Condensed Matter Physics, 2012, Vol. 15, No 1, 14001: 1–6
DOI: 10.5488/CMP.15.14001
http://www.icmp.lviv.ua/journal

Rapid Communication

On the problem of a consistent description of kinetic and hydrodynamic processes in dense gases and liquids: Collective excitations spectrum

B.B. Markiv, I.P. Omelyan, M.V. Tokarchuk

Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine,
1 Svientsitskii Str., 79011 Lviv, Ukraine

Received December 21, 2011, in final form March 5, 2012

Based on the generalized non-Markovian equations obtained earlier for a nonequilibrium one-particle distribution function and potential part of the averaged enthalpy density [Markiv B.B., Omelyan I.P, Tokarchuk M.V., Condens. Matter Phys., 2010, **13**, 23005] a spectrum of collective excitations is investigated, where the potential of interaction between particles is presented as a sum of the potential of hard spheres and a certain long-range potential.

Key words: *kinetics, hydrodynamics, kinetic equations, memory functions, collective modes*

PACS: *05.20.Dd, 05.60.+w, 52.25.Fi, 82.20.M*

1. Introduction

A number of investigations [1–10] were devoted to the problem of constructing a consistent description of kinetic and hydrodynamic processes in dense gases, liquids, and plasma. For instance, the importance of taking into account the kinetic processes connected with irreversible collision processes at the scale of short-ranged interparticle interactions was pointed out in [11]. Short-wavelength collective modes in liquids were investigated therein based on the linearized kinetic equation of the revised Enskog theory for the hard spheres model.

In this paper we investigate a spectrum of collective excitations within a consistent description of kinetic and hydrodynamic processes in a system in which the potential of interaction between particles consists of two parts: the hard spheres potential and a long-range part.

2. Transport equations

Using the ideas presented in papers [3, 4] the nonequilibrium statistical operator consistently describing the kinetic and hydrodynamic processes for a system of classical interacting particles was obtained in [7, 8] by means of nonequilibrium statistical operator method. Using this operator, a set of kinetic equations for the nonequilibrium one-particle distribution function $f_{\vec{k}}(\vec{p};t) = \langle \hat{n}_{\vec{k}}(\vec{p})\rangle^t$ and the potential part of the averaged enthalpy density $h^{\rm int}_{\vec{k}}(t) = \langle \hat{h}^{\rm int}_{\vec{k}}\rangle^t$ was obtained in the case of weakly nonequilibrium processes:

$$\frac{\partial}{\partial t} f_{\vec{k}}(\vec{p};t) + \frac{\mathrm{i}\vec{k}\cdot\vec{p}}{m} f_{\vec{k}}(\vec{p};t) = -\frac{\mathrm{i}\vec{k}\cdot\vec{p}}{m} n f_0(p) c_2(k) \int \mathrm{d}\vec{p}\,' f_{\vec{k}}(\vec{p}\,';t) + \mathrm{i}\Omega_{nh}(\vec{k};\vec{p}) h^{\rm int}_{\vec{k}}(t)$$
$$- \int \mathrm{d}\vec{p}\,' \int_{-\infty}^{t} \mathrm{e}^{\varepsilon(t'-t)} \varphi_{nn}(\vec{k};\vec{p},\vec{p}\,';t,t') f_{\vec{k}}(\vec{p}\,';t')\mathrm{d}t' - \int_{-\infty}^{t} \mathrm{e}^{\varepsilon(t'-t)} \varphi_{nh}(\vec{k};\vec{p};t,t') h^{\rm int}_{\vec{k}}(t')\mathrm{d}t', \qquad (1)$$

© B.B. Markiv, I.P. Omelyan, M.V. Tokarchuk, 2012

$$\frac{\partial}{\partial t}h^{\rm int}_{\vec k}(t)=\int{\rm d}\vec p\,'{\rm i}\Omega_{hn}(\vec k;\vec p\,')f_{\vec k}(\vec p\,';t)$$
$$-\int{\rm d}\vec p\,'\int_{-\infty}^{t}{\rm e}^{\varepsilon(t'-t)}\varphi_{hn}(\vec k;\vec p\,';t,t')f_{\vec k}(\vec p\,';t'){\rm d}t'-\int_{-\infty}^{t}{\rm e}^{\varepsilon(t'-t)}\varphi_{hh}(\vec k;t,t')h^{\rm int}_{\vec k}(t'){\rm d}t', \tag{2}$$

where ${\rm i}\Omega_{nh}(\vec k;\vec p)=\langle\hat n_{\vec k}(\vec p)\hat h^{\rm int}_{-\vec k}\rangle_0\Phi^{-1}_{hh}(\vec k)$ and ${\rm i}\Omega_{hn}(\vec k;\vec p)=\int{\rm d}\vec p\,'\langle\dot{\hat h}^{\rm int}_{\vec k}\hat n_{-\vec k}(\vec p\,')\rangle_0\Phi^{-1}_{\vec k}(\vec p\,',\vec p)$ are the normalized static correlation functions.

