistical operator) $f_r(t)$. The obtained exact kernel of TC-HGME (12) may serve as a starting point for consecutive perturbation expansions. In many cases such expansions of the homogeneous equations (like (12)) have much broader range of validity than that for the inhomogeneous ones (like (9)), when the expansions of the functions $(f_r,\ f_i)$, rather than equation, are involved (see also ref. 1).

However, the problem of the existence (convergency) of $R(t-t_0)$ may be raised. The function $R(t-t_0)$ behaves properly at all times. Moreover, the expansion of the kernel of (12) may result in canceling the pole in function $R(t-t_0)$. In the classical physics case it has been shown in ref. 6 in the linear approximation on the small density for a dilute gas of particles (see Eq. (32) in ref. 6)). As we will see below, the same is also valid in the case of quantum particles. In such cases there is no problem with the existence of $R(t-t_0)$.

3. TIME-CONVOLUTIONLESS HOMOGENEOUS GENERALIZED MASTER EQUATION

Now, let us turn to the case of the so called time-convolutionless (time-local) GME. It is believed that such TCL-GME can be more easily solved and be more convenient for studying the non-Markovian processes than the integral time-convolution GME (9) (see refs. 7,9,10).

Using the identity $F_N(\tau)=\exp[-L(t-\tau)][f_r(t)+f_i(t)]$, we turn Eq. (8) into the form

$$\begin{aligned} f_i(t) &= [1+A(t-t_0)]^{-1}\left[-A(t-t_0)f_r(t)+e^{QL(t-t_0)}f_i(t_0)\right], \\ A(t-t_0) &= -\int_0^{t-t_0} e^{QL\tau}QLPe^{-L\tau}d\tau = e^{QL(t-t_0)}Qe^{-L(t-t_0)}-Q. \end{aligned} \tag{14}$$

Inserting Eq. (14) for $f_i(t)$ into Eq. (6), we get the TCL-GME$^{(9,10)}$

$$\frac{\partial}{\partial t}f_r(t)=PL[1+A(t-t_0)]^{-1}\left[f_r(t)+e^{QL(t-t_0)}f_i(t_0)\right], \tag{15}$$

which contains the undesirable inhomogeneous initial condition term $\propto f_i(t_0)$.

Solving Eqs. (14) and (10), we get for $f_i(t_0)$

$$f_i(t_0) = \chi^{-1} C_0 e^{-L(t-t_0)} (1 + A(t - t_0))^{-1} f_r(t), \tag{16}$$

where

$$\chi^{-1} = \left[1 - C_0 e^{-L(t-t_0)} (1 + A(t - t_0))^{-1} e^{QL(t-t_0)}\right]^{-1}. \tag{17}$$

The inverse operator (17), needed for obtaining $f_i(t_0)$ from Eq. (16), is defined by expanding it into the series in the term $\propto C_0$. At $t = t_0$, $A(t - t_0) = 0$ and there is no singularity at the initial moment of time if $|C_0| < 1$. From the existence of $(1 + A(t - t_0))^{-1(9,10)}$ it follows that χ^{-1} will exist at any time if $|C_0| < 1$. As for the function $R(t - t_0)$ (13) in TC-HGME (12), an expansion in some small parameter may result in canceling the pole in (17) and, therefore, the condition $|C_0| < 1$ may be not necessary.

Inserting Eq. (16) into Eq. (15) and using (17), we obtain a desired time-convolutionless (time-local) homogeneous generalized master equation (TCL-HGME) for the relevant part of the distribution function (statistical operator) $f_r(t)$

$$\frac{\partial}{\partial t} f_r(t) = PL\,[1 + A(t - t_0)]^{-1} \left\{1 - C_0(t - t_0)\,[1 + A(t - t_0)]^{-1}\right\}^{-1} f_r(t). \tag{18}$$

Based on the above mentioned arguments, one may expect that all operators entering Eq. (18) exist (more attention to this issue will be paid in the next publications).

Thus, using the introduced identity (10), we have transferred the inhomogeneous initial correlations term of Eq. (15) into the operator acting on the relevant part of a distribution function (statistical operator). Equation (18) is exact homogeneous time-local equation for the relevant part of a distribution function (statistical operator) which accounts for initial correlations via the time-dependent parameter of initial correlations $C_0(t - t_0)$ defined by (13). This equation is expected to work on any timescale and describe the entire evolution process. It may appear more convenient for studying the non-Markovian processes than the time-convolution HGME (12).

4. THE CLASSICAL PHYSICS CASE

How the proposed approach works for the case of a homogeneous dilute gas of $N \gg 1$ interacting classical particles was demonstrated in ref. 6. In this case, the Liouville operator L may be presented as

$$\begin{aligned} &L = L^0 + L^{'} \;, \\ &L^0 = \sum_{i=1}^{N} L_i^0, \, L_i^0 = -\mathbf{v}_i \cdot \nabla_i, \quad \mathbf{v}_i = \frac{\mathbf{p}_i}{m} \;, \quad \nabla_i = \frac{\partial}{\partial \mathbf{x}_i} \;, \\ &L^{'} = \sum_{i<j=1}^{N} L_{ij}^{'}, \, L_{ij}^{'} = (\nabla_i V_{ij}) \cdot \left(\frac{\partial}{\partial \mathbf{p}_i} - \frac{\partial}{\partial \mathbf{p}_j} \right), \end{aligned} \tag{19}$$

where L^0 corresponds to the kinetic energy of particles with the mass m, and $L^{'}$ describes the interaction between particles with the pair interaction $V_{ij} = V(|\mathbf{x}_i - \mathbf{x}_j|)$.

By selecting the projection operator in the form

$$P = \left[\prod_{i=2}^{N} f_1(x_i) \right] \frac{1}{V^{N-1}} \int dx_2 \ldots \int dx_N, \tag{20}$$

where $f_1(x_i) = f_1(x_i, t_0)$ is the one-particle distribution function

$$f_1(x_i, t) = V \int dx_1 \ldots \int dx_{i-1} \int dx_{i+1} \ldots \int dx_N F_N(x_{1,\ldots,}x_N, t), \tag{21}$$

taken at $t = t_0$, and V is the volume of the system, we choose the relevant part of the N-particle distribution function as

$$f_r(t) = P f_N(t) = \left[\prod_{i=2}^{N} f_1(x_i) \right] f_1(x_i, t). \tag{22}$$

Here, $f_N(t) = V^N F_N(t)$ is the N-particle distribution function satisfying the same Liouville equation (1) and defined in accordance with the following definition for the s-particle ($s \leqslant N$) distribution function

$$f_s(x_1, \ldots, x_s, t) = V^s \int dx_{s+1} \ldots \int dx_N F_N(x_1, \ldots, x_N, t), \tag{23}$$

which satisfies the normalization condition

$$\int dx_1 \ldots \int dx_s f_s(x_1, \ldots, x_s, t) = V^s. \tag{24}$$

The irrelevant part of the N-particle distribution function at t_0, $f_i(t_0) = f_N(t_0) - f_r(t_0)$, may be always represented by the following cluster expansion

$$f_i(t_0) = \sum_{i<j=1}^{N} g_2(x_i, x_j) \prod_{k \neq i,j}^{N-2} f_1(x_k) + \sum_{i<j<k=1}^{N} g_3(x_i, x_j, x_k) \prod_{l \neq i,j,k}^{N-3} f_1(x_l) + \ldots, \tag{25}$$

where $\prod_{k \neq i,j}^{N-2} f_1(x_k)$ and $\prod_{l \neq i,j,k}^{N-3} f_1(x_l)$ stand for the products of $N-2$ and $N-3$ one-particle distribution functions with $k \neq i, j$ and $l \neq i, j, k$, respectively, whereas $g_2(x_i, x_j)$ and $g_3(x_i, x_j, x_k)$ are the irreducible two-particle and three-particle correlation functions (further terms in (25) are defined in the same way).

