Kinetic equation for liquids with a multistep potential of interaction: Calculation of transport coefficients

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(Received 15 May 2000)

Using the boundary conditions method, we find normal solutions to a kinetic equation proposed recently by us [Physica A **234**, 89 (1996)] to describe nonequilibrium properties of classical liquids. As a result, explicit expressions for the transport coefficients and macroscopic conservation laws are obtained in the first order for gradients of hydrodynamic parameters. In some particular cases, these expressions are reduced to those corresponding to the well-known Enskog, Davis-Rice-Sengers, and mean-field kinetic theories. It is demonstrated that our approach allows an accurate reproduction of experimental and molecular dynamics data for the transport coefficients of liquid argon in a wide density-temperature range.

PACS number(s): 05.20.Dd, 05.60.−k, 05.70.Ln, 52.25.Fi

I. INTRODUCTION

In 1872, Boltzmann has proposed a kinetic theory [1] for the description of nonequilibrium processes in dilute gases and proved the *H*-theorem. However, until now there is no consequent kinetic approach for dense gases and liquids with a realistic interparticle potential of interaction. The derivation and solution of kinetic equations for dense classical systems still remains an important and unresolved problem in nonequilibrium statistical mechanics.

In 1946, Bogolubov had suggested an approach [2] to the problem of derivation of kinetic equations which allows a generalization to higher densities. Within this theory, the Boltzmann equation corresponds to zeroth approximation in the power series with respect to density. But, it was soon realized that the second- and higher-order terms are divergent [3]. The reason for such a divergence can be explained by the fact that the expansions used were based on dynamics of isolated groups of particles in an infinite space without taking into consideration the media, i.e., all others particles in the system. In contrast to systems at equilibrium, the velocity correlations in a nonequilibrium state include long-range correlations between particles. This does not allow to generalize the Boltzmann kinetic equation to high densities within such expansions.

A successful empirical kinetic theory of dense gases was developed by Enskog in 1922 at least for the case of hard spheres (standard Enskog theory SET) [4]. His arguments were similar to Boltzmann's. In 1961 Davis *et al.* [5] suggested the Davis-Rice-Sengers (DRS) kinetic theory, where the so-called ''square-well'' potential of interaction is considered. DRS theory is an analog of the usual SET theory for a specific type of interaction potential. Here an attractive part of real interaction potential is approximated by some finite attractive wall. A revised Enskog theory (RET) [6–8] and a revised version of DRS–RDRS [9] have been obtained. The necessity of the revised versions could be explained as follows. (1) Kinetic equations of the initial versions of those theories cannot be derived consistently. (2) The exact entropy functional cannot be constructed, hence the *H*-theorem cannot be proved. But some recipe of construction of entropy functional for the SET theory was suggested in Refs. [10–12]. For the revised versions RET [7,8] and RDRS [9] the exact entropy functional was constructed and the *H*-theorem was proved. Furthermore, the RET kinetic equation has been obtained successfully within the frame of some theoretical scheme, which is analogous to Bogolubov's [2], but uses a modification of boundary conditions. The last one takes into account the local conservation laws in the solution of the BBGKY hierarchy [13].

In order to apply the results of the SET theory to real systems, Enskog suggested to change the hydrostatic pressure of a system of hard spheres to a thermodynamic pressure of a real system. Having this assertion in mind, Hanley *et al.* [14] built a kinetic theory called later the modified Enskog theory (MET) where the hard sphere diameter σ is defined via the second virial coefficient of the system equation of state. In such a way, σ becomes dependent on temperature and density. Using different equations of state: BH [15], WCA [16], MC/RS [17,18] and others, one obtains the corresponding versions of MET.

In the kinetic mean-field theory (KMFT) [19], along with the hard sphere interaction potential one considers also some smooth attractive ''tail.'' It is noted in Ref. [20] that in this case the quasiequilibrium binary correlation function of hard spheres should be replaced with one which takes into account, explicitly or implicitly, the total interaction potential. The main conclusion of KMFT is that the smooth part of interaction potential in the first approximation in gradients of hydrodynamic parameters does not contribute explicitly into transport coefficients. There is only an indirect contribution via the binary correlation function. Its dependence on temperature is defined by a smooth part of the interaction potential.

In our recent paper [21] we suggested a kinetic equation for systems with a multistep potential of interaction (MSPI). This potential consists of the hard sphere part and of a system of attractive and repulsive walls. Such a model is a generalization of SET (RET, MET), DRS (RDRS) and KMFT theories. We also proved the *H*-theorem for this equation. However, a normal solution has not been published yet. In

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this article, going to the schema of construction of normal solutions of kinetic equations with the help of boundary conditions method [22], a normal solution to the kinetic equation has been obtained and the integral conservation laws linear in gradients of hydrodynamic parameters have been derived. The expressions for such transport coefficients as bulk and shear viscosity and thermal conductivity are calculated for the case of stationary process. We also consider limiting cases for this kinetic equation. For specific parameters of model interaction potential in shape of the multistep function, the obtained results rearrange to those of the SET (RET, MET), DRS (RDRS) or KMFT theories by means of the standard Chapman-Enskog method [23]. In view of this, the theory can be considered as a generalized one which in some specific cases arrives at the results of previous ones and in such a way displays the connection between these theories. At the end of this article we present results of numerical computation of transport coefficients for argon and their comparison with the available experimental data and MD simulations.

II. MULTISTEP POTENTIAL OF INTERACTION: KINETIC EQUATION

Let us consider a system of N classical particles in volume V when $N\to\infty$ and $V\to\infty$, provided $N/V=\text{const}$. The Hamiltonian of this system reads:

$$H_N=\sum_{i=1}^{N}\frac{p^2}{2m}+\sum_{i<j}^{N}\varphi_{ij}. \tag{2.1}$$

Our purpose is the most detailed analysis of nonequilibrium processes in dense systems. To do this let us define MSPI $\varphi_{ij}\equiv\varphi(|\vec{r}_i-\vec{r}_j|)\equiv\varphi(|\vec{r}_{ij}|)\equiv\varphi(r_{ij})$ in a form of the multistep function:

$$\varphi_{ij}=\begin{cases}\infty; & r_{ij}<\sigma_0,\\ \varepsilon_k; & \sigma_{k-1}<r_{ij}<\sigma_k; \quad k=1,\dots,N^*,\\ 0; & \sigma_{N^*}<r_{ij}.\end{cases} \tag{2.2}$$

Here N^* is the total number of attractive and repulsive walls except the hard sphere one. For our convenience we distinguish systems of attractive and repulsive walls. Let one have n^* repulsive walls, separated by the distances σ_{li} and having heights $\Delta\varepsilon_{li}$, $i=1,\dots,n^*$; and m^* attractive walls with the parameters σ_{rj} and $\Delta\varepsilon_{rj}$, $j=1,\dots,m^*$, respectively, σ_0 is the location of the hard sphere wall. It is obvious that $n^*+m^*=N^*$, $\Delta\varepsilon_{li}=\varepsilon_{li}-\varepsilon_{li+1}$, $\Delta\varepsilon_{rj}=\varepsilon_{rj+1}-\varepsilon_{rj}$. In such a way the parameters σ_0, n^*, σ_{li}, $\Delta\varepsilon_{li}$, m^*, σ_{rj}, $\Delta\varepsilon_{rj}$ define the multistep potential of interaction completely (see Fig. 1).

Going similarly to the derivation of the kinetic equation of the RET theory [7,8,24] and taking into account the system of attractive and repulsive walls, one obtains the following kinetic equation:

$$\left(\frac{\partial}{\partial t}+\vec{v}_1\frac{\partial}{\partial\vec{r}_1}\right)f_1(x_1;t)=\int dx_2\hat{T}f_2(x_1,x_2;t), \tag{2.3a}$$

$$f_2(x_1,x_2;t)=g_2^q f_1(x_1;t)f_1(x_2;t), \tag{2.3b}$$

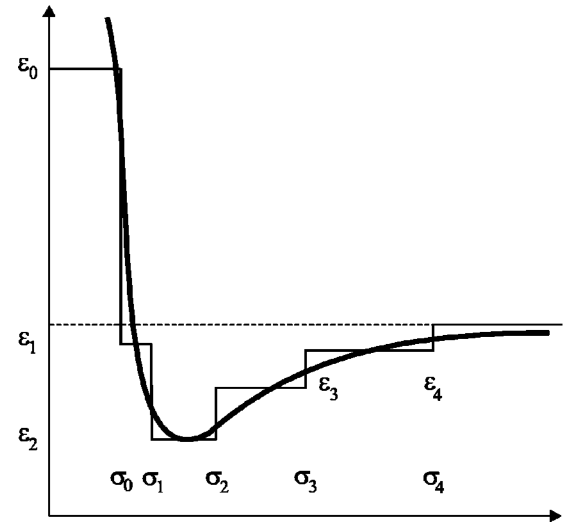

FIG. 1. Multistep potential of interaction with $n^*=1$, $m^*=3$.

where $g_2^q\equiv g_2^q(\vec{r}_1,\vec{r}_2|n(t),\beta(t))$ is defined in the usual way from the maximum of the entropy functional and in its turn is the functional of local values of density $n(\vec{r}_1;t)$ and inverse temperature $\beta(\vec{r}_1;t)=1/(k_BT)$, k_B is the Boltzmann constant and T is the local temperature. In (2.3) $\hat{T}$ is an operator which describes interaction of two particles in presence of MSPI:

$$\hat{T}=\hat{T}^a_{hs}+\sum_{i=1}^{n^*}\hat{T}_{li}+\sum_{j=1}^{m^*}\hat{T}_{rj}, \tag{2.4}$$

$$\hat{T}^a_{hs}=\sigma_0^2\int d\hat{\sigma}\,\hat{\sigma}\vec{g}\,\theta(\hat{\sigma}\vec{g})\{\delta(\vec{r}_1-\vec{r}_2+\hat{\sigma}\sigma_0^+)B_a(\hat{\sigma}) - \delta(\vec{r}_1-\vec{r}_2-\hat{\sigma}\sigma_0^+)\}. \tag{2.5}$$