$$\begin{aligned}\varphi_{nn}(\vec k;\vec p,\vec p\,';t,t') &= \int{\rm d}\vec p\,''\langle I_n(\vec k;\vec p)T_0(t,t')I_n(-\vec k;\vec p\,'')\rangle_0\Phi^{-1}_{\vec k}(\vec p\,'',\vec p\,'),\\ \varphi_{hn}(\vec k;\vec p;t,t') &= \int{\rm d}\vec p\,'\langle I^{\rm int}_h(\vec k)T_0(t,t')I_n(-\vec k;\vec p\,')\rangle_0\Phi^{-1}_{\vec k}(\vec p\,',\vec p),\\ \varphi_{nh}(\vec k;\vec p;t,t') &= \langle I_n(\vec k;\vec p)T_0(t,t')I^{\rm int}_h(-\vec k)\rangle_0\Phi^{-1}_{hh}(\vec k),\\ \varphi_{hh}(\vec k;t,t') &= \langle I^{\rm int}_h(\vec k)T_0(t,t')I^{\rm int}_h(-\vec k)\rangle_0\Phi^{-1}_{hh}(\vec k)\end{aligned} \tag{3}$$

are the generalized transport kernels (memory functions) describing kinetic and hydrodynamic processes. In [12], the inner structure of generalized transport kernels for a consistent description of kinetic and hydrodynamic processes was analyzed in detail. It was shown that they are expressed in terms of time correlation functions related to the basic set of dynamical variables, phase density $\hat n_{\vec k}(\vec p)$ and potential part of the enthalpy density $\hat h^{\rm int}_{\vec k}$ along with the transport kernels describing diffusive and visco-thermal processes. Here, $\hat n_{\vec k}(\vec p)=\int{\rm d}\vec r{\rm e}^{-{\rm i}\vec k\vec r}\hat n_1(\vec r,\vec p)$ are the Fourier-components of microscopic phase density of particles number, $\hat n_1(\vec r,\vec p)=\sum_{l=1}^N\delta(\vec p-\vec p_l)\delta(\vec r-\vec r_l)$, $\hat h^{\rm int}_{\vec k}=\hat\varepsilon^{\rm int}_{\vec k}-\langle\hat\varepsilon^{\rm int}_{\vec k}\hat n_{-\vec k}\rangle_0S^{-1}(k)\hat n_{\vec k}$ are the Fourier-components of the potential part of the enthalpy density, $\hat\varepsilon^{\rm int}_{\vec k}=\frac12\sum_{l\neq j=1}^N\Phi(|\vec r_{lj}|){\rm e}^{-{\rm i}\vec k\vec r_j}$ and $\hat n_{\vec k}=\sum_{l=1}^N{\rm e}^{-{\rm i}\vec k\vec r_l}$ are the Fourier-components of the potential energy and particle number densities, respectively, $\vec k$ is the wave-vector. $\Phi^{-1}_{hh}(\vec k)$ is the function inverse to the equilibrium correlation function $\Phi_{hh}(\vec k)=\langle\hat h^{\rm int}_{\vec k}\hat h^{\rm int}_{-\vec k}\rangle_0$, $\langle\ldots\rangle_0=\int{\rm d}\Gamma_N\ldots\varrho_0(x^N)$, where ϱ_0 is an equilibrium statistical operator. $I_n(\vec k;\vec p)=(1-P_0){\rm i}L_N\hat n_{\vec k}(\vec p)=(1-P_0)\dot{\hat n}_{\vec k}(\vec p)$ and $I^{\rm int}_h(\vec k)=(1-P_0){\rm i}L_N\hat h^{\rm int}_{\vec k}=(1-P_0)\dot{\hat h}^{\rm int}_{\vec k}$ are the generalized flows in linear approximation, $T_0(t,t')={\rm e}^{(t-t')(1-P_0){\rm i}L_N}$ is the evolution operator with regard to projection. P_0 is the linear approximation of the Mori projection operator constructed on the orthogonal dynamic variables $\hat n_{\vec k}(\vec p)$, $\hat h^{\rm int}_{\vec k}$ [8]: $P_0\hat A_{\vec k}=\sum_{\vec k}\langle\hat A_{\vec k}\hat h^{\rm int}_{-\vec k}\rangle_0\Phi^{-1}_{hh}(\vec k)\hat h^{\rm int}_{\vec k}+\sum_{\vec k}\int{\rm d}\vec p\int{\rm d}\vec p\,'\langle\hat A_{\vec k}\hat n_{-\vec k}(\vec p)\rangle_0\Phi^{-1}_{\vec k}(\vec p,\vec p\,')\hat n_{\vec k}(\vec p\,')$. It possesses the following properties: $P_0P_0=P_0$, $P_0(1-P_0)=0$, $P_0\hat n_{\vec k}(\vec p)=\hat n_{\vec k}(\vec p)$, $P_0\hat h^{\rm int}_{\vec k}=\hat h^{\rm int}_{\vec k}$. $\Phi^{-1}_{\vec k}(\vec p,\vec p\,')$ is the function inverse to $\Phi_{\vec k}(\vec p,\vec p\,')=\langle\hat n_{\vec k}(\vec p)\hat n_{-\vec k}(\vec p\,')\rangle_0=n\delta(\vec p-\vec p\,')f_0(p')+n^2f_0(p)f_0(p')h_2(\vec k)$. It is equal to $\Phi^{-1}_{\vec k}(\vec p,\vec p\,')=\frac{\delta(\vec p-\vec p\,')}{nf_0(p')}-c_2(k)$, where $n=N/V$, $f_0(p)=\left(\beta/2\pi m\right)^{3/2}{\rm e}^{-\beta\frac{p^2}{2m}}$ is the Maxwellian distribution, $\beta=1/k_{\rm B}T$ is an inverse temperature and $k_{\rm B}$ is Boltzmann constant. $c_2(k)$ is the direct correlation function related to the correlation function $h_2(k)$: $h_2(k)=c_2(k)[1-nc_2(k)]^{-1}$. $S(k)=\langle\hat n_{\vec k}\hat n_{-\vec k}\rangle_0$ denotes the static structure factor. It is important to note that dynamical variables $\hat h^{\rm int}_{\vec k}$ and $\hat n_{\vec k}(\vec p)$ are orthogonal in the sense that $\langle\hat h^{\rm int}_{\vec k}\hat n_{\vec k}(\vec p)\rangle_0=0$.

