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ON THE THEORY OF DYNAMIC PROPERTIES FOR SEMI–QUANTUM FLUIDS

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#### До теорії динамічних властивостей напівквантових рідин

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Анотація. На основі методу нерівноважного статистичного оператора запропоновано загальну структуру теоретичного підходу до вивчення динамічних властивостей напівквантових рідин. Отримано систему рівнянь узагальненої гідродинаміки та проаналізовано частковий випадок т. зв. термов'язкоеластичної моделі в гідродинамічній границі. Обговорюються кілька наближених підходів розрахунку ядер переносу, що дає змогу отримати замкнуту систему рівнянь для часових кореляційних функцій. Задача розглядається в контексті взаємозв'язку з експериментами з розсіяння нейтронів та з відомими теоретичними результатами.

#### On the theory of dynamic properties for semi-quantum fluids

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Abstract. On the basis of nonequilibrium statistical operator method a general theoretical framework for the study of dynamic properties of semi-quantum fluids is developed. We derive the set of equations of generalized hydrodynamics and analyse the particular case of so-called thermo-viscoelastic dynamical model of a fluid in more detail considering hydrodynamic limit. We discuss also some approximate procedures for evaluation of transport kernels which allow to obtain a closed set of equations for time correlation functions. The problem is considered in the context of relation with neutron scattering experiment data and theoretical results known previously in the literature.

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### 1. Introduction.

Liquid <sup>4</sup>He is a sample of quantum liquid that excites permanent interest both for theoretical physicists and experimentalists [1–4]. Being the system that obeys Bose statistics a liquid <sup>4</sup>He, together with a number of Fermi systems [3–5] such as <sup>3</sup>He, various compounds of hydrogen, electronic gas, needs applying of quantum mechanics apparatus for its description.

It is well known that any quantum system may be characterized by the set of some typical temperatures to be very important for understanding of its dynamical properties. One of them is a temperature of quantum degeneration  $T_d = \hbar/\tau$  which can be estimated both for Bose and Fermi cases as follows  $T_d \sim n^{\frac{2}{3}}/m^*$  where n and  $m^*$  are the number density and the effective mass of particle, respectively. The value  $\tau$ may be considered as a quantum delocalization time. Another temperature, characterizing quantum systems, in which phonon processes are dominant in low-temperature region (what one has, in fact, in quantum <sup>4</sup>He and <sup>3</sup>He [4]) is a Debye temperature  $T_D = \hbar\Omega_D$ . This temperature can be simply estimated using the well know formula for solids, namely,  $T_D \sim cn^{\frac{1}{3}}$ , where c is an adiabatic sound velocity, and may characterize the frequency of the vibrational degrees of freedom in a quantum system.

For quantum liquids mentioned above the inequality  $T_d \ll T_D$  takes usually place. Depending on the value of equilibrium temperature Tconsidered, all the quantum fluids (for which the melting point is far less then  $T_D$ ) could be arbitrarily divided into two main classes:

(i) quantum fluids for which an equality  $T < T_d$  is satisfied, so that the quantum effects plays crucial role;

(ii) quantum fluids considered within region  $T_d \ll T \ll T_D$ .

Estimations, performed for some quantum systems by Andreev [6], give us for the pressure P = 0 atm, P = 25 atm, P = 64.6 atm, the following values of Debye temperatures: 13.7 K for <sup>3</sup>He; 32.7 K for <sup>4</sup>He; 155 K for H<sub>2</sub>, respectively. The temperature  $T_d$  is  $T_d \approx 3$  K for <sup>3</sup>He and <sup>4</sup>H and has been estimated as  $T_d \approx 10$  K for H<sub>2</sub> [7]. So that a number of quantum fluids being considered as the fluids (ii) with  $T_d \ll T \ll T_d$  is much larger. Besides <sup>3</sup>He and <sup>4</sup>He, to this class of fluids belong isotopes of hydrogen as well as its solutions.

Let us discuss now what is the reasons and the physical meaning for such a division.

According to Frenkel picture of kinetic phenomena in liquids [8], in case (ii) a vibrational frequency  $\Omega$  of the atoms near equilibrium position is large in comparison with inverse time  $\tau^{-1}$  of the jump of the particles between local positions of equilibrium ( $\Omega \tau \gg 1$ ). Thus, a phenomenological model of the liquid as a system of particles trapped at the bottom of the potential well which vibrate very frequently and during certain period of time  $\tau$  jump in the closest position of equilibrium can be constructed. In the Frenkel picture tunnel transitions of the particles in nonsymmetric potential well, created by neighbouring surrounding, play the role of elementary excitations. Because of assumption  $\Omega \tau \gg 1$  these phonon–like excitation are well–defined and they should contribute essentially both to thermodynamic and dynamic properties.

For a system to remain in a liquid state at  $T \ll T_D$  it is necessary that the amplitude of vibrations to be sufficiently large comparatively with interatomic distance, or, what is nearly the same, the Debye temperature to be comparative with interparticle interaction energy U. So far as there is not long-range order and equilibrium positions are distributed irregularly in space, such a liquid resembles a glass. The only difference consists in the fact that in quantum liquids all potential barriers are penetrable, so that a small concentration of excitations may be conditioned only by low temperatures in comparison with typical difference of energies in the neighbouring equilibrium positions. Such phenomenological treatment has been developed by Andreev who introduced in the literature (after Lifshitz proposal) the term "semi-quantum" liquid for description of the object for which the conditions (ii) are valid. Let us consider one from the thermodynamical results which obtained by Andrevev. Taking into account that the main contribution to the thermodynamics is related to the phonon-like excitations, the free energy per atom can be written in the form [6]:

$$f(T) = -T \int_{0}^{\infty} \ln\left(1 + \exp(-\epsilon/T)\right) \nu(\epsilon) d\epsilon, \qquad (1.1)$$

where  $\nu(\epsilon) d\epsilon$  denotes the probability for some particle to occupy neighbouring equilibrium position with excitation energies in the interval  $\epsilon$  and  $\epsilon + d\epsilon$ . When  $\epsilon \ll U$  the density of levels does not depend on energy  $(\nu(\epsilon) = \nu = const)$  and could be estimated as z/U, where z denotes an effective number of neighbouring vacancies. Then free energy per atom equals

$$f(T) = -\frac{\pi^2}{12}\nu T^2 \,,$$

where from specific heat  $c_V(T)$  could be obtained:

$$c_V(T) = \frac{\pi^2}{6} \nu T$$
. (1.2)

Hence, instead of phonon-like contribution to  $c_V(T) \sim T^3$  observed in quantum liquids for low temperature region  $(T < T_d)$  we got linear dependence. This very simple and nice formula has been verified for <sup>3</sup>He, <sup>4</sup>He and H<sub>2</sub> liquids and it was shown that the expression (1.2) could be applied for up to temperatures of order  $T/T_D \approx 0.07$ . There were also found the estimations for the value of  $1/\nu$ : 3.5 K for <sup>3</sup>He (P = 0 atm); 6 K for <sup>4</sup>He (P = 25 atm) and 110 K for H<sub>2</sub> (P = 64.6 atm), respectively, to be seem quite reasonable. In the section 4 the expression for generalized specific heat via quantum static correlation functions of enthalpy density will be presented. It may be expected that in microscopic approach, due to essential anharmonicity of a model Hamiltonian, the linear behaviour might be also found while in case of degenerated non-perfect Bose gas one has the well-known dependence  $c_V(T) \sim T^3$  [9].

Hence, having an example when phonon-like non-dispersive excitations influence on thermodynamic properties of semi-quantum liquid. one can asked himself whether these excitations could be observed in kinetic properties? So the next natural step in investigation of semiquantum helium was the study of dynamic properties. This was performed partly in [10] where on the basis of 2- and 3-levels model the transport coefficients were calculated. A remarkable feature, founded in this study, consists in the fact that in low frequency limit  $\hbar\omega \ll T$  shear viscosity and thermal conductivity behave as  $T^{-1}$  and  $T^{1}$ , respectively. A comparison with experimental data supported these results. In the paper [7] ultrasound damping in semi-quantum liquids was studied. Kinetic equations were written and solved assuming that  $\nu(\epsilon) \approx \nu$  and diffusion character of relaxation mechanism is dominant. One obtained frequency dependence of damping coefficient both in high frequency limit and in case  $\omega \tau \ll 1$ . Frequency dependence occurs to be proportional  $\omega^2$  in the first case and linear in  $\omega$  in low frequency limit. Now, the next question naturally arises. Could these non-dispersion excitations be observed in scattering experiments and in which range of k one can expect to find them?

The history of the study of quantum liquids has a long tradition. We restrict themselves only by a short discussion of the results for a quantum <sup>4</sup>He liquid related to our topic. What might one expected to find? The first point, we should consider the temperatures higher than  $T/T_D \approx 0.07$  and this means for <sup>4</sup>He that we are interested in cases  $T \geq 4$  K depending on the density or pressure. The second point, one may hope to find the excitations with a weak dispersion located about the frequency  $\omega = \Omega$ . For <sup>4</sup>He one has  $\Omega \approx 5$  ps<sup>-1</sup>. And these excitations have to appear when k increases in order to rich the range where the

excitations are located. Taking into account the viscoelastic properties of medium to be crucial usually, when k is about the position  $k_0$  of the first maximum of the static structural factor, one may expect to find these excitations for  $k > k_0$  only as additional side peaks in the symmetrized dynamic structural factor. According to the conditions formulated above we should state that the most part of scattering data known in the literature were obtained for the temperatures and the  $(k, \omega)$ -regions which are outside of our interest in this study.