The last expression is nothing but the operator of hard spheres interaction [25], $\hat{\sigma}$ is the unit vector directed from the second particle to the first one, $\vec{g}=\vec{v}_2-\vec{v}_1$ is the relative velocity. $B_a(\hat{\sigma})$ is the velocities shift operator as in the classical mechanics of elastic collisions. $\hat{T}_{li}=\Sigma_{k=b,c,d}\hat{T}_{lik}$ is an interaction operator at the ith repulsive wall;

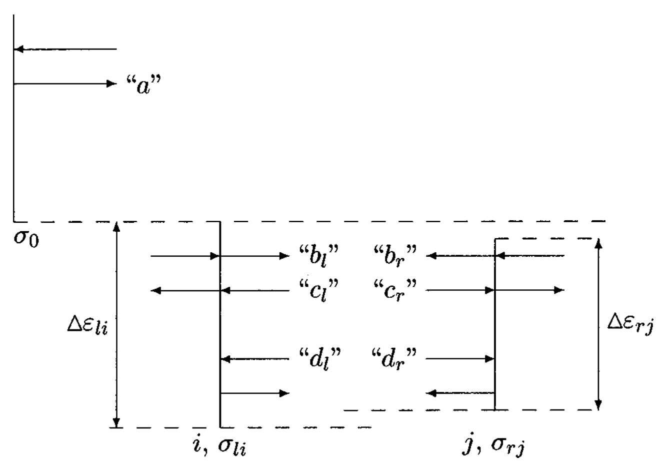

FIG. 2. Types of possible interactions (schematic draw).

$\hat{T}_{rj}=\Sigma_{k=b,c,d}\hat{T}_{rjk}$ is an interaction operator at the jth attractive wall; a,b,c,d are types of possible interactions (see Fig. 2).

$$\hat{T}_{{}^{li}_{rj}k}=\sigma^2_{{}^{li}_{rj}}\int d\hat{\sigma}\,\hat{\sigma}\vec{g}\,\theta_{{}^{li}_{rj}k}(\dots)\{\delta(\vec{r}_1-\vec{r}_2+\hat{\sigma}\sigma^+_{{}^{li}_{rj}})B_{{}^{li}_{rj}k}(\hat{\sigma}) - \delta(\vec{r}_1-\vec{r}_2-\hat{\sigma}\sigma^+_{{}^{li}_{rj}})\}, \tag{2.6}$$

where

$$\theta_{lib}\equiv\theta(-\hat{\sigma}\vec{g}), \tag{2.7a}$$

$$\theta_{lic}\equiv\theta\left(\hat{\sigma}\vec{g}-\sqrt{\frac{4\Delta\varepsilon_{li}}{m}}\right), \tag{2.7b}$$

$$\theta_{lid}\equiv\theta\left(\sqrt{\frac{4\Delta\varepsilon_{li}}{m}}-\hat{\sigma}\vec{g}\right)\theta(\hat{\sigma}\vec{g}), \tag{2.7c}$$

$$\theta_{rjb}\equiv\theta(\hat{\sigma}\vec{g}), \tag{2.7d}$$

$$\theta_{rjc}\equiv\theta\left(-\hat{\sigma}\vec{g}-\sqrt{\frac{4\Delta\varepsilon_{rj}}{m}}\right), \tag{2.7e}$$

$$\theta_{rjd}\equiv\theta\left(\sqrt{\frac{4\Delta\varepsilon_{li}}{m}}+\hat{\sigma}\vec{g}\right)\theta(-\hat{\sigma}\vec{g}). \tag{2.7f}$$

Expressions (2.7) are nothing but conditions for specific type of interaction [$\theta(z)$ is the unit step function].

$B_{{}^{li}_{rj}k}(\hat{\sigma})$ is an operator which acts on velocities and changes them in accordance with the interaction of a specific type at each wall:

$$B_{{}^{li}_{rj}k}(\hat{\sigma})Y(\vec{v}_1,\vec{v}_2)=Y(\vec{v}_{1{}^l_r k},\vec{v}_{{}^i_j k}) \tag{2.8}$$

where Y is some arbitrary function of $\vec{v}_1$, $\vec{v}_2$.
Type ''*a*:''

$$\vec{v}\,'_1=\vec{v}_1+\hat{\sigma}(\hat{\sigma}\vec{g}); \tag{2.9a}$$

$$\vec{v}\,'_2=\vec{v}_2-\hat{\sigma}(\hat{\sigma}\vec{g}); \tag{2.9b}$$

type ''*b*:''

$$\vec{v}\,''_{1l}=\vec{v}_1+\frac{1}{2}\hat{\sigma}\left(\hat{\sigma}\vec{g}+\sqrt{(\hat{\sigma}\vec{g})^2+\frac{4\Delta\varepsilon_{li}}{m}}\right); \tag{2.10a}$$

$$\vec{v}\,''_{1r}=\vec{v}_1+\frac{1}{2}\hat{\sigma}\left(\hat{\sigma}\vec{g}-\sqrt{(\hat{\sigma}\vec{g})^2+\frac{4\Delta\varepsilon_{rj}}{m}}\right); \tag{2.10b}$$

type ''*c*:''

$$\vec{v}\,'''_{1l}=\vec{v}_1+\frac{1}{2}\hat{\sigma}\left(\hat{\sigma}\vec{g}-\sqrt{(\hat{\sigma}\vec{g})^2-\frac{4\Delta\varepsilon_{li}}{m}}\right); \tag{2.11a}$$

$$\vec{v}\,'''_{1r}=\vec{v}_1+\frac{1}{2}\hat{\sigma}\left(\hat{\sigma}\vec{g}+\sqrt{(\hat{\sigma}\vec{g})^2-\frac{4\Delta\varepsilon_{rj}}{m}}\right); \tag{2.11b}$$

type ''*d*:''

$$\vec{v}\,''''_{1{}^l_r}=\vec{v}_1+\hat{\sigma}(\hat{\sigma}\vec{g})\equiv\vec{v}\,'_1. \tag{2.12}$$

Now kinetic equation (2.3) can be written explicitly:

$$\begin{aligned}
\left(\frac{\partial}{\partial t}+\vec{v}_1\frac{\partial}{\partial\vec{r}_1}\right)f_1(x_1;t)&=\sigma_0\int d\hat{\sigma}d\vec{v}_2\hat{\sigma}\vec{g}\,\theta(\hat{\sigma}\vec{g})\{f_2(\vec{r}_1,\vec{v}\,'_1,\vec{r}_1+\hat{\sigma}\sigma_0^+,\vec{v}\,'_2;t)-f_2(x_1,\vec{r}_1-\hat{\sigma}\sigma_0^+,\vec{v}_2;t)\}\\
&+\sum_{i=1}^{n^*}\sigma_{li}^2\int d\hat{\sigma}d\vec{v}_2\hat{\sigma}\vec{g}\Big[\theta(-\hat{\sigma}\vec{g})\{f_2(\vec{r}_1,\vec{v}\,''_{1l},\vec{r}_1+\hat{\sigma}\sigma_{li}^+,\vec{v}\,''_{2l};t)-f_2(x_1,\vec{r}_1-\hat{\sigma}\sigma_{li}^-,\vec{v}_2;t)\}\\
&+\theta\left(\hat{\sigma}\vec{g}-\sqrt{\frac{4\Delta\varepsilon_{li}}{m}}\right)\{f_2(\vec{r}_1,\vec{v}\,'''_{1l},\vec{r}_1+\hat{\sigma}\sigma_{li}^-,\vec{v}\,'''_{2l};t)-f_2(x_1,\vec{r}_1-\hat{\sigma}\sigma_{li}^+,\vec{v}_2;t)\}\\
&+\theta(\hat{\sigma}\vec{g})\theta\left(\sqrt{\frac{4\Delta\varepsilon_{li}}{m}}-\hat{\sigma}\vec{g}\right)\{f_2(\vec{r}_1,\vec{v}\,''''_{1l},\vec{r}_1+\hat{\sigma}\sigma_{li}^+,\vec{v}\,''''_{2l};t)-f_2(x_1,\vec{r}_1-\hat{\sigma}\sigma_{li}^+,\vec{v}_2;t)\}\Big]\\
&+\sum_{j=1}^{m^*}\sigma_{rj}^2\int d\hat{\sigma}d\vec{v}_2\hat{\sigma}\vec{g}\Big[\theta(\hat{\sigma}\vec{g})\{f_2(\vec{r}_1,\vec{v}\,''_{1r},\vec{r}_1+\hat{\sigma}\sigma_{rj}^-,\vec{v}\,''_{2r};t)-f_2(x_1,\vec{r}_1-\hat{\sigma}\sigma_{rj}^+,\vec{v}_2;t)\}\\
&+\theta\left(-\hat{\sigma}\vec{g}-\sqrt{\frac{4\Delta\varepsilon_{rj}}{m}}\right)\{f_2(\vec{r}_1,\vec{v}\,'''_{1r},\vec{r}_1+\hat{\sigma}\sigma_{rj}^+,\vec{v}\,'''_{2r};t)-f_2(x_1,\vec{r}_1-\hat{\sigma}\sigma_{rj}^-,\vec{v}_2;t)\}\\
&+\theta(-\hat{\sigma}\vec{g})\theta\left(\sqrt{\frac{4\Delta\varepsilon_{rj}}{m}}+\hat{\sigma}\vec{g}\right)\{f_2(\vec{r}_1,\vec{v}\,''''_{1r},\vec{r}_1+\hat{\sigma}\sigma_{rj}^-,\vec{v}\,''''_{2r};t)-f_2(x_1,\vec{r}_1-\hat{\sigma}\sigma_{rj}^-,\vec{v}_2;t)\}\Big]\\
&=J_E(f_1,f_1)+\sum_{i=1}^{n^*}(J_{lib}+J_{lic}+J_{lid})+\sum_{j=1}^{m^*}(J_{rjb}+J_{rjc}+J_{rjd}),
\end{aligned} \tag{2.13}$$

$J_{\rm E}$ denotes ordinary Enskog collision integral of hard spheres.