Projecting the set of equations (1), (2) onto the first moments of the nonequilibrium one-particle distribution function $\Psi_1(\vec p)=1$, $\Psi_\alpha(\vec p)=\sqrt2p_\alpha/2k_{\rm B}T$ (where $\alpha=x,y,z$), $\Psi_\varepsilon(\vec p)=\sqrt{2/3}(p^2/2mk_{\rm B}T-3/2)$, one can obtain a set of equations for the averaged values of densities of particles number $n_{\vec k}(t)$, momentum $\vec J_{\vec k}(t)$, kinetic $h^{\rm kin}_{\vec k}(t)$ and potential $h^{\rm int}_{\vec k}(t)$ parts of enthalpy [8], where the Fourier-components of the kinetic part of enthalpy density defined as $\hat h^{\rm kin}_{\vec k}=\hat\varepsilon^{\rm kin}_{\vec k}-\langle\hat\varepsilon^{\rm kin}_{\vec k}\hat n_{-\vec k}\rangle_0\langle\hat n_{\vec k}\hat n_{-\vec k}\rangle_0^{-1}\hat n_{\vec k}$. For this purpose, we introduce the projection operator constructed on the eigenfunctions $|\Psi_\nu(\vec p)\rangle$ of the nonequilibrium one-particle function such that $\mathscr P|\Psi\rangle=\sum_{\nu=1}^n|\Psi_\nu\rangle\langle\Psi_\nu|\Psi\rangle$. Here, $\langle\Psi|\Psi_\nu\rangle=\int d\vec p\Psi(\vec p)f_0(p)\Psi_\nu(\vec p)$, while $\Psi_\nu(\vec p)$ satisfies the conditions $\langle\Psi_\mu|\Psi_\nu\rangle=\delta_{\mu\nu}$ and $\sum_\nu|\Psi_\nu\rangle\langle\Psi_\nu|=1$. Then, let us act by the projection operator $\mathscr P$ onto the set of equation (1), (2). Repeat this operation acting by the operator $\mathscr Q=1-\mathscr P$ complementary to $\mathscr P$. Then, substituting the unknown quantity from the second equation into the first one we obtain the necessary set of equations with separated contributions of kinetic and potential energies. Using the

Laplace transform, let us represent it in a matrix form:

$$z\tilde{a}_{\vec{k}}(z) - \tilde{\Sigma}_{\mathrm{G}}(\vec{k};z)\tilde{a}_{\vec{k}}(z) = -\langle \tilde{a}_{\vec{k}}(t=0)\rangle^{t}. \tag{4}$$

$\tilde{\Sigma}_{\mathrm{G}}(\vec{k};z)$ is the matrix of memory kernels

$$\tilde{\Sigma}_{\mathrm{G}}(\vec{k};z) = \mathrm{i}\tilde{\Omega}_{\mathrm{G}}(\vec{k}) - \tilde{\Pi}(\vec{k};z), \tag{5}$$

where $\tilde{a}_{\vec{k}}(z) = [n_{\vec{k}}(z), \vec{J}_{\vec{k}}(z), h^{\mathrm{kin}}_{\vec{k}}(z), h^{\mathrm{int}}_{\vec{k}}(z)]$ is the column-vector.

$$\mathrm{i}\tilde{\Omega}_{\mathrm{G}}(\vec{k}) = \begin{pmatrix} 0 & \mathrm{i}\Omega_{nJ} & 0 & 0 \\ \mathrm{i}\Omega_{Jn} & 0 & \mathrm{i}\Omega^{\mathrm{kin}}_{Jh} & \mathrm{i}\Omega^{\mathrm{int}}_{Jh} \\ 0 & \mathrm{i}\Omega^{\mathrm{kin}}_{hJ} & 0 & 0 \\ 0 & \mathrm{i}\Omega^{\mathrm{int}}_{hJ} & 0 & 0 \end{pmatrix}, \quad \tilde{\Pi}(\vec{k};z) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \Pi_{JJ} & \Pi^{\mathrm{kin}}_{Jh} & \Pi^{\mathrm{int}}_{Jh} \\ 0 & \Pi^{\mathrm{kin}}_{hJ} & \Pi^{\mathrm{kin,kin}}_{hh} & \Pi^{\mathrm{kin,int}}_{hh} \\ 0 & \Pi^{\mathrm{int}}_{hJ} & \Pi^{\mathrm{int,kin}}_{hh} & \Pi^{\mathrm{int,int}}_{hh} \end{pmatrix} \tag{6}$$

are the frequency matrix and the matrix of transport kernels. The elements of the latter have the following structure:

$$\Pi_{\mu\nu}(\vec{k};z) = \langle \Psi_{\mu}|\tilde{\varphi}(\vec{k};z) + \tilde{\Sigma}(\vec{k};z)\mathcal{Q}[z\tilde{I} - \mathcal{Q}\tilde{\Sigma}(\vec{k};z)\mathcal{Q}]^{-1}\mathcal{Q}\tilde{\Sigma}(\vec{k};z)|\Psi_{\nu}\rangle. \tag{7}$$