The most interesting data related to our topic are obtained by group of experimentalists from Delft Interfaculty Reactor Institute [11,12]. They performed two sets of experiments for helium at the states T = 4 K, P = 1 bar and T = 8 K, P = 18.7 bar and determined the dynamic structure factor  $S(k,\omega)$  in the range 1 < k < 30 nm<sup>-1</sup>. The subject of our interest is the symmetrized dynamic structure factor  $S_{sym}(k,\omega)$  of liquid helium at T = 4 K and gaseous helium at T = 8 K which are presented on figures 1 and 2. One can see in these figures that:

(i) For small k ( $k < 2 \text{ nm}^{-1}$ ) the usual hydrodynamic behaviour is observed what is quite similar to classical fluids. It is clearly that  $S_{sym}(k,\omega)$  consists of three lines which form the Rayleigh-Brillouin triplet, namely, a central line corresponding to entropy diffusion, which disappears for  $k > 3 \text{ nm}^{-1}$  and two side peaks representing all the mechanisms which normally related to the propagation of sound waves.

(ii) When k increases one may see that at first the central peak is disappearing for both temperatures, and then the sound modes become overdamped and form two broad peaks getting to be indistinguishable for  $k > 10 \text{ nm}^{-1}$ . It is worth to note that for T = 4 K all these effects are started to be visible for smaller k.

(iii) For the wave-numbers about the value of  $k_0 = 20 \text{ nm}^{-1}$  (where the first maximum of static structural factor is approximately located) the spectrum, much like the behaviour in classical fluids, gets narrow (de Gennes' narrowing). For large k the width of the spectrum increases again with increasing of k.

(iv) For larger values of k the side peaks appear again and their position is increasing weakly when k increases, so that we face with new propagating damped sound-like modes which characterize mainly the dynamic properties of the liquid helium for large k. It should be emphasised that such behaviour is rather special and is not typical for any classical fluid.



Figure 1. Symmetrized dynamic structure factor  $S_{sym}(q,\omega)$  of He<sup>4</sup> at T = 4K (left) and T = 8K (right) as function of  $\omega$  for different q. Experiment (error bars), best fits using 3-variables generalized hydrodynamics model (solid line) and best fits using 2-variables model of damped harmonic oscillators (dashed line) [12].



Figure 2. The same as on figure 4 for  $q \ge 4$  nm<sup>-1</sup>.

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In the same series of papers [11,12] a semi-phenomenological theoretical model, based on the generalized mode approach (see, e.g., [13,14]), has been developed for a description of experimental data. Within this framework the model parameters has been considered as adjustable parameters giving the best fit of dynamic structure factor. In particulary, it was shown that all the data could be described using a small number lof basic dynamic variables (l < 3) for all k, namely, in the hydrodynamic range a three Lorentzians scheme was used for description of Rayleigh-Brillouin triplet; for intermediate range of k so-called damped harmonic oscillator model has been applied (l = 2), and the viscoelastic model (l = 3) was utilized for describing of the experimental data when k is large enough. It is worth to point out that these results have little to use for understanding of the real dynamic properties in a liquid helium. Some anzats has been applied just to fit of experimental data. Hence, one may agree with a conclusion of Griffin [15] that "the overdamped phonon spectrum may well be an artifact of the particular formula used in the fits".

Another paper [16] to be important for our discussion reported the results of a neutron-scattering experiments on dense helium at T = 13.3 K, P = 203 bar in the range  $3 < k < 11 \text{ nm}^{-1}$ . It was found that the dynamic structure factor  $S(k, \omega)$  has a clearly visible additional peak which can not be considered as sound modes. Moreover, the directly related scattering spectrum  $C(k, \omega) = \omega^2 S(k, \omega)$  showed a four-peaked structure, so that it was necessary to consider at least five Lorentzians for a description of experimental data consistently (i.e., four side lines and one central line). Two additional peaks were treated as the propagating temperature waves, which are not seen in dense classical fluids. Unfortunately, this study has been only performed for  $k < 11 \text{ nm}^{-1}$ , so that it is impossible to say anything about the behaviour of a central peak as well as side propagating excitations when k increases.

The last scattering data that we would like to mention were presented in Ref. [17] and obtained for dense helium at T = 39 K, P = 114 bar in the range 3 < k < 24 nm<sup>-1</sup>. In fact this temperature is nearly the same as Debye temperature  $T_D$  for <sup>4</sup>He, so that one could expected to find herein the behaviour to be very similar to classical fluids. The main conclusion of this paper is that the dynamic structure factor can be described completely by the viscoelastic model. We note that such conclusion is typical for classical fluids for intermediate values of k. Because of large values of k, the presented results do not allow to discuss the hydrodynamic behaviour of  $S(k, \omega)$  where Rayleigh-Brillouin triplet have to be visible.

Now let us summarize our introductory part and underline the main

problems which still wait to be solved.

(a) There are a lot of reasons to consider semi-quantum fluids as a separate class of fluids. These fluids possess some special properties which could be recognized in thermodynamics, kinetics, and dynamic behaviour;

(b) one can expect that the most part of their typical properties are closely related with the existence of weak dispersive excitations, which play crucial role both for thermodynamics and dynamics;

(c) in order to understand the interplay of collective excitations, which are observed in scattering experiments, the additional study has to be preformed taking into account all the processes to be important from the physical point of view, namely, entropy fluctuations, viscoelastic properties as well as their mutual interaction. This study should base on the unified dynamical model to have been applied for all temperatures from the range  $T_d \ll T \ll T_d$ . Here the main problems are: a decrease of central peak in the dynamic structure factor and an appearance of new propagating phonon–like excitations when k increases.

The goal of this paper is to develop a general microscopic framework for the next *ab initio* study of generalized collective mode spectrum, time correlation functions and generalized transport coefficients for semi-quantum fluids. We use for this purpose the generalized mode approach developed [14,18] for the investigation of a dense classical fluid. Moreover, comparing the results obtained for the spectrum of generalized collective modes of a Lennard-Jones fluid [19], one may assume that weak dispersive excitations observed in scattering experiments are indeed kinetic propagating modes which appear due of coupling thermal and viscous processes. In classical fluids these modes are usually overdamped and can not be observed in scattering experiment. However, they become to be visible in some binary mixtures [20–22] with a large distinction in the masses of components and are known in the literature as "fast" sound.

#### 2. Initial relations.

We shall deal in this study with the time correlation functions (TCFs)  $\Phi_{AB}(\mathbf{k}, t)$  defined by

$$\Phi_{AB}(\boldsymbol{k},t) = \left(\hat{A}(\boldsymbol{k},t), \hat{B}(-\boldsymbol{k})\right)_{0} = \int_{0}^{1} d\tau \operatorname{Sp}\left(\Delta \hat{A}(\boldsymbol{k},t) \rho_{0}^{\tau} \Delta \hat{B}(-\boldsymbol{k}) \rho_{0}^{1-\tau}\right), \quad (2.3)$$
$$\Delta \hat{A}(\boldsymbol{k},t) = \hat{A}(\boldsymbol{k},t) - \operatorname{Sp}\rho_{0} \hat{A}(0,0),$$

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where the time dependence is in the Heisenberg representation

$$\hat{A}(\boldsymbol{k},t) = \exp(\imath\hat{\mathcal{H}})\hat{A}(\boldsymbol{k})\exp(-\imath\hat{\mathcal{H}}), \quad \hat{\mathcal{H}} = \hat{H} - \mu\hat{N}.$$
(2.4)

Here  $\hat{H}$  means Hamiltonian of the system (see eqn. (3.1) for its explicit form),  $\hat{N}$  denotes particle number operator,  $\rho_0$  is an equilibrium statistical operator  $\rho_0(x^N) = \exp\left\{-\Phi - \beta(\hat{H} - \hat{N}\mu)\right\}$  of Bose–system with equilibrium inverse temperature  $\beta$  and chemical potential  $\mu$ .

TCF  $\Phi_{AB}(\mathbf{k}, t)$  appear in natural way in the nonequilibrium statistical operator method and are directly related to the so-called correlation Green's function.

The Fourier transform  $\Phi_{nn}(\mathbf{k},\omega)$  of the time correlation function  $\Phi_{nn}(\mathbf{k},t)$  constructed on number density operators  $\hat{n}_{\mathbf{k}}$ ,

$$\Phi_{AB}(\boldsymbol{k},\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \, \exp(\imath\omega t) \Phi_{AB}(\boldsymbol{k},t), \quad A,B = n, \qquad (2.5)$$

is straightforwardly related to the experimentally determined dynamic structure factor  $S(\mathbf{k},\omega)$  as

$$\Phi_{nn}(\boldsymbol{k},\omega) = \frac{1 - \exp(-\beta\hbar\omega)}{\beta\hbar\omega} S(\boldsymbol{k},\omega).$$
(2.6)

Taking into account that  $\Phi_{nn}(\mathbf{k},\omega)$  is a function of  $\omega$ , one may see that the detailed balance relation

$$S(\boldsymbol{k},-\omega) = e^{-\beta\hbar\omega}S(\boldsymbol{k},\omega)$$

follows directly from (2.6), and  $\Phi_{nn}(\mathbf{k},\omega)$  can be considered as symmetrized dynamic structure factor  $S_{sym}(\mathbf{k},\omega)$  introduced in Ref. [11,12], so that

$$S_{sym}(\boldsymbol{k},\omega) \equiv \Phi_{nn}(\boldsymbol{k},\omega).$$

Another expression to be useful for the next consideration establishes the relation between the Laplace transform  $\tilde{\Phi}_{nn}(\mathbf{k}, z)$  of  $\Phi_{nn}(\mathbf{k}, t)$ ,

$$\tilde{\Phi}_{AB}(\boldsymbol{k},z) = \int_{0}^{\infty} dt \ e^{-zt} \Phi_{AB}(\boldsymbol{k},t), \quad A,B = n,$$
(2.7)

where  $z = i\omega + \epsilon$ ,  $\epsilon = +0$ , and the symmetrized dynamic structure factor

$$S_{sym}(\boldsymbol{k},\omega) = \frac{1}{\pi} \operatorname{Re} \,\tilde{\Phi}_{nn}(\boldsymbol{k},z)$$