Using these definitions, the following homogeneous equation for a one-particle momentum distribution function $f_1(x_i, t) = f_1(\mathbf{p}_i, t)$ retaining initial correlations was derived in ref. 6 from TC-HGME (12) for the space homogeneous case in the linear approximation on the small density of particles parameter γ

$$\begin{aligned} \frac{\partial}{\partial t} f_1(\mathbf{p}_1, t) &= n \int dx_2 L_{12}^{'} G_{12}(t) f_1(\mathbf{p}_2) f_1(\mathbf{p}_1, t) \\ &\quad + n \int dx_2 \int_0^t dt_1 L_{12}^{'} [1 + G_{12}(t)] e^{L_{12} t_1} L_{12}^{'} f_1(\mathbf{p}_2) f_1(\mathbf{p}_1, t - t_1), \\ \gamma &= r_0^3 n \ll 1. \end{aligned} \tag{26}$$

Here, r_0 is the effective radius of inter-particle interaction, $n = \frac{N}{V}$ is the particles' density, $t_0 = 0$ is selected as the initial moment of time (Eq. (12) is valid for any t_0), $L_{12} = L_{12}^0 + L_{12}^{'}$ is the two-particle Liouvillian (19) L_{ij} $(i = 1, j = 2)$, and

$$\begin{aligned} G_{12}(t) &= R_{12} - 1 \\ &= e^{L_{12} t} \frac{g_2(x_1, x_2)}{f_1(\mathbf{p}_1) f_1(\mathbf{p}_2)} e^{-L_{12} t} \end{aligned} \tag{27}$$

is the parameter of initial correlations in the linear in γ approximation which is defined by the time evolution of a two-particle correlation function. It is interesting to note that the expression like (27) appears as an additional term in the (correlation) entropy caused by two-particle correlation function and obtained by means of quasi-equilibrium statistical operator (see, e.g. ref. 8). This additional contribution to entropy is essential when a two-particle correlation function damps slowly.

Equation (26) is a new equation for a one-particle distribution function obtained from TC-HGME (12) in the linear approximation in n which accounts for both initial correlations and collisions in this approximation exactly. First term in the right-hand side of this equation (linear in L'_{12}) is exclusively defined by initial correlations evolving with time. Initial correlations also modify the collision integral (second term in the right-hand side of this equation). It contains, except the term related to an interaction between particles (described by Liouvillian L'_{12}), also time-dependent initial correlations described by two-particle correlation function (27)). Evolution in time of initial correlations as well as of the collision term is defined by the exact two-particle propagator only, and in this sense Eq. (26) is closed. This equation describes the entire evolution process and is expected to switch from initial (reversible) regime into the kinetic (irreversible) one, automatically. It was shown in ref. 6 that Eq. (26) converts on the appropriate timescale into the conventional Boltzmann equation if all correlations (initial and caused by collisions) damp with time.

5. THE QUANTUM CASE

Let us now test the general scheme outlined in Section 2 by applying it to the system of interacting quantum particles. In the quantum physics case the derived HGMEs hold in the forms obtained above but the Liouville operator L in Eq. (1) (and elsewhere) as well as the operator $\exp(Lt)$ are now the superoperators acting according to (4) on any operator $A(t)$ (particularly on the statistical operator $F_N(t)$ of N interacting quantum particles) as

$$LA(t)=\frac{1}{i\hbar}[H,A(t)],\ e^{Lt_1}A(t)=e^{\frac{1}{i\hbar}Ht_1}A(t)e^{-\frac{1}{i\hbar}Ht_1}, \tag{28}$$

respectively. Accordingly, Eqs. (12) and (18) for the relevant part of the statistical operator $f_r(t)=PF_N(t)$ hold with the appropriate redefinitions of the symbols and operations used in these equations. The order of operators in these equations also matters.

Let us consider the quantum physics case in more detail. In the space representation the system of N quantum particles is described by the density matrix $F_N(\mathbf{r}_1,\dots,\mathbf{r}_N,\mathbf{r}'_1,\dots,\mathbf{r}'_N,t)$. This matrix should satisfy the symmetry conditions which reflect the statistics of the particles under consideration, i.e.

$$\begin{gathered}P_{ij}F_N=F_NP_{ij}=\theta F_N,\\ \theta=\pm 1,\end{gathered} \tag{29}$$

where P_{ij} is the operator of transmutation of any two variables $\mathbf{r}_i$ and $\mathbf{r}_j$, when it stands to the left of F_N, or of $\mathbf{r}_i'$and $\mathbf{r}_j'$, when it acts from the write side of F_N (this rule holds for any operators acting on the matrixes). The sign plus is applicable for bosons and minus should be used for fermions.

We will focus on the derivation of the evolution equation for a one-particle density matrix $f_1(\mathbf{r}_1, \mathbf{r}_1', t)$, which is defined according to the following definition of the s-particle ($s \leqslant N$) density matrix

$$f_s(\mathbf{r}_1, \dots, \mathbf{r}_s, \mathbf{r}_1', \dots, \mathbf{r}_s', t) = V^s Tr_{(s+1,\dots,N)} F_N(\mathbf{r}_1, \dots, \mathbf{r}_N, \mathbf{r}_1', \dots, \mathbf{r}_N', t), \tag{30}$$

where $Tr_{(s+1,\dots,N)}$ denotes the trace taken over the coordinates of N–s particles $(s+1, \dots, N)$. From the normalization condition (2) $Tr F_N = 1$ it follows that $\frac{1}{V} Tr f_1 = 1$.