$\tilde{I}$ denotes a unit matrix, $\tilde{\varphi}(\vec{k};z)$ is the matrix whose elements are the generalized transport kernels $\varphi_{nn}(\vec{k};\vec{p},\vec{p}\,';z)$, $\varphi_{hn}(\vec{k};\vec{p}\,';z)$, $\varphi_{nh}(\vec{k};\vec{p};z)$, $\varphi_{hh}(\vec{k};z)$ in the set of equations (1), (2), and $\tilde{\Sigma}(\vec{k};z) = \mathrm{i}\tilde{\Omega}(\vec{k}) - \tilde{\varphi}(\vec{k};z)$. Here, $\mathrm{i}\tilde{\Omega}(\vec{k})$ is the matrix of static correlation functions $\mathrm{i}\Omega_{nh}(\vec{k};\vec{p})$, $\mathrm{i}\Omega_{hn}(\vec{k};\vec{p})$. For the sake of simplicity the dependence of $\tilde{\varphi}(\vec{k};z)$, $\tilde{\Sigma}(\vec{k};z)$ on $\vec{p},\vec{p}\,'$ was omitted. As we can see from the structure of elements of the matrices $\mathrm{i}\tilde{\Omega}_{\mathrm{G}}(\vec{k})$ and $\tilde{\Pi}(\vec{k};z)$, the contributions of kinetic and potential parts of enthalpy are separated. Herewith, a question arises regarding the study of time correlation functions and collective modes for liquids based on the set of transport equations (4).

3. Spectrum of collective excitations

Let us consider the system of kinetic equations (1), (2) in the case where the potential of interaction is presented as follows:

$$\Phi(|\vec{r}_{ij}|) = \Phi^{\mathrm{hs}}(|\vec{r}_{ij}|) + \Phi^{\mathrm{l}}(|\vec{r}_{ij}|), \tag{8}$$

where $\Phi^{\mathrm{hs}}(|\vec{r}_{ij}|)$ is the hard sphere interaction potential, and $\Phi^{\mathrm{l}}(|\vec{r}_{ij}|)$ is the long-range potential. Taking into account the features of the hard sphere model dynamics [4] and the results of investigations [11, 13, 14], one can separate Enskog-Boltzmann collision integral from the function $\varphi_{nn}(\vec{k};\vec{p},\vec{p}\,';t,t')$. Indeed, an infinitesimal time of a collision $\tau_0 \to +0$ within an infinitesimal region $\sigma \pm \Delta r_0$, $\Delta r_0 \sim |\tau_0||\vec{p}_2 - \vec{p}_1|/m \to +0$ being a feature of the hard sphere model dynamics (σ is the hard sphere diameter). Taking this into account in the kinetic equation (1) we can obtain the kinetic equation of the revised Enskog theory for the hard sphere model and the kinetic Enskog-Landau equation for the charged hard sphere model in a pair collision approximation, respectively [4]. In the latter case, when $\Phi^{\mathrm{l}}(|\vec{r}_{ij}|)$ is the Coulomb potential of interaction, taking into account the features $\tau_0 \to +0$, $\Delta r_0 \to +0$ makes it possible to separate a collision integral of the revised Enskog theory and a Landau-like collision integral in the limits $\tau \to -0$ and $\tau \to -\infty$, respectively. In the case of potential (8), in the region of $\tau_0 \to +0$, $\Delta r_0 \to +0$, $\sigma \pm \Delta r_0$ where the main contribution to a dynamics is defined by pair collisions of hard spheres, the memory function $\varphi_{nn}(\vec{k};\vec{p},\vec{p}\,';t,t')$ can be calculated by expanding it over the density (a pair collision approximation), which was scrupulously done in papers by Mazenko [13–17].

Then, the kinetic equation (1) can be represented in the following form:

$$\begin{aligned}
\frac{\partial}{\partial t} f_{\vec{k}}(\vec{p};t) + \frac{\mathrm{i}\vec{k}\cdot\vec{p}}{m} f_{\vec{k}}(\vec{p};t) &= -\frac{\mathrm{i}\vec{k}\cdot\vec{p}}{m} n f_0(\vec{p})\left[c_2(k) - g_2(\sigma)c^0_2(k)\right]\int \mathrm{d}\vec{p}\,' f_{\vec{k}}(\vec{p}\,';t) \\
&- \int \mathrm{d}\vec{p}\,'\varphi^{\mathrm{hs}}_{nn}(\vec{k},\vec{p},\vec{p}\,')f_{\vec{k}}(\vec{p}\,';t) + \mathrm{i}\Omega_{nh}(\vec{k};\vec{p})h^{\mathrm{int}}_{\vec{k}}(t) \\
&- \int \mathrm{d}\vec{p}\,'\int\limits_{-\infty}^{t} \mathrm{d}t'\mathrm{e}^{\varepsilon(t-t')}\varphi^{\mathrm{l}}_{nn}(\vec{k};\vec{p},\vec{p}\,';t,t')f_{\vec{k}}(\vec{p}\,';t') - \int\limits_{-\infty}^{t}\mathrm{d}t'\mathrm{e}^{\varepsilon(t-t')}\varphi_{nh}(\vec{k};\vec{p};t,t')h^{\mathrm{int}}_{\vec{k}}(t').
\end{aligned} \tag{9}$$