Similary to the static structure factor S(k) defined by

$$S(\mathbf{k}) = \int_{-\infty}^{\infty} d\omega \, S(\mathbf{k}, \omega) \,, \qquad (2.8)$$

the symmetrized static correlation factor can be defined as  $^{1}$ 

$$S_{sym}(\boldsymbol{k}) = \int_{-\infty}^{\infty} d\omega \, S_{sym}(\boldsymbol{k}, \omega) \,. \tag{2.9}$$

It would be useful to write down some additional relations for higher frequency moments of dynamic structure factor which were given in Ref. [12]. The frequency moments  $S(\mathbf{k}, \omega)$  and  $S_{sym}(\mathbf{k}, \omega)$  are in general defined by

$$M^{(l)}(\boldsymbol{k}) = \int_{-\infty}^{\infty} d\omega \,\omega^{l} S(\boldsymbol{k}, \omega)$$
(2.10)

 $\operatorname{and}$ 

$$M_{sym}^{(l)}(\boldsymbol{k}) = \int_{-\infty}^{\infty} d\omega \,\omega^{l} S_{sym}(\boldsymbol{k},\omega), \qquad (2.11)$$

where  $l \geq 0$ . Because  $S_{sym}(\mathbf{k}, \omega)$  is an even function of  $\omega$ , all the odd moments  $M_{sym}^{(2l+1)}(\mathbf{k})$  are equal to zero. The additional exact relations follow straightforwardly from the detailed balance relation and Eqn. (2.6)

$$M^{(2l+1)}(\mathbf{k}) = \frac{\hbar\beta}{2} M^{(2l+2)}_{sym}(\mathbf{k}).$$
(2.12)

In a similar manner the even moments of  $S(\mathbf{k},\omega)$  can be expressed as a series expansion in the small parameter  $(\hbar\beta)^2$ 

$$M^{(2l)}(\mathbf{k}) = M^{(2l)}_{sym}(\mathbf{k}) + \frac{(\hbar\beta)^2}{12} M^{(2l+2)}_{sym}(\mathbf{k}) - \frac{(\hbar\beta)^4}{720} M^{(2l+4)}_{sym}(\mathbf{k}) + O((\hbar\beta)^6).$$
(2.13)

It is clear from expressions presented above that in low frequency region  $\hbar\omega \ll T$  we face with purely classical behaviour while as in collisionless high–frequency domain  $\hbar\omega > T$  quantum features become essential.

 $<sup>^{1}</sup>$ Due to definition (2.3) we shall deal with symmetrized static correlation functions only in all subsequent expressions.

# 3. Nonequilibrium statistical operator of liquid <sup>4</sup>He above Bose-condensation point.

Hydrodynamic state of helium above  $T_d$  will be described on the basis of the model of Bose–system with Hamiltonian

$$\hat{H} = \sum_{p} \frac{p^{2}}{2m} \hat{a}_{p}^{\dagger} \hat{a}_{p} + \frac{1}{2V} \sum_{k} \sum_{p} \nu(k) \hat{a}_{p+\frac{k}{2}}^{\dagger} \hat{n}_{k} \hat{a}_{p-\frac{k}{2}}, \qquad (3.1)$$

where  $\hat{a}_{p}^{\dagger}$ ,  $\hat{a}_{p}$  denote creation and annihilation operators in the state with momentum p,  $\nu(q) = \int \exp(i q r) \Phi(|r|) dr$  denotes Fourier-component of the interaction potential  $\Phi(|r|)$  between helium particles, V means volume of the system.

$$\hat{n}_{k} = \frac{1}{\sqrt{N}} \sum_{p} \hat{a}_{p-\frac{k}{2}}^{\dagger} \hat{a}_{p+\frac{k}{2}}$$
(3.2)

is a Fourier–component of the number density operator,  ${\cal N}$  denotes total particle number.

Nonequilibrium state of such a quantum system is described by nonequilibrium statistical operator (NSO)  $\rho(x^N, t)$  obeying quantum Liouville equation:

$$\frac{\partial}{\partial t}\rho(x^N,t) + i\hat{L}_N\rho(x^N,t) = 0, \qquad (3.3)$$

where  $i\hat{L}_N$  denotes Liouville operator determined as  $i\hat{L}_N\hat{A} = \frac{i}{\hbar} \left[\hat{A}, \hat{H}\right]$ . Within Zubarev's method of NSO [23], the retarded solutions of the Liouville equation can be obtained by introduction an infinitesimal source in the right hand side of (3.3):

$$\frac{\partial}{\partial t}\rho(x^N,t) + i\hat{L}_N\rho(x^N,t) = -\varepsilon \left(\rho(x^N,t) - \rho_q(x^N,t)\right) , \qquad (3.4)$$

 $(\varepsilon \to 0 \text{ after thermodynamic transition})$ , where  $\rho_q(x^N, t)$  is so-called quasi-equilibrium statistical operator is known to be functional of the mean values of the certain set of dynamic operators  $\hat{P}_n(\mathbf{k})$ . So far as we investigate hydrodynamic state of the system one can choose as parameters of abbreviated description the most slowly physical quantities  $\hat{P}_n(\mathbf{k})$ , which are thought to determine the nonequilibrium state. One can select among them Fourier-transforms of the number density  $\hat{n}_k$ (see eqn.(3.2)), momentum density  $\hat{J}_k$ :

$$\hat{J}_{k} = \frac{1}{\sqrt{N}} \sum_{p} p \, \hat{a}_{p-\frac{k}{2}}^{\dagger} \hat{a}_{p+\frac{k}{2}}$$
(3.5)

and total energy density  $\hat{\varepsilon}_{k}$ :

$$\hat{\varepsilon}_{\boldsymbol{k}} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{p}} \left( \frac{\boldsymbol{p}^2}{2m} - \frac{\boldsymbol{k}^2}{8m} \right) \hat{a}^{\dagger}_{\boldsymbol{p} - \frac{\boldsymbol{k}}{2}} \hat{a}_{\boldsymbol{p} + \frac{\boldsymbol{k}}{2}}$$
$$+ \frac{1}{2V} \sum_{\boldsymbol{p}} \sum_{\boldsymbol{q}} \nu(\boldsymbol{q}) \hat{a}^{\dagger}_{\boldsymbol{p} + \frac{\boldsymbol{q} - \boldsymbol{k}}{2}} \hat{n}_{\boldsymbol{q}} \hat{a}_{\boldsymbol{p} - \frac{\boldsymbol{q} - \boldsymbol{k}}{2}}$$
(3.6)

which obey conservation laws

$$\dot{\hat{P}}_{n}(\boldsymbol{k}) \equiv i\hat{L}_{N}\hat{P}_{n}(\boldsymbol{k}) = -i\boldsymbol{k}\hat{\boldsymbol{I}}_{n}(\boldsymbol{k}), \qquad (3.7)$$
$$\hat{P}_{n}(\boldsymbol{k}) = \left\{\hat{n}_{\boldsymbol{k}}, \hat{\boldsymbol{J}}_{\boldsymbol{k}}, \hat{\varepsilon}_{\boldsymbol{k}}\right\}, \quad \hat{\boldsymbol{I}}_{n}(\boldsymbol{k}) = \left\{\frac{1}{m}\hat{\boldsymbol{J}}_{\boldsymbol{k}}, \hat{\boldsymbol{\Pi}}_{\boldsymbol{k}}, \hat{\boldsymbol{J}}_{\varepsilon\boldsymbol{k}}\right\},$$

where  $\hat{\Pi}_{k}$  is a stress tensor operator and  $\hat{J}_{\varepsilon k}$  denotes operator of energy current.

Accordingly [23], quasiequilibrium statistical operator  $\rho_q(x^N, t)$  is being determined from maximum entropy principle under fixed mean values  $\langle \hat{P}_n(\mathbf{k}) \rangle^t$  and normalization condition  $Sp \rho_q(x^N, t) = 1$  and has the following form:

$$\rho_q(x^N, t) = \exp\left\{-\Phi(t) - \sum_{\boldsymbol{k}} \left(\beta_{-\boldsymbol{k}}(t)\hat{\varepsilon}_{\boldsymbol{k}} - (\beta\boldsymbol{v})_{-\boldsymbol{k}}(t)\hat{\boldsymbol{J}}_{\boldsymbol{k}} - (\beta(\mu - \frac{m}{2}\boldsymbol{v}^2))_{-\boldsymbol{k}}(t)\hat{n}_{\boldsymbol{k}}\right)\right\}, \qquad (3.8)$$
$$\Phi(t) = \ln Sp \exp\left\{-\sum_{\boldsymbol{k}} \left(\beta_{-\boldsymbol{k}}(t)\hat{\varepsilon}_{\boldsymbol{k}} - (\beta\boldsymbol{v})_{-\boldsymbol{k}}(t)\hat{\boldsymbol{J}}_{\boldsymbol{k}}\right)\right\}$$

$$-\left(\beta(\mu-\frac{m}{2}\boldsymbol{v}^{2})\right)_{-\boldsymbol{k}}(t)\hat{n}_{\boldsymbol{k}}\right)\Big\}$$
(3.9)

denotes Massier–Planck functional, where  $\beta_{k}(t)$ ,  $v_{k}(t)$ ,  $\mu_{k}(t)$  denote Fourier–components of the local values of inverse temperature, hydrodynamic velocity and chemical potential which are being determined from self–consistency conditions:

$$\langle \hat{n}_{\boldsymbol{k}} \rangle^{t} = \langle \hat{n}_{\boldsymbol{k}} \rangle_{q}^{t}, \quad \langle \hat{\boldsymbol{J}}_{\boldsymbol{k}} \rangle^{t} = \langle \hat{\boldsymbol{J}}_{\boldsymbol{k}} \rangle_{q}^{t}, \quad \langle \hat{\varepsilon}_{\boldsymbol{k}} \rangle^{t} = \langle \hat{\varepsilon}_{\boldsymbol{k}} \rangle_{q}^{t}, \quad (3.10)$$
$$\langle \dots \rangle^{t} = Sp\left(\dots \rho(x^{N}, t)\right), \quad \langle \dots \rangle_{q}^{t} = Sp\left(\dots \rho_{q}(x^{N}, t)\right).$$