One can draw the following conclusions regarding the form of (2.13). In the absence of attractive and repulsive walls ($\Delta\varepsilon_{li}=0$, $i=1,\dots,n^*$, $\Delta\varepsilon_{rj}=0$, $j=1,\dots,m^*$) this kinetic equation transfers to that one of the RET theory [7,8]. In the presence of only one finite attractive wall ($\Delta\varepsilon_{li}=0$, $i=1,\dots,n^*$, $\Delta\varepsilon_{rj}=0$, $j=2,\dots,m^*$, $\Delta\varepsilon_{r1}\neq 0$) one obtains the kinetic equation of the RDRS theory [9]. Moreover, it can be shown, that in the third special case when the set of walls is merged with some smooth potential ϕ_t and $\Delta\sigma_{li}=\sigma_{li}-\sigma_{li-1}\to 0$, $i=1,\dots,n^*-1$, $\Delta\varepsilon_{li}\to 0$, $n^*\to\infty$, $\Delta\sigma_{rj}=\sigma_{rj+1}-\sigma_{rj}\to 0$, $j=1,\dots,m^*-1$, $\delta\varepsilon_{rj}\to 0$, $m^*\to\infty$, and

$$-\frac{\Delta\varepsilon_{li}}{\Delta\sigma_{li}}\to\phi_t'(\sigma_{li}),$$

$$\frac{\Delta\varepsilon_{rj}}{\Delta\sigma_{rj}}\to\phi_t'(\sigma_{rj}),$$

the kinetic equation (2.13) transfers to that of the KMFT theory [19].

III. MACROSCOPIC CONSERVATION LAWS: THE ZEROTH APPROXIMATION

Let us introduce the following set of hydrodynamic parameters: particles number density $n(\vec r;t)$, hydrodynamic velocity $\vec u(\vec r;t)$, densities of kinetic $\omega_{\rm k}$ and interaction $\omega_{\rm i}$ energies:

$$n(\vec r_1;t)=\int d\vec v_2 f_1(x_1;t), \tag{3.1a}$$

$$\vec u(\vec r_1;t)=\int d\vec v_2 f_1(x_1;t)\frac{\vec v_1}{n(\vec r_1;t)}, \tag{3.1b}$$

$$\omega_{\rm k}(\vec r_1;t)=\int d\vec v_2 f_1(x_1;t)\frac{c_1^2}{2n(\vec r_1;t)}, \tag{3.1c}$$

$$\omega_{\rm i}(\vec r_1;t)=\int d\vec r_2 n(\vec r_2;t) g_2^q(\vec r_1,\vec r_2|n(t),\beta(t))\frac{1}{2m}\Phi(|\vec r_{12}|). \tag{3.1d}$$

Here $\vec c(\vec r;t)=\vec u(\vec r;t)-\vec v$ is the heat velocity. We also introduce the set of interaction invariants $\vec\Psi\equiv\{m,m\vec v,\frac{1}{2}mv^2+\phi(r_{12})\}$ [23]. Multiplying initial kinetic equation (2.13) by each component of the vector $\vec\Psi$ and integrating with respect to $\vec v_2$, one obtains the equation of continuity, the equation of motion, and equation of kinetic energy balance, respectively:

$$\frac{1}{n}\frac{dn}{dt}=-\frac{\partial}{\partial r_{1\alpha}}u_\alpha, \tag{3.2a}$$

$$\frac{du_\alpha}{dt}=-\frac{1}{mn}\frac{\partial}{\partial r_{1\beta}}P_{\alpha\beta}, \tag{3.2b}$$

$$\frac{d\omega_{\rm k}}{dt}=-\frac{1}{mn}\left\{\frac{\partial}{\partial r_{1\alpha}}q_\alpha+P_{\alpha\beta}\frac{\partial}{\partial r_{1\beta}}u_\alpha\right\}, \tag{3.2c}$$

and

$$\frac{d}{dt}=\frac{\partial}{\partial t}+u_\gamma\frac{\partial}{\partial r_{1\gamma}}.$$

The equation for interaction energy density is obtained automatically by differentiating the expression for $\omega_{\rm i}$ with taking into account the conservation laws for $n(\vec r;t)$, $\vec u(\vec r;t)$, and $\omega_{\rm k}$ (3.2). Stress tensor $P_{\alpha\beta}$ and heat flow vector consist of the kinetic and interaction parts:

$$P_{\alpha\beta}=P^{\rm k}_{\alpha\beta}+P^{\rm i}_{\alpha\beta},$$

$$q_\alpha=q^{\rm k}_\alpha+q^{\rm i}_\alpha. \tag{3.3}$$

In its turn, the potential parts consist of the hard sphere term and components caused by the set of attractive and repulsive walls:

$$\begin{aligned}P^{\rm i}_{\alpha\beta}&=P^{\rm i}_{1\alpha\beta}+\sum_{i=1}^{n^*}(P^{\rm i}_{i2\alpha\beta}+P^{\rm i}_{i3\alpha\beta}+P^{\rm i}_{i4\alpha\beta})\\&\quad+\sum_{j=1}^{m^*}(P^{\rm i}_{j2\alpha\beta}+P^{\rm i}_{j3\alpha\beta}+P^{\rm i}_{j4\alpha\beta}),\\q^{\rm i}_\alpha&=q^{\rm i}_{1\alpha}+\sum_{i=1}^{n^*}(q^1_{i2\alpha}+q^{\rm i}_{i3\alpha}+q^{\rm i}_{i4\alpha})\\&\quad+\sum_{j=1}^{m^*}(q^{\rm i}_{j2\alpha}+q^{\rm i}_{j3\alpha}+q^{\rm i}_{j4\alpha}),\end{aligned} \tag{3.4}$$

where indices 1, 2, 3, and 4 correspond to the types of interactions ''*a*,'' ''*b*,'' ''*c*,'' and ''*d*,'' respectively. Now let us write down the expressions for the stress tensor $P_{\alpha\beta}$ and heat flow vector q_α in an explicit form:

$$\begin{aligned}P^{\rm k}_{\alpha\beta}&=\int d\vec v_1 f_1(x_1;t) m c_{1\alpha}c_{1\beta},\\q^{\rm k}_\alpha&=\int d\vec v_1 f_1(x_1;t)\frac{mc_1^2}{2}c_{1\alpha},\end{aligned} \tag{3.5}$$

$$\begin{aligned}P^{\rm i}_{1\alpha\beta}=&\frac{1}{2}m\sigma_0^3\int d\vec v_1 d\vec v_2 d\hat\sigma\,\hat\sigma\vec g\,\theta(\hat\sigma\vec g)(v'_{1\alpha}-v_{1\alpha})\hat\sigma_\beta\\&\times\int_0^1 d\lambda f_2(\vec r_1+\lambda\hat\sigma\sigma_0^+,\vec v_1,\vec r_1+\lambda\hat\sigma\sigma_0^+-\hat\sigma\sigma_0^+,\vec v_2;t),\end{aligned} \tag{3.6}$$

$$\begin{aligned}q^{\rm i}_{1\alpha}=&\frac{1}{2}m\sigma_0^3\int d\vec v_1 d\vec v_2 d\hat\sigma\,\hat\sigma\vec g\,\theta(\hat\sigma\vec g)\left(\frac{(c_1')^2}{2}-\frac{c_1^2}{2}\right)\hat\sigma_\alpha\\&\times\int_0^1 d\lambda f_2(\vec r_1+\lambda\hat\sigma\sigma_0^+,\vec v_1,\vec r_1+\lambda\hat\sigma\sigma_0^+-\hat\sigma\sigma_0^+,\vec v_2;t),\end{aligned} \tag{3.7}$$

$$P^{\rm i}_{i2\alpha\beta}=\frac{1}{2}m\sigma^3_{li}\int d\vec{v}_1 d\vec{v}_2 d\hat{\sigma}\,\hat{\sigma}\vec{g}\,\theta(-\hat{\sigma}\vec{g})(v''_{1l\alpha}-v_{1\alpha})\hat{\sigma}_\beta \times\int_0^1 d\lambda f_2(\vec{r}_1+\lambda\hat{\sigma}\sigma^-_{li},\vec{v}_1,\vec{r}_1+\lambda\hat{\sigma}\sigma^-_{li} -\hat{\sigma}\sigma^-_{li},\vec{v}_2;t), \quad (3.8)$$