Here,

$$\int \mathrm{d}\vec{p}'\varphi^{\mathrm{hs}}_{nn}(\vec{k},\vec{p},\vec{p}')f_{\vec{k}}(\vec{p}';t) = ng_2(\sigma)\sigma^2\int \mathrm{d}\Omega_\sigma \int \mathrm{d}\vec{p}'\frac{(\vec{p}-\vec{p}')\cdot\hat{\vec{\sigma}}}{m}\Theta_-\left(\hat{\vec{\sigma}}\cdot[\vec{p}-\vec{p}']\right)$$
$$\times\left[f_0(p'^*)f_{\vec{k}}(\vec{p};t) - f_0(p')f_{\vec{k}}(\vec{p}^*;t) + \mathrm{e}^{\mathrm{i}\vec{k}\cdot\hat{\vec{\sigma}}\sigma}f_0(p'^*)f_{\vec{k}}(\vec{p}'^*;t) - \mathrm{e}^{\mathrm{i}\vec{k}\cdot\hat{\vec{\sigma}}\sigma}f_0(p)f_{\vec{k}}(\vec{p}';t)\right] \tag{10}$$

is the Enskog-Boltzmann collision integral, where $c_2^0(\vec{k})$ is the low-density limit of the direct correlation function and $g_2(\sigma)$ is the pair distribution function. The step function $\Theta_-(x)$ is unity for $x<0$ and vanishes otherwise. $\mathrm{d}\Omega_\sigma$ is the differential solid angle, $\hat{\vec{\sigma}}$ is unity vector. The precollision and postcollision momenta of the colliding hard spheres are denoted as $(\vec{p},\vec{p}')$ and $(\vec{p}^*,\vec{p}'^*)$, respectively. $\varphi^{\mathrm{l}}_{nn}(\vec{k};\vec{p},\vec{p}';t,t')$ is the part of the transport kernel related to the long-range interaction potential $\Phi^{\mathrm{l}}(|\vec{r}_{ij}|)$. Notably, the presented equation contains the Enskog-Boltzmann collision integral describing short-time dynamics of the hard sphere model. The collective effects related to the long-range interactions between particles are described by the functions $\mathrm{i}\Omega_{nh}(\vec{k};\vec{p})$, $\varphi^{\mathrm{l}}_{nn}(\vec{k};\vec{p},\vec{p}';t,t')$, $\varphi_{nh}(\vec{k};t,t')$ and by the equation for $h^{\mathrm{int}}_{\vec{k}}(t)$. Since the collective modes for the Enskog-Boltzmann model are well studied [11], the investigation of time correlation functions and collective modes for the system of particles interacting through the potential (8) turns out to be of great interest. In the case of the hard spheres system, the set of kinetic equations (2), (9) reduces to the Enskog-Boltzmann kinetic equation [11].

$$\frac{\partial}{\partial t}f_{\vec{k}}(\vec{p};t) + \frac{\mathrm{i}\vec{k}\cdot\vec{p}}{m}f_{\vec{k}}(\vec{p};t) = -\frac{\mathrm{i}\vec{k}\cdot\vec{p}}{m}nf_0(\vec{p})\left[c_2(k) - g_2(\sigma)c_2^0(k)\right]\int \mathrm{d}\vec{p}'f_{\vec{k}}(\vec{p}';t)$$
$$- ng_2(\sigma)\sigma^2\int \mathrm{d}\Omega_\sigma\int \mathrm{d}\vec{p}'\frac{(\vec{p}-\vec{p}')\cdot\hat{\vec{\sigma}}}{m}\Theta_-\left(\hat{\vec{\sigma}}\cdot[\vec{p}-\vec{p}']\right)$$
$$\times\left[f_0(p'^*)f_{\vec{k}}(\vec{p};t) - f_0(p')f_{\vec{k}}(\vec{p}^*;t) + \mathrm{e}^{\mathrm{i}\vec{k}\cdot\hat{\vec{\sigma}}\sigma}f_0(p'^*)f_{\vec{k}}(\vec{p}'^*;t) - \mathrm{e}^{\mathrm{i}\vec{k}\cdot\hat{\vec{\sigma}}\sigma}f_0(p)f_{\vec{k}}(\vec{p}';t)\right]. \tag{11}$$

Projecting the Enskog-Boltzmann equation (11) onto the first moments of the nonequilibrium one-particle distribution function a spectrum of collective excitations for the hard sphere model was obtained in [11, 18]. Herewith, it is important to note that for the kinetic Enskog-Boltzmann equation we can consider two typical limits: $k\sigma \ll 1$ and $k\sigma \gg 1$. In the hydrodynamic limit ($k\sigma \ll 1$) the spectrum includes: **heat mode** $z_{\mathrm{H}}(k) = -D_{\mathrm{TE}}k^2$, where D_{TE} is the thermal diffusivity coefficient in the Enskog transport theory [19]; **two sound modes** with eigenvalues given by $z_\pm(k) = \pm\mathrm{i}ck - \Gamma_{\mathrm{E}}k^2$, where Γ_{E} is the sound damping coefficient and c is the sound velocity in the Enskog theory; **two shear modes** with eigenvalues given by $z_{\nu_1}(k) = z_{\nu_2}(k) = z_\nu(k) = -\nu_{\mathrm{E}}k^2$, ν_{E} is the kinematic viscosity in the Enskog dense gas theory. In the limit $k\sigma \gg 1$ the Enskog-Boltzmann collision integral (10) is transformed [11] into the Lorentz-Boltzmann collision integral which has only one eigenfunction $\Psi_1(\vec{p}) = 1$. Consequently, we obtain the **diffusion mode** only with the eigenvalue $z_{\mathrm{D}}(k) = -D_{\mathrm{E}}k^2$, where D_{E} is the self-diffusion coefficient as given by the Enskog dense gas theory.