One can point out that values  $\beta_{\mathbf{k}}(t)$ ,  $(\beta \boldsymbol{v})_{\mathbf{k}}(t)$  and  $(\beta(\mu - \frac{m}{2}\boldsymbol{v}^2))_{\mathbf{k}}(t)$  play the role of Lagrange multipliers in the problem of conditioned maximum of entropy and due to local thermodynamic relations should be attributed to corresponding thermodynamic forces [23].

NSO method allows to solve equation (3.4) and to write down the explicit form of  $\rho(x^N, t)$  as retarded solution of Liouville equation:

$$\rho(x^{N},t) = \rho_{q}(x^{N},t) + \sum_{\boldsymbol{k}} \int_{-\infty}^{t} dt' \exp(\varepsilon(t'-t))T(t,t') \int_{0}^{1} d\tau \rho_{q}^{\tau}(x^{N},t')$$
$$\times \left\{ \beta_{-\boldsymbol{k}}(t')\hat{\boldsymbol{J}}_{\varepsilon\boldsymbol{k}} - (\beta\boldsymbol{v})_{-\boldsymbol{k}}(t')\hat{\boldsymbol{\Pi}}_{\boldsymbol{k}} \right\} \rho_{q}^{1-\tau}(x^{N},t').$$
(3.11)

Here time evolution is being described by evolution operator

$$T(t,t') = \exp_{+} \left\{ -\int_{t'}^{t} (1 - \mathcal{P}_{q}(\tau)) i \hat{L}_{N} d\tau \right\} , \qquad (3.12)$$

where  $\mathcal{P}_{q}(\tau)$  denotes generalized Kawasaki–Gunton operator [23].

The first term of (3.11) doesn't contribute to entropy production. On the contrary, integral term in the right-hand side of NSO (3.11) describes dissipative processes. Generalized transport coefficients - viscosity, thermal conductivity and thermoelasticity are being constructed on dissipative fluxes  $\hat{I}_{\varepsilon}(\boldsymbol{k},t)$  and  $\hat{I}_{J}(\boldsymbol{k},t)$  that are of the following structure:

$$\hat{I}_{\varepsilon}(\boldsymbol{k},t) = (1 - \mathcal{P}(t)) \dot{\varepsilon}_{\boldsymbol{k}}, \qquad (3.13)$$

$$\hat{I}_j(\boldsymbol{k},t) = (1 - \mathcal{P}(t)) \, \dot{\boldsymbol{j}}_{\boldsymbol{k}}, \qquad (3.14)$$

where  $\mathcal{P}(t)$  denotes Mori projection operator, constructed on basic variables  $\{\hat{n}_{k}, \hat{J}_{k}, \hat{\varepsilon}_{k}\}$ , which acts on arbitrary operator  $\hat{A}$  accordingly rule:

$$\mathcal{P}(t)\hat{A} = \langle \hat{A} \rangle_{q}^{t} + \sum_{k} \left\{ \frac{\delta \langle \hat{A} \rangle_{q}^{t}}{\delta \langle \hat{n}_{k} \rangle^{t}} \left( \hat{n}_{k} - \langle \hat{n}_{k} \rangle^{t} \right) + \frac{\delta \langle \hat{A} \rangle_{q}^{t}}{\delta \langle \hat{J}_{k} \rangle^{t}} \left( \hat{J}_{k} - \langle \hat{J}_{k} \rangle^{t} \right) + \frac{\delta \langle \hat{A} \rangle_{q}^{t}}{\delta \langle \hat{\varepsilon}_{k} \rangle^{t}} \left( \hat{\varepsilon}_{k} - \langle \hat{\varepsilon}_{k} \rangle^{t} \right) \right\}$$
(3.15)

and has the following properties:  $\mathcal{P}(t)\mathcal{P}(t) = \mathcal{P}(t), (1 - \mathcal{P}(t))\mathcal{P}(t) = 0,$  $\mathcal{P}(t)\hat{P}_n(\mathbf{k}) = \hat{P}_n(\mathbf{k}).$  Mori projection operator is connected with Kawasaki–Gunton operator appearing in (3.12) by relation

$$\mathcal{P}_q(t)\hat{A}\rho_q(x^N,t) = \int_0^1 d\tau \,\rho_q^\tau(x^N,t)\mathcal{P}(t)\hat{A}\rho_q^{1-\tau}(x^N,t).$$

Local energy conservation laws (3.7) averaged by nonequilibrium statistical operator  $\rho(x^N, t)$  form generalized equations of hydrodynamics. These equations together with equations for time correlation functions will be obtained in the next section.

#### 4. Transport equations and time correlation functions.

So far as thermodynamic parameters  $\beta_{\mathbf{k}}(t)$ ,  $\mathbf{v}_{\mathbf{k}}(t)$ ,  $\mu_{\mathbf{k}}(t)$  are being defined from self-consistency conditions (3.10) at every step of their determination, NSO becomes the functional of mean values  $\langle \hat{n}_{\mathbf{k}} \rangle^t$ ,  $\langle \hat{J}_{\mathbf{k}} \rangle^t$  and  $\langle \hat{\varepsilon}_{\mathbf{k}} \rangle^t$ . Given mean values obey generalized transport equations, which could be obtained by averaging of local conservation laws (3.7) with NSO (3.11) taking into consideration identities  $\frac{\partial}{\partial t} \langle \tilde{P}_n(\mathbf{k}) \rangle^t = \langle \tilde{P}_n(\mathbf{k}) \rangle_q^t + \langle (1 - \mathcal{P}(t)) \dot{\tilde{P}}_n(\mathbf{k}) \rangle^t$ . In general case such a system of equations can be represented in the matrix form:

$$\frac{\partial}{\partial t} \langle \tilde{P}(\boldsymbol{k}) \rangle^{t} = \langle \dot{\tilde{P}}(\boldsymbol{k}) \rangle_{q}^{t} + \sum_{\boldsymbol{k}'} \int_{-\infty}^{t} \exp(\varepsilon(t'-t)) \tilde{\varphi}(\boldsymbol{k}, \boldsymbol{k}', t, t) \tilde{F}(\boldsymbol{k}', t') dt', \quad (4.1)$$

where  $\tilde{P}(\mathbf{k}) = col\left(\hat{n}_{\mathbf{k}}, \hat{\mathbf{J}}_{\mathbf{k}}, \hat{\varepsilon}_{\mathbf{k}}\right)$  is vector-column of the operators of number, momentum and energy densities;  $\tilde{F}(\mathbf{k}, t) = \left\{-\left(\mu - \frac{m}{2}\mathbf{v}^{2}\right)\beta_{\mathbf{k}}(t), -\left(\beta\mathbf{v}\right)_{\mathbf{k}}(t), \beta_{\mathbf{k}}(t)\right\}$  denotes vector-row of thermodynamic parameters;  $\tilde{\varphi}(\mathbf{k}, \mathbf{k}', t, t')$  denotes generalized transport kernels matrix:

$$\tilde{\varphi}(\boldsymbol{k}, \boldsymbol{k}', t, t') = \begin{bmatrix} 0 & 0 & 0\\ 0 & \varphi_{JJ} & \varphi_{J\varepsilon}\\ 0 & \varphi_{\varepsilon J} & \varphi_{\varepsilon\varepsilon} \end{bmatrix}_{(\boldsymbol{k}, \boldsymbol{k}', t, t')}$$
(4.2)

with nonzero elements of the following structure:

$$\varphi_{mn}(\boldsymbol{k}, \boldsymbol{k}', t, t') = Sp\left((1 - \mathcal{P}(t))\dot{\tilde{P}}_m(\boldsymbol{k})T(t, t')\right)$$

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$$\times \int_{0}^{1} d\tau \rho_{q}^{\tau}(t') (1 - \mathcal{P}(t')) \dot{\tilde{P}}_{n}(k') \rho_{q}^{1-\tau}(t') \bigg).$$
(4.3)