It is convenient to introduce the following projection operator (compare with the definition (20))

$$P = \left[\prod_{i=2}^{N} f_1(\mathbf{r}_i, \mathbf{r}_i')\right] \frac{1}{V^{N-1}} Tr_{(2,\dots,N)}, \tag{31}$$

where $f_1(r_i, r_i') = f_1(r_i, r_i', t_0)$ is the one-particle density matrix taken at the initial moment of time t_0. Therefore, the chosen relevant density matrix under consideration is (in accordance with the definition (30) for the N-particle density matrix $f_N = V^N F_N$)

$$P f_N(t) = f_r(t) = \left[\prod_{i=2}^{N} f_1(\mathbf{r}_i, \mathbf{r}_i')\right] f_1(\mathbf{r}_1, \mathbf{r}_1', t). \tag{32}$$

As it is seen from Eq. (32), the selected relevant part of the N-particle density matrix does not contain any correlations. In order to define the irrelevant part of the density matrix $f_i(t_0) = (1 - P) f_N(t_0)$, which enters Eqs. (12) and (18) and comprise all initial correlations, we have also to take into account the quantum correlations arising due to the symmetry condition (29). These correlations exist independently of the interaction between particles, which we introduce by means of the following Hamiltonian

$$\begin{aligned} H &= H^0 + H', \\ H^0 &= \textstyle\sum_{i=1}^{N} K_i, \quad H' = \sum_{i<j=1}^{N} \Phi_{i,j}, \\ K_i &= -\tfrac{\hbar^2}{2m} \nabla_{\mathbf{r}_i}^2, \quad \Phi_{i,j} = \Phi(|\mathbf{r}_i - \mathbf{r}_j|). \end{aligned} \tag{33}$$

Thus, $f_N(t_0) = f_r(t_0) + f_i(t_0)$ may be presented in the form of the cluster expansion with

$$f_r(t_0) = \prod_{i=1}^{N} f_1(i), \tag{34}$$

and

$$f_i(t_0) = \sum_{i<j=1}^{N} \tilde{g}_2(i,j) \prod_{k \neq i,j}^{N-2} f_1(k) + \sum_{i<j<k=1}^{N} \tilde{g}_3(i,j,k) \prod_{l \neq i,j,k}^{N-3} f_1(l) + \dots, \tag{35}$$

where we have used the short notation $f_1(i) = f_1(\mathbf{r}_i, \mathbf{r}_i')$ (i.e. $i = \mathbf{r}_i, \mathbf{r}_i', i = 1, \dots, N$) and, e.g. $\prod_{k \neq i,j}^{N-2} f_1(k)$ stands for the product of $N-2$ one-particle functions $f_1(k)$ with k taking values $1, \dots, N$ but $k \neq i, j$. A two-particle $\tilde{g}_2(i,j)$ and a three-particle $\tilde{g}_3(i,j,k)$ correlation functions are defined as (the correlation functions for more particles may be written down in the same way)

$$\begin{aligned} \tilde{g}_2(i,j) &= \theta P_{ij} f_1(i) f_1(j) + g_2(i,j), \\ \tilde{g}_3(i,j,k) &= (P_{ij} P_{jk} + P_{ij} P_{ik}) f_1(i) f_1(j) f_1(k) + (\theta P_{ik} + \theta P_{jk}) g_2(i,j) f_1(k) \\ &\quad + (\theta P_{ij} + \theta P_{ik}) g_2(j,k) f_1(i) + (\theta P_{ij} + \theta P_{jk}) g_2(i,k) f_1(j) \\ &\quad + g_3(i,j,k). \end{aligned} \tag{36}$$

The terms in the right-hand sides of Eq. (36) with one, two, etc. permutation operators, P_{ij}, represent a two-, three-particle, etc. quantum correlations emerging due to the proper symmetry properties of $f_N(0)$ guaranteed by the symmetrization operators, e.g.

$$f_2(i,j) = \theta P_{ij} f_2(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_i', \mathbf{r}_j'). \tag{37}$$

The irreducible two-, three-, etc. correlation functions, $g_2(i,j)$, $g_3(i,j,k)$, etc., are caused by the interaction between particles, $\Phi_{i,j}$, and are proportional to an interaction parameter ε in some power. Note, that in contrast to the classical physics case (see (25)), each correlation functions (36) contains correlations of all possible orders in ε, e.g. $\widetilde{g}_2(i,j)$ includes two-particle quantum correlations (existing even in the absence of interaction, when $\varepsilon=0$) and two-particle correlations of the first order in ε ($g_2(i,j)$). The same is valid for $\widetilde{g}_3(i,j,k)$, which contains a three-particle correlations of the zero, first and second ($g_3(i,j,k)$) orders in ε.

The following useful relations hold for the permutation operators

$$\begin{aligned} P_{ij}P_{jk} &= P_{ik}P_{ij}, \\ P_{jk}P_{ij} &= P_{ij}P_{ik}. \end{aligned} \tag{38}$$

Let us now derive the evolution equation for a gas of interacting quantum particles in the lowest (first) order in the small density of particles parameter n. The corresponding dimensionless small parameter is

$$\gamma = r_0^3 n \sim t_{\mathrm{cor}}/t_{\mathrm{rel}} \ll 1. \tag{39}$$

We will use the TC-HGME given by Eqs.(12) and (13) with appropriate redefinitions of the symbols, as it was mentioned above.

The Liouville (super)operator $L=L^0+L^{'}$, corresponding to the Hamiltonian (33), is easily defined by Eq. (28) as

$$\begin{aligned} L^0 &= \sum_{i=1}^{N} L_i^0,\, L_i^0 = \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\right)\left(\nabla^2_{\mathbf{r}_i} - \nabla^2_{\mathbf{r}_i^{'}}\right), \\ L^{'} &= \sum_{i<j=1}^{N} L_{ij}^{'},\, L_{ij}^{'} = \frac{1}{i\hbar}\left[\Phi(|\mathbf{r}_i - \mathbf{r}_j|) - \Phi(|\mathbf{r}_i^{'} - \mathbf{r}_j^{'}|)\right], \end{aligned} \tag{40}$$

where we have used the abovementioned rule, that an operator standing on the right side (in the commutator) acts on the primed variables.

Using the definitions (40), one can easily show that the following relations hold (similar to the classical physics case)

$$\begin{aligned} &Tr_{(i)} L_i^0 \varphi_N(1,\ldots,i,\ldots,N) = 0, \\ &Tr_{(i,j)} L_{ij}^{'} \varphi_N(1,\ldots,i,\ldots,j,\ldots,N) = 0, \end{aligned} \tag{41}$$

where $\varphi_N(1,\ldots,i,\ldots,N)$ is some matrix, defined for the N-particle system, which in the space representation takes the form $\varphi_N(1,\ldots,i,\ldots,N) = \varphi_N(\mathbf{r}_1,\ldots,\mathbf{r}_i,\ldots,\mathbf{r}_N,\mathbf{r}_1^{'},\ldots,\mathbf{r}_i^{'},\ldots,\mathbf{r}_N^{'})$ and possesses the necessary boundary conditions.

Therefore, using the projection operator (31) and the relevant density matrix (32), the first two terms in TC-HGME (12), $P(L^0+L^{'})f_r(t)$ (which coincide with those in TC-GME (9)), may be presented as follows

$$\begin{aligned} PL^0 f_r(t) &= \left[\prod_{i=2}^{N} f_1(i)\right] \frac{1}{i\hbar}\left[-\frac{\hbar^2}{2m}\left(\nabla^2_{\mathbf{r}_1} - \nabla^2_{\mathbf{r}_1^{'}}\right)\right] f_1(\mathbf{r}_1, \mathbf{r}_1^{'}, t), \\ PL^{'} f_r(t) &= \left[\prod_{i=2}^{N} f_1(i)\right] \frac{n}{i\hbar}\int d\mathbf{r}_2[\Phi(|\mathbf{r}_1 - \mathbf{r}_2|) \\ &\quad -\Phi(|\mathbf{r}_1^{'} - \mathbf{r}_2|)] f_1(\mathbf{r}_2, \mathbf{r}_2) f_1(\mathbf{r}_1, \mathbf{r}_1^{'}, t)\}. \end{aligned} \tag{42}$$

