Unification of kinetic and hydrodynamic approaches in the theory of dense gases and liquids far from equilibrium

Tokarchuk M. V.$^{1,2}$

$^1$Institute for Condensed Matter Physics of NAS of Ukraine, 1 Svientsitskii Str., 79011, Lviv, Ukraine
$^2$Lviv Polytechnic National University, 12 S. Bandera Str., 79013, Lviv, Ukraine

(Received 12 September 2022; Revised 15 February 2023; Accepted 20 February 2023)

A system of non-Markovian transport equations is obtained for the non-equilibrium one-particle distribution function of particles and the non-equilibrium average value of the density of the potential energy of the interaction of the system particles far from the equilibrium state. Expressions for entropy, the partition function of the non-equilibrium state of the system, as well as non-equilibrium thermodynamic relations were obtained. The generalized structure of transfer nuclei is revealed in detail with the selection of short-range and long-range contributions of interactions between particles. The connection of transport nuclei with generalized diffusion coefficients, friction in the space of coordinates and momentum and the potential part of the thermal conductivity coefficient is established.

Keywords: non-Markov equations; the method of nonequilibrium statistical operator; entropy; partition function of the non-equilibrium state; transport nuclei.

2010 MSC: 82C05, 82C70

DOI: 10.23939/mmc2023.02.272

1. Introduction

A whole series of works is dedicated to problems and approaches to the agreed description of kinetic and hydrodynamic processes in dense gases, liquids, and plasma [1–17]. In [7], it is justified the necessity and the possibility of a single description of kinetic and hydrodynamic processes in gases for values of the Knudsen number of the order of unity. Based on this, a generalized kinetic equation was proposed for the description of non-equilibrium processes under arbitrary conditions Knudsen numbers. The collision integral of such an equation, in particular, includes the diffusion coefficient in the velocity space.

Based on ideas [3, 5], by the method of non-equilibrium statistical operator, the generalized transport equations for hydrodynamic variables (density of the number of particles, momentum, and total energies) consistent with the kinetic equation for non-equilibrium of the single-particle distribution function were obtained in [8, 11]. This approach studied time correlation functions for fluids that describe the dynamics systems in the states close to equilibrium. The results of this approach are equivalent research of works [1, 2] based on the Mori projective operators method. An important and common problem with data research is the calculation of generalized transfer kernels (functions memory), which are defined as integrals of the collision between particles for different models [1, 18–29], and generalized viscosity transfer coefficients, thermal conductivity [1, 8, 11].

A special problem is the area of short-range interactions since at short distances in dynamics of particles not only spatio-temporal characteristics change but also pulses when particles collide in the region of the physical volume $V_{ph}$ at times $\tau_{ph}$, respectively Klimontovych [6, 7]. In the hydrodynamic region, that is, for small values of frequency and wave vector, the results correspond to molecular equation hydrodynamics in the case of simple fluids [2, 30]. In a recent work [31], there is discussed the important issue of the hydrodynamic boundary based on the classical equations of hydrodynamics in comparison with the molecular dynamics method for four models of liquid systems. Such a description corresponds to linear approximations by kinetic and hydrodynamic fluctuations, which leads, in par-
particularly, to equilibrium temporal correlation functions of the densities of the number of particles, their momentum and energy, and memory functions that determine the generalized transfer coefficients of viscosity, thermal conductivity, diffusion, friction, and they are the equilibrium temporal correlation functions of the corresponding flows. In the case of non-equilibrium states far from equilibrium, the description of kinetic and hydrodynamic fluctuations becomes much more complicated. Here, in temporal correlation functions and memory functions, averaging is performed not according to the equilibrium distribution of particles but according to the time-dependent distribution of particles, which can be found from the principle of the maximum of the corresponding information entropy.

A consistent description of kinetic and hydrodynamic processes is necessary for dust plasma [12, 32–39]. The non-equilibrium state of such a multicomponent system of charges and neutral particles is connected with the dynamics of each of the components and the interaction between them. Different components can be in the kinetic or hydrodynamic, stationary, or non-stationary states; and the condition of local electroneutrality may be violated due to the charging and recharging of powders.

The combination of kinetic and hydrodynamic approaches is also relevant to research of non-equilibrium properties of systems of active particles [40–46]. A vivid example of such systems is molecular, biological fluids, and suspensions, in which the movement and behavior of various components can change due to the transformation of accumulated energy or under the influence of external sources (pressure, light, temperature gradients). At the same time, various components, depending on their properties, can be at the kinetic or hydrodynamic stages of non-equilibrium processes. As a rule, the solvent is considered from the point of view of hydrodynamic processes, when the visco-thermal properties can change significantly due to the kinetic behavior of individual active components of the system.

The various non-equilibrium statistical theory methods for describing nonlinear kinetic and hydrodynamic fluctuations we discussed in the works [47–49].

In the second section, we will obtain the non-equilibrium statistical operator of the non-equilibrium state of the far-from-equilibrium system of particles, when the parameters of a reduced description are the non-equilibrium one-particle distribution function of particles, non-equilibrium average value of the potential energy density of the interaction of particles. The method of non-equilibrium statistical operator [8,10,50] is applied. At the same time, the energy of interaction between particles is presented as the sum of short-range and long-range interactions between particles. To describe collective dynamic processes in the system as collective variables, we introduce the Fourier components of the density, the number of particles that are related to the Fourier components of the particle momentum density by the continuity equation, and also through them, the long-range part of the potential energy of the interaction of particles is expressed. At the same time, the density of the kinetic energy and the short-lived part of the potential of the interaction of particles are described in the coordinate–momentum space. The issue of entropy and the partition function of the non-equilibrium state of the system, as well as non-equilibrium thermodynamic relations, are discussed.

In the third section, we derive the generalized transport equations for the non-equilibrium one-particle distribution function of particles and non-equilibrium average value of the potential energy density of particle interaction. The structure of generalized transfer nuclei is revealed in detail, with the contributions of short-range and long-range interactions between particles being highlighted. Their connection with the generalized diffusion transfer coefficients, friction in the space of momentum and coordinates, and the potential part of the thermal conductivity coefficient has been established. As a result of the exclusion using self-consistency conditions of the Lagrangian parameter \( a(x;t) \) conjugated to the non-equilibrium one-particle distribution function \( f_1(x;t) \) made it possible to write the kinetic equation for \( f_1(x;t) \) in the closed form with the contribution of the generalized mean field and the generalized integral of collisions of the Fokker–Planck type with generalized coefficients of diffusion, friction in the momentum–coordinate space. In addition, using the self-consistency condition and integral transformations, the Lagrange parameter \( \beta(r;t) \) is the time-dependent local inverse temperature, it is also determined. As a result, a closed system of non-Markov transport equations for the non-equilibrium single-particle distribution function of particles and of the non-equilibrium average value of the potential energy density of the interaction of the system’s particles far from the state of equilibrium is obtained.