Components of transport kernels  $\varphi_{JJ}(\mathbf{k}, \mathbf{k}', t, t')$  are dealt with generalized shear and bulk viscosities,  $\varphi_{\varepsilon\varepsilon}(\mathbf{k}, \mathbf{k}', t, t')$  defines generalized thermal conductivity and  $\varphi_{J\varepsilon}(\mathbf{k}, \mathbf{k}', t, t')$  describes correlation between viscous and thermal processes. Transport equations (4.1) are not closed, so on every step of their solution thermodynamic parameters are to be determined from self-consistency conditions (3.10). In the case when hydrodynamic processes are characterized by slight deviations of mean values  $\langle \tilde{P}_n(\mathbf{k}) \rangle^t$  or corresponding thermodynamic forces  $\tilde{F}_n(\mathbf{k}, t)$  from their equilibrium values, generalized transport equations (4.1) could be simplified essentially due to linearization on deviations  $\delta\beta_{\mathbf{k}}(t), \, \delta v_{\mathbf{k}}(t),$  $\delta\mu_{\mathbf{k}}(t)$ . Moreover, in spatially homogeneous case longitudinal (parallel to wave-vector) and transverse (orthogonal to wave-vector) dynamic variables are independent and can be studied separately. In particular, we present momentum density as sum of two terms:

$$\hat{\boldsymbol{J}}_{\boldsymbol{k}} = \hat{\boldsymbol{J}}_{\boldsymbol{k}}^{||} + \hat{\boldsymbol{J}}_{\boldsymbol{k}}^{\perp}$$

$$(4.4)$$

and in all subsequent expressions for TCF shall take longitudinal part  $\hat{J}_{k}^{||}$ . Hence, in linear approximation on fluctuations matrix equation (4.1) can be presented in the form:

$$\frac{\partial}{\partial t} \langle \delta \tilde{B}(\boldsymbol{k}) \rangle^{t} - i \tilde{\Omega}(\boldsymbol{k}) \langle \delta \tilde{B}(\boldsymbol{k}) \rangle^{t} + \int_{\infty}^{t} \exp(\varepsilon (t'-t)) \tilde{\varphi}(\boldsymbol{k}, t, t') \langle \delta \tilde{B}(\boldsymbol{k}) \rangle^{t'} dt' = 0, \qquad (4.5)$$

where  $\delta \tilde{B}(\mathbf{k}) = \tilde{B}(\mathbf{k}) - \langle \tilde{B}(\mathbf{k}) \rangle_0$ ,  $\tilde{B}(\mathbf{k}) = col\left(\hat{n}_{\mathbf{k}}, \hat{J}_{\mathbf{k}}^{||}, \hat{h}_{\mathbf{k}}\right)$  denotes vectorcolumn,  $\hat{h}_{\mathbf{k}}$  denotes Fourier-component of enthalpy density operator

$$\hat{h}_{\boldsymbol{k}} = \hat{\varepsilon}_{\boldsymbol{k}} - (\hat{\varepsilon}_{\boldsymbol{k}}, \hat{n}_{-\boldsymbol{k}})_0 (\hat{n}_{\boldsymbol{k}}, \hat{n}_{-\boldsymbol{k}})_0 \hat{n}_{\boldsymbol{k}}, \qquad (4.6)$$

that appears due to exclusion of thermodynamic force  $1/2 \beta (\mu - mv^2)_{k}(t)$ accordingly to self-consistency condition. In (4.6)  $(\hat{c}_{k}, \hat{n}_{-k})_{0}$ ,  $(\hat{n}_{k}, \hat{n}_{-k})_{0}$ are equilibrium quantum correlation functions defined as

$$\left(\hat{A},\hat{B}\right)_{0} = Sp\left(\Delta\hat{A}\int_{0}^{1}d\tau\rho_{0}^{\tau}\Delta\hat{B}\rho_{0}^{1-\tau}\right)$$
(4.7)

(see eqn.(2.3) for comparison). Equation (4.5) forms a basis of molecular hydrodynamics of semi–quantum helium. Frequency matrix  $i\tilde{\Omega}(\mathbf{k})$  in (4.5) has a structure:

$$i\tilde{\Omega}(\boldsymbol{k}) = \begin{bmatrix} 0 & i\Omega_{Jn} & 0 \\ i\Omega_{nJ} & 0 & i\Omega_{hn} \\ 0 & i\Omega_{Jh} & 0 \end{bmatrix}_{(\boldsymbol{k})}, \qquad (4.8)$$

with elements

$$i\Omega_{Jn}(\boldsymbol{k}) = \left(\hat{\boldsymbol{J}}^{||}_{\boldsymbol{k}}, \hat{n}_{-\boldsymbol{k}}\right)_{0} \left(\hat{n}_{\boldsymbol{k}}, \hat{n}_{-\boldsymbol{k}}\right)_{0}^{-1} = \frac{i\boldsymbol{k}}{\beta S(\boldsymbol{k})},$$

$$i\Omega_{nJ}(\boldsymbol{k}) = \left(\dot{\hat{n}}_{\boldsymbol{k}}, \hat{\boldsymbol{J}}^{||}_{-\boldsymbol{k}}\right)_{0} \left(\hat{\boldsymbol{J}}^{||}_{\boldsymbol{k}}, \hat{\boldsymbol{J}}^{||}_{-\boldsymbol{k}}\right)_{0}^{-1} = \frac{i\boldsymbol{k}}{m},$$

$$i\Omega_{Jh}(\boldsymbol{k}) = \left(\hat{\boldsymbol{J}}^{||}_{\boldsymbol{k}}, \hat{h}_{-\boldsymbol{k}}\right)_{0} \left(\hat{h}_{\boldsymbol{k}}, \hat{h}_{-\boldsymbol{k}}\right)_{0}^{-1} = i\boldsymbol{k}\frac{1}{nc_{V}(\boldsymbol{k})}\frac{\alpha(\boldsymbol{k})}{k_{T}(\boldsymbol{k})}, \qquad (4.9)$$

$$i\Omega_{hJ}(\boldsymbol{k}) = \left(\dot{\hat{h}}_{\boldsymbol{k}}, \hat{\boldsymbol{J}}^{||}_{-\boldsymbol{k}}\right)_{0} \left(\hat{\boldsymbol{J}}^{||}_{\boldsymbol{k}}, \hat{\boldsymbol{J}}^{||}_{-\boldsymbol{k}}\right)_{0}^{-1} = \frac{i\boldsymbol{k}}{mn\beta}\frac{\alpha(\boldsymbol{k})}{k_{T}(\boldsymbol{k})}.$$

We have used in (4.9) the following denotations for generalized thermodynamic quantities:  $S(\mathbf{k})$  for static structure factor,  $c_V(\mathbf{k})$  for generalized specific heat at constant volume,  $\alpha(\mathbf{k})$  for generalized thermal expansion coefficient and  $k_T(\mathbf{k})$  for generalized compressibility

Matrix of the kernels from (4.5) has the structure similar to (4.3), however its elements are normalized TCF:

$$\varphi_{JJ}(\mathbf{k}, t, t') = \left(\hat{I}_{J}(\mathbf{k}), T_{0}(t, t')\hat{I}_{J}(-\mathbf{k})\right)_{0} \left(\hat{\mathbf{J}}_{\mathbf{k}}^{||}, \hat{\mathbf{J}}_{-\mathbf{k}}^{||}\right)_{0}^{-1},$$
  

$$\varphi_{Jh}(\mathbf{k}, t, t') = \left(\hat{I}_{J}(\mathbf{k}), T_{0}(t, t')\hat{I}_{h}(-\mathbf{k})\right)_{0} \left(\hat{h}_{\mathbf{k}}, \hat{h}_{-\mathbf{k}}\right)_{0}^{-1},$$
  

$$\varphi_{hJ}(\mathbf{k}, t, t') = \left(\hat{I}_{h}(\mathbf{k}), T_{0}(t, t')\hat{I}_{J}(-\mathbf{k})\right)_{0} \left(\hat{\mathbf{J}}_{\mathbf{k}}^{||}, \hat{\mathbf{J}}_{-\mathbf{k}}^{||}\right)_{0}^{-1},$$
  

$$\varphi_{hh}(\mathbf{k}, t, t') = \left(\hat{I}_{h}(\mathbf{k}), T_{0}(t, t')\hat{I}_{h}(-\mathbf{k})\right)_{0} \left(\hat{h}_{\mathbf{k}}, \hat{h}_{-\mathbf{k}}\right)_{0}^{-1}.$$
  
(4.10)

Dissipative fluxes  $I_J(\mathbf{k})$ ,  $I_h(\mathbf{k})$  in (4.10) are of the following structure:

$$I_J(\mathbf{k}) = (1 - \mathcal{P}_0) \dot{\mathbf{j}}_{\mathbf{k}}^{||}, \quad I_h(\mathbf{k}) = (1 - \mathcal{P}_0) \dot{\hat{h}}_{\mathbf{k}}.$$
 (4.11)

Here  $\mathcal{P}_0$  denotes Mori projection operator constructed on basic operators  $\hat{n}_k$ ,  $\hat{J}_k^{||}$ ,  $\hat{h}_k$ , which are mutually orthogonal, and its action is defined as

$$\mathcal{P}_{0}\hat{A} = \sum_{l} \sum_{\boldsymbol{k}} \left( \hat{A}, \tilde{B}_{l}(-\boldsymbol{k}) \right)_{0} \left( \tilde{B}_{l}(\boldsymbol{k}), \tilde{B}_{l}(-\boldsymbol{k}) \right)_{0}^{-1} \tilde{B}_{l}(\boldsymbol{k}).$$
(4.12)