To simplify the derivation, we will restrict ourself to the space homogeneous case, when all matrixes are invariant under translations and, particularly, the matrix $f_1(\mathbf{r}_i, \mathbf{r}_i^{'})$ should be of the form

$$f_1(\mathbf{r}_i, \mathbf{r}_i^{'}, t) = f_1(\mathbf{r}_i - \mathbf{r}_i^{'}, t). \tag{43}$$

Then, it is easy to see that for functions (43), H^0 commutes with $f_r(t)$ and Eq. (42) vanish, i.e.

$$L^0 f_r(t) = 0, \; PL^{'} f_r(t) = 0. \tag{44}$$

Also, in this space homogeneous case for any matrix $\varphi_N(1, \dots, N)$

$$PL^0 \varphi_N(1, \dots, N) = 0. \tag{45}$$

Let us now consider the terms in TC-HGME (12) caused by initial correlations. It is worth noting, that in the considered case of identical interacting quantum particles it is impossible to simply disregard the inhomogeneous term in the exact TC-GME (9) (assuming that correlations damp with the distance between particles) due to always existing (at any distances) quantum initial correlations (see (36)). Bogoliubov$^{(1)}$ tackled this problem by introducing a special boundary (initial) condition to the BBGKY chain at $t_0 \to -\infty$ implying that at this limiting moment of time the particles are located at distances beyond the correlation radius r_0, which means that correlation functions in (36), $g_2(i, j)$, $g_3(i, j, k)$, etc., caused by interaction between particles (and proportional to some power of ε), vanish, and

$$\lim_{t_0 \to -\infty} f_i(t_0) = \gamma_N \prod_{i=1}^{N} f_1(i), \tag{46}$$

where

$$\gamma_N = (1 + \theta P_{1N} + \ldots + \theta P_{N-1,N}) \ldots (1 + \theta P_{12}) \tag{47}$$

is the symmetrization operator for N particles. Therefore, in the Bogoliubov approach, the multi-particle density matrix at $t_0 \to -\infty$ is the properly symmetrized product of one-particle density matrixes (compare with (34)–(36)). As in the classical physics case, this boundary condition introduces irreversibility into an evolution of the system and thus allows for obtaining the quantum kinetic equations.(11) Also, as in the case of a dilute gas of classical particles, in order to obtain the closed kinetic equation for a one-particle density matrix, Bogoliubov used the specific form of time-dependence of the multi-particle density matrix (valid only at $t - t_0 \gg t_{\mathrm{cor}}$), i.e. he assumed that on this timescale the dependence on time of the multi-particle density matrices is defined by the time-dependence of an one-particle density matrix.

In this paper we are not using any of the abovementioned Bogoliubov's assumptions. Thus, let us consider the (super)operator (see (13))

$$C(t) = R(t) - 1 = e^{QLt} \frac{1}{1 - C_0 e^{-Lt} e^{QLt}} C_0 e^{-Lt} \tag{48}$$

defining the influence of initial correlations in Eq. (12) on the evolution process (hereinafter we put $t_0 = 0$, because the HGMEs are valid for any initial moment t_0). In order to expand exponential (super)operators in a power series, we will use the following relation valid for any (super)operators A and B

$$e^{(A+B)t} = e^{At} + \int_0^t d\tau e^{A(t-\tau)} B e^{(A+B)\tau}. \tag{49}$$

Making use of (49) and expanding (48) in PL^0 and $QL^{'}$, it is seen that all terms with PL^0 vanish due to Eq. (45) and, therefore, all QL in (48) may be replaced by $L^0 + QL^{'}$. Taking into account that the terms containing $PL^{'}$ result in the expressions proportional to at least the first power of n (see, e.g.(42)) and looking for the lowest (first) order approximation in n of Eq. (12), we can substitute $Q = 1 - P$ in (48) with unity and simplify it to

$$C(t) = e^{Lt} \frac{1}{1 - C_0} C_0 e^{-Lt}. \tag{50}$$

Using expression (11) for C_0, we have

$$\frac{1}{1 - C_0} C_0 = f_i(0) f_r^{-1}(0). \tag{51}$$

This is a remarkable result showing that in this approximation there is no problem with the existence (convergence/invertability) of $R(t)$ (13) (the same has been shown for the classical physics case in ref. 6). In connection with that it is worth reminding that if in some part of the definition space $f_r(0)$ goes to zero, so should $f_i(0)$ (at the same rate or more promptly than the relevant part). It follows from the possibility of breaking the statistical operator into the uncorrelated (f_r) and correlated (f_i) parts (see (34)–(36)), which in turn caused by the fact that if an interaction between particles is switched off ($\varepsilon = 0$), the statistical operator should be given by symmetrized product of one-particle operators. Moreover, in the equations for the relevant part of statistical operator obtained below, as a result of approximation (51), the factor $f_i(0) f_r^{-1}(0)$ is always multiplied by $f_r(0)$ (see (69) below and take into account that in the approximation under consideration the relevant part changes slowly). This fact additionally guarantees an absence of any divergencies (in other words, any manipulations with initial condition term should result in terms behaving like $f_i(0)$ in accordance with the identity (10)).

Now, it is necessary to define $f_r^{-1}(0)$. In the space homogeneous case under consideration, it is convenient to work in the momentum representation. The relation between the space and momentum representations for a one-particle density matrix of interest is

$$\begin{aligned} f_1(\mathbf{r}, \mathbf{r}^{'}, t) &= \frac{1}{(2\pi\hbar)^3} \int f_1(\mathbf{p}, \mathbf{p}^{'}, t) e^{i\mathbf{pr}/\hbar} e^{-i\mathbf{p}^{'}\mathbf{r}^{'}/\hbar} d\mathbf{p} d\mathbf{p}^{'}, \\ f_1(\mathbf{p}, \mathbf{p}^{'}, t) &= (2\pi\hbar)^3 w(\mathbf{p}, \mathbf{t}) \delta(\mathbf{p} - \mathbf{p}^{'}), \end{aligned} \tag{52}$$

where a function $w(\mathbf{p})$ (with dimension $[p^{-3}]$) is normalized to unity and corresponds to a classical momentum distribution function. According to the definition

$$\int f_1(\mathbf{p},\mathbf{p}'',t)f_1^{-1}(\mathbf{p}'',\mathbf{p}',t)d\mathbf{p}''=\delta(\mathbf{p}-\mathbf{p}'), \tag{53}$$

we may take for $f_1^{-1}(\mathbf{p},\mathbf{p}')$ the following matrix

$$f_1^{-1}(\mathbf{p},\mathbf{p}',t)=(2\pi\hbar)^{-3}w^{-1}(\mathbf{p},\mathbf{t})\delta(\mathbf{p}-\mathbf{p}'). \tag{54}$$

Note that the δ-functions in (52)–(54) (related to the fact that a one-particle distribution function is diagonal in the space homogeneous case) always stay under the integrals or are divided out.