Let us now project the system of equations (2), (9) onto the first moments of the nonequilibrium one-particle distribution function. Thereafter, we perform simple transformations consisting in the transition from the set of equations (4) for averages $n_{\vec{k}}(z), \vec{J}_{\vec{k}}(z), h^{\mathrm{kin}}_{\vec{k}}(z), h^{\mathrm{int}}_{\vec{k}}(z)$ to the equations of generalized hydrodynamics for averages $\tilde{b}_{\vec{k}}(z) = [n_{\vec{k}}(z), \vec{J}_{\vec{k}}(z), h_{\vec{k}}(z) = h^{\mathrm{kin}}_{\vec{k}}(z) + h^{\mathrm{int}}_{\vec{k}}(z)]$. This permits to correctly define (see below) the generalized viscosity coefficient via the transport kernel (13) and the heat conductivity coefficient via the transport kernel $\Pi_{hh}(k,z)$. The averages $\tilde{b}_{\vec{k}}(z)$ satisfy the set of equations $z\tilde{b}_{\vec{k}}(z) - \tilde{\Sigma}_{\mathrm{G}}(\vec{k};z)\tilde{b}_{\vec{k}}(z) = -\langle\tilde{b}_{\vec{k}}(t=0)\rangle^t$. In the limit $k\sigma \gg 1$, the latter reduces to a single equation of diffusion for $n_{\vec{k}}(z)$ in which the transport kernel $\Sigma_{\mathrm{G}}(\vec{k};z) = \langle\Psi_1|\varphi^{\mathrm{L-B}}_{nn}(\vec{k})|\Psi_1\rangle$ corresponds to the Lorentz-Boltzmann collision integral (10). In the opposite case, when $k\sigma \ll 1$, the matrix $\tilde{\Sigma}_{\mathrm{G}}(\vec{k};z)$ is defined as follows: $\tilde{\Sigma}_{\mathrm{G}}(\vec{k};z) = \tilde{\Sigma}_{\mathrm{H}}(\vec{k};z) = \mathrm{i}\tilde{\Omega}_{\mathrm{H}}(\vec{k}) - \tilde{\Pi}_{\mathrm{H}}(\vec{k};z)$,

$$\tilde{\Sigma}_{\mathrm{H}}(\vec{k};z) = \begin{pmatrix} 0 & \mathrm{i}\Omega_{nJ} & 0 \\ \mathrm{i}\Omega_{Jn} & -\langle\Psi_2|\varphi^{\mathrm{hs}}_{nn}|\Psi_2\rangle - \Sigma^{\mathrm{l}}_{jj} & \mathrm{i}\Omega_{Jh} - \Pi_{Jh} \\ 0 & \mathrm{i}\Omega_{hJ} - \Pi_{hJ} & -\langle\Psi_3|\varphi^{\mathrm{hs}}_{nn}|\Psi_3\rangle - \Pi^{\mathrm{l}}_{hh}\end{pmatrix}_{(k,z)}. \tag{12}$$

Here we use the notations

$$\Sigma_{jj}(k,z) = \Pi_{jj}(k,z) - \Sigma^{\rm int}_{jh}(k,z)\left[\Sigma^{\rm kin,kin}_{hh}(k,z)\right]^{-1}\left\{{\rm i}\Omega^{\rm kin}_{hj}(k) + \Pi^{kin,int}_{hh}(k,z)\right. \times \left.\left[z-\Sigma^{\rm int,int}_{hh}(k,z)\right]^{-1}\Sigma^{\rm int}_{hj}(k,z)\right\} - \Sigma^{\rm kin}_{jh}(k,z)\left[z-\Sigma^{\rm int,int}_{hh}(k,z)\right]^{-1}\Sigma^{\rm int}_{hj}(k,z), \tag{13}$$

$$\Pi_{hh}(k,z) = \Pi^{\rm kin,kin}_{hh}(k,z) + \Pi^{\rm kin,int}_{hh}(k,z) + \Pi^{\rm int,kin}_{hh}(k,z) + \Pi^{\rm int,int}_{hh}(k,z), \tag{14}$$