 $\mathcal{P}_0$  has the properties of Mori projector:  $\mathcal{P}_0\mathcal{P}_0 = \mathcal{P}_0$ ,  $(1 - \mathcal{P}_0)\mathcal{P}_0 = 0$ ,  $\mathcal{P}_0\tilde{B}_n(\mathbf{k}) = \tilde{B}_n(\mathbf{k})$ ;  $T_0(t, t')$  means time evolution operator with projection acting as

$$T_0(t, t') = \exp\left\{-(t - t')(1 - \mathcal{P}_0)i\hat{L}_N\right\}.$$

In molecular (or linear) hydrodynamics the system of equations (4.5) plays very important role because gives possibility to calculate hydrodynamic modes spectrum (heat diffusion and sound propagation) and to investigate TCF of hydrodynamic variables  $\hat{n}_{k}$ ,  $\hat{J}_{k}^{||}$ ,  $\hat{h}_{k}$ , which could be presented in a matrix form:

$$\tilde{\Phi}(\boldsymbol{k},t) = \begin{bmatrix} \Phi_{nn} & \Phi_{nJ} & \Phi_{nh} \\ \Phi_{Jn} & \Phi_{JJ} & \Phi_{Jh} \\ \Phi_{hn} & \Phi_{hJ} & \Phi_{hh} \end{bmatrix}_{(\boldsymbol{k},t)}.$$
(4.13)

On the basis of the system of transport equations (4.5) one can show TCF to obey the system of equations analogous to (4.5):

$$\frac{\partial}{\partial t}\tilde{\Phi}(\boldsymbol{k},t) - \imath\tilde{\Omega}(\boldsymbol{k})\tilde{\Phi}(\boldsymbol{k},t) + \int_{-\infty}^{t} \exp(\varepsilon(t'-t))\tilde{\varphi}(\boldsymbol{k},t-t')\tilde{\Phi}(\boldsymbol{k},t')dt' = 0. \quad (4.14)$$

Using Laplace transformation matrix equation (4.14) can be rewritten as

$$z\tilde{\Phi}(\boldsymbol{k},z) - \imath\tilde{\Omega}(\boldsymbol{k})\tilde{\Phi}(\boldsymbol{k},z) + \tilde{\varphi}(\boldsymbol{k},z)\tilde{\Phi}(\boldsymbol{k},z) = \tilde{\Phi}(\boldsymbol{k}), \qquad (4.15)$$

where  $\tilde{\Phi}(\boldsymbol{k})$  is a diagonal matrix of static correlation functions

$$\tilde{\Phi}(\boldsymbol{k}) = \left(\tilde{B}_n(\boldsymbol{k}), \tilde{B}_m(-\boldsymbol{k})\right)_0 \delta_{mn}$$
(4.16)

with elements

$$\Phi_{nn}(\boldsymbol{k}) = (\hat{n}_{\boldsymbol{k}}, \hat{n}_{-\boldsymbol{k}})_0 = S(\boldsymbol{k}),$$
  

$$\Phi_{JJ}(\boldsymbol{k}) = \left(\hat{\boldsymbol{J}}_{\boldsymbol{k}}^{||}, \hat{\boldsymbol{J}}_{-\boldsymbol{k}}^{||}\right)_0 = m/\beta,$$
(4.17)

$$\Phi_{hh}(\boldsymbol{k}) = \left(\hat{h}_{\boldsymbol{k}}, \hat{h}_{-\boldsymbol{k}}\right)_0 = \frac{1}{\beta^2} c_V(\boldsymbol{k}).$$

In matrix equation (4.15) the elements of transport kernels  $\tilde{\varphi}(\mathbf{k}, z)$  define generalized transport coefficients

$$\varphi_{JJ}(\boldsymbol{k}, z) = \boldsymbol{k}^2 \left( \frac{4}{3} \eta(\boldsymbol{k}, z) + \zeta(\boldsymbol{k}, z) \right) / mn,$$
  
$$\varphi_{Jh}(\boldsymbol{k}, z) = \imath \boldsymbol{k}^2 \xi(\boldsymbol{k}, z) / nc_V(\boldsymbol{k}),$$
  
$$\varphi_{hh}(\boldsymbol{k}, z) = \boldsymbol{k}^2 \lambda(\boldsymbol{k}, z) / nc_V(\boldsymbol{k}).$$
  
(4.18)

Here  $\eta(\mathbf{k}, z)$ ,  $\zeta(\mathbf{k}, z)$  and  $\lambda(\mathbf{k}, z)$ , are, correspondingly, generalized coefficients of shear, bulk viscosity and thermal conductivity. Coefficient  $\xi(\mathbf{k}, z)$  describes correlation between viscous and heat processes in semiquantum helium. In hydrodynamic limit  $k \to 0$ ,  $\omega \to 0$  ( $z = \omega + i\varepsilon$ ,  $\varepsilon \to 0$ ) generalized transport coefficients  $\eta(\mathbf{k}, z)$ ,  $\zeta(\mathbf{k}, z)$  and  $\lambda(\mathbf{k}, z)$  tend to their hydrodynamic values while  $\xi(\mathbf{k}, z)$  vanishes (we have introduced imaginary unit factor in the expression for  $\varphi_{Jh}(\mathbf{k}, z)$  to show that  $\xi(\mathbf{k}, z)$ is pure imaginary when  $k \neq 0$  and z = 0).

From the system of equations (4.15) we can define nine time correlation functions  $\Phi_{\alpha\beta}(\mathbf{k}, z)$ ,  $\alpha$ ,  $\beta = \{n, J, h\}$ . The functions of greatest interest are  $\Phi_{nn}(\mathbf{k}, z)$ ,  $\Phi_{JJ}(\mathbf{k}, z)$ ,  $\Phi_{hh}(\mathbf{k}, z)$  that are expressed via static correlation functions of frequency matrix (4.9) and generalized transport coefficients (4.18) because first of them is directly dealt with dynamic structure factor and the second one – with its frequency moments. Hence, the problem of calculation of generalized transport coefficients as functions of wave-vector k and frequency  $\omega$  becomes very important.

In [18,19] the method of extension of abbreviated description parameters, when TCF (4.13) and transport coefficients (4.18) were expressed through the same generalized (higher memory functions) transport kernels, had been proposed. Using scheme considered above we shall find relation between generalized transport coefficients of Bose–system and higher–order memory functions, whose time evolutions is being described on the extended space of the operators orthogonal to operators of generalized fluxes  $I_J(\mathbf{k})$ ,  $I_h(\mathbf{k})$  that form generalized transport coefficients. For this purpose we supplement the set of reduced description parameters  $\{\hat{n}_k, \hat{J}_k, \hat{h}_k\}$  by generalized fluxes  $\hat{\pi}_k, \hat{Q}_k$ :

$$\hat{\pi}_{\boldsymbol{k}} = (1 - \mathcal{P}_0) \hat{\boldsymbol{J}}_{\boldsymbol{k}} , \qquad (4.19)$$

$$\hat{Q}_{k} = (1 - \mathcal{P}_{0})\hat{h}_{k}$$
 (4.20)

As a result we obtain the extended set of abbreviated description parameters  $\hat{Y}_m(\mathbf{k}) = col\left(\hat{n}_{\mathbf{k}}, \hat{\mathbf{J}}_{\mathbf{k}}, \hat{h}_{\mathbf{k}}, \hat{\pi}_{\mathbf{k}}, \hat{Q}_{\mathbf{k}}\right)$ , which are mutually orthogonal:

$$\left(\hat{Y}_i(\boldsymbol{k}), \hat{Y}_l(-\boldsymbol{k})\right)_0 = 0, \qquad i \neq l.$$

Now using NSO method we can obtain the system of equations for averaged operators  $\langle \hat{n}_{k} \rangle^{t}$ ,  $\langle \hat{J}_{k} \rangle^{t}$ ,  $\langle \hat{h}_{k} \rangle^{t}$ ,  $\langle \hat{\pi}_{k} \rangle^{t}$ ,  $\langle \hat{Q}_{k} \rangle^{t}$  in Laplace transform representation that can be written down in matrix form

$$z\langle \hat{Y}(\boldsymbol{k})\rangle_{z} - \imath \tilde{\Omega}_{1}(\boldsymbol{k})\langle \hat{Y}(\boldsymbol{k})\rangle_{z} + \tilde{\varphi}_{1}(\boldsymbol{k},z)\langle \hat{Y}(\boldsymbol{k})\rangle_{z} = -\langle \hat{Y}(\boldsymbol{k})\rangle^{t=0}, \quad (4.21)$$

where

$$i\tilde{\Omega}_{1}(\boldsymbol{k}) = \left(i\hat{L}_{N}\hat{Y}(\boldsymbol{k}), \hat{Y}(-\boldsymbol{k})\right)_{0} \left(\hat{Y}(\boldsymbol{k}), \hat{Y}(-\boldsymbol{k})\right)_{0} = \left[ \begin{array}{ccc} 0 & i\Omega_{nJ} & 0 & 0 & 0\\ i\Omega_{Jn} & 0 & i\Omega_{Jh} & i\Omega_{J\pi} & 0\\ 0 & i\Omega_{hJ} & 0 & 0 & i\Omega_{hQ}\\ 0 & i\Omega_{\pi J} & 0 & 0 & i\Omega_{\pi Q}\\ 0 & 0 & i\Omega_{Qh} & i\Omega_{Q\pi} & 0 \end{array} \right]_{(\boldsymbol{k})}$$
(4.22)

denotes the frequency matrix;  $\tilde{\varphi}_1(\mathbf{k}, z)$  means the matrix of Laplacetransforms of higher-order memory functions with non-zero elements

$$\varphi_{\pi\pi}(\boldsymbol{k},t,t') = \left(\hat{I}_{\pi}(\boldsymbol{k}), \bar{T}(t,t')\hat{I}_{\pi}(-\boldsymbol{k})\right)_{0} \left(\hat{\pi}(\boldsymbol{k}), \hat{\pi}(-\boldsymbol{k})\right)_{0}^{-1},$$