In correspondence with (52) and (54), an invert one-particle matrix in the space representation may be defined as

$$\begin{aligned} f_1^{-1}(\mathbf{r},\mathbf{r}',t) &= \frac{1}{(2\pi\hbar)^3}\int f_1^{-1}(\mathbf{p},\mathbf{p}',t)e^{i\mathbf{pr}/\hbar}e^{-i\mathbf{p}'\mathbf{r}'/\hbar}d\mathbf{p}d\mathbf{p}' \\ &= \frac{1}{(2\pi\hbar)^6}\int w^{-1}(\mathbf{p},\mathbf{t})e^{i\mathbf{p}(\mathbf{r}-\mathbf{r}')}d\mathbf{p}. \end{aligned} \tag{55}$$

It satisfies the necessary relation

$$\int f_1(\mathbf{r},\mathbf{r}'',t)f_1^{-1}(\mathbf{r}'',\mathbf{r}',t)d\mathbf{r}''=\delta(\mathbf{r}-\mathbf{r}'). \tag{56}$$

Now,we may define an operator, invert to the relevant operator (34), as following

$$f_r^{-1}(0)=\prod_{i=1}^{N}f_1^{-1}(i), \tag{57}$$

because, due to (53) and (56),

$$[f_r(0)f_r^{-1}(0)]=\prod_{i=1}^{N}I(i). \tag{58}$$

Here and further (i) stands for $(\mathbf{r}_i,\mathbf{r}_i')$ or $(\mathbf{p}_i,\mathbf{p}_i')$ depending on the representation used, and $I(i)$ is the unity matrix in the space of i-particle

$$\begin{aligned} I(\mathbf{r}_i,\mathbf{r}_i') &= \delta(\mathbf{r}_i-\mathbf{r}_i'), \\ I(\mathbf{p}_i,\mathbf{p}_i') &= \delta(\mathbf{p}_i-\mathbf{p}_i'), \end{aligned} \tag{59}$$

in the space and momentum representations, respectively.

Applying the introduced definitions for invert matrixes and using Eq. (35) for the irrelevant density matrix, the correlation parameter (51) may be rewritten in the following way

$$f_i(0)f_r^{-1}(0) = \sum_{i<j=1}^{N} \tilde{g}(i,j)f_1^{-1}(i)f_1^{-1}(j) \prod_{k\neq i,j}^{N-2} I(k) + \sum_{i<j<k=1}^{N} \tilde{g}(i,j,k)f_1^{-1}(i)f_1^{-1}(j)f_1^{-1}(k) \prod_{l\neq i,j,k}^{N-3} I(l) + \dots, \tag{60}$$

where, e.g. the two-particle part of (60), according to the expressions for correlation functions (36), is

$$\tilde{g}(i,j)f_1^{-1}(i)f_1^{-1}(j) = \theta P_{ij} + g(i,j)f_1^{-1}(i)f_1^{-1}(j), \tag{61}$$

and the matrix elements of the permutation operator P_{ij} are defined in the space and momentum representations as

$$\begin{aligned} P_{ij}(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_i^{'},\mathbf{r}_j^{'}) &= \delta(\mathbf{r}_i-\mathbf{r}_j^{'})\delta(\mathbf{r}_j-\mathbf{r}_i^{'}),\\ P_{ij}(\mathbf{p}_i,\mathbf{p}_j,\mathbf{p}_i^{'},\mathbf{p}_j^{'}) &= \delta(\mathbf{p}_i-\mathbf{p}_j^{'})\delta(\mathbf{p}_j-\mathbf{p}_i^{'}). \end{aligned} \tag{62}$$

Let us consider the additional (to the flow) term in TC-HGME (12), $F(t) = PL^{'}C(t)f_r(t)$, caused by initial correlations, in the linear approximation in n. Using (50), (51) and (60), (61), one may obtain in this approximation

$$\begin{aligned} F(t) &= PL^{'}e^{Lt}\frac{1}{1-C_0}C_0e^{-Lt}f_r(t)\\ &= \left[\prod_{i=2}^{N} f_1(i)\right]\frac{n}{i\hbar}Tr_{(2)}L_{12}^{'}e^{-\frac{i}{\hbar}(H_{12}^0+H_{12}^{'})t}[\theta P_{12}\\ &\quad +g(1,2)f_1^{-1}(1)f_1^{-1}(2)]e^{\frac{i}{\hbar}(H_{12}^0+H_{12}^{'})t}f_1(2)f_1(1,t). \end{aligned} \tag{63}$$

Deriving (63), we have taken into consideration that each additional integration over the coordinate or momentum space adds an additional power of n and, therefore, in the linear approximation in n all formulae can contain no more than one integration (as in (63)). Thus, Eq. (63) is defined only by the two-particle dynamics described by the Hamiltonian $H_{12} =$

$H_{12}^0+H_{12}^{'}$ (and the corresponding Liouvillian $L_{12}=L_{12}^0+L_{12}^{'}$). It is worth noting that (63) is different from the corresponding additional (to flow) term (caused by initial correlations) obtained in ref. 6 for the classical physics case: except a two-particle correlation function, Eq. (63) contains a symmetrization operator P_{12} responsible for quantum correlations.

Taking into account (62) and invariance of the Hamiltonian H_{12} with regard to renaming the particles, i.e. $H_{12}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1^{'},\mathbf{p}_2^{'})=H_{12}(\mathbf{p}_2,\mathbf{p}_1,\mathbf{p}_2^{'},\mathbf{p}_1^{'})$, it may be shown that in the operator form it looks like (see, e.g. ref. 12)

$$P_{12}H_{12}P_{12}^{-1}=H_{12} \tag{64}$$

(i.e. a symmetrization operator commutes with the Hamiltonian) and, therefore, $e^{-\frac{i}{\hbar}(H_{12}^0+H_{12}^{'})t}P_{12}e^{\frac{i}{\hbar}(H_{12}^0+H_{12}^{'})t}=P_{12}$. Now, it is easy to show that the first term in (63), caused by the symmetrization operator P_{12}, vanishes in the space homogeneous case (for non-symmetrized $f_r(t)$ it is demonstrated by Eq. (44)). Thus,

$$\begin{aligned} PL_{12}^{'}P_{12}f_r(t) &= n\left[\prod_{i=2}^{N} f_1(i)\right]\int d\mathbf{r}_2\frac{1}{i\hbar}[\Phi(|\mathbf{r}_1-\mathbf{r}_2|) \\ &\quad -\Phi(|\mathbf{r}_1^{'}-\mathbf{r}_2|)]f_1(\mathbf{r}_1-\mathbf{r}_2)f_1(\mathbf{r}_2-\mathbf{r}_1^{'},t)=0. \end{aligned} \tag{65}$$

That may be easily proven, if we substitute the integration variable $\mathbf{r}_2$ in (65) by $\rho=\mathbf{r}_1-\mathbf{r}_2$ and $\rho^{'}=\mathbf{r}_2-\mathbf{r}_1^{'}$ in the first and second integrals, respectively, and take into consideration, that in the adopted approximation (first order in n) the time-dependence of an one-particle density matrix may be disregarded due to the fact that the change with time is described by the (super)operator which is already of the first order in n for the space homogeneous system.

