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Chain of kinetic equations for the distribution functions of particles in simple liquid taking into account nonlinear hydrodynamic fluctuations

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HIGHLIGHTS

- Consistent description of kinetic and hydrodynamic fluctuations in a classical simple fluid is proposed.
- Chain of kinetic equations for non-equilibrium single, double and *s*-particle distribution functions of particles is obtained.
- We applied the method of collective variables to calculate the structure function and hydrodynamic velocities.

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ABSTRACT

Chain of kinetic equations for non-equilibrium single, double and *s*-particle distribution functions of particles is obtained taking into account nonlinear hydrodynamic fluctuations. Non-equilibrium distribution function of non-linear hydrodynamic fluctuations satisfies a generalized Fokker–Planck equation. The method of non-equilibrium statistical operator by Zubarev is applied. A way of calculating the structural distribution function of hydrodynamic collective variables and their hydrodynamic velocities (above Gaussian approximation) contained in the generalized Fokker–Planck equation for the non-equilibrium distribution function of hydrodynamic collective variables is proposed.

1. Introduction

The study of nonlinear kinetic and hydrodynamic fluctuations in dense gases, liquids and plasma, in turbulence phenomena and dynamics of phase transitions, in chemical reactions and self-organizing processes are relevant both on kinetic and hydrodynamic levels of description in statistical theory of non-equilibrium processes [1–20]. The non-equilibrium states of such systems are far from equilibrium. Therefore the study of both the processes establishing the stationary states with characteristic times of life and the relaxation processes to the known equilibrium states, that are described by means of molecular hydrodynamics [21–25], is of great importance. An important feature of theoretical modeling of non-equilibrium phenomena in dense gases, liquids, dense plasmas (dusty plasmas) is a consistent description of kinetic and hydrodynamic processes [25–29] and taking into account the characteristic short and long-range interactions between the particles of the systems. In particular, the non-equilibrium gas–liquid phase transition is characterized by nonlinear hydrodynamic fluctuations of mass, momentum and particle energy, which describe a collective nature of the process and define the spatial and temporal behavior of the transport coefficients (viscosity, thermal conductivity), time correlation functions and dynamic structure factor. At the same time, due to heterogeneity in collective dynamics of these

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fluctuations, liquid drops emerge in the gas phase (in case of transition from the gas phase to the liquid phase), or the gas bubbles emerge in the liquid phase (in case of transition from the liquid phase to the gas phase), formation of which has a kinetic nature described by a redistribution of momentum and energy, i.e. when a certain group of particles in the system receives a significant decrease (in the case of drops), or increase (in the case of bubbles) of kinetic energy. The particles, that form bubbles or droplets, diffuse out of their phases in the liquid or the gas and vice versa. They have different values of momentum, energy and pressure in different phases. All these features are related to the non-equilibrium unary, binary and s-particle distribution functions (which depend on coordinate, momentum and time) that satisfy the BBGKY chain of equations. These problems concern the consistent description of kinetic and hydrodynamic processes in heterophase systems [30–33].

Therefore, the construction of kinetic equations that take into account nonlinear hydrodynamic fluctuations [34–38] is an important problem in the theory of transport processes in dense gases and liquids. In particular, this problem arises in the description of low-frequency anomalies in the kinetic equations and related "long tail" correlation functions [39–41].

The main difficulty of the problem is that the kinetics and hydrodynamics of these processes are strongly related and should be considered simultaneously. Zubarev, Morozov, Omelyan and Tokarchuk [42,43,25] proposed the consistent description of kinetic and hydrodynamic processes in dense gases and liquids on the basis of Zubarev non-equilibrium statistical operator [44,45]. In particular, this approach was used to obtain the kinetic equation of the revised Enskog theory [43,46] for a system of hard spheres and kinetic Enskog–Landau equations for one-component system of charged hard spheres from the BBGKY chain of equations.