$$q^{\rm i}_{i2\alpha}=\frac{1}{2}m\sigma^3_{li}\int d\vec{v}_1 d\vec{v}_2 d\hat{\sigma}\,\hat{\sigma}\vec{g}\,\theta(-\hat{\sigma}\vec{g}) \times\left(\frac{(c''_{1l})^2}{2}-\frac{c_1^2}{2}-\frac{\Delta\varepsilon_{li}}{m}\right)\hat{\sigma}_\alpha \times\int_0^1 d\lambda f_2(\vec{r}_1+\lambda\hat{\sigma}\sigma^-_{li},\vec{v}_1,\vec{r}_1+\lambda\hat{\sigma}\sigma^-_{li}-\hat{\sigma}\sigma^-_{li},\vec{v}_2;t), \quad (3.9)$$

$$P^{\rm i}_{i3\alpha\beta}=\frac{1}{2}m\sigma^3_{li}\int d\vec{v}_1 d\vec{v}_2 d\hat{\sigma}\,\hat{\sigma}\vec{g} \times\theta\left(\hat{\sigma}\vec{g}-\sqrt{\frac{4\Delta\varepsilon_{li}}{m}}\right)(v'''_{1l\alpha}-v_{1\alpha})\hat{\sigma}_\beta \times\int_0^1 d\lambda f_2(\vec{r}_1+\lambda\hat{\sigma}\sigma^+_{li},\vec{v}_1,\vec{r}_1+\lambda\hat{\sigma}\sigma^+_{li} -\hat{\sigma}\sigma^+_{li},\vec{v}_2;t), \quad (3.10)$$

$$q^{\rm i}_{i3\alpha}=\frac{1}{2}m\sigma^3_{li}\int d\vec{v}_1 d\vec{v}_2 d\hat{\sigma}\,\hat{\sigma}\vec{g}\,\theta\left(\hat{\sigma}\vec{g}-\sqrt{\frac{4\Delta\varepsilon_{li}}{m}}\right) \times\left[\frac{(c'''_{1l})^2}{2}-\frac{c_1^2}{2}+\frac{\Delta\varepsilon_{li}}{2m}\right]\hat{\sigma}_\alpha \times\int_0^1 d\lambda f_2(\vec{r}_1+\lambda\hat{\sigma}\sigma^+_{li},\vec{v}_1,\vec{r}_1+\lambda\hat{\sigma}\sigma^+_{li}-\hat{\sigma}\sigma^+_{li},\vec{v}_2;t), \quad (3.11)$$

$$P^{\rm i}_{i4\alpha\beta}=\frac{1}{2}m\sigma^3_{li}\int d\vec{v}_1 d\vec{v}_2 d\hat{\sigma}\,\hat{\sigma}\vec{g}\,\theta(\hat{\sigma}\vec{g})\,\theta\left(\sqrt{\frac{4\Delta\varepsilon_{li}}{m}}-\hat{\sigma}\vec{g}\right) \times(v''''_{1l\alpha}-v_{1\alpha})\hat{\sigma}_\beta\int_0^1 d\lambda f_2(\vec{r}_1+\lambda\hat{\sigma}\sigma^+_{li},\vec{v}_1,\vec{r}_1 +\lambda\hat{\sigma}\sigma^+_{li}-\hat{\sigma}\sigma^+_{li},\vec{v}_2;t), \quad (3.12)$$

$$q^{\rm i}_{i4\alpha}=\frac{1}{2}m\sigma^3_{li}\int d\vec{v}_1 d\vec{v}_2 d\hat{\sigma}\,\hat{\sigma}\vec{g}\,\theta(\hat{\sigma}\vec{g})\,\theta\left(\sqrt{\frac{4\Delta\varepsilon_{li}}{m}}-\hat{\sigma}\vec{g}\right) \times\left(\frac{(c''''_{1l})^2}{2}-\frac{c_1^2}{2}\right)\hat{\sigma}_\alpha\int_0^1 d\lambda f_2(\vec{r}_1+\lambda\hat{\sigma}\sigma^+_{li},\vec{v}_1,\vec{r}_1 +\lambda\hat{\sigma}\sigma^+_{li}-\hat{\sigma}\sigma^+_{li},\vec{v}_2;t). \quad (3.13)$$

Expressions for $P_{j2\alpha\beta}$, $P_{j3\alpha\beta}$, $P_{j4\alpha\beta}$, $q_{j2\alpha}$, $q_{j3\alpha}$, and $q_{j4\alpha}$ look similar to (3.6)–(3.13) $P_{i2\alpha\beta}$, $P_{i3\alpha\beta}$, $P_{i4\alpha\beta}$, $q_{i2\alpha}$, $q_{i3\alpha}$, and $q_{i4\alpha}$, respectively, at formal replacing $\sigma^{\pm}_{li}\to\sigma^{\mp}_{rj}$, $\hat{\sigma}\vec{g}\to-\hat{\sigma}\vec{g}$, $\vec{v}_{1l}\to\vec{v}_{1r}$, $\Delta\varepsilon_{li}\to\Delta\varepsilon_{rj}$.

At the end of this section we consider the macroscopic conservation laws in the zeroth approximation. Let us suppose that the one-particle distribution function in this case is equal to the local-equilibrium Maxwell one:

$$f_1\equiv f_1^{(0)}(x_1;t) =n(\vec{r}_1;t)\left(\frac{m}{2\pi k_B T(\vec{r}_1;t)}\right)^{3/2}\exp\left\{-\frac{mc_1^2(\vec{r}_1;t)}{2k_B T(\vec{r}_1;t)}\right\}. \quad (3.14)$$

Neglecting any spatial gradient one obtains

$$g_2^q(\vec{r}_1,\vec{r}_2|n(\vec{r}_1;t),\beta(\vec{r}_1;t)) \simeq g_2^{\rm eq}\left(r_{12};n\left(\frac{\vec{r}_1+\vec{r}_2}{2};t\right),\beta\left(\frac{\vec{r}_1+\vec{r}_2}{2};t\right)\right), \quad (3.15a)$$

$$\int_0^1 d\lambda f_2(x_1;x_2;t)\simeq\int_0^1 d\lambda f_2^{(0)}(\dots) =g_2^{\rm eq}(\sigma|n,\beta)f_1^{(0)}(x_1;t)f_1^{(0)}(\vec{r}_1,\vec{v}_2;t). \quad (3.15b)$$

It is well-known from the equilibrium statistical mechanics [26] that any sharp jump of interaction potential results in a corresponding jump of binary correlation function:

$$\frac{g_2^{\rm eq}(\sigma^+_{li}|n,\beta)}{g_2^{\rm eq}(\sigma^-_{li}|n,\beta)}=\exp\{\beta\Delta\varepsilon_{li}\}, \quad (3.16a)$$

$$\frac{g_2^{\rm eq}(\sigma^-_{rj}|n,\beta)}{g_2^{\rm eq}(\sigma^+_{rj}|n,\beta)}=\exp\{\beta\Delta\varepsilon_{rj}\}. \quad (3.16b)$$

Substituting these relations into (3.5)–(3.13), one obtains that $P_{\alpha\beta}=p\,\delta_{\alpha\beta}$, where p is the hydrostatic pressure which consists of the kinetic $p^{\rm k}$ and interaction $p^{\rm i}$ parts; $q_\alpha=0$:

$$p=p^{\rm k}+p^{\rm i},$$

$$p^{\rm k}=nk_BT,$$

$$p^{\rm i}=\frac{2}{3}\pi n^2 k_B T\Lambda, \quad (3.17)$$

$$\Lambda=\sigma_0^3 g_2(\sigma_0^+)-\sum_{i=1}^{n^*}\sigma^3_{li}g_2(\sigma^+_{li})\{e^{-\beta\Delta\varepsilon_{li}}-1\} +\sum_{j=1}^{m^*}\sigma^3_{rj}g_2(\sigma^-_{rj})\{e^{-\beta\Delta\varepsilon_{rj}}-1\},$$

$$g_2^{\rm eq}\equiv g_2^{\rm eq}(\sigma|n(\vec{r}_1;t),\beta(\vec{r}_1;t)).$$

Then, starting from (3.2), one has the conservation laws in the zeroth approximation (Euler laws):

$$\frac{1}{n}\frac{dn}{dt}=-\frac{\partial\vec{u}}{\partial\vec{r}_1}, \tag{3.18a}$$

$$\frac{d\vec{u}}{dt}=-\frac{1}{mn}\frac{\partial P}{\partial\vec{r}_1}, \tag{3.18b}$$

$$\frac{d\omega_{\rm k}}{dt}=-\frac{1}{mn}p\frac{\partial\vec{u}}{\partial\vec{r}_1},\quad \omega_{\rm k}=\frac{3}{2m\beta}, \tag{3.18c}$$

$$\omega_{\rm i}^{(0)}(\vec{r}_1;t)=\frac{1}{2m}\int d\vec{r}_{12}n(\vec{r}_1;t)g_2^{\rm eq}i \times(|\vec{r}_{12}|;n(\vec{r}_1;t),\beta(\vec{r}_1;t))\Phi(|\vec{r}_{12}|). \tag{3.18d}$$

IV. THE PRINCIPLE OF CONSTRUCTION OF HIGHER ORDER APPROXIMATIONS: NORMAL SOLUTIONS BY MEANS OF BOUNDARY CONDITIONS METHOD