Thus, the contribution of initial correlations to the flow term of Eq. (12) in the first order in n and for the space homogeneous system is

$$PL^{'}C(t)f_r(t)=\left[\prod_{i=2}^{N} f_1(i)\right]nTr_{(2)}L_{12}^{'}G_{12}^{q}(t)f_1(2)f_1(1,t), \tag{66}$$

where

$$G_{12}^{q}(t)=e^{-\frac{i}{\hbar}H_{12}t}g(1,2)f_1^{-1}(1)f_1^{-1}(2)e^{\frac{i}{\hbar}H_{12}t} \tag{67}$$

is a time-dependent (quantum) two-particle correlation function. This result is similar to that obtained in ref. 6 for the classical physics case (see also (26) and (27)): initial correlations lead to the appearance of the additional, linear in interaction between particles (H'_{12}), term which is defined by the evolution with time of a two-particle correlation function. Moreover, this result is closed in the sense that the time-evolution is also completely defined by a two-particle dynamics with the Hamiltonian H_{12}.

The collision term of equation (12) in the adopted approximation may be obtained in the same way. Accounting for Eqs. (44), (45), (49)–(51), (60), (61), (64) and remembering that any additional power of PL' and any additional integration (taking a trace) over the coordinate or momentum space adds an additional power of density n, it is not difficult to show that in the linear approximation in n the collision integral of (12) reduces to

$$K(t) = \left[\prod_{i=2}^{N} f_1(i)\right] n \int_0^t dt_1 Tr_{(2)} L'_{12}\left[1+\theta P_{12}+G^q_{12}(t)\right] e^{L_{12}t_1} \times L'_{12} f_1(2) f_1(1, t-t_1). \tag{68}$$

This result is different from that obtained in ref. 6 for the classical physics case due to the presence of quantum correlations stipulated by a symmetrization operator P_{12}.

Collecting the obtained results (formulae (66) and (68)) and accounting for the definition of the relevant statistical operator (32), we get from the TC-HGME (12) the following equation for a one-particle density matrix in the linear approximation in n and for the space homogeneous case

$$\frac{\partial}{\partial t} f_1(1,t) = nTr_{(2)} L'_{12} G^q_{12}(t) f_1(2) f_1(1,t) + n\int_0^t dt_1 Tr_{(2)} L'_{12}\left[1+\theta P_{12}+G^q_{12}(t)\right] e^{L_{12}t_1} L'_{12} f_1(2) f_1(1,t-t_1). \tag{69}$$

Equation (69) is the central result of this section. We have obtained a new closed homogeneous integra-differential equation for a one-particle density matrix retaining initial correlations which is valid on any timescale (i.e. we may use Eq. (69) for considering all stages of evolution of a one-particle density matrix). No approximation like the Bogoliubov principle of weakening of initial correlations (valid only on a large timescale $t-t_0 \gg t_{\mathrm{cor}}$) has been used for deriving equation (69). This equation is exact in the linear approximation in n and, therefore, accounts for initial correlations and collisions in this approximation exactly. The first term in the right-hand side of (69), linear in interaction ($L_{12}^{'}$), is defined by initial correlations caused by interaction between particles (this term is absent if we apply the boundary condition (46)). Initial correlations, both quantum and caused by interaction, also modify the second (collision) term of (69). Note, that the symmetrization operator θP_{12} (accounting for the particles' statistics) appears in this term as a result of a regular procedure outlined above but not as a result of using the boundary condition (46), as it is the case when one applies the Bogoliubov principle of weakening of initial correlations.$^{(1)}$ Also, when this principle is applied, the correlation function $G_{12}^{q}(t)$ does not show up in the second term of the right-hand side of (69)). Evolution with time in (69) is completely defined by the exact two-particle dynamics, described by the Hamiltonian H_{12} (which is quite natural for the considered linear in n approximation), and in this sense this equation is closed.

6. CONNECTION TO THE QUANTUM BOLTZMANN EQUATION

Equation (69) is not a kinetic equation in the conventional sense because it is time reversible (if the correlation function $g_2(i,j)f_1^{-1}(i)$ $f_1^{-1}(j)$ does not change when the particles' velocities are reversed). Thus, one of the possibilities to secure a time-asymmetric behaviour may be the special choice of an initial condition (e.g. the factorizing one, like (46)).

It is instructive to consider the transition from Eq. (69) to an irreversible kinetic equation describing the evolution, say, into the future ($t > 0$). As it is seen from (69), in order to enter the kinetic (irreversible) stage of the evolution, the reversible terms caused by initial correlations, $G_{12}^{q}(t)$, should vanish on some timescale. Let us suppose that this is the case, when $t \gg t_{\rm cor}$, i.e.

$$G_{12}^{q}(t) = 0, t \gg t_{\rm cor}. \tag{70}$$

Here, the correlation time may be estimated as $t_{\rm cor} \sim r_0/\overline{v}$, where r_0 is the radius of inter-particle interaction and $\overline{v}$ is a typical mean particle velocity. Thus, if a dynamics of the system of particles under consideration is such (e.g. a mixing ergodic flow) that **all** initial correlations caused by inter-particle interaction vanish at the timescale $t \gg t_{\rm cor}$, as it is supposed by condition (70), then Eq. (69) reduces to

$$\begin{aligned} \frac{\partial}{\partial t} f_1(1,t) &= n\int_0^t dt_1 Tr_{(2)} L_{12}^{'} e^{L_{12}t_1} L_{12}^{'}(1+\theta P_{12}) f_r^{12}(t-t_1), \\ f_r^{12}(t-t_1) &= f_1(2) f_1(1,t-t_1), t \gg t_{\rm cor}, \end{aligned} \tag{71}$$

where (64) is also taken into account. Making use of the definitions (28), this equation may be rewritten as

$$\frac{\partial f_1(1,t)}{\partial t} = -\frac{n}{\hbar^2}\int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dE'$$
$$\times \int_0^t dt_1 e^{\frac{1}{i\hbar}(E-E')t_1} Tr_{(2)}\Phi_{12}(E,E',t-t_1), t \gg t_{\mathrm{cor}},$$
$$\Phi_{12}(E,E',t-t_1) = \left[H'_{12}, \delta(E-H_{12})\left[H'_{12}, (1+\theta P_{12})f_r^{12}(t-t_1)\right]\right. \quad (72)$$
$$\left.\times\delta(E'-H_{12})\right].$$

In the adopted first approximation in n, we may consider $f_r^{12}(t-t_1)$ under the integral in the zero approximation in n, in which it does not change with time. Thus, one can approximate the two-particle relevant part of a density matrix under the integral in (72) as $f_r^{12}(t-t_1) = f_1(1,t)f_1(2,t)$. Now, the integral in (72) over t_1 may be calculated. Note, that for finite t Eq. (72) is time reversible and integral over t_1 is a periodic function of t for a finite volume of a system V. This equation becomes time irreversible if the upper limit of integral may be extended to infinity, $t \to \infty$, and this limiting value of the integral over t_1 exists. However, this limiting value of the integral may evidently exist only for a large enough volume of the system under consideration. In other words, in order to exclude the long Poincare's cycles, the thermodynamic limiting procedure ($V \to \infty, N \to \infty, n = \frac{N}{V}$–finite) is needed before calculating the integral. If the mentioned limiting value of the integral exists, then the integral may be considered in the Abel's sense, i.e.