2. Non-equilibrium distribution function

For a consistent description of kinetic and hydrodynamic fluctuations in classical dense gases and liquids, it is necessary to select the basic parameters of a reduced description single-particle and collective processes. As such parameters, we choose [1–3, 8, 11] the nonequilibrium one-particle distribution function \( f_1(x; t) = \langle \hat{n}_1(x) \rangle^t \) and the non-equilibrium mean value, the energy of interaction of particles \( \langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t \), in which the microscopic phase density of the number of particles \( \hat{n}_1(x) \) and microscopic potential energy density interactions of the particles of the system \( \hat{\varepsilon}_{\text{int}}(r) \) are given by the expressions:

\[
\hat{n}_1(x) = \sum_{j=1}^{N} \delta(x - x_j) = \sum_{j=1}^{N} \delta(r - r_j)\delta(p - p_j),
\]

\[
\hat{\varepsilon}_{\text{int}}(r) = \frac{1}{2} \sum_{j \neq l=1}^{N} \Phi(|r_{lj}|)\delta(r - r_j),
\]

where \( x_j = (r_j, p_j) \) are the coordinates and momenta of the particles in the phase space, \( N \) is the total number of system particles in the volume \( V \). In the pair potential of interaction between particles \( \Phi(|r_{lj}|) = \Phi(|r_l - r_j|) \), selected the short-term \( \Phi_{\text{sh}}(|r_{lj}|) \) and the long-range \( \Phi_{\text{long}}(|r_{lj}|) \) part:

\[
\Phi(|r_{lj}|) = \Phi_{\text{sh}}(|r_{lj}|) + \Phi_{\text{long}}(|r_{lj}|). \tag{1}
\]

Accordingly, the non-equilibrium value of the potential energy of the interacting particles will have the form:

\[
\langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t = \langle \hat{\varepsilon}_{\text{int}}^{\text{sh}}(r) \rangle^t + \frac{1}{2V^2} \sum_{q,k} \nu(q,k) e^{iqr} \left( \langle \rho_{q+k} \hat{\rho}_{-k} \rangle^t - \langle \hat{\rho}_q \rangle^t \right),
\]

where \( \nu(q,k) \) is the Fourier component of the long-range part of the particle interaction potential, \( q \) and \( k \) are wave vectors.

\[
\hat{\rho}_k = \sum_{j=1}^{N} e^{-ikr_j}
\]

is the Fourier component of the density of the number of particles, \( \langle \hat{\varepsilon}_{\text{int}}^{\text{sh}}(r) \rangle^t \) is the non-equilibrium average value of the energy density of short-range interactions between particles. Non-equilibrium particle scattering function \( \langle \hat{\rho}_{q+k} \hat{\rho}_{-k} \rangle^t = F(q,k; t) \) is related to the non-equilibrium dynamic structural factor \( S(q,k; \omega) \), which is measured in neutron scattering processes. The non-equilibrium mean values \( \langle \hat{n}_1(x) \rangle^t \) and \( \langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t \) are calculated with the non-equilibrium function distribution of \( N \)-particles \( \varrho(x^N; t) \)

\[
\varrho(x^N; t) = \varrho(\ldots, f_1(x; t), \langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t, \ldots).
\]

At the same time, the moments of the non-equilibrium one-particle function, which form the basis of the hydrodynamic description [11] for both weakly and strongly non-equilibrium processes, have the form:

\[
n(r; t) = \int dp \varrho_{f_1}(p, r; t),
\]

\[
p(r; t) = \int dp \varrho_{f_1}(p, r; t)p,
\]

\[
\langle \hat{\varepsilon}_{\text{kin}}(r) \rangle^t = \int dp \varrho_{f_1}(p, r; t) \frac{p^2}{2m},
\]

there are non-equilibrium mean values of particle number densities \( n(r; t) \), momentum \( p(r; t) \), kinetic energy \( \langle \hat{\varepsilon}_{\text{kin}}(r) \rangle^t \) together with \( \langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t \).

To find the non-equilibrium distribution function \( \varrho(x^N; t) \), we will use Zubarev’s method [10, 50], in which the general solution the Liouville equation, taking into account the design procedure, can be
where the relevant distribution function can be written as $\varrho_{\text{rel}}(x^N; t) = \varrho_{\text{rel}}(x^N; t) - \int_{-\infty}^{t} dt' e^{\varepsilon(t'-t)} T_{\text{rel}}(t, t')(1 - P_{\text{rel}}(t')) i L_N \varrho_{\text{rel}}(x^N; t')$, where $\varepsilon \to +0$ after the limiting thermodynamic transition, which selects the lagging solutions of the Liouville equation with the operator $i L_N$. $T_{\text{rel}}(t, t') = \exp \left( - \int_{t'}^{t} dt' \left( 1 - P_{\text{rel}}(t') \right) i L_N \right)$ is a generalized evolution operator dependent on time taking into account the Kawasaki–Gunton design $P_{\text{rel}}(t)$. The structure of $P_{\text{rel}}(t)$ depends on the relevant distribution function $\varrho_{\text{rel}}(x^N; t)$, which in the Zubarev method is from the extremum of the information entropy (in particular, the Gibbs entropy) at fixed values of the basic parameters of a reduced description, in our case $f_1(x; t)$, $\langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t$ and preserved rationing conditions:

$$\int d\Gamma_N \varrho_{\text{rel}}(x^N; t) = 1, \quad \text{where} \quad d\Gamma_N = \frac{(dx)^N}{N!} = \frac{(dx_1 \ldots dx_N)}{N!}, \quad dx = dr \, dp.$$  

Thus, the relevant distribution function can be written as [3, 5, 8, 11]:

$$\varrho_{\text{rel}}(x^N; t) = \exp \left[ - \Phi(t) - \int dr \beta(r; t) \hat{\varepsilon}_{\text{int}}(r) - \int dx a(x; t) \hat{n}_1(x) \right],$$  

where $\Phi(t)$ is the Massier–Planck functional, which is determined from the normalization condition of the relevant distribution function

$$\Phi(t) = \ln Z_{\text{rel}}(t),$$

where

$$Z_{\text{rel}}(t) = \int d\Gamma_N \exp \left[ - \int dr \beta(r; t) \hat{\varepsilon}_{\text{int}}(r) - \int dx a(x; t) \hat{n}_1(x) \right]$$

is the partition function of the relevant distribution function. The Lagrange multipliers $a(x; t)$ and $\beta(r; t)$ are from self-consistency conditions:

$$f_1(x; t) = \langle \hat{n}_1(x) \rangle^t = \langle \hat{n}_1(x) \rangle_{\text{rel}}^t, \quad \langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t = \langle \hat{\varepsilon}_{\text{int}}(r) \rangle_{\text{rel}}^t,$$

where $\langle \ldots \rangle_{\text{rel}} = \int d\Gamma_N \ldots \varrho_{\text{rel}}(x^N; t)$.

The relevant distribution function (3) corresponds to the Gibbs entropy

$$S(t) = - \langle \ln \varrho_{\text{rel}}(x^N; t) \rangle_{\text{rel}}^t = \Phi(t) + \int dr \beta(r; t) \langle \hat{\varepsilon}_{\text{int}}(r) \rangle_{\text{rel}}^t + \int dx a(x; t) \langle \hat{n}_1(x) \rangle_{\text{rel}}^t,$$

which, in combination with self-consistency conditions (4), can be considered as the entropy of the non-equilibrium state:

$$S(t) = \Phi(t) + \int dr \beta(r; t) \langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t + \int dx a(x; t) \langle \hat{n}_1(x) \rangle^t,$$

and for which the Boltzmann theorem must hold:

$$\frac{dS(t)}{dt} \geq 0.$$  

As we can see, the change in entropy over time is described both by the Lagrange parameters $\beta(r; t)$, $a(x; t)$ and by the parameters of the shortening description $\langle \hat{n}_1(x) \rangle^t$, $\langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t$, and also depends on the non-equilibrium partition function $\Phi(t) = \ln Z_{\text{rel}}(t)$ taking into account the self-consistency conditions for the Lagrangian parameters. From this point of view, in the general formulation of the problem of statistical description, an important issue is the calculation of the partition function $Z_{\text{rel}}(t)$ both for the calculation of non-equilibrium entropy and Lagrange multipliers. In work [51], one of the methods of calculating $Z_{\text{rel}}(t)$ using the method of collective variables [47–49] was proposed. At the same time, contributions from short-range and long-range interactions were separated between particles. This led to the fact that short-range interactions (for example, the hard-sphere model) were described in the coordinate-momentum space, and long-range ones in the space of collective variables of the particle number density. Moreover, the short-acting component was considered the basic one, to which the chain of BBGKl equations for non-equilibrium distribution functions corresponds, in particular, in the case of the hard-sphere model [52].