Let us consider initial kinetic equation (2.3) [or (2.13)]

$$\left(\frac{\partial}{\partial t}+\vec{v}_1\frac{\partial}{\partial\vec{r}_1}\right)f_1(x_1;t)=\int dx_2\hat{T}f_2(x_1,x_2;t)=J(f_1,f_1), \tag{4.1}$$

where the collision integral $J(f_1,f_1)$ consists of the usual one of the RET theory—$J_E(f_1,f_1)$ and collision integrals demanding on interaction on each wall. Such a structure of $J(f_1,f_1)$ is caused by the structure of $\hat{T}$-operator:

$$J(f_1,f_1)=J_E(f_1,f_1)+\sum_{i=1}^{n*}[J_{lib}+J_{lic}+J_{lid}] +\sum_{j=1}^{m*}[J_{rjb}+J_{rjc}+J_{rjd}]. \tag{4.2}$$

Going to the schema of construction of normal solutions to kinetic equations with the help of boundary conditions [22], let us introduce in the right-hand side of (4.1) an infinitely small source $-\overline{\epsilon}(f_1-f_1^{(0)})$, where $\overline{\epsilon}\to 0$:

$$\left(\frac{\partial}{\partial t}+\vec{v}_1\frac{\partial}{\partial\vec{r}_1}\right)f_1(x_1;t)=J(f_1,f_1)-\overline{\epsilon}(f_1-f_1^{(0)}). \tag{4.3}$$

For deviation $\delta f=f_1-f_1^{(0)}$ this equation reads:

$$\left(\frac{\partial}{\partial t}+\vec{v}_1\frac{\partial}{\partial\vec{r}_1}+\overline{\epsilon}\right)\delta f=-\left(\frac{\partial}{\partial t}+\vec{v}_1\frac{\partial}{\partial\vec{r}_1}\right)f_1^{(0)}+J(f_1^{(0)},f_1^{(0)}) +J(f_1^{(0)},\delta f)+J(\delta f,f_1^{(0)})+J(\delta f,\delta f).$$

First and foremost it should be noted that the collision integral in the usual Boltzmann equation is local (f_1 is a function of the same Cartesian coordinate $\vec{r}_1$). In our case the $J(f_1,f_1)$ is a nonlocal collision integral. f_1 is calculated in points $\vec{r}_1$ and $\vec{r}_1\pm\hat{\sigma}\sigma$, integration with respect to $\hat{\sigma}$ (surface of unit sphere) is performed. As a result, in one way or another, we will find solutions in some approximation, and there is no need ‘‘to draw’’ the whole nonlocal collision integral. It is much more convenient to use its approximate expression. This approximation should be of the same order as within the frame for the solution of total kinetic equation. In such a way, let us expand functions f_1 and g_2^q in the vicinity of $\vec{r}_1$ into series in deviations $\pm\hat{\sigma}\sigma$. This results in:

$$J\equiv\sum_{k=0}^{\infty}J_k=J_0+J^*,\quad J^*=\sum_{k=1}^{\infty}J_k, \tag{4.5}$$

$$I\equiv\sum_{k=0}^{\infty}I_k=I_0+I^*,\quad I^*=\sum_{k=1}^{\infty}I_k, \tag{4.6}$$

where k is the expansion order. All J_k here are local functionals of f_1. We also use the following notations: $I(\delta f)=J(f_1^{(0)},\delta f)+J(\delta f,f_1^{(0)})$ for the linearized nonlocal collision operator. We have similar expansion for this operator—the relation (4.6). Here $I_0(\delta f)=J_0(f_1^{(0)},\delta f)+J_0(\delta f,f_1^{(0)})$ is a linearized local collision operator which coincides with that of the usual Boltzmann kinetic equation within a factor of $g_2^{\rm eq}(\sigma_0^+)$ if one neglects the set of walls except hard sphere wall. Then equation (4.4) transfers to

$$\frac{\partial}{\partial t}\delta f+\overline{\epsilon}\delta f-I_0(\delta f)=-\frac{D}{Dt}f_1^{(0)}+J(f_1^{(0)},f_1^{(0)})+I^*(\delta f) +J(\delta f,\delta f)-\vec{v}_1\frac{\partial}{\partial\vec{r}_1}\delta f. \tag{4.7}$$

To solve this equation by means of the boundary conditions method, we need its integral form. To this end let us introduce operator $S(t,t')$ with the following properties:

$$\frac{\partial}{\partial t}S(t,t')=I_0S(t,t'),\quad S(t,t)=1. \tag{4.8}$$

Using the limiting condition $\lim_{t\to-\infty}\delta f(t)=0$ one obtains:

$$\delta f(t)=\int_{-\infty}^{t}dt'e^{\overline{\epsilon}(t'-t)}S(t,t')\left[\frac{D}{Dt}f_1^{(0)}+J(f_1^{(0)},f_1^{(0)}) +I^*(\delta f)+J(\delta f,\delta f)-\vec{v}_1\frac{\partial}{\partial\vec{r}_1}\delta f\right]_{t'}. \tag{4.9}$$

Equation (4.9) is completely ready for the iteration procedure. This procedure can be organized as follows:

$$\delta f^{(k+1)}(t)=\int_{-\infty}^{t}dt'e^{\overline{\epsilon}(t'-t)}S(t,t')\left[\frac{D}{Dt}f_1^{(0)} +J^{(k+1)}(f_1^{(0)},f_1^{(0)})+I^{*(k+1)}(\delta f^{(k)}) +J^{(k+1)}(\delta f^{(k)},\delta f^{(k)})-\vec{v}_1\frac{\partial}{\partial\vec{r}_1}\delta f^{(k)}\right]_{t'}, \tag{4.10}$$

where

$$J^{(k+1)}=\sum_{k'=0}^{k+1}J_{k'},$$

$$I^{*(k+1)}=\sum_{k'=0}^{k+1} I_{k'}.$$

Each $(k+1)$th step uses conservation laws in kth approximation.

V. ONE-PARTICLE DISTRIBUTION FUNCTION IN THE FIRST APPROXIMATION

The expression for the distribution function f_1 in the first approximation is obtained if one puts $k=0$ in (3.5) and takes into account the equality $\delta f^{(0)}=0$. Then we have:

$$\delta f^{(1)}(t)=\int_{-\infty}^{t} dt' e^{\epsilon(t'-t)} S(t,t') \times\left[\frac{D}{Dt} f_1^{(0)}+J_0(f_1^{(0)},f_1^{(0)})+J_1(f_1^{(0)},f_1^{(0)})\right]_{t'}. \tag{5.1}$$

It can be shown that

$$J_0(f_1^{(0)},f_1^{(0)})=0. \tag{5.2}$$

Making the expansion up to the linear terms in gradients of hydrodynamic parameters

$$g_2^q(\vec{r}_1,\vec{r}_2|n(t),\beta(t))\simeq g_2^{\mathrm{eq}}\left(r_{12};n\left(\frac{\vec{r}_1+\vec{r}_2}{2};t\right),\beta\left(\frac{\vec{r}_1+\vec{r}_2}{2};t\right)\right) =\frac{1}{2}\vec{r}_{12}\frac{\partial}{\partial\vec{r}_1} g_2^{\mathrm{eq}}+\dots, \tag{5.3a}$$

$$f_1(\vec{r}_1\pm\hat{\sigma}\sigma)=f_1(\vec{r}_1)\pm\frac{\partial}{\partial\vec{r}_1} f_1\hat{\sigma}\sigma+\dots \tag{5.3b}$$

and taking into account the conservation laws (3.18), one obtains after very unwieldy calculations the following:

$$-\frac{D}{Dt} f_1^{(0)}+J_1(f_1^{(0)},f_1^{(0)})=K_\alpha\frac{\partial}{\partial r_{1\alpha}}\ln T+L_{\alpha\beta}\frac{\partial}{\partial r_{1\beta}} u_\alpha, \tag{5.4}$$

$$K_\alpha=-f_1^{(0)}\left[1+\frac{3}{5}\frac{p^{\mathrm{i}}}{nk_BT}\right]\left[\frac{mc_1^2}{2k_BT}-\frac{5}{2}\right]c_{1\alpha} +\sum_{i=1}^{n*} K_{\alpha li}+\sum_{j=1}^{m*} K_{\alpha rj}, \tag{5.5}$$

$$L_{\alpha\beta}=-f_1^{(0)}\left[1+\frac{2}{5}\frac{p^{\mathrm{i}}}{nk_BT}\right]\frac{m}{k_BT}\left[c_{1\alpha}c_{1\beta}-\frac{1}{3}c_1^2\delta_{\alpha\beta}\right] +\sum_{i=1}^{n*} L_{\alpha\beta li}+\sum_{j=1}^{m*} L_{\alpha\beta rj}, \tag{5.6}$$

where

$$\begin{aligned} K_{\alpha{}^{li}_{rj}}=&\mp\frac{8}{\pi^2}n^2\sigma_{{}^{li}_{rj}}g_2^{\mathrm{eq}}(\sigma^{\pm}_{{}^{rj}_{li}})\frac{m}{2k_BT}\left[\frac{1}{30}e^{-s^2}\int d\vec{x}_2\exp\{-h^2-v^2\}h_\beta\left(v_\alpha v_\beta-\frac{1}{3}v^2\delta_{\alpha\beta}\right)\right.\\ &\times\left\{4+\frac{s^3}{v^5}(5v^2+6s^2)+\frac{1}{v^5}(v^2+s^2)^{3/2}(4v^2-6s^2)\right\}-\frac{1}{30}\int_{v>s}d\vec{x}_2\exp\{-h^2-v^2\}h_\beta\left(v_\alpha v_\beta-\frac{1}{3}v^2\delta_{\alpha\beta}\right)\\ &\times\left\{4+\frac{s^3}{v^5}(5v^2-9s^2)+\frac{1}{v^5}(v^2-s^2)^{3/2}(4v^2+6s^2)\right\}+\frac{1}{9}e^{-s^2}\int d\vec{x}_2\exp\{-h^2-v^2\}h_\alpha\left(v^2-\frac{s^3}{v}+\frac{1}{v}(v^2+s^2)^{3/2}\right)\\ &\left.-\frac{1}{9}\int_{v>s}d\vec{x}_2\exp\{-h^2-v^2\}h_\alpha\left(v^2-\frac{s^3}{v}+\frac{1}{v}(v^2+s^2)^{3/2}\right)\right], \end{aligned} \tag{5.7}$$