$$\lim_{t\to\infty}\int_0^t dt_1 e^{\frac{1}{i\hbar}(E-E')t_1}$$
$$= \lim_{\varepsilon\to 0^+}\lim_{t\to\infty}\int_0^t dt_1 e^{-\epsilon t_1} e^{\frac{1}{i\hbar}(E-E')t_1} = -i\hbar\frac{\mathrm{Pr}}{E-E'} + \pi\hbar\delta(E-E'), \quad (73)$$

where the order of taking limits matters and Pr is a symbol of taking a principal value of an integral. The procedure given by (73) may also be considered as a coarse-graining (smoothing) procedure over the coarse-graining time interval Δt. This interval, which can be interpreted as the "observation time" (see, for example, ref. 13), should be, naturally, much larger than t_{cor} and much less than the relaxation time t_{rel}

$$t_{\mathrm{cor}} \ll \Delta t \ll t_{\mathrm{rel}}. \quad (74)$$

The existing of interval Δt is guaranteed by the condition (39). Using (73), Eq. (72) may be rewritten as following

$$\begin{gathered}\frac{\partial f_1(1,t)}{\partial t}=-\frac{\pi n}{\hbar}\int dE\,Tr_{(2)}\Phi_{12}(E,t),\, t\gg t_{\mathrm{rel}}\\ \Phi_{12}(E,t)=\left[H_{12}^{'},\delta(E-H_{12})\left[H_{12}^{'},(1+\theta P_{12})f_1(1,t)f_1(2,t)\right]\delta(E-H_{12})\right].\end{gathered}\tag{75}$$

Obtaining (75), we have taken into account that Eq. (72) contains only the diagonal matrix element $\Phi_{12}(E,E^{'},\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1,\mathbf{p}_2,t)$ as it should be because of taking a trace over $\mathbf{p}_2$ and because the left hand side of (72) is diagonal relatively to $\mathbf{p}$ and $\mathbf{p}^{'}$(see (52)). The latter property of $Tr_{(2)}\Phi_{12}(E,t)$ may also be proven explicitly. This diagonal element possesses the symmetry property $\Phi_{12}(E,E^{'},\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1,\mathbf{p}_2,t)=\Phi_{12}(E^{'},E,\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1,\mathbf{p}_2,t)$ and, therefore, the imaginary (principal) part of the integral over E and $E^{'}$ vanishes, as it follows from (72) and (73). The mentioned symmetry of $\Phi_{12}(E,E^{'},\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1,\mathbf{p}_2,t)$ (72) is a consequence of the symmetry of matrix elements of H_{12}^0 and $H_{12}^{'}$ (and, therefore, of H_{12}). The latter symmetry follows from the definition (33) and means that $H_{12}^0(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1^{'},\mathbf{p}_2^{'})=H_{12}^0(\mathbf{p}_1^{'},\mathbf{p}_2^{'},\mathbf{p}_1,\mathbf{p}_2)$ and $H_{12}^{'}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1^{'},\mathbf{p}_2^{'})=H_{12}^{'}(\mathbf{p}_1^{'},\mathbf{p}_2^{'},\mathbf{p}_1,\mathbf{p}_2)$, where

$$\begin{aligned}H_{12}^0(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1^{'},\mathbf{p}_2^{'})&=[K(\mathbf{p}_1)+K(\mathbf{p}_2)]\delta(\mathbf{p}_1-\mathbf{p}_1^{'})\delta(\mathbf{p}_2-\mathbf{p}_2^{'}),\quad K(\mathbf{p}_i)=\tfrac{\mathbf{p}_i^2}{2m},\\ H_{12}^{'}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1^{'},\mathbf{p}_2^{'})&=\tfrac{1}{(2\pi\hbar)^3}\nu(\mathbf{p}_1-\mathbf{p}_1^{'})\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_1^{'}-\mathbf{p}_2^{'}),\\ \nu(\mathbf{p})&=\int\Phi(|\mathbf{r}|)\exp(-\tfrac{i}{\hbar}\mathbf{p}\mathbf{r})d\mathbf{r},\nu(\mathbf{p})=\nu(-\mathbf{p}).\end{aligned}\tag{76}$$

The (operator) δ-function with some Hamiltonian H (entering Eq. (75) with a two-particle Hamiltonian H_{12}) may be expressed via the imaginary part of Green's function $G(E)$:

$$\begin{aligned}\delta(E-H)&=\mp\tfrac{1}{\pi}\mathrm{Im}G(E^{\pm}),\quad G(E^{\pm})=\tfrac{1}{E^{\pm}-H},\\ E^{\pm}&=E\pm i\varepsilon,\quad \varepsilon=0^{+}.\end{aligned}\tag{77}$$

On the other hand, there is the so called optical theorem relating $\delta(E-H)$ (the imaginary part of Green's function $G(E^{\pm})$ for the full Hamiltonian $H=H^0+H^{'}$) and the interaction Hamiltonian $H^{'}$to $\delta(E-H^0)$ (the imaginary part of Green's function $G^0(E^{\pm})=(E^{\pm}-H^0)^{-1}$) and the T-matrix (see, e.g. ref. 8):

$$H'\delta(E-H)H^{'}=T^{+}\delta(E-H^0)T^{-}=T^{-}\delta(E-H^0)T^{+},\tag{78}$$

where the T-matrix is defined as

$$T^{\pm}=T(E^{\pm})=H^{'}G(E^{\pm})G^{0^{-1}}(E^{\pm}), \tag{79}$$

and satisfies the equations

$$T^{\pm}=H^{'}+H^{'}G^{0}(E^{\pm})T^{\pm}=H^{'}+T^{\pm}G^{0}(E^{\pm})H^{'}. \tag{80}$$

The relations (77)–(79) allow for converting $\Phi_{12}(E,t)$ (75) into the following form

$$\Phi_{12}(E,t)=\left[H_{12}^{'-1},T_{12}^{+}\delta(E-H_{12}^{0})T_{12}^{-}\left[H_{12}^{'-1},(1+\theta P_{12})f_{1}(1,t)f_{1}(2,t)\right]T_{12}^{-}\delta(E-H_{12}^{0})T_{12}^{+}\right], \tag{81}$$

where $T_{12}^{\pm}$ refers to the T-matrix (79) defined for the two-particle Hamiltonian $H_{12}=H_{12}^{0}+H_{12}^{'}$. Using (80), it is not difficult to show that

$$T_{12}^{-}\left[H_{12}^{'-1},(1+\theta P_{12})f_{1}(1,t)f_{1}(2,t)\right]T_{12}^{-}=-\left[T_{12}^{-},(1+\theta P_{12})f_{1}(1,t)f_{1}(2,t)\right], \tag{82}$$

where we have also taken into account that $G_{12}^{0}(E^{\pm})=(E^{\pm}-H_{12}^{0})^{-1}$ commutes with $(1+\theta P_{12})f_{1}(1,t)f_{1}(2,t)$ for the space homogeneous case (see also (44)).