Hence, varying the entropy (10) by the mean values $\langle \cdot \rangle$, we will find non-equilibrium thermodynamic relations:

$$
\dot{\varepsilon}'(r) = \dot{\varepsilon}(r) - \dot{p}(r)\mathbf{v}(r; t) + \frac{1}{2}m^2 \mathbf{v}(r; t)\dot{n}(r).
$$

Parameters $\beta(r; t)$ and $a'(x; t)$ in (5) are determined from the self-consistency conditions — equalities of quasi-means $\langle \dot{n}_1(x) \rangle_{rel}^t$, $\langle \varepsilon'(r) \rangle_{rel}^t$ is true by the mean $\langle \dot{n}_1(x) \rangle^t$, $\langle \varepsilon'(r) \rangle^t$:

$$
\langle \dot{n}_1(x) \rangle^t = \langle \dot{n}_1(x) \rangle_{rel}^t,
$$

$$
\langle \varepsilon'(r) \rangle^t = \langle \varepsilon'(r) \rangle_{rel}^t,
$$

where the parameter $a'(x; t)$ is related to the $a(x; t)$ relation:

$$
a'(x; t) = a(x; t) - \beta(r; t) \left( \frac{p^2}{2m} - \mathbf{p} \cdot \mathbf{v}(r; t) + \frac{1}{2}m^2 \mathbf{v}(r; t) \right)
= a(x; t) - \beta(r; t) \frac{m}{2} \left( \mathbf{p} - m\mathbf{v}(r; t) \right)^2.
$$

If the self-consistency conditions (6) and (7) are performed by taking the variational derivatives of the functional Massier–Planck

$$
\Phi(t) = \ln \int d\Gamma_N \exp \left( -\int dr \beta(r; t)\varepsilon'(r) - \int dx a'(x; t)\dot{n}_1(x) \right),
$$

according to the parameters $\beta(r; t)$ and $a'(x; t)$, we obtain non-equilibrium thermodynamic relations taking into account the conditions of self-consistency:

$$
\frac{\delta\Phi(t)}{\delta\beta(r; t)} = -\langle \varepsilon'(r) \rangle_{rel}^t = -\langle \varepsilon'(r) \rangle^t,
$$

$$
\frac{\delta\Phi(t)}{\delta a'(x; t)} = -\langle \dot{n}_1(x) \rangle_{rel}^t = -\langle \dot{n}_1(x) \rangle^t,
$$

this means that $\beta(r; t)$ is conjugate to the average energy accompanying coordinate system, and $a'(x; t)$ is conjugate $f_1(x; t)$ is a non-equilibrium one-particle particle distribution function. According to (8) and (9), the calculation of the partition function of the relevant distribution makes it possible to calculate the exact parameters of a reduced description $f_1(x; t)$ and $\langle \varepsilon'(r) \rangle^t$.

Next, we write the entropy of the system, taking into account (5) in the form:

$$
S(t) = \Phi(t) + \int dr \beta(r; t)\varepsilon'(r) + \int dx a'(x; t)\dot{n}_1(x)\dot{t}.
$$

Hence, varying the entropy (10) by the mean values $\langle \varepsilon'(r) \rangle^t$ and $\langle \dot{n}_1(x) \rangle^t$ at fixed corresponding values medium, we will find non-equilibrium thermodynamic relations:

$$
\frac{\delta S(t)}{\delta \langle \varepsilon'(r) \rangle^t} = \beta(r; t),
$$

$$
\frac{\delta S(t)}{\delta \langle \dot{n}_1(x) \rangle^t} = a'(x; t),
$$

from which we get that the function $\beta(r; t)$ is an analogue of the inverse local temperature. The Lagrangian parameter $a(x; t)$ can be determined from the self-consistency condition (4) by defining it by the relation [3, 4, 8, 11]

$$
\exp \left( -a(x; t) \right) = \frac{f_1(x; t)}{u(r; t)},
$$

where the function $u(r; t)$ satisfies the equation:

$$
uu(r; t) = \int \frac{dr^N}{(N-1)!} \exp \left( -\Phi(t) - U_N(r, r^{N-1}; t) \right) \prod_{i=2}^N \frac{n(r_i, t)}{u(r_i; t)},
$$

in which
\[ U_N(r^N; t) = U_N(r_1, \ldots, r_N; t) = \frac{1}{2} \sum_{i,j=1}^N \Phi(|r_ij|)\beta(r_j; t). \]

Next, using (11) and the relevant distribution in the form:
\[ \rho_{\text{rel}}(x^N; t) = \exp \left( -\Phi(t) - U_N(r^N; t) \right) \prod_{l=1}^N \exp(-a(x_l; t)), \]
for \( \rho_{\text{rel}}(x^N; t) \) we get
\[ \rho_{\text{rel}}(x^N; t) = \exp \left( -\Phi(t) - U_N(r^N; t) \right) \prod_{l=1}^N \frac{f_l(x_l, t)}{u(r_l; t)}. \] (12)

If \( u(r; t) \) is found, then from (12), one can obtain an explicit expression for of the relevant distribution function through the non-equilibrium one-particle function distribution. In (12) the function \( U_N(r^N; t) \) is explicit, and \( u(r_l; t) \) is implicit depend on hydrodynamic parameters \( u(r, t), \beta(r; t) \) (or \( (\hat{\varepsilon}'(r))^t \)). Therefore, the Lagrangian parameter can be defined as
\[ a(x; t) = -\ln \frac{f_l(x, t)}{u(r; t)}. \] (13)

The expression for non-equilibrium entropy (12), taking into account (13), can be given as
\[ S(t) = \Phi(t) + \int dx \beta(r; t)\hat{\varepsilon}_{\text{int}}(r)^t - \int dx f_l(x; t) \ln \frac{f_l(x; t)}{u(r; t)}. \] (14)

Moreover, if we neglect contributions of potential energy \( \hat{\varepsilon}_{\text{int}}(r) \), which is true for rare gases, then expression (14) for the non-equilibrium entropy of the agreed description of kinetics and hydrodynamics is transformed into the Boltzmann entropy \( (u = e) \).

We will use the corresponding self-consistency condition to determine the Lagrangian parameter \( \beta(r; t) \). We will perform the following actions:
\[ \frac{\partial}{\partial t} (\hat{\varepsilon}_{\text{int}}(r))^t = \frac{\partial}{\partial t} (\hat{\varepsilon}_{\text{int}}(r))^t_{\text{rel}} = \frac{\partial}{\partial \beta(r; t)} (\hat{\varepsilon}_{\text{int}}(r))^t_{\text{rel}} = K_{\varepsilon}(r, r; t) \frac{\partial}{\partial \beta(r; t)} \beta(r; t), \]
where
\[ K_{\varepsilon}(r, r; t) = (\hat{\varepsilon}_{\text{int}}(r)\hat{\varepsilon}_{\text{int}}(r))^t_{\text{rel}} - ((\hat{\varepsilon}_{\text{int}}(r))^t_{\text{rel}})^2 = \frac{\partial^2}{\partial \beta(r; t)^2} \ln Z_{\text{rel}}(t) \]
is a dispersion of the random value of the interaction energy density between the particles of the system. From the obtained equation, we determine \( \frac{\partial}{\partial \beta(r; t)} \), after which we integrate the obtained expression over time within \( (-\infty \div t) \). As a result, we get the following:
\[ \beta(r; t) = \int_{-\infty}^t K_{\varepsilon}^{-1}(r, r; t') \frac{\partial}{\partial t'} (\hat{\varepsilon}_{\text{int}}(r))^{t'} dt' + \beta(r; -\infty), \] (15)
where \( \beta(r; -\infty) \) is the local inverse temperature at \( t = -\infty \) (past). Calculation of the variance \( K_{\varepsilon}(r, r; t) \) requires the calculation of the partition function \( Z_{\text{rel}}(t) \) [51].