$$\begin{aligned} L_{\alpha\beta{}^{li}_{rj}}=&\mp\frac{8}{\pi^2}n^2\sqrt{2}\sigma_{{}^{li}_{rj}}g_2^{\mathrm{eq}}(\sigma^{\pm}_{{}^{li}_{rj}})\left(\frac{m}{2k_BT}\right)^{3/2}\left[\frac{1}{30}e^{-s^2}\int d\vec{x}_2\exp\{-h^2-v^2\}\left(v_\alpha v_\beta-\frac{1}{3}v^2\delta_{\alpha\beta}\right)\right.\\ &\times\left\{4+\frac{s^3}{v^5}(5v^2+6s^2)+\frac{1}{v^5}(v^2+s^2)^{3/2}(4v^2-6s^2)\right\}-\frac{1}{30}\int_{v>s}d\vec{x}_2\exp\{-h^2-v^2\}\left(v_\alpha v_\beta-\frac{1}{3}v^2\delta_{\alpha\beta}\right)\\ &\times\left\{4+\frac{s^3}{v^5}(5v^2-9s^2)+\frac{1}{v^5}(v^2-s^2)^{3/2}(4v^2+6s^2)\right\}+\frac{1}{9}e^{-s^2}\int d\vec{x}_2\exp\{-h^2-v^2\}\left(v^2-\frac{s^3}{v}+\frac{1}{v}(v^2+s^2)^{3/2}\right)\delta_{\alpha\beta}\\ &\left.-\frac{1}{9}\int_{v>s}d\vec{x}_2\exp\{-h^2-v^2\}\left(v^2-\frac{s^3}{v}+\frac{1}{v}(v^2+s^2)^{3/2}\right)\delta_{\alpha\beta}\right]. \end{aligned} \tag{5.8}$$

Here

$$s=\begin{cases}(\beta\Delta\epsilon_{li})^{1/2},\\(\beta\Delta\epsilon_{rj})^{1/2},\end{cases}\quad \vec{x}_2=\left(\frac{m}{4k_BT}\right)^{1/2}\vec{c}_2, \tag{5.9}$$

$$\vec{v}=\frac{1}{2}\left(\frac{m}{k_BT}\right)^{1/2}(\vec{c}_2-\vec{c}_1), \tag{5.10a}$$

$$\vec{h}=\frac{1}{2}\left(\frac{m}{k_BT}\right)^{1/2}(\vec{c}_1+\vec{c}_2). \tag{5.10b}$$

Then

$$f_1\equiv f_1^{(1)}=f_1^{(0)}+\delta f^{(1)}, \tag{5.11a}$$

$$\delta f^{(1)}(t)=\int_{-\infty}^{t}dt'\,e^{\epsilon(t'-t)}S(t,t')\times\left\{K_\alpha\frac{\partial}{\partial r_{1\alpha}}\ln T+L_{\alpha\beta}\frac{\partial}{\partial r_{1\beta}}u_\alpha\right\}_{t'}. \tag{5.11b}$$

It can be shown that $\int d\vec{v}_1\,\delta f^{(1)}(\vec{r}_1,\vec{v}_1;t)\vec{\Psi}=0$, i.e., the hydrodynamic parameters $n(\vec{r}_1;t)$, $\vec{u}(\vec{r}_1;t)$, β, $\omega_{\rm i}$ are completely defined by the local one-particle distribution function $f_1^{(0)}$ (3.14).

VI. CONSERVATION LAWS IN THE FIRST APPROXIMATION: STATIONARY PROCESS

First, let us calculate kinetic parts of the stress tensor and heat flux vector. Substituting one-particle distribution function f_1 (5.11) into (3.5) one obtains:

$$P_{\alpha\beta}^{{\rm k}(1)}=p^{\rm k}\delta_{\alpha\beta}+\int dt'\,e^{\epsilon(t'-t)}M^{\rm k}(t,t')[S_{\alpha\beta}]_{t'}, \tag{6.1}$$

$$S_{\alpha\beta}=\frac{\partial}{\partial r_{1\alpha}}u_\alpha+\frac{\partial}{\partial r_{1\beta}}u_\beta-\frac{2}{3}\frac{\partial}{\partial r_{1\gamma}}u_\gamma\delta_{\alpha\beta},$$
$$q_\alpha^{{\rm k}(1)}=\int dt'\,e^{\epsilon(t'-t)}L^{\rm k}(t,t')\left[\frac{\partial}{\partial r_{1\alpha}}\ln T\right]_{t'}, \tag{6.2}$$

where cores of kinetic parts of transport laws read:

$$M^{\rm k}(t,t')=\frac{1}{10}\int d\vec{v}_1 m c_{1\alpha}c_{1\beta}S(t,t')\{L_{\alpha\beta}\}_{t'}, \tag{6.3}$$

$$L^{\rm k}(t,t')=\frac{1}{3}\int d\vec{v}_1 c_{1\alpha}\frac{mc_1^2}{2}S(t,t')\{K_\alpha\}_{t'}. \tag{6.4}$$

To calculate the potential (interaction) parts of $P_{\alpha\beta}^{{\rm i}(1)}$ and $q_\alpha^{{\rm i}(1)}$, the expression $\int_0^1 d\lambda\, f_2(\vec{r}_1+\lambda\hat{\sigma}\sigma,\vec{v}_1,\vec{r}_1+\lambda\hat{\sigma}\sigma-\hat{\sigma}\sigma,\vec{v}_2;t)=z_1+z_2$ should be expanded into series in, first of all, inhomogeneity of distribution function, then in deviation $\delta f^{(1)}$. In both cases one should keep only the linear terms in gradients. Calculations give:

$$z_1=\frac{1}{2}\sigma g_2^{\rm eq}(\sigma)f_1^{(0)}(x_1;t)f_1^{(0)}(\vec{r}_1,\vec{v}_2;t)\hat{\sigma}\frac{\partial}{\partial\vec{r}_1}\ln\frac{f_1^{(0)}(\vec{r}_1,\vec{v}_1;t)}{f_1^{(0)}(\vec{r}_1,\vec{v}_2;t)}, \tag{6.5}$$

$$z_2=g_2^{\rm eq}(\sigma)\{f_1^{(0)}(x_1;t)\,\delta f^{(1)}(\vec{r}_1,\vec{v}_2;t)+\delta f^{(1)}(x_1;t)f_1^{(0)}(\vec{r}_1,\vec{v}_2;t)\}. \tag{6.6}$$

z_1 is the expansion of $f_1^{(0)}$ in inhomogeneity (the inhomogeneity of $\delta f^{(1)}$ is considered as a negligibly small quantity), z_2 is the expansion in deviation $\delta f^{(1)}$. Then, general expressions (3.6)–(3.13) with taking into account (6.5) and (6.6) transfer to

$$P_{\alpha\beta}^{\rm i1}=\int dt'\,e^{\epsilon(t'-t)}M^{\rm i}(t,t')[S_{\alpha\beta}]_{t'}-\frac{4}{9}n^2\sqrt{\pi mk_BT}H_2\left\{\frac{6}{5}S_{\alpha\beta}+\frac{\partial}{\partial r_{1\gamma}}u_\gamma\delta_{\alpha\beta}\right\}, \tag{6.7}$$

$$q_\alpha^{\rm i1}=\int dt'\,e^{\epsilon(t'-t)}L^{\rm i}(t,t')\left[\frac{\partial}{\partial r_{1\alpha}}\ln T\right]_{t'}-\frac{2}{3}n^2k_B\sqrt{\frac{nk_BT}{m}}H_2\frac{\partial T}{\partial r_{1\alpha}}, \tag{6.8}$$

where $M^{\rm i}$, $L^{\rm i}$ are cores of the potential parts of transfer laws. Their structure is very complicated. To save space, these expressions are not presented here in their explicit form.

$$H_2=\sigma_0^4g_2^{\rm eq}(\sigma_0^+)+\sum_{i=1}^{n^*}\sigma_{li}^4g_2(\sigma_{li}^+)e^{-\beta\Delta\epsilon_{li}}\Xi(\beta\Delta\epsilon_{li})+\sum_{j=1}^{m^*}\sigma_{rj}^4g_2^{\rm eq}(\sigma_{rj}^+)e^{-\beta\Delta\epsilon_{rj}}\Xi(\beta\Delta\epsilon_{rj}), \tag{6.9}$$

$$\Xi(s)=e^s-\tfrac{1}{2}s-K_1^*(s), \tag{6.10a}$$

$$K_1^*(s)=2\int_0^\infty dx\; x^2e^{-x^2}\sqrt{x^2+s}. \tag{6.10b}$$

In such a way, the transport laws in the first approximation are in an integral form only partially. They are in an integral form completely in the case of solution of the usual Boltzmann kinetic equation [22]. There are also local-time terms [second terms in (6.7) and (6.8)], caused by the inhomogeneity of $f_1^{(0)}$ and, therefore, not sensitive to the "memory" effects.