Zubarev et al. [25] obtained the generalized hydrodynamic equations for the hydrodynamic variables (densities of the particle, momentum and the total energy) connected with the kinetic equation for the non-equilibrium one-particle distribution function. Later [26,28], these equations were used to study time correlation functions and the collective excitation spectrum of the weakly non-equilibrium processes in liquids.

Obviously, the approach proposed by Zubarev et al. [42,43,25] and Tokarchuk et al. [26,28] can be used to describe both weakly and strongly non-equilibrium systems. At the same time, in order to consistently describe kinetic processes and nonlinear hydrodynamic fluctuations it is convenient to reformulate this theory so that a set of equations for non-equilibrium one-particle distribution function and the distribution functional of hydrodynamic variables, particle number densities as well as momentum and energy densities could be obtained.

In this contribution we will develop an approach for consistent description of kinetic and hydrodynamic processes that are characterized by non-linear fluctuations and are especially important for the description of non-equilibrium gas–liquid phase transition. In Section 2 we will obtain the non-equilibrium statistical operator for non-equilibrium state of the system when the parameters of the reduced description are a non-equilibrium one-particle distribution function and the distribution function of non-equilibrium nonlinear hydrodynamic variables. Using this operator we construct the kinetic equations for the non-equilibrium single, double, s-particle distribution functions which take into account nonlinear hydrodynamic fluctuations, for which the non-equilibrium distribution function satisfies a generalized Fokker–Planck equation. In Section 3, we will consider one of the ways to calculate the structural distribution function of hydrodynamic collective variables and their hydrodynamic velocities (in higher than Gaussian approximation), which enter the generalized Fokker–Planck equation for the non-equilibrium distribution function of hydrodynamic collective variables.

2. Non-equilibrium distribution function

For a consistent description of kinetic and hydrodynamic fluctuations in a classical one-component fluid it is necessary to select the description parameters for one-particle and collective processes. As these parameters we choose the non-equilibrium one-particle distribution function $f_1(x;t) = \langle \hat{n}_1(x)\rangle^t$ and distribution function of hydrodynamic variables $f(a;t) = \langle \delta(\hat{a}-a)\rangle^t$. Here the phase function

$$\hat{n}_1(x) = \sum_{j=1}^{N} \delta(x-x_j) = \sum_{j=1}^{N} \delta(\mathbf{r}-\mathbf{r}_j)\delta(\mathbf{p}-\mathbf{p}_j) \tag{1}$$

is the microscopic particle number density. $x_j = (\mathbf{r}_j, \mathbf{p}_j)$ is the set of phase variables (coordinates and momentums), N is the total number of particles in a volume V. A microscopic phase distribution of hydrodynamic variables is given by

$$\hat{f}(a) = \delta(\hat{a}-a) = \prod_{m=1}^{3}\prod_{\mathbf{k}} \delta(\hat{a}_{m\mathbf{k}} - a_{m\mathbf{k}}), \tag{2}$$

where $\hat{a}_{1\mathbf{k}} = \hat{n}_{\mathbf{k}}$, $\hat{a}_{2\mathbf{k}} = \hat{\mathbf{J}}_{\mathbf{k}}$, $\hat{a}_{3\mathbf{k}} = \hat{\varepsilon}_{\mathbf{k}}$ are the Fourier components of the densities of particle number, momentum and energy:

$$\hat{n}_{\mathbf{k}} = \sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{r}_j}, \qquad \hat{\mathbf{J}}_{\mathbf{k}} = \sum_{j=1}^{N} \mathbf{p}_j \mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{r}_j}, \tag{3}$$

$$\hat{\varepsilon}_{\mathbf{k}} = \sum_{j=1}^{N}\Big[\frac{p_j^2}{2m} + \frac{1}{2}\sum_{l\neq j=1}^{N} \Phi(|\mathbf{r}_{lj}|)\Big]\mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{r}_j},$$