It is important to note that in previous works [8, 11, 53–55], there were no problems calculating \( \Phi(t) = \ln Z_{\text{rel}}(t) \) in non-equilibrium entropy since we studied in detail weak non-equilibrium transport processes, in particular the spectrum of collective excitations, time correlation functions for simple liquid and dense plasma. In the case of weakly non-equilibrium processes, only the partition function of the equilibrium distribution contributes to the non-equilibrium entropy, and the evolution in time is described by non-equilibrium fluctuations of the parameters of a reduced description \( (\delta \hat{n}(x))^t, (\delta \hat{\varepsilon}_{\text{int}}(r))^t \) relative to their equilibrium average values \( (\bar{n}(x))_0, (\bar{\varepsilon}_{\text{int}}(r))_0 \), where \( \delta \hat{n}(x) = \hat{n}(x) - \bar{n}(x) \), \( \delta \hat{\varepsilon}_{\text{int}}(r) = \hat{\varepsilon}_{\text{int}}(r) - \bar{\varepsilon}_{\text{int}}(r) \), \( f_0(p) = (\beta/2\pi m)^{3/2} \exp \{-\beta p^2/2m\} \) is the Maxwell distribution, \( \{x\} = \int d\Gamma x \cdots \rho_0(x^N) \) and \( \rho_0(x^N) = Z^{-1} e^{-\beta(\hat{H} - \mu N)} \) is the grand canonical Gibbs distribution of system particles, \( \beta = 1/k_B T, \mu \) is the equilibrium temperature value, \( Z = \int d\Gamma_N e^{-\beta(\hat{H} - \mu N)} \) is grand partition function, \( \mu \) is the equilibrium value of the chemical potential (see Appendix 1).
Therefore, for a consistent description of kinetic and hydrodynamic processes in dense gases and liquids, an important issue is the calculation of the partition function \( Z_{\text{rel}}(t) \) (taking into account the self-consistency conditions for the Lagrangian parameters \( \beta(r; t), a(x; t) \)), which is included in the expression for the non-equilibrium entropy of the system, and also makes it possible to calculate the parameters of a reduced description \( \langle \varepsilon'(r) \rangle^t \) and \( \langle \dot{n}_1(x) \rangle^t \) according to nonequilibrium thermodynamic relations (8) and (9).

To obtain a clear form of the non-equilibrium distribution function according to (2), it is necessary to perform the action of Liouville and Kawasaki–Gunton operators on the function \( \varrho_{\text{rel}}(x^N; t) \). The Kawasaki–Gunton projection operator according to (3) has the following structure:

\[
P_q(t)\varrho' = \varrho_{\text{rel}}(x^N; t) \int d\Gamma_N \varrho' + \int dx \frac{\partial \varrho_{\text{rel}}(x^N; t)}{\partial \dot{\varrho}_1(x)^{t}} \left[ \int d\Gamma_N \dot{\varrho}_1(x)^{t} - \langle \dot{\varrho}_1(x) \rangle^t \int d\Gamma_N \varrho' \right] + \int d\mathbf{r} \frac{\partial \varrho_{\text{rel}}(x^N; t)}{\partial \langle \dot{\varepsilon}_{\text{int}}(\mathbf{r}) \rangle^t} \left[ \int d\Gamma_N \langle \dot{\varepsilon}_{\text{int}}(\mathbf{r}) \rangle^t - \langle \dot{\varepsilon}_{\text{int}}(\mathbf{r}) \rangle^t \int d\Gamma_N \varrho' \right].
\]

First, we will reveal the action of the Liouville operator on the relevant distribution function (3). As a result, we get the following:

\[
i_{LN} \varrho_{\text{rel}}(x^N; t) = - \int dx a(x; t) \dot{\varrho}_1(x) \varrho_{\text{rel}}(x^N; t) - \int d\mathbf{r} \beta(r; t) \dot{\varepsilon}_{\text{int}}(\mathbf{r}) \varrho_{\text{rel}}(x^N; t),
\]

where \( \dot{\varrho}_1(x) = i_{LN} \dot{\varrho}_1(x), \dot{\varepsilon}_{\text{int}}(\mathbf{r}) = i_{LN} \dot{\varepsilon}_{\text{int}}(\mathbf{r}) \). By substituting this expression into (2), we find the non-equilibrium distribution function in the form:

\[
\varrho(x^N; t) = \varrho_{\text{rel}}(x^N; t) + \int d\mathbf{r} \int_{-\infty}^{t} dt' e^{\varepsilon(t'-t)} T_{\text{rel}}(t, t') (1 - P_{\text{rel}}(t')) \dot{\varepsilon}_{\text{int}}(\mathbf{r}) \varrho_{\text{rel}}(x^N; t) \beta(r; t') + \int dx \int_{-\infty}^{t} dt' e^{\varepsilon(t'-t)} T_{\text{rel}}(t, t') (1 - P_{\text{rel}}(t')) \dot{\varrho}_1(x) \varrho_{\text{rel}}(x^N; t') a(x; t').
\]

Let us write the expression for (16) in a more explicit form, revealing the action of operators \((1 - P_{\text{rel}}(t'))\) and \(i_{LN}\) on \(\varrho_{\text{rel}}(x^N; t')\):

\[
(1 - P_{\text{rel}}(t))i_{LN}\varrho_{\text{rel}}(x^N; t) = - \int d\mathbf{r} \beta(r; t)((1 - P_{\text{rel}}(t))i_{LN} \dot{\varepsilon}_{\text{int}}(\mathbf{r})) \varrho_{\text{rel}}(x^N; t)
\]

or

\[
(1 - P_{\text{rel}}(t))i_{LN}\varrho_{\text{rel}}(x^N; t) = -( \int d\mathbf{r} \beta(r; t)(1 - P(t))i_{LN} \dot{\varepsilon}_{\text{int}}(\mathbf{r})
\]

\[
+ \int dx b(x; t)(1 - P(t))i_{LN} \dot{n}_1(x) \varrho_{\text{rel}}(x^N; t),
\]

where \(P(t)\) is the generalized Mori projection operator acting on dynamic variables \(A(\mathbf{r})\) and has the following structure:

\[
P(t)A(\mathbf{r}) = \langle A(\mathbf{r}) \rangle^t_{\text{rel}} + \int d\mathbf{r}' \frac{\delta(A(\mathbf{r}))/\delta(\dot{\varepsilon}_{\text{int}}(\mathbf{r}'))}{\delta(\dot{\varepsilon}_{\text{int}}(\mathbf{r})')} (\dot{\varepsilon}_{\text{int}}(\mathbf{r}') - \langle \dot{\varepsilon}_{\text{int}}(\mathbf{r}') \rangle^t) + \int dx \frac{\delta(A(\mathbf{r}))/\delta(\dot{n}_1(\mathbf{r}))/\delta(\dot{n}_1(\mathbf{r}'))}{\delta(\dot{n}_1(\mathbf{r}'))} (\dot{n}_1(\mathbf{r}) - \langle \dot{n}_1(\mathbf{r}) \rangle^t).
\]

The projection operator \(P(t)\) has the following properties:

\[
P(t)n_1(x) = \dot{n}_1(x), \quad P(t)\dot{\varepsilon}_{\text{int}}(\mathbf{r}) = \dot{\varepsilon}_{\text{int}}(\mathbf{r}),
\]

\[
P(t)P(t') = P(t), \quad P(t)(1 - P(t)) = 0.
\]

Now, taking into account (17), we write the expression for \(\varrho(x^N; t)\) (16) as

\[
\varrho(x^N; t) = \varrho_{\text{rel}}(x^N; t) + \int d\mathbf{r} \int_{-\infty}^{t} e^{\varepsilon(t'-t)} \beta(r; t') T(t, t') \dot{\varepsilon}_{\text{int}}^t (\mathbf{r}) \varrho_{\text{rel}}(x^N; t') \rho_{\text{rel}}(x^N; t') dt' + \int dx \int_{-\infty}^{t} e^{\varepsilon(t'-t)} a(x; t') T(t, t') \dot{n}_1(x; t') \rho_{\text{rel}}(x^N; t') dt',
\]

where
\[ I_e^{\text{int}}(r; t') = (1 - P(t')) iL_N \hat{\varepsilon}^{\text{int}}(r), \quad I_n(x; t') = (1 - P(t')) iL_N \hat{n}_1(x) \]
are generalized flows that describe dissipative processes in the system. To analyze the structure of generalized flows, it is necessary to calculate \( iL_N \hat{\varepsilon}^{\text{int}}(r) \) and \( iL_N \hat{n}_1(x) \) taking into account that the complete particle interaction potential is divided into short-range and long-range contributions (1).