In the stationary case, the operator I_0 does not depend on time explicitly:

$$S(t,t')=e^{I_0(t-t')}.$$

Then

$$\delta f^{(1)}=\int d\tau\; e^{\epsilon\tau}e^{-I_0\tau}\left\{K_\alpha\frac{\partial}{\partial r_{1\alpha}}\ln T+L_{\alpha\beta}\frac{\partial}{\partial r_{1\beta}}u_\alpha\right\}, \tag{6.11}$$

$$\tau = t' - t.$$

Let us define the following quantities:

$$a_\alpha(\tau) = e^{-I_0\tau}\left\{ K_\alpha \frac{\partial}{\partial r_{1\alpha}} \ln T \right\}, \quad (6.12a)$$

$$b_{\alpha\beta}(\tau) = e^{-I_0\tau}\left\{ L_{\alpha\beta} \frac{\partial}{\partial r_{1\beta}} u_\alpha \right\}, \quad (6.12b)$$

with the initial conditions

$$a_\alpha(0) = K_\alpha \frac{\partial}{\partial r_{1\alpha}} \ln T, \quad (6.12c)$$

$$b_{\alpha\beta}(0) = L_{\alpha\beta} \frac{\partial}{\partial r_{1\beta}} u_\alpha . \quad (6.12d)$$

It can be shown that the operator I_0 has the same mathematical properties that the corresponding operator of the usual Boltzmann kinetic equation:

$$I_0(f_1^{(0)}\vec{\Psi}) = 0, \quad (6.13a)$$

$$I_0(\xi) = \lambda \xi, \quad \lambda < 0. \quad (6.13b)$$

Then, for $\tau < 0$, $\lambda_{\max} \equiv \max\{\lambda\}$:

$$\|a_\alpha(\tau)\| \leqslant \|a_\alpha(0)\| \exp\{\lambda_{\max}\tau\}, \quad (6.14a)$$

$$\|b_{\alpha\beta}(\tau)\| \leqslant \|b_{\alpha\beta}(0)\| \exp\{\lambda_{\max}\tau\}, \quad (6.14b)$$

and

$$\|\varphi\| = \int d\vec{v}_1 [f^{(0)}]^{-1} \varphi^2.$$

Using last transformations, equation (6.11) transfers to:

$$\delta f^{(1)} = \lim_{\epsilon \to +0} \int_{-\infty}^{0} d\tau\, e^{\epsilon\tau} [a_\alpha(\tau) + b_{\alpha\beta}(\tau)]$$
$$= \int_{-\infty}^{0} d\tau [a_\alpha(\tau) + b_{\alpha\beta}(\tau)], \quad (6.15)$$

or, introducing $\delta f^{(1)} = \phi^{(1)} f_1^{(0)}$, it can be rewritten in the following final form:

$$\phi^{(1)} = A_\alpha \frac{\partial}{\partial r_{1\alpha}} \ln T + B_{\alpha\beta} \frac{\partial}{\partial r_{1\beta}} u_\alpha . \quad (6.16)$$

A_α and $B_{\alpha\beta}$ satisfy the integral equations like:

$$I_0(A_\alpha) = K_\alpha , \quad (6.17a)$$

$$I_0(B_{\alpha\beta}) = L_{\alpha\beta} . \quad (6.17b)$$

Operator I_0 has the following structure:

$$I_0 = I_a + \sum_{i=1}^{n^*} \{I_{ib} + I_{ic} + I_{id}\} + \sum_{j=1}^{m^*} \{I_{jb} + I_{jc} + I_{jd}\}, \quad (6.18)$$

where

$$I_\alpha(\phi_1) = \sigma_0^2 g_2^{\mathrm{eq}}(\sigma_0^+) \int d\vec{v}_2 d\hat{\sigma}\ \hat{\sigma}\vec{g}\,\theta(\hat{\sigma}\vec{g}) f_1^{(0)}(\vec{v}_1) f_1^{(0)}(\vec{v}_2)$$
$$\times \{\phi_1 + \phi_2 - \phi_1' - \phi_2'\}, \quad (6.19)$$

$$I_{ib}(\phi_1) = \sigma_{li}^2 g_2^{\mathrm{eq}}(\sigma_{li}^-) \int d\vec{v}_2 d\hat{\sigma}\ \hat{\sigma}\vec{g}\,\theta(-\hat{\sigma}\vec{g}) f_1^{(0)}(\vec{v}_1) f_1^{(0)}(\vec{v}_2)$$
$$\times \{\phi_1 + \phi_2 - \phi_{1i}'' - \phi_{2i}''\}, \quad (6.20)$$

$$I_{ic}(\phi_1) = \sigma_{li}^2 g_2^{\mathrm{eq}}(\sigma_{li}^+) \int d\vec{v}_2 d\hat{\sigma}\ \hat{\sigma}\vec{g}\,\theta\left(\hat{\sigma}\vec{g} - \sqrt{\frac{4\Delta\epsilon_{li}}{m}} \right)$$
$$\times f_1^{(0)}(\vec{v}_1) f_1^{(0)}(\vec{v}_2) \{\phi_1 + \phi_2 - \phi_1''' - \phi_{2i}'''\}, \quad (6.21)$$

$$I_{id}(\phi_1) = \sigma_{li}^2 g_2^{\mathrm{eq}}(\sigma_{li}^+) \int d\vec{v}_2 d\hat{\sigma}\ \hat{\sigma}\vec{g}\,\theta(\hat{\sigma}\vec{g})\,\theta\left(\sqrt{\frac{4\Delta\epsilon_{li}}{m}} - \hat{\sigma}\vec{g} \right)$$
$$\times f_1^{(0)}(\vec{v}_1) f_1^{(0)}(\vec{v}_2) \{\phi_1 + \phi_2 - \phi_{1i}'''' - \phi_{2i}''''\}, \quad (6.22)$$

$$I_{jb}(\phi_1) = \sigma_{rj}^2 g_2^{\mathrm{eq}}(\sigma_{rj}^+) \int d\vec{v}_2 d\hat{\sigma}\ \hat{\sigma}\vec{g}\,\theta(\hat{\sigma}\vec{g}) f_1^{(0)}(\vec{v}_1) f_1^{(0)}(\vec{v}_2)$$
$$\times \{\phi_1 + \phi_2 - \phi_{1j}'' - \phi_{2j}''\}, \quad (6.23)$$

$$I_{jc}(\phi_1) = \sigma_{rj}^2 g_2^{\mathrm{eq}}(\sigma_{rj}^-) \int d\vec{v}_2 d\hat{\sigma}\hat{\sigma}\vec{g}\,\theta\left(-\hat{\sigma}\vec{g} - \sqrt{\frac{4\Delta\epsilon_{rj}}{m}} \right)$$
$$\times f_1^{(0)}(\vec{v}_1) f_1^{(0)}(\vec{v}_2) \{\phi_1 + \phi_2 - \phi_{1j}''' - \phi_{2j}'''\}, \quad (6.24)$$

$$I_{jd}(\phi_1) = \sigma_{rj}^2 g_2^{\mathrm{eq}}(\sigma_{rj}^+) \int d\vec{v}_2 d\hat{\sigma}\hat{\sigma}\vec{g}\,\theta(-\hat{\sigma}\vec{g})$$
$$\times \theta\left(\sqrt{\frac{4\Delta\epsilon_{rj}}{m}} + \hat{\sigma}\vec{g} \right) f_1^{(0)}(\vec{v}_1) f_1^{(0)}(\vec{v}_2)$$
$$\times \{\phi_1 + \phi_2 - \phi_{1j}'''' - \phi_{2j}''''\}, \quad (6.25)$$

$$\phi_1 \equiv \phi(\vec{r}_1, \vec{v}_1; t), \quad (6.26a)$$

$$\phi_2 \equiv \phi(\vec{r}_1, \vec{v}_2; t), \quad (6.26b)$$

$$\phi_{1_j^i} \equiv \phi(\vec{r}_1, \vec{v}^*_{1_r^l}; t), \quad (6.26c)$$

$$\phi_{2_j^i} \equiv \phi(\vec{r}_1, \vec{v}^*_{2_r^l}; t), \quad (6.26d)$$

$$* \equiv (', '', ''', ''''). \quad (6.26e)$$

In the case of SET (RET) theory, the linearized local integral operator $I_0 = I_a$, whereas in the case of the Boltzmann kinetic equation there is the usual Boltzmann's linearized operator and I_a tends to that one in the low density limit: $n \to 0$, $g_2^{\mathrm{eq}}(\sigma_0^+) \to 1$, $I_a \to I_B$.

In such a way, to find one-particle distribution function in the first approximation in stationary case one should analyze integral equations (6.17) and solve them.