$$\varphi_{\pi Q}(\boldsymbol{k},t,t') = \left(\hat{I}_{\pi}(\boldsymbol{k}), \bar{T}(t,t')\hat{I}_{Q}(-\boldsymbol{k})\right)_{0} \left(\hat{Q}(\boldsymbol{k}), \hat{Q}(-\boldsymbol{k})\right)_{0}^{-1},$$

$$\varphi_{Q\pi}(\boldsymbol{k},t,t') = \left(\hat{I}_{Q}(\boldsymbol{k}), \bar{T}(t,t')\hat{I}_{\pi}(-\boldsymbol{k})\right)_{0} \left(\hat{\pi}(\boldsymbol{k}), \hat{\pi}(-\boldsymbol{k})\right)_{0}^{-1}, \quad (4.23)$$

$$\varphi_{QQ}(\boldsymbol{k},t,t') = \left(\hat{I}_{Q}(\boldsymbol{k}), \bar{T}(t,t')\hat{I}_{Q}(-\boldsymbol{k})\right)_{0} \left(\hat{Q}(\boldsymbol{k}), \hat{Q}(-\boldsymbol{k})\right)_{0}^{-1},$$

where dissipative fluxes are determined in the following way:

$$\hat{I}_{\pi}(\boldsymbol{k}) = (1 - \mathcal{P}_{H}) \dot{\hat{\pi}}_{\boldsymbol{k}},$$
$$\hat{I}_{Q}(\boldsymbol{k}) = (1 - \mathcal{P}_{H}) \dot{\hat{Q}}_{\boldsymbol{k}}.$$
(4.24)

Here Mori projection operator  $\mathcal{P}_H$  is defined as

$$\mathcal{P}_H = \mathcal{P}_0 + \mathcal{P}_1 \,, \tag{4.25}$$

where the first term is determined in (4.12) while the second term accordingly to

$$\mathcal{P}_{1}\hat{A} = \sum_{\boldsymbol{k}} \left\{ \left( \hat{A}, \hat{\pi}_{-\boldsymbol{k}} \right)_{0} \left( \hat{\pi}_{\boldsymbol{k}}, \hat{\pi}_{-\boldsymbol{k}} \right)_{0}^{-1} \hat{\pi}_{\boldsymbol{k}} + \left( \hat{A}, \hat{Q}_{\boldsymbol{k}} \right)_{0} \left( \hat{Q}_{\boldsymbol{k}}, \hat{Q}_{-\boldsymbol{k}} \right)_{0}^{-1} \hat{Q}_{\boldsymbol{k}} \right\}.$$

$$(4.26)$$

Projection operator  $\mathcal{P}_H$  possesses properties

$$\mathcal{P}_H(1-\mathcal{P}_H)=0, \quad \mathcal{P}_H\mathcal{P}_H=\mathcal{P}_H, \quad \mathcal{P}_H\hat{Y}_i(\boldsymbol{k})=\hat{Y}_i(\boldsymbol{k})$$

and forms time evolution operator  $\bar{T}(t,t') = \exp\{-(t-t')(1-\mathcal{P}_H)i\hat{L}_N\}$ .

On the basis of transport equations (4.21) one can obtain the system of equations for 25 TCF  $\tilde{\Phi}_H(\mathbf{k}, t) = (\hat{Y}(\mathbf{k}, t), \hat{Y}(-\mathbf{k}))_0$ , constructed on operators  $\hat{Y}_i(\mathbf{k})$ . In Laplace–transform representation they can be written in the matrix form very similarly to (4.15):

$$z\tilde{\Phi}_{H}(\boldsymbol{k},z) - i\tilde{\Omega}_{1}(\boldsymbol{k})\tilde{\Phi}_{H}(\boldsymbol{k},z) + \tilde{\varphi}_{1}(\boldsymbol{k},z)\tilde{\Phi}_{H}(\boldsymbol{k},z) = \tilde{\Phi}_{H}(\boldsymbol{k}), \quad (4.27)$$

where

$$\tilde{\Phi}_{H}(\boldsymbol{k}) = \left(\hat{Y}(\boldsymbol{k}), \hat{Y}(-\boldsymbol{k})\right)_{0}$$
(4.28)

is a diagonal matrix of static correlation functions.

Some remarks concerning relations of our results with those of [12] ought to be done.

- (i) An explicit form of dynamic matrix in [12] directly follows from (4.15) and (4.21).
- (ii) Nondiagonal elements in memory kernels were neglected in [12] while these elements (as shown by the calculations for Lennard–Jones fluid [14]) become very important for intermediate values of k and ω.
- (iii) Reduction of the number of dynamical variables was performed in [12] in nonconsistent way when passing to viscoelastic and damped harmonic oscillators approximations. In fact, "rolling-up procedure" of elimination of redundant variables leads to the appearance of time-spatial dispersion of transport coefficients and had been used in a number of papers [18,19,24,25].

In the next section we present the results for collective modes spectrum in hydrodynamic limit taking into account kinetic excitations in semi-quantum helium. We shall consider Markovian approximation for transport kernels in the system of equations (4.27), when memory functions (4.23) are being approximated by expressions

$$\varphi_{\pi\pi}(\boldsymbol{k}, z) \approx \varphi_{\pi\pi}(\boldsymbol{k}, 0) = \int_{0}^{\infty} \varphi_{\pi\pi}(\boldsymbol{k}, t) dt,$$
  

$$\varphi_{\pi Q}(\boldsymbol{k}, z) \approx \varphi_{\pi Q}(\boldsymbol{k}, 0) = \int_{0}^{\infty} \varphi_{\pi Q}(\boldsymbol{k}, t) dt,$$
  

$$\varphi_{Q\pi}(\boldsymbol{k}, z) \approx \varphi_{Q\pi}(\boldsymbol{k}, 0) = \int_{0}^{\infty} \varphi_{Q\pi}(\boldsymbol{k}, t) dt,$$
  

$$\varphi_{QQ}(\boldsymbol{k}, z) \approx \varphi_{QQ}(\boldsymbol{k}, 0) = \int_{0}^{\infty} \varphi_{QQ}(\boldsymbol{k}, t) dt.$$
  
(5.1)

Under this condition the system of transport equations (4.21) can be written down in the following manner:

$$z\langle \hat{Y}(\boldsymbol{k})\rangle_{z} + \tilde{T}(\boldsymbol{k})\langle \hat{Y}(\boldsymbol{k})\rangle_{z} = -\langle \hat{Y}(\boldsymbol{k})\rangle^{t=0}, \qquad (5.2)$$

where matrix  $\tilde{T}(\mathbf{k})$  has the structure:

$$\tilde{T}(\boldsymbol{k}) = \begin{bmatrix} 0 & i\Omega_{nJ} & 0 & 0 & 0\\ i\Omega_{Jn} & 0 & i\Omega_{Jh} & i\Omega_{J\pi} & 0\\ 0 & i\Omega_{hJ} & 0 & 0 & i\Omega_{hQ}\\ 0 & i\Omega_{\pi J} & 0 & \varphi_{\pi\pi} & 0\\ 0 & 0 & i\Omega_{Qh} & 0 & \varphi_{QQ} \end{bmatrix}_{(\boldsymbol{k},z=0).}$$
(5.3)

In the limit  $k \to 0$  linear system of equations allows solutions on eigenvalues, which are the following:

<u>heat mode</u>:

$$z_h(k) = D_T k^2 + o(k^4); (5.4)$$

two complex conjugated <u>sound modes</u>:

$$z_{\pm}(k) = \pm ic \, k + \Gamma k^2 + o(k^4) \,; \tag{5.5}$$

two nonvanishing in the limit  $k \to 0$  kinetic modes:

$$z_{\pi}(k) = \varphi_{\pi\pi}(0,0) + o(k^2), \qquad (5.6)$$

$$z_Q(k) = \varphi_{QQ}(0,0) + o(k^2).$$
(5.7)

In (5.4)-(5.7)  $D_T$  means temperature diffusion coefficient:

$$D_T = \frac{v_{TQ}^2}{\gamma \varphi_{QQ}(0,0)} = \frac{\lambda(0,0)}{nmc_p(0)}$$
(5.8)

$$v_{TQ}^2 = \frac{m\Phi_{QQ}(0,0)\beta^2}{c_V(0)}, \qquad \gamma = c_p(0)/c_V(0), \qquad (5.9)$$

 $c_p(0)$  and  $c_V(0)$  denote, correspondingly, thermodynamic values of the specific heats at constant pressure and volume,  $\lambda(0,0)$  means generalized thermal conductivity coefficient at k = 0, z = 0,  $c = \frac{\gamma}{nmS(k=0)}$  denotes adiabatic sound velocity,

$$\Gamma = \frac{1}{2}(\gamma - 1)D_T + \frac{1}{2}\eta^{||}$$
(5.10)

is the sound damping coefficient with

$$\eta^{||} = \frac{v_{J\pi}^2}{\varphi_{\pi\pi}(0,0)} = \left(\frac{4}{3}\eta(0,0) + \zeta(0,0)\right)/n\,m\tag{5.11}$$

$$v_{J\pi}^2 = \frac{\beta \Phi_{\pi\pi}(0,0)}{m},\tag{5.12}$$

where  $\eta(0,0)$  and  $\zeta(0,0)$  are generalized shear and bulk viscosities at k = 0, z = 0. Expressions (5.6)-(5.7) and (5.8)-(5.12) give us relations between kinetic modes  $z_{\pi}, z_Q$  and transport coefficients:

$$z_Q^{-1} = \frac{\lambda}{mnc_V(0)v_{TQ}^2},$$
 (5.13)

$$z_{\pi}^{-1} = \left(\frac{4}{3}\eta(0,0) + \zeta(0,0)\right) / mnv_{J_{\pi}}^2.$$
 (5.14)

It should be mentioned that kinetic modes (5.6)-(5.7) are very important in the context of the study of non-dispersive phonon-like excitations. For instance, it was found that for a Lennard-Jones fluid the interplay of these two kinetic modes forms (starting from some fixed value of k) propagating excitations, the dispersion of which for larger k is very small [19]. A similar situation was found recently for a binary mixture [22]. Hence, on the basis of the system of TCF (4.27) in hydrodynamic limit  $k \to 0$ ,  $\omega \to 0$  we obtained collective excitations spectrum, which is being formed by heat mode  $z_h(k)$ , two sound modes  $z_{\pm}(k)$  and two kinetic modes  $z_{\pi}(k)$ ,  $z_Q(k)$ .