So, we get
\[ iL_N \hat{\varepsilon}^{\text{int}}(r) = iL_N \hat{\varepsilon}^{\text{sh}}^{\text{int}}(r) + iL_N \hat{\varepsilon}^{\text{long}}^{\text{int}}(r) \]
\[ = -\frac{\partial}{\partial r} \cdot \hat{\mathbf{j}}^{\text{int}}(r) + \frac{1}{2V^2} \sum_{q,k} \nu(k) e^{iqr} \left( -i(q + k) \cdot \hat{\mathbf{p}}_{q+k} \hat{\rho}_{-k} + i(k \cdot \hat{\mathbf{p}}_{q+k} + i\mathbf{q} \cdot \hat{\mathbf{p}}_q) \right), \]
where
\[ \hat{\mathbf{p}}_q = \sum_{j=1}^N \mathbf{p}_j e^{-iq \cdot r_j} \]
is the Fourier component of the microscopic momentum density of the system particles,
\[ \hat{\mathbf{j}}^{\text{sh}}^{\text{int}}(r) = \frac{1}{2} \sum_{j,l=1}^N \frac{\mathbf{p}_j - \mathbf{p}_l}{m} \Phi_{rl}(\mathbf{r}_j, \mathbf{r}_l)\delta (\mathbf{r} - \mathbf{r}_j) + \frac{1}{2} \sum_{j,l=1}^N \frac{\mathbf{p}_j + \mathbf{p}_l}{m} \cdot \mathbf{F}^{\text{sh}}_{jl}(\mathbf{r}_j, \mathbf{r}_l) \delta (\mathbf{r} - \mathbf{r}_j) \]
is the vector of the microscopic energy flow density of short-range particle interactions,
\[ \mathbf{F}^{\text{sh}}_{jl}(\mathbf{r}_j, \mathbf{r}_l) = -\frac{\partial}{\partial |\mathbf{r}_{jl}|} \Phi_{rl}(\mathbf{r}_j, \mathbf{r}_l) \frac{1}{|\mathbf{r}_{jl}|} \mathbf{r}_{jl} \]
is a short-acting microscopic force between the \( j \)-th and \( l \)-th particles of the system. It can be seen from this that the generalized flow \( I_e^{\text{int}}(r; t') \) contains short-range and long-range contributions of the potential part of the particle interaction energy flow density:
\[ I_e^{\text{int}}(r; t') = I_e^{\text{sh}}(r; t') + I_e^{\text{long}}(r; t'), \]
where
\[ I_e^{\text{sh}}(r; t') = -\frac{\partial}{\partial r}(1 - P(t')) \hat{\mathbf{j}}^{\text{sh}}^{\text{int}}(r), \]
\[ I_e^{\text{long}}(r; t') = (1 - P(t')) \frac{1}{2V^2} \sum_{q,k} \nu(k) e^{iqr} \left( -i(q + k) \cdot \hat{\mathbf{p}}_{q+k} \hat{\rho}_{-k} + i(k \cdot \hat{\mathbf{p}}_{q+k} + i\mathbf{q} \cdot \hat{\mathbf{p}}_q) \right). \]
Moreover, the long-range contribution is related to the product of modes \( \hat{\mathbf{p}}_{q+k} \hat{\rho}_{-k}, \hat{\mathbf{p}}_{q+k} \hat{\rho}_{-k} \), which will obviously be reflected in the structure of generalized transfer kernels. Similar calculations for
\[ iL_N \hat{n}_1(x) = -\frac{1}{m} \frac{\partial}{\partial \mathbf{r}} \hat{\mathbf{j}}(\mathbf{p}, r) + \frac{\partial}{\partial \mathbf{p}} \mathbf{F}(\mathbf{p}, r), \]
where
\[ \hat{\mathbf{j}}(\mathbf{p}, r) = \sum_{j=1}^N \mathbf{p}_j \delta (\mathbf{r} - \mathbf{r}_j) \delta (\mathbf{p} - \mathbf{p}_j) \]
is the microscopic particle momentum density in the space of coordinates and momentum,
\[ \mathbf{F}(\mathbf{p}, r) = \sum_{j=1}^N \mathbf{F}_j \delta (\mathbf{r} - \mathbf{r}_j) \delta (\mathbf{p} - \mathbf{p}_j) \]
is the microscopic density of forces acting on particles in the space of coordinates and momentum,
\[ \mathbf{F}_j(\mathbf{r}_j) = \sum_{l=1}^N \frac{\partial}{\partial \mathbf{r}_j} \Phi(|\mathbf{r}_{jl}|) = \sum_{l=1}^N \frac{\partial}{\partial \mathbf{r}_j} \Phi_{rl}(\mathbf{r}_j, \mathbf{r}_l) + \sum_{l=1}^N \frac{\partial}{\partial \mathbf{r}_j} \Phi^{\text{long}}(\mathbf{r}_j, \mathbf{r}_l) \]
indicate that the generalized flux \( I_n(x; t') \) is related to the momentum and force densities in the space of coordinates and momentum:
\[ I_n(x; t') = -\frac{\partial}{\partial x} I_f(x; t) + \frac{\partial}{\partial \mathbf{p}} I_f(x; t), \quad (19) \]
where
\[ I_j(x; t') = (1 - P(t')) j(p, r); \]
there is a difference between the microscopic momentum density in the space coordinates and momentum and its projection onto the space of selected parameters of a reduced description \( \hat{n}_1(x), \hat{\varepsilon}_{\text{int}}(r) \),

\[ I_F(x; t') = (1 - P(t')) F(p, r), \]

is a difference between the microscopic force density in the space of momentum and coordinates and its projection onto the space of selected parameters of a reduced description \( \hat{n}_1(x), \hat{\varepsilon}_{\text{int}}(r) \). The generalized flux framework (19) will generate the transport kernels (generalized transport coefficients) in the corresponding transport equations, which will be considered in the next section.

3. Generalized transport equations of the agreed description of kinetic and hydrodynamic processes

Using the solution of the Liouville equation (18), we obtain system of coupled equations for non-equilibrium one-particle distribution functions \( \langle \hat{n}_1(x) \rangle^t \) and of the average interaction energy density \( \langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t \). For this, it is necessary to calculate the following:

\[ \frac{\partial}{\partial t} \langle \hat{n}_1(x) \rangle^t = \frac{\partial}{\partial t} f_1(x; t) = \langle iL_N \hat{n}_1(x) \rangle^t, \]

\[ \frac{\partial}{\partial t} \langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t = \frac{\partial}{\partial t} \varepsilon_{\text{int}}(r; t) = \langle iL_N \varepsilon_{\text{int}}(r) \rangle^t. \]