where $\Sigma^{\rm kin,kin}_{hh}(k,z) = z - \Pi^{\rm kin,kin}_{hh}(k,z)$, $\Sigma^{\rm int,int}_{hh}(k,z) = \Pi^{\rm int,int}_{hh}(k,z) + \Pi^{\rm int,kin}_{hh}(k,z)\left[\Sigma^{\rm kin,kin}_{hh}(k,z)\right]^{-1}$ $\times\Pi^{\rm kin,int}_{hh}(k,z)$, $\Sigma^{\rm int}_{hj}(k,z) = {\rm i}\Omega^{\rm int}_{hj}(k) + \Pi^{\rm int,kin}_{hh}(k,z)\left[\Sigma^{\rm kin,kin}_{hh}(k,z)\right]^{-1}{\rm i}\Omega^{\rm kin}_{hj}(k)$. We can separate real and imaginary parts in memory functions (13) and (14) as follows: $\Sigma_{jj}(k,z) = \Sigma'_{jj}(k,\omega) + {\rm i}\Sigma''_{jj}(k,\omega)$ and $\Pi_{hh}(k,z) = \Pi'_{hh}(k,\omega) + {\rm i}\Pi''_{hh}(k,\omega)$. Herewith, the contributions from the hard sphere dynamics with typical spatial-temporal scale $\tau_0 \to +0$, $\Delta r_0 \to +0$ are separated in the transport kernel $\varphi_{nn}(\vec{k};\vec{p},\vec{p}\,';t,t')$ only in the first term in the right-hand side of elements (7) and hence in (13). After these transformations we can obtain a spectrum of collective excitations in the hydrodynamic limit $k\sigma \ll 1$: **heat mode** $z_{\rm H}(k) = -D_{\rm T}k^2$, where $D_{\rm T}$ is the thermal diffusivity coefficient for the system with the potential of interaction (8). It has the following structure: $D_{\rm T} = D_{\rm TE} + D^{\rm l}_{\rm T}$, $D^{\rm l}_{\rm T}$ is determined through the corresponding elements (7) of matrix of transport kernels (6). $D^{\rm l}_{\rm T} = \frac{\lambda^{\rm l}}{nmc_p}$, c_p is a heat capacity at constant pressure, $\lambda^{\rm l}$ is the heat conductivity coefficient in the hydrodynamic limit: $\lambda^{\rm l} = \lim_{k\to0,\omega\to0}\lambda^{\rm l}(k,\omega)$. $\lambda^{\rm l}(k,\omega)$ is the generalized heat conductivity coefficient defined via elements of the matrix (6): $\lambda^{\rm l}(k,\omega) = \frac{c_V(k)}{k_{\rm B}\beta^2}\frac{1}{k^2}\Pi''_{hh}(k,\omega)$, where $c_V(k)$ is the generalized heat capacity at constant volume dependent on the wave vector $\vec{k}$; **two sound modes** $z_\pm(k) = \pm{\rm i}ck - \Gamma k^2$, where Γ is the sound damping and $c = \frac{c_p}{c_V\beta mS(0)}$ is the sound velocity in the system with the potential of interaction (8), $S(0) = S(k=0)$, $S(k)$ is a static structure factor of the system with potential (8). $\Gamma = \frac{1}{2}(c_p/c_V - 1)D_{\rm T} + \frac{1}{2}\eta^{\rm L}$, where $c_V = c_V(k=0)$, $\eta^{\rm L} = \left(\frac{4}{3}\eta^\perp + \eta^{\rm b}\right)/mn$ is the longitudinal viscosity defined via the bulk viscosity $\eta^{\rm b} = \eta^{\rm b}_{\rm E} + \eta^{\rm b}_{\rm l}$ and the shear viscosity $\eta^\perp = \eta^\perp_{\rm E} + \eta^\perp_{\rm l}$ coefficients. $\eta^\perp_{\rm E}$ is the shear viscosity in Enskog theory, and $\eta^\perp_{\rm l}$ is calculated in the hydrodynamic limit $\eta^\perp_{\rm l} = \lim_{k\to0,\omega\to0}\eta^\perp_{\rm l}(k,\omega)$. $\eta^\perp_{\rm l}(k,\omega)$ is the generalized shear viscosity coefficient defined via elements of the matrix (6) $\eta^\perp_{\rm l}(k,\omega) = \frac{mn}{\beta}\frac{1}{k^2}\Sigma''^{\perp}_{jj}(k,\omega)$. $\Sigma^\perp_{jj}(k,z)$ is the transverse component of the generalized transport kernel $\Sigma_{jj}(k,z)$, where the wave vector $\vec{k}$ is directed along the $0Z$ axis. The longitudinal viscosity coefficient $\eta^{\rm L}_{\rm l}$ is calculated in the hydrodynamic limit $\eta^{\rm L}_{\rm l} = \lim_{k\to0,\omega\to0}\eta^{\rm L}_{\rm l}(k,\omega)$, where $\eta^{\rm L}_{\rm l}(k,\omega)$ is the generalized longitudinal viscosity coefficient defined via longitudinal components of the generalized transport kernel $\Sigma_{jj}(k,z)$: $\eta^{\rm L}_{\rm l}(k,\omega) = \frac{mn}{\beta}\frac{1}{k^2}\Sigma''^{\rm L}_{jj}(k,\omega)$; **two shear modes** with the eigenvalues given by $z_\nu(k) = -\nu k^2$. $\nu = \nu_{\rm E} + \nu_{\rm l}$ is the kinematic viscosity $\nu = \eta^\perp/nm$ for the system with the potential of interaction (8). Here, ν_l is a contribution determined by the corresponding elements (7) of the matrix of transport kernels (6). In the limit $k\sigma \gg 1$, we obtain a **diffusion mode**, with the eigenvalue $z_{\rm D}(k) = -D_{\rm E}k^2$, which is the same as in the Enskog theory.

As we can see from the above expressions, presence of the long-range part in the potential of interaction entails a renormalization of all the damping coefficients in the collective modes spectrum. In particular, contributions related to long-range potential appear in heat and sound modes as well as in shear modes. Nevertheless, diffusion mode remains unchanged.