In Markovian approximation for memory functions solutions of TCF (4.27) can be expressed via eigenvalues  $z_{\alpha}$  and eigenvectors  $X_{\alpha} = ||X_{i\alpha}||$  of matrix  $\tilde{T}(\mathbf{k})$ :

$$\Phi_{il}(k,z) = \sum_{\alpha=1}^{5} \frac{G_{\alpha}^{il}(k)}{z + z_{\alpha}(k)}, \qquad (5.15)$$

where

$$G_{\alpha}^{ij}(k) = \sum_{l=1}^{5} X_{i\alpha} X_{l\alpha}^{-1} \tilde{\Phi}_{lj}(k,0)$$
(5.16)

and  $X^{-1}$  denotes matrix inverse to  $X = ||X_{i\alpha}||$ . In time representation (5.15) has the form

$$\Phi_{ij}(k,t) = \sum_{\alpha=1}^{5} G_{\alpha}^{ij}(k) \exp\{-z_{\alpha}(k) t\}, \qquad (5.17)$$

so TCF in Markovian approximation appear to be the sum of weighted exponents related with collective modes of semi–quantum  ${}^{4}$ He.

TCF "density–density", which has been expressed in our approximation via sum of five Lorenz lines (5.15), gives us possibility to study the behaviour of dynamic structure factor. Each of the modes can more or less contribute to  $S(\mathbf{k}, \omega)$ . For instance, half-width on half-height of the central peak of dynamic structure factor at small wave–number (see Fig.2) is being determined by (5.4), whose value, in its turn, is renormalized via kinetic mode (5.7). Hence, hydrodynamic limits of corresponding TCF  $\Phi_{QQ}(0,0)$  together with memory kernel  $\varphi_{QQ}(0,0)$  as well as some thermodynamic values completely define central resonance clearly distinguishable at  $k = 1 \div 2$  nm<sup>-1</sup>.

Localization of the sound peak is being determined by sound frequency and its half-width is a result of interplay of two processes: heat diffusion (first term in (5.10)) and shear flow (second term), whose value is defined by kinetic mode (5.6). It should be stressed that one can easily derive from (5.8)-(5.9) and (5.10)-(5.12) the explicit forms of heat conductivity  $\lambda(0,0)$  and longitudinal viscosity  $\eta^{||}(0,0)$  and these results coincide with those for simple fluids [26].

What about kinetic modes (5.6)-(5.7) themselves, that are being determined in the limit  $k \to 0$ ,  $\omega \to 0$  by memory kernels  $\varphi_{\pi\pi}(0,0)$ ,  $\varphi_{QQ}(0,0)$ , their role becomes important in the intermediate region of wave-vectors and can results in phenomena mentioned on previous pages.

Hence, the main difference of our approach from [12] is the following: we would like to study the system within five-variables set for the whole range of k and  $\omega$ . The role of each mode may be established by calculations of generalized collective modes spectrum as well as weight coefficients (5.16). In such a way one may conclude about the disappearance of heat mode or application of damped phonon model much more based on a microscopic treatment.

#### 6. Discussion.

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In previous sections the set of equations for TCFs within a five- variables thermo-elastic model is derived. In the hydrodynamic limit we use Markovian approximation for memory functions, which is indeed exact in this case, and study the hydrodynamic spectrum of collective modes. As it was shown for a simple fluid [14] as well as for a binary mixture [22], the Markovian anzats for the higher-order memory functions could be applied for the subsequent calculations of dynamic quantities for all k and  $\omega$ , and not only the low frequency domain. To simplify the scheme for a classical fluid the inverse transformation to initial non-orthogonal set of dynamic variables has been performed after Markovian approximation, and it was shown [14,18,19] that the matrix  $T(\mathbf{k})$ - matrix (see Eq.(5.3) could be presented in a more simple and computer-adapted form. In such a case the main input of the theory are static correlation functions and the hydrodynamic correlation times. All these quantities for a classical fluid can be calculated by either integral equations method or computer simulations. We note also that recently for the calculations of correlation times a new iterating procedure, based on the knowledge of static correlation functions only, has been developed [27]. In a such a way the problem of calculations of generalized collective modes, TCFs and generalized transport coefficients can be reduced on the first stage to the obtaining of corresponding static correlation functions.

The problem becomes much more complicated for a quantum fluid where the computer methods for the study of higher-order static correlation functions are not so developed. From this point of view one may understand the approach used in [12] based on a fitting procedure for all the parameters of the theory. However, as it was mentioned above, the physical meaning of some interesting phenomena remains outside of our understanding in such a case. Hence, a continuation of this study may follow by several main ways. (i) Semi-phenomenological approach. For small values of k, taking into account the next order with respect to k, all the elements of generalized hydrodynamic matrix (5.3) can be written via thermodynamic quantities (such as specific heats, thermal expansion coefficient, compressibility, etc.), transport coefficients (kinematic viscosity and thermal conductivity), and some parameters to have been treated as phenomenological. For thermodynamic quantities as well as for transport coefficients the experimental data may be used. Phenomenological coefficients may be considered as fitting parameters. Thus, one may to study the dynamical properties of a semi-quantum fluid within thermoelastic model. We note that similar schemes are widely used in the theory of complex classical fluids, i. e. see Ref. [16,28].

For a semi-quantum liquid some semi-microscopic models have been developed. As has been noted in the Introduction, for a semi-quantum fluid it is important to take into account kinetic jumping processes. To do it, Andreyev proposed to consider 2- and 3-level models [6,7,10] and obtained reasonable results for entropy, specific heat, shear viscosity and thermal conductivity. However, in this case many processes have to be important for scattering were not incorporated into the theory.

(ii) Statistical mechanics approach. Developing the previous point the static correlation functions can be calculated using one from the methods of quantum statistical physics applied for approximate calculations. For instance, in [9] one has calculated a set of generalized thermodynamic values (specific heat, static structure factor etc.) of slightly nonideal Bose gas using Green's functions methods for evaluation of static susceptibilities. Well known  $c_V(T) \sim T^3$  was found as well as small wave-number corrections to corresponding static correlation functions. A similar approach had been used in [29] in application to investigation of generalized hydrodynamics equations. In [30] the authors calculated single particle density matrix using pair correlation functions method and presented formulae for evaluation of Bose condensation temperature. Other problems dealt with  $\lambda$ -transition in <sup>4</sup>He have been examined in [31,32].

(iii) Decoupling of memory functions. It should be stressed that quantum case occurs to be even somewhat easier for investigation then classical one because it gives us clear picture how to take into consideration the relation between kinetics and hydrodynamics on the stage of decoupling of memory kernels. It ought to be mentioned that decoupling of mass operator could be performed in terms of either single particle Green's function [33] or many particle correlation functions [34,35]. Of course, both way can be followed separately thought our assumption about intermixing between kinetics and hydrodynamics can be applied.

Though above  $\lambda$ -point there is not direct coupling between single particle and collective modes on microscopic level [2], one may consider correlation between these processes on the stage of decoupling of memory kernels representing them via convolution integrals of Laplacetransforms of nonequilibrium single particle time correlation function  $\left(\hat{a}_{\boldsymbol{k}}^{\dagger}, \hat{a}_{\boldsymbol{k}}\right)_{\tilde{z}}$  together with integrals of TCF constructed on hydrodynamic variables. Then, corresponding memory kernel or "collision integral" in the kinetic equation can be decomposed in the same approximation taking into account the order of operators. Thus, an interesting question about the contributions from one-particle kinetic and hydrodynamic processes into dispersion of generalized transport coefficient appears.

We note there are also alternative ways to construct a closed chain of equations for TCFs. In one of them the hydrodynamic velocities and thermodynamic forces are presented as an expansion in terms of higherorder fluctuations with further closure of memory functions in form of convolution integrals of TCFs. This method is known as mode-coupling theory and is widely used for an analysis of time-spatial dispersion of transport coefficients as well as for the study of TCFs behaviour. However, a decoupling procedure is known to be valid, generally speaking, in low-wavelength and low-frequency limit only [36,37] and allows one to obtain nonanalytical corrections to transport coefficients, e.g. the wellknown  $k^{5/2}$  contribution to sound velocity [38]. Generalization of modecoupling theory on high  $k, \omega$  region was considered in a number of papers and was shown to give reliable results in some cases [34,35,39-41]. In majority of cases viscoelastic approach was applied (in this framework knowledge of triple static structure factor only is necessary). Consideration of energy fluctuation gives more correct description of the processes outside roton minimum region, where viscoelastic description is quite sufficient. For instance, in [41] the total energy density has been considered in addition and the dynamic structure factor of a simple Lennard-Jones liquid was calculated using mode-coupling approach up to  $k = 0.9 \text{\AA}^{-1}$ . However, using the mode coupling theory for a quantum fluid we face once again with the problem of calculations of higher-order static correlation functions.

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