Using the identities:

\[ \langle (1 - P(t)) iL_N \hat{n}_1(x) \rangle^t = \langle iL_N \hat{n}_1(x) \rangle^t - \langle iL_N \hat{n}_1(x) \rangle^t_{\text{rel}}, \]

\[ \langle (1 - P(t)) iL_N \varepsilon_{\text{int}}(r) \rangle^t = \langle iL_N \varepsilon_{\text{int}}(r) \rangle^t - \langle iL_N \varepsilon_{\text{int}}(r) \rangle^t_{\text{rel}}, \]

in which, on the left-hand sides, we will perform the averaging on the non-equilibrium basis by the distribution function (18) for the system of equations (20), (21). We find

\[ \frac{\partial}{\partial t} \langle \hat{n}_1(x) \rangle^t = - \frac{1}{2} \frac{\partial}{\partial r} \left( \frac{p(r; t)}{m} \right) W^{\text{sh}}(r; t) + \frac{1}{2} \frac{p(r; t)}{m} F^{\text{sh}}(r; t) \]

\[ + \frac{1}{2V^2} \sum_{a,k} \nu(k) e^{i\mathbf{q} \cdot \mathbf{r}} \left( -i(\mathbf{q} + \mathbf{k}) \cdot \langle \hat{\mathbf{p}}_{\mathbf{q} + \mathbf{k} \hat{\mathbf{p}} - \mathbf{k}} \rangle_{\text{rel}} + i\mathbf{k} \cdot \langle \hat{\mathbf{p}}_{\mathbf{q} + \mathbf{k} \hat{\mathbf{p}} - \mathbf{k}} \rangle_{\text{rel}} + i\mathbf{q} \cdot \langle \hat{\mathbf{p}}_{\mathbf{q}} \rangle_{\text{rel}} \right) \]

\[ + \int \mathbf{d}x' \int_{-\infty}^{t} dt' e^{i(t' - t) \phi_{\text{int}}(x, r'; t') \beta(r'; t')} + \int dx' \int_{t'}^{t} dt' e^{i(t' - t) \phi_{\text{int}}(r, x'; t) \beta(r'; t')} + \int \mathbf{d}x' \int_{-\infty}^{t} dt' e^{i(t' - t) \phi_{\text{int}}(x, r'; t) \beta(r'; t')} = \]

\[ \frac{\partial}{\partial t} \langle \hat{\varepsilon}_{\text{int}}(r) \rangle^t = - \frac{1}{2} \frac{\partial}{\partial r} \left( \frac{p(r; t)}{m} \right) W^{\text{sh}}(r; t) + \frac{1}{2} \frac{p(r; t)}{m} F^{\text{sh}}(r; t) \]

\[ + \frac{1}{2} n(r; t) \int \mathbf{d}r' F^{\text{sh}}(|r - r'|) g_2(r, r'; t) \]

\[ + \frac{1}{2} \mathbf{n}(r; t) \int \mathbf{d}r' F^{\text{sh}}(|r - r'|) g_2(r, r'; t) \]

\[ + \frac{1}{2} \int_{-\infty}^{t} dt' e^{i(t' - t) \phi_{\text{int}}(x, r'; t) \beta(r'; t')} + \int dx' \int_{t}^{t} dt' e^{i(t' - t) \phi_{\text{int}}(r, x'; t) \beta(r'; t')} = \]

\[ \frac{1}{n(r; t) n(r'; t)} \int d\Gamma_N(x) \hat{n}(r) \hat{n}(r') \rho_{\text{rel}}(x^N; t) \]

(24)

is a time-dependent even coordinate distribution function. It takes into account both short-range and long-range interactions between the particles of the system and is calculated through the relevant distribution function, or through the partition function of the relevant distribution:

\[ g_2(r, r'| n, \beta; t) = \frac{1}{n(r, t), n(r'; t)} \left( \int \mathbf{d}p \int \mathbf{d}p' \frac{\delta}{\delta a(p, r, t)} \frac{\delta}{\delta a(p', r', t)} \ln Z_{\text{rel}}(t) \right) \]

According to these definitions, \( g_2(\mathbf{r}, \mathbf{r}'; n, \beta; t) \) is a function of non-equilibrium mean values of particle number densities \( n(\mathbf{r}; t) \) and the inverse temperature \( \beta(\mathbf{r}; t) \). In (24) \( \dot{n}(\mathbf{r}') = \sum_{j=1}^{N} \delta(\mathbf{r} - \mathbf{r}_j) \) is the microscopic density of the number of particles. The equation (23) includes \( W^{sh}(\mathbf{r}; t) = \int d\mathbf{r}' \Phi^{sh}(\mathbf{r} - \mathbf{r}') g_2(\mathbf{r}, \mathbf{r}'; t) n(\mathbf{r}'; t) \) is a non-equilibrium mean field of short-range interactions, and 

\[
W^{sh}(\mathbf{r}; t) = \int d\mathbf{r}' \Phi^{sh}(\mathbf{r} - \mathbf{r}') g_2(\mathbf{r}, \mathbf{r}'; t) n(\mathbf{r}'; t)
\]

is a non-equilibrium average strength of short-range interactions between system particles. For their calculation, an even coordinate distribution function is required (24), which takes into account both short-range and long-range interactions between system particles. The generalized transport equations (22), (23) also contain generalized transport kernels

\[
\phi_{\alpha\gamma}(t, t') = \langle I_{\alpha}(t) T_{rel}(t, t') I_{\gamma}(t) \rangle_{rel}, \quad \alpha, \gamma = \{ n, \varepsilon \}
\]

that describe non-Markov processes and are non-equilibrium correlation functions. They are built on generalized flows. In particular, the transfer kernel \( \phi_{nn}(x, x'; t, t') \) can be expressed in the form

\[
\phi_{nn}(x, x'; t, t') = -\frac{\partial}{\partial x} \cdot D_{jj}(x, x', t') \cdot \frac{\partial}{\partial x} + \frac{\partial}{\partial x} \cdot D_{jF}(x, x'; t') \cdot \frac{\partial}{\partial x'} + \frac{\partial}{\partial x} \cdot D_{Fj}(x, x'; t') \cdot \frac{\partial}{\partial x'} - \frac{\partial}{\partial x} \cdot D_{FF}(x, x'; t') \cdot \frac{\partial}{\partial x'}, \quad (25)
\]

where

\[
D_{jj}(x, x'; t', t') = \langle I_{j}(x; t) T_{rel}(t, t') I_{j}(x'; t') \rangle_{rel}
\]

is the generalized diffusion coefficient in the space of coordinates and momentum,

\[
D_{Fj}(x, x'; t', t') = \langle I_{j}(x; t) T_{rel}(t, t') I_{j}(x'; t') \rangle_{rel}
\]

is the generalized coefficient of friction in the space of coordinates and momentum,

\[
D_{jj}(x, x'; t', t') = \langle I_{j}(x; t) T_{rel}(t, t') I_{j}(x'; t') \rangle_{rel}
\]

is a cross-generalized coefficient “momentum–force” in the space of coordinates and momentum. Moreover, it should be noted that the generalized diffusion coefficients \( D_{jj}(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}'; t, t') \) and friction \( D_{Fj}(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}'; t, t') \) describe the corresponding non-Markov processes in the space of momentums, coordinates and time. The values of the \( \mathbf{p} \) and \( \mathbf{p}' \) momentums of the particles in the non-equilibrium state can differ greatly in magnitude. In particular, in the case of multicomponent systems, for example, dust plasma, the components of which differ significantly in terms of energy and, therefore, in the values of momentums. The transfer kernel \( \phi_{ee}^{\text{int}}(\mathbf{r}, \mathbf{r}'; t, t') \), built on generalized interaction energy flows, can be expressed as

\[
\phi_{ee}^{\text{int}}(\mathbf{r}, \mathbf{r}'; t, t') = \langle I_{e}^{\text{sh}}(\mathbf{r}; t) T_{rel}(t, t') I_{e}^{\text{sh}}(\mathbf{r}'; t') \rangle_{rel} + \langle I_{e}^{\text{sh}}(\mathbf{r}; t) T_{rel}(t, t') I_{e}^{\text{long}}(\mathbf{r}'; t') \rangle_{rel}
\]

with selected contributions from short-range and long-range interactions of system particles (see Appendix 2).