Using (82), (81), (80), diagonality of $G^{0}(E^{\pm})$ and of both sides of Eq. (75) in the momentum representation, we may transform this equation into the following form

$$\frac{\partial f_{1}(1,t)}{\partial t}=-\frac{\pi n}{\hbar}\int dETr_{(2)}\left[T_{12}^{+},\delta(E-H^{0})[T_{12}^{-},(1+\theta P_{12})f_{1}(1,t)f_{1}(2,t)]\delta(E-H^{0})\right]. \tag{83}$$

To calculate the trace (integral over $\mathbf{p}_2$) in (83), one need to have the matrix elements of T-matrix in the $\mathbf{p}$-representation. Iterating Eq. (80) and calculating the matrix elements in the momentum representation, one may show that the T_{12}-matrix (describing the particles' collisions) secures the momentum conservation, i.e. $T_{12}^{\pm}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1^{'},\mathbf{p}_2^{'})\sim\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_1^{'}-\mathbf{p}_2^{'})$. For example, in the first approximation in $H_{12}^{'}$, we have $T_{12}^{\pm(1)}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1^{'},\mathbf{p}_2^{'})=H_{12}^{'}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1^{'},\mathbf{p}_2^{'})$, where the matrix element of the interaction Hamiltonian is given by (76). In general, it is not difficult to obtain from (80) and

(76) the following expression for the matrix element of T_{12} in the momentum representation:

$$\begin{aligned} T_{12}^{\pm}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2') &= \tfrac{1}{(2\pi\hbar)^3}t^{\pm}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2')\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_1'-\mathbf{p}_2'), \\ t^{\pm}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2') &= \nu(\mathbf{p}_1-\mathbf{p}_1') \\ &\quad +\tfrac{1}{(2\pi\hbar)^3}\textstyle\int d\mathbf{p}_1''\int d\mathbf{p}_2''\tfrac{\nu(\mathbf{p}_1-\mathbf{p}_1'')\nu(\mathbf{p}_1''-\mathbf{p}_1')}{E^{\pm}-K(\mathbf{p}_1'')-K(\mathbf{p}_2'')} \\ &\quad \times\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_1''-\mathbf{p}_2'') \\ &\quad +\ldots \end{aligned} \tag{84}$$

This T-matrix obeys the following symmetry conditions

$$\begin{aligned} T_{12}^{\pm}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2') &= T_{12}^{\pm}(\mathbf{p}_2,\mathbf{p}_1,\mathbf{p}_2',\mathbf{p}_1'), \\ T_{12}^{\pm}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2') &= T_{12}^{\pm}(\mathbf{p}_1',\mathbf{p}_2',\mathbf{p}_1,\mathbf{p}_2). \end{aligned} \tag{85}$$

Calculating the trace (integral over $\mathbf{p}_2$) in (83) with the use of (84), (85), (52) and (62), we get the following equation for the momentum distribution function

$$\begin{aligned} \frac{\partial w(\mathbf{p}_1,t)}{\partial t} = \frac{\pi n}{(2\pi\hbar)^3\hbar}\int & d\mathbf{p}_2 d\mathbf{p}_1' d\mathbf{p}_2' \delta\left[K(\mathbf{p}_1)+K(\mathbf{p}_2)-K(\mathbf{p}_1')-K(\mathbf{p}_2')\right] \\ & \times\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_1'-\mathbf{p}_2')\left|t^{+}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2')+\theta t^{+}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_2',\mathbf{p}_1')\right|^2 \\ & \times\left[w(\mathbf{p}_1',t)w(\mathbf{p}_2',t)-w(\mathbf{p}_1,t)w(\mathbf{p}_2,t)\right]. \end{aligned} \tag{86}$$

Equation (86) is the quantum Boltzmann equation in the linear approximation in the particles' density n (only binary collisions have been accounted for). It includes (as it should be) the quantum mechanical processes of particles' exchange at scattering (the term proportional to θ), which are caused by the quantum statistics of particles. This irreversible kinetic equation has been obtained with no use of a factorizing initial condition (which introduces irreversibility) for the density matrix of the system under consideration. In the suggested here approach the kinetic Eq. (86) follows from the evolution Eq. (69), which is exact in the linear approximation in n and describes an evolution process at any timescale treating the initial correlations and correlations caused by collisions on the equal footing. The described procedure of obtaining the time-irreversible Eq. (86) from Eq. (69) clearly indicates that irreversibility emerges on the macroscopic timescale (74) as a result of the damping of both the initial correlations caused by interaction and correlations caused by collisions (see also ref. 14). The latter may be secured by the appropriate properties (e.g. ergodic mixing flow) of the system's dynamics. One may, therefore, expect that Eq. (69) will switch automatically from a reversible behaviour to an irreversible one (described by the Boltzmann Eq. (86)) if all correlations vanish with time while going from microscopic to a large enough timescale. Thus, the influence of initial correlations on an evolution process may be revealed.

7. CONCLUSION

We have rederived the exact time-convolution homogeneous generalized master equation (TC-HGME) and obtained the exact time-convolutionless homogeneous generalized master equation (TCL-HGME) which are valid for both the classical and quantum physics cases. In the derivation we have not used any approximation (like a factorizing initial condition or RPA) or principle (like the Bogoliubov principle of weakening of initial correlations). These equations have several advantages as compared to the generalized master equations (GMEs). The HGMEs contain the parameter of initial correlations depending on time in the "mass" (super)operator acting on the relevant part of a distribution function (statistical operator). Thus, these equations allow for treating the initial correlations consistently and on the equal footing with the collision integral by expanding the "mass" (super)operator into the series on the appropriate small parameter. The obtained equations are valid on any timescale, particularly on the initial stage of evolution $t_0 \leqslant t \leqslant t_{\text{cor}}$, which may be important for studying the irreversibility problem and the ultrafast and non-Markovian relaxation processes. The HGMEs enable the consideration of the entire evolution process of the relevant part of a distribution function (statistical operator) and of the influence of initial correlations on this process, because these equations can switch, in principle, e.g. from the initial (reversible) regime into the kinetic (irreversible) one, automatically. Special consideration has been given to the existence of the parameter of initial correlations. It has been shown that the corresponding inverse operators exist (at least) in the considered first approximation in the density of particles.

To test the developed general formalism in the quantum physics case, we have focused in this work on the application of the TC-HGME to a dilute gas of quantum particles. By appropriate selection of the projection operator, we have obtained a new evolution Eq. (69) for a one-particle density matrix, which retains initial correlations and is exact in the linear approximation in n for the space homogeneous case. In this approximation the evolution equation for a one-particle momentum distribution function contains only binary collisions and a two-particle time-dependent (through only two-particle dynamics) correlation function as well as the symmetrization operator P_{ij} (caused by quantum statistics) in the parameter accounting for initial correlations. It has been shown that on the macroscopic timescale this equation (valid on any timescale) may become equivalent to the quantum Boltzmann Eq. (86) if all correlations caused by interaction between particles vanish on this timescale. All stages of evolution described by Eq. (69) may be numerically modelled for some specific interaction between particles, specific initial two-particle correlation function $g(1, 2)$ and initial values $f_1(i)$ $(i = 1, 2)$.

Next approximation in n will evidently result in the additional, nonlinear in f_1, terms, which account for the Fermi or Bose statistics of the particles in the scattering processes.

The developed formalism may be applied to an open quantum system like a subsystem interacting with an environment (heat bath). This will be done in the next paper.

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