4. Conclusions

In this brief report within the framework of consistent description of kinetic and hydrodynamic processes we considered a set of kinetic equations for the potential of interaction of the system presented by the sum of hard spheres potential $\Phi^{\rm hs}(|\vec{r}_{ij}|)$ and a certain smooth one $\Phi^{\rm l}(|\vec{r}_{ij}|)$. In this case, we separated the Enskog-Boltzmann collision integral describing a collision dynamics at short distances from the collision integral of the kinetic equation for the nonequilibrium distribution function. Applying the procedure of projecting onto the moments of the nonequilibrium distribution function to the equations (2), (9) we obtain a set of equations for hydrodynamic variables. Based on this set of equations a spectrum of collective excitations was obtained in the limits $k\sigma \ll 1$ and $k\sigma \gg 1$. We showed that, besides the contribution from the hard spheres potential, all hydrodynamic modes contain contributions from the long-range part of potential. These contributions make the damping coefficients closer to the ones known from the hydrodynamic theory. Here, we formally presented the contribution from the long-ranged part of potential, since the latter, for example the Coulomb one, will contribute into the transport kernels (3). Moreover, we can separate the linearized Landau-like collision integral describing pair collisions in $\varphi_{nn}(\vec{k};\vec{p},\vec{p}';t,t')$, while $\varphi_{hn}(\vec{k};\vec{p};t,t')$, $\varphi_{nh}(\vec{k};\vec{p};t,t')$, $\varphi_{hh}(\vec{k};\vec{p};t,t')$ take into account collective Coulombic interactions. Evidently, calculation of the elements (7) of matrix $\tilde{\Pi}(\vec{k};z)$ will depend on the model of time dependence (exponential, Gaussian etc.) for transport kernels (3). When a spectrum of collective excitations is known, a whole set of time correlation functions can be investigated. In particular, it makes possible to investigate the behaviour of the dynamic structure factor and, in the case of potential (8), to separate a contributions from the hard spheres potential and the long-range part of potential in it.

References

1. Jhon M.S., Forster D., Phys. Rev. A, 1975, **12**, 254; doi:10.1103/PhysRevA.12.254.
2. Boon J.P., Yip S., Molecular Hydrodynamics, Dover, New York, 1991.
3. Zubarev D.N., Morozov V.G., Theor. Math. Phys., 1984, **60**, 814; doi:10.1007/BF01018982.
4. Zubarev D.N., Morozov V.G., Omelyan I.P., Tokarchuk M.V., Theor. Math. Phys., 1991, **87**, 412; doi:10.1007/BF01016582.
5. Klimontovich Yu.L., Theor. Math. Phys., 1992, **92**, 909; doi:10.1007/BF01015557.
6. Tokarchuk M.V., Theor. Math. Phys., 1993, **97**, 1126; doi:10.1007/BF01014805.
7. Zubarev D.N., Morozov V.G., Omelyan I.P., Tokarchuk M.V., Theor. Math. Phys., 1993, **96**, 997; doi:10.1007/BF01019063.
8. Tokarchuk M.V., Omelyan I.P., Kobryn A.E., Condens. Matter Phys., 1998, **1**, 687.
9. Zubarev D.N., Morozov V.G., Röpke G., Statistical Mechanics of Nonequilibrium Processes. Vol. 1: Basic Concepts, Kinetic Theory, Alademie Verlag, Berlin, 1996.
10. Tokarchuk M.V., Markiv B.B., Collected Physical Papers, Shevchenko Scientific Society, 2008, **7**, 100 (in Ukrainian).
11. De Schepper I.M., Cohen E.G.D., J. Stat. Phys., 1982, **27**, 223; doi:10.1007/BF01008939.
12. Markiv B.B., Omelyan I.P, Tokarchuk M.V., Condens. Matter Phys., 2010, **13**, 23005; doi:10.5488/CMP.13.23005.
13. Furtado P.M., Mazenko G.F., Yip S., Phys. Rev. A, 1975, **12**, 1653; doi:10.1103/PhysRevA.12.1653.
14. Mazenko G.F., Phys. Rev. A, 1974, **9**, 360; doi:10.1103/PhysRevA.9.360.
15. Mazenko G.F., Phys. Rev. A, 1971, **3**, 2121; doi:10.1103/PhysRevA.3.2121.
16. Mazenko G.F., Phys. Rev. A, 1972, **5**, 2545; doi:10.1103/PhysRevA.5.2545.
17. Mazenko G.F., Tomas Y.S., Yip S., Phys. Rev. A, 1972, **5**, 1981; doi:10.1103/PhysRevA.6.1981.
18. De Schepper I.M., Cohen E.G.D., Phys. Rev. A, 1980, **22**, 287; doi:10.1103/PhysRevA.22.287.
19. Chapman S., Cowling T.G., The Mathematical Theory of Non Uniform Gases, Cambrige University Press, London, 1970.

До проблеми узгодженого опису кінетичних та гідродинамічних процесів у густих газах та рідинах: спектр колективних збуджень

Б.Б. Марків, І.П. Омелян, М.В. Токарчук

Інститут фізики конденсованих систем НАН України, вул. І. Свєнціцького, 1, 79011 Львів, Україна

На основі отриманих раніше узагальнених немарківських рівнянь для нерівноважної одночастинкової функції розподілу та середнього значення густини потенціальної частини ентальпії [Markiv B.B., Omelyan I.P, Tokarchuk M.V., Condens. Matter Phys., 2010, **13**, 23005] досліджується спектр колективних збуджень, коли потенціал взаємодії між частинками представлено сумою потенціалу твердих сфер та деякого далекосяжного потенціалу.

Ключові слова: *кінетика, гідродинаміка, кінетичні рівняння, функції пам'яті, колективні моди*