Now, taking into account the defined Lagrange parameters (13), (15) and the expression for the transfer kernel (25) for the non-equilibrium one-particle distribution function, we obtain a kinetic equation in the form

\[
\left[ \frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \cdot \frac{\partial}{\partial \mathbf{r}} \right] f_1(x; t) - \int dx' \frac{\partial}{\partial \mathbf{r}} \Phi(\mathbf{r} - \mathbf{r}') \cdot \left[ \frac{\partial}{\partial \mathbf{p}} - \frac{\partial}{\partial \mathbf{p}'} \right] g_2(\mathbf{r}, \mathbf{r}'; t)f_1(x; t)\]

\[
= \int dx' \int_{-\infty}^{t'} e^{\varepsilon(t'-t)} \phi_{ne}^{\text{int}}(x, \mathbf{r}'; t, t') \left( \int_{-\infty}^{t'} K_{ee}^{-1}(\mathbf{r}'', t'') \frac{\partial}{\partial t''} (\varepsilon_{\text{int}}(\mathbf{r}''))'' + \beta(\mathbf{r}', -\infty) \right) dt''
\]

\[ + \int dx' \int_{-\infty}^{t} dt' e^{(t'-t)} \left( \frac{\partial}{\partial r} D_{JJ}(x, x', t, t') \cdot \frac{\partial}{\partial p} \right) + \int dx' \int_{-\infty}^{t} dt' e^{(t'-t)} \left( \frac{\partial}{\partial r} D_{JF}(x, x', t, t') \cdot \frac{\partial}{\partial p} + \frac{\partial}{\partial p} D_{FF}(x, x', t, t') \cdot \frac{\partial}{\partial p} \right) \ln \frac{f_1(x'; t')}{u(r'; t')} \] 

\[ \frac{\partial}{\partial t} \langle \hat{z}_{\text{int}}(r) \rangle = -\frac{1}{2} \frac{\partial}{\partial r} \left( \frac{p(r; t)}{m} W^{\text{sh}}(r; t) + \frac{1}{2} \frac{p(r; t)}{m} F^\text{sh}(r; t) \right) + \frac{1}{2} m \dot{r}(r; t) \int d\mathbf{r}' F^\text{sh}([r - r'][r - r')] g_2(r, r'; t) \frac{p(r'; t)}{m} \] 

\[ + \frac{1}{2} \sum_{q, k} \nu(k) e^{i\mathbf{q} \cdot \mathbf{r}} \left( -i(q + k) \cdot (\hat{p}_q + k \hat{p}_k)_{\text{rel}}^\dagger + i\mathbf{k} \cdot (\hat{p}_q + k \hat{p}_k)_{\text{rel}}^\dagger \right) + \frac{1}{2} \int dt' \int_{-\infty}^{t} e^{(t'-t)} \phi_{\text{int}}(r, r', t, t') \left( \int_{-\infty}^{t''} K^{-1}_{\text{el}}(r', r''; t'') \frac{\partial}{\partial t''} \langle \hat{z}_{\text{int}}(r') \rangle \right) + \beta(r', -\infty) dt'' dt' 

- \int dx' \int_{-\infty}^{t} dt' e^{(t'-t)} \phi_{\text{int}}(r, x', t, t') \ln \frac{f_1(x'; t')}{u(r'; t')} \] 

(27)

4. Conclusion

The resulting system of non-Markovian transport equations (26)–(27) provides a consistent description of kinetic and hydrodynamic processes in classical liquids and dense gases far from equilibrium. This system of equations is closed according to the basic parameters of a reduced description.

The kinetic equation (26) contains the contribution of the generalized mean-field, in which the coordinate quasi-equilibrium distribution function \( g_2(r, r'; t) \) can be calculated through the partition function \( Z_{\text{el}}(t) \) [51]. The transfer kernel \( \phi_{\text{int}}(r, r', t; t') \), variance \( K_{\text{el}}(r', r''; t') \) and generalized diffusion coefficients \( D_{JJ}(x, x'; t, t') \), friction \( D_{FF}(x, x'; t, t') \) and transverse transfer coefficients \( D_{JF}(x, x'; t, t') \) are calculated through the relevant distribution \( \rho_{\text{el}}(x; t) \). The potential energy transfer equation (27) includes the nonequilibrium mean field of short-range interactions \( W^{\text{sh}}(r; t) \), the nonequilibrium mean force of short-range interactions \( F^\text{sh}(r - r') \), which are calculated via \( g_2(r, r'; t) \). In addition, the temporal correlation functions \( \langle \hat{p}_q + k \hat{p}_k \rangle_{\text{rel}}^\dagger \) and \( \langle \hat{p}_q \rangle_{\text{rel}}^\dagger \) can be expressed in terms of the partition function of the relevant distribution

\[ \theta_{\text{el}}(x; t) = \exp \left[ -\Phi(t) - \int dr \beta(r; t) \hat{z}_{\text{int}}(r) - \int dr \lambda(r; t) \hat{m}(r) - \int dx a(x; t) \hat{n}_1(x) \right] \]

in the case \( A(r) = \hat{p}(r) \). The calculation of such a partition function can be carried out by the method of collective variables [51]. In this case, the collective variables will be the Fourier components of the particle number density \( \rho_q \) and the momentum \( \mathbf{p}_q \). Such calculations require separate consideration in subsequent works. It is obvious that time correlation functions, transfer kernels, and the partition function \( Z_{\text{el}}(t) \) cannot be calculated exactly. However, certain approximations of the RPA type (Gaussian approximation) for \( Z_{\text{el}}(t) \), as well as higher approximations by cumulative averages [51], can be implemented.

Appendix 1

Indeed, in the case of weakly nonequilibrium processes, the relevant distribution \( \rho_{\text{el}}(x; t) \) can be obtained in the form [8, 11, 53–55] (by excluding the Lagrangian parameters using the conditions self-concordance):

\[ \rho_{\text{el}}^0(x; t) = \rho_0(x) \left( 1 + \int dx \int dx' (\delta \hat{n}(x')) \Phi_{\text{el}}^{-1}(x', x) \hat{n}(x) + \int dr \int dr' (\delta \hat{h}_{\text{int}}(r')) \Phi_{\text{el}}^{-1}(r', r) \hat{h}_{\text{int}}(r') \right) \]

where the $\Phi_{nn}(x',x)$ function is inverted to the equilibrium correlation function $\Phi_{nn}(x',x) = \langle \hat{n}(x')\hat{n}(x') \rangle_0$ and is found using the relation:

$$\int dx'' \Phi_{nn}^{-1}(x,x'') \Phi_{nn}(x'',x') = \delta(x-x').$$

As a result of excluding the parameter $\beta(t;r)$, using self-consistency conditions, fluctuations of the potential part of the generalized enthalpy $\hat{h}_{int}(\mathbf{r}') = \hat{h}_{int}(\mathbf{r}') - \langle \hat{h}_{int}(\mathbf{r}') \rangle_0$, which has the following structure:

$$\hat{h}_{int}(\mathbf{r}) = \hat{\varepsilon}_{int}(\mathbf{r}) - \int dx \int dx' \langle \hat{\varepsilon}_{int}(\mathbf{r})\hat{n}(x') \rangle_0 \Phi_{nn}^{-1}(x',x)\hat{n}(x),$$

and the dynamic variables $\hat{h}_{int}(\mathbf{r}')$ and $\hat{n}(x)$ are orthogonal in the sense of the means $\langle \hat{h}_{int}(\mathbf{r}')\hat{n}(x) \rangle_0 = 0$.

**Appendix 2**

In particular, the contributions of short-range interactions give

$$\langle I^{sh}_e(\mathbf{r};t)T_{rel}(t,t')I^{sh}_e(\mathbf{r};t') \rangle_{rel}^{t'} = \frac{1}{2V^2} \sum_{q',k'} \nu(k') e^{i q' \cdot \mathbf{r'}} \times \left( \frac{\partial}{\partial t} \langle (1-P(t))\hat{h}_{int}(\mathbf{r})T_{rel}(t,t')(1-P(t'))\hat{\rho}_{q+k\hat{p}} \hat{\rho}_{-k} \rangle_{rel}^{t'} \cdot i(q + k') \right)$$

$$- \frac{\partial}{\partial t} \left( (1-P(t))\hat{h}_{int}(\mathbf{r})T_{rel}(t,t')(1-P(t'))\hat{\rho}_{q+k\hat{p}} \hat{\rho}_{-k} \right)_{rel}^{t'} \cdot i k'$$

$$- \frac{\partial}{\partial t} \langle (1-P(t))\hat{h}_{int}(\mathbf{r})T_{rel}(t,t')(1-P(t'))\hat{\rho}_{q+k\hat{p}} \hat{\rho}_{-k} \rangle_{rel}^{t'} \cdot i q'. $$

Exciting is the averaged correlations between the flows of short-range interactions and the flows of long-range interactions according to the relevant distribution have the following structure:

$$\langle I^{long}_e(\mathbf{r};t)T_{rel}(t,t')I^{long}_e(\mathbf{r};t') \rangle_{rel}^{t'} = \frac{1}{4V^4} \sum_{q,k,q',k'} \nu(k) \nu(k') e^{i q \cdot \mathbf{r}} e^{i q' \cdot \mathbf{r'}} \left( - (q + k) \cdot \langle (1-P(t))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} T_{rel}(t,t')(1-P(t'))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} \rangle_{rel}^{t'} \cdot (q' + k') + (q + k) \cdot \langle (1-P(t))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} T_{rel}(t,t')(1-P(t'))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} \rangle_{rel}^{t'} \cdot k' \right)$$

$$+ (q + k) \cdot \langle (1-P(t))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} T_{rel}(t,t')(1-P(t'))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} \rangle_{rel}^{t'} \cdot q'$$

$$+ k \cdot \langle (1-P(t))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} T_{rel}(t,t')(1-P(t'))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} \rangle_{rel}^{t'} \cdot (q' + k') - k \cdot \langle (1-P(t))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} T_{rel}(t,t')(1-P(t'))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} \rangle_{rel}^{t'} \cdot k'$$

$$- k \cdot \langle (1-P(t))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} T_{rel}(t,t')(1-P(t'))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} \rangle_{rel}^{t'} \cdot q'$$

$$+ q \cdot \langle (1-P(t))\hat{p}_{q} T_{rel}(t,t')(1-P(t'))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} \rangle_{rel}^{t'} \cdot (q' + k') - q \cdot \langle (1-P(t))\hat{p}_{q} T_{rel}(t,t')(1-P(t'))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} \rangle_{rel}^{t'} \cdot k'$$

$$- q \cdot \langle (1-P(t))\hat{p}_{q} T_{rel}(t,t')(1-P(t'))\hat{p}_{q+k\hat{p}} \hat{\rho}_{-k} \rangle_{rel}^{t'} \cdot q'. $$

First of all, the last application:
\[
\langle (1 - P(t))\hat{p}_q T_{rel}(t, t') (1 - P(t'))\hat{p}_{q'} \rangle^{\prime \prime}_{rel} = D(q, q'; t, t')
\]
is the generalized diffusion coefficient in the space of wave vectors and time. Other temporal correlation functions
\[
\langle (1 - P(t))\hat{p}_{q+k} \hat{\rho}_{-k} T_{rel}(t, t') (1 - P(t'))\hat{p}_{q'+k'} \hat{\rho}_{-k'} \rangle^{\prime \prime}_{rel},
\]
\[
\langle (1 - P(t))\hat{p}_{q+k} \hat{\rho}_{-k} T_{rel}(t, t') (1 - P(t'))\hat{p}_{q'+k'} \hat{\rho'}_{-k'} \rangle^{\prime \prime}_{rel},
\]
\[
\langle (1 - P(t))\hat{\rho}^{q+k} \hat{\rho}_{-k} T_{rel}(t, t') (1 - P(t'))\hat{\rho}^{q'+k'} \hat{\rho'}_{-k'} \rangle^{\prime \prime}_{rel},
\]
are higher-order functions of the dynamic variables \(\rho^{q+k}\) and \(\hat{\rho}_{-k}\). For them, a similar approximation can be applied as in the theory of interacting modes
\[
\approx \langle \rho^{q+k} T_{rel}(t, t') \rangle^{\prime \prime}_{rel} D(k, k'; t, t'),
\]
where
\[
\langle \rho^{q+k} T_{rel}(t, t') \rangle^{\prime \prime}_{rel} = E_{\rho\rho}((q + k), (q' + k'); t, t')
\]
can be defined as a non-equilibrium scattering function associated with a non-equilibrium dynamic structural factor of a system far from equilibrium. Time correlation functions
\[
\langle (1 - P(t))\hat{p}_{q+k} \hat{\rho}_{-k} T_{rel}(t, t') (1 - P(t'))\hat{p}_{q'-k'} \hat{\rho}_{-k'} \rangle^{\prime \prime}_{rel}
\]
is of the third order in the dynamic variables \(\rho^{q+k}\) and \(\hat{\rho}_{-k}\). For them, the following approximation through the generalized diffusion coefficient can be applied
\[
\approx D(q + k, q' + k'; t, t') \langle \hat{\rho}_{-k} \rangle^{\prime \prime}_{rel}.
\]
The applied approximations include the generalized diffusion coefficient \(D(q, q'; t, t')\), which describes non-Markov collective diffusion processes. Taking into account the approximation data for the long-range part of the energy transfer core \(\langle I^{\text{long}}(r; t) T_{rel}(t, t') I^{\text{long}}(r'; t') \rangle^{\prime \prime}_{rel}\), we get
\[
\langle I^{\text{long}}(r; t) T_{rel}(t, t') I^{\text{long}}(r'; t') \rangle^{\prime \prime}_{rel} = 1 \frac{1}{4\pi^2} \sum_{q, k} \sum_{q', k'} \nu(k) \nu(k') e^{i\mathbf{q} \cdot \mathbf{r}} e^{i\mathbf{q'} \cdot \mathbf{r'}}
\]
\[
\times \left( - (q + k) \cdot D(q + k, q' + k'; t, t') \cdot (q' + k') F(k, k'; t, t') + (q + k) \cdot D(q + k, k'; t, t') \cdot k' F(q + k, q'; t, t')
\]
\[
+ k \cdot D(k, q' + k'; t, t') \cdot (q' + k') F(q + k, k'; t, t') - k \cdot D(k, k'; t, t') \cdot k' F(q + k, q' + k'; t, t')
\]
\[
+ (q + k) \cdot D(q + k, q' + k'; t, t') \cdot q' \langle \hat{p}_{q+k} \rangle^{\prime \prime}_{rel} - k \cdot D(k, q' + k'; t, t') \cdot k' \langle \hat{\rho}_{-k} \rangle^{\prime \prime}_{rel} - q \cdot D(q, q' + k'; t, t') \cdot k' \langle \hat{\rho}_{q+k} \rangle^{\prime \prime}_{rel} - q \cdot D(q, q'; t, t') \cdot q' \right).
\]


Unification of kinetic and hydrodynamic approaches in the theory of dense gases and liquids...


Ob’єднання кінетичного та гідродинамічного підходів у теорії густих газів і рідин, далеких від рівноваги

Токарчук М. В.1,2

1 Інститут фізики конденсованих систем НАН України,
вулиця Сянціцького, 1, 79011, Львів, Україна
2 Національний університет “Львівська політехніка”,
вулиця С. Бандери, 12, 79013, Львів, Україна

Отримано систему немарковських рівнянь переносу для нерівноважної одночастинкової функції розподілу частинок і нерівноважного середнього значення густини потенціальної енергії взаємоіонних частинон системи, далеких від стану рівноваги. Отримано вирази для ентропії, статистичної суми нерівноважного стану системи, а також нерівноважні термодинамічні співвідношення. Детально розкрито узагальнену структуру ядер переносу з виділенням короткодіючих і далекодіючих вкладів взаємодії між частинонами. Встановлено зв’язок ядер переносу із узагальненими коефіцієнтами дифузії, тертя в просторі координат та імпульсів і потенціальною частиною коефіцієнта теплопровідності.

Ключові слова: немарковські рівняння; метод нерівноважного статистичного оператора; ентропія; статистична сума нерівноважного стану; ядра переносу.