VII. SOLUTIONS TO THE INTEGRAL EQUATIONS

To find quantities A_α and $B_{\alpha\beta}$ we have set of integral equations (6.17). Let us define the dimensionless self-velocity: $\vec{w}=(m/2k_BT)^{1/2}\vec{c}$. Using the property of isotropy (in the velocity space) of the operator I_0 and structures of K_α (5.7) and $L_{\alpha\beta}$ (5.8) solutions to (6.17) can be presented as follows:

$$A_\alpha = w_{1\alpha}A(w_1), \tag{7.1}$$

$$B_{0\alpha\beta}=B_{1\alpha\beta}+B_{2\alpha\beta}(w_1)\,\delta_{\alpha\beta}, \tag{7.2}$$

$$B_{1\alpha\beta}=\left(w_{1\alpha}w_{1\beta}-\frac{1}{3}w_1^2\delta_{\alpha\beta}\right)B_1(w_1).$$

The structure of $B_{0\alpha\beta}$ is caused by the structure of $L_{\alpha\beta}$: $L_{\alpha\beta}=L_{1\alpha\beta}+L_{2\alpha\beta}$, where in $L_{1\alpha\beta}$ are all terms with $(w_{1\alpha}w_{1\beta}-\frac{1}{3}w_1^2\delta_{\alpha\beta})$, in $L_{2\alpha\beta}$ are all terms with $\delta_{\alpha\beta}$. Then

$$I_0(w_{1\alpha}A(w_1))=K_\alpha, \tag{7.3a}$$

$$I_0\left(\left(w_{1\alpha}w_{1\beta}-\frac{1}{3}w_1^2\delta_{\alpha\beta}\right)B_1(w_1)\right)=L_{1\alpha\beta}, \tag{7.3b}$$

$$I_0(B_2(w_1))=L_2. \tag{7.3c}$$

Following the standard Chapman-Enskog method [23], let us represent $A(w_1)$, $B_1(w_1)$ and $B_2(w_1)$ via the Sonine-Laguerre polynomials

$$S_n^m(z)=\sum_{j=0}^{m}(-z)^j\frac{\Gamma(n+m+1)}{j!(m-j)!\Gamma(n+j+1)}, \tag{7.4}$$

i.e., in the form

$$A(w_1)=\sum_{m=0}^{\infty}a^{(m)}S_{3/2}^{(m)}(w_1^2), \tag{7.5a}$$

$$B_1(w_1)=\sum_{m=0}^{\infty}b_1^{(m)}S_{5/2}^{(m)}(w_1^2), \tag{7.5b}$$

$$B_2(w_1)=\sum_{m=0}^{\infty}b_2^{(m)}S_{1/2}^{(m)}(w_1^2). \tag{7.5c}$$

Fredgolm condition puts limitations on expansion coefficients $a^{(m)}$ and $b^{(m)}$: the correction in the first approximation does not contribute to hydrodynamic parameters $\int d\vec{w}_1 f_1^{(0)}\phi^{(1)}=0$. By this means:

$$a^{(0)}=0, \tag{7.6a}$$

$$b^{(0)}=0, \tag{7.6b}$$

$$b^{(1)}=0. \tag{7.6c}$$

It is known that the Sonine-Laguerre polynomials converge quickly. Therefore only the first nonzero term is considered in expansion. This is as a rule and we will follow the procedure. Such an approximation gives the error for transport coefficients (practically for all types of interaction potentials) not exceeding 2%. Thus, we have:

$$A(w_1)\simeq a^{(1)}S_{3/2}^{(1)}(w_1^2)=a^{(1)}(\tfrac{5}{2}-w_1^2), \tag{7.7a}$$

$$B_1(w_1)\simeq b_1^{(0)}S_{5/2}^{(0)}(w_1^2)=b_1^{(0)}, \tag{7.7b}$$

$$B_2(w_1)\simeq b_2^{(0)}S_{1/2}^{(2)}(w_1^2)=b_2^{(2)}(\tfrac{15}{8}-\tfrac{5}{2}w_1^2+\tfrac{1}{2}w_1^4), \tag{7.7c}$$

and

$$I_0(w_{1\alpha}a^{(1)}(\tfrac{5}{2}-w_1^2))=K_\alpha, \tag{7.8a}$$

$$I_0((w_{1\alpha}w_{1\beta}-\tfrac{1}{3}\,w_1^2\delta_{\alpha\beta})b_1^{(0)})=L_{1\alpha\beta}, \tag{7.8b}$$

$$I_0(b_2^{(2)}(\tfrac{15}{8}-\tfrac{5}{2}\,w_1^2+\tfrac{1}{2}\,w_1^4))=L_2. \tag{7.8c}$$

Multiplying these equations by $w_{1\alpha}S_{3/2}^{(1)}(w_1^2)$, $(w_{1\alpha}w_{1\beta}-\frac{1}{3}w_1^2\delta_{\alpha\beta})$, $S_{1/2}^{(2)}(w_1^2)$, respectively, and integrating with respect to $\vec{w}_1$, one finds:

$$a^{(1)}=\frac{\int d\vec{w}_1K_\alpha w_{1\alpha}S_{3/2}^{(1)}(w_1^2)}{\int d\vec{w}_1I_0(w_{1\alpha}S_{3/2}^{(1)}(w_1^2))w_{1\alpha}S_{3/2}^{(1)}(w_1^2)}, \tag{7.9}$$

$$b_1^{(0)}=\frac{\int d\vec{w}_1L_{1\alpha\beta}(w_{1\alpha}w_{1\beta}-\frac{1}{3}w_1^2\delta_{\alpha\beta})}{\int d\vec{w}_1I_0(w_{1\alpha}w_{1\beta}-\frac{1}{3}w_1^2\delta_{\alpha\beta})(w_{1\alpha}w_{1\beta}-\frac{1}{3}w_1^2\delta_{\alpha\beta})}, \tag{7.10}$$

$$b_2^{(0)}=\frac{\int d\vec{w}_1L_2S_{1/2}^{(2)}(w_1^2)}{\int d\vec{w}_1I_0(S_{1/2}^{(2)}(w_1^2))S_{1/2}^{(2)}(w_1^2)}. \tag{7.11}$$

First-hand calculations for $a^{(1)}$ and $b^{(0)}$ give the following:

$$a^{(1)}=\frac{\frac{15}{4}n(1+\frac{2}{5}\pi n\Lambda)-\frac{3}{2}\sqrt{\pi}n^2D_1}{8\sqrt{2\pi}n^2\{\lambda^*+\frac{11}{32}D_2\}}, \tag{7.12}$$

$$b_1^{(0)}=-\frac{5n(1+\frac{4}{15}\pi n\Lambda)-\frac{4}{3}\sqrt{\pi}n^2D_1}{8\sqrt{2\pi}n^2\{\lambda^*+\frac{1}{12}D_2\}}\left(\frac{m}{2k_BT}\right)^{1/2}, \tag{7.13}$$

where

$$D_1=-\sum_{i=1}^{n^*}\sigma_{li}^3g_2^{\rm eq}(\sigma_{li}^+)\Delta s_ie^{-\Delta s_i}H_s(\Delta s_i)+\sum_{j=1}^{m^*}\sigma_{rj}^3g_2^{\rm eq}(\sigma_{rj}^-)\Delta s_je^{-\Delta s_j}H_s(\Delta s_j),$$

$$D_2=\sum_{i=1}^{n^*}\sigma_{li}^3g_2^{\rm eq}(\sigma_{li}^+)\Delta s_i^2e^{-\Delta s_i}+\sum_{j=1}^{m^*}\sigma_{rj}^3g_2^{\rm eq}(\sigma_{rj}^-)\Delta s_j^2e^{-\Delta s_j},$$

$$\Delta s_i=\beta\Delta\epsilon_{li},\quad i=1,\ldots,n^*,$$

$$\Delta s_j=\beta\Delta\epsilon_{rj},\quad j=1,\ldots,m^*,$$

$$\lambda^* = \frac{1}{2}\left[\sigma_0 g_2^{\rm eq}(\sigma_0^+) + \sum_{i=1}^{n^*} \sigma_{li}^3 g_2^{\rm eq}(\sigma_{li}^+) e^{\Delta s_i} \Xi(\Delta s_i) + \sum_{j=1}^{m^*} \sigma_{rj}^3 g_2^{\rm eq}(\sigma_{rj}^-) e^{\Delta s_j} \Xi(\Delta s_j) \right],$$

$$H_s(z) = \frac{\sqrt{\pi}}{2} + e^s \Gamma\left(\frac{3}{2}, z\right), \qquad (7.14)$$

$\Gamma(r,s) = \int_s^\infty dx\, x^{r-1} e^{-x}$ is the incomplete Γ-function. Since $b_2^{(2)}$ does not contribute into transport coefficients, we did not calculate it.

In this manner, one-particle distribution function in stationary case reads:

$$f_1^{(1)} = f_1^{(0)}(1 + \phi^{(1)}), \qquad (7.15a)$$

$$\phi^{(1)} \simeq a^{(1)}\left(\tfrac{5}{2} - w_1^2\right) w_{1\alpha} \frac{\partial}{\partial r_{1\alpha}} \ln T + b_1^{(0)}\left(w_{1\alpha} w_{1\beta} - \tfrac{1}{3} w_1^2 \delta_{\alpha\beta}\right) \times \frac{\partial}{\partial r_{1\beta}} u_\alpha + b_2^{(2)}\left(\tfrac{15}{8} - \tfrac{5}{2} w_1^2 + \tfrac{1}{2} w_1^4\right) \frac{\partial}{\partial r_{1\alpha}} u_\alpha, \qquad (7.15b)$$

where $a^{(1)}$ and $b^{(2)}$ are defined by (7.12) and (7.13), correspondingly.

VIII. CALCULATION OF TRANSPORT COEFFICIENTS: SOME LIMITING CASES

General expressions for the stress tensor and heat flux vector for nonstationary process were obtained in Sec. VI. But explicit calculations were performed for only one part of it which is inhomogeneous on $f_1^{(0)}$ and local-time next to other integral terms. In the stationary case, the integral terms transfers to local-time ones. The explicit calculation of these terms becomes possible. Substituting one-particle distribution function f_1 (7.15) into the general expressions (3.5)–(3.13) and taking into account new structure for (6.6):

$$z_2 = g_2^{\rm eq}(\sigma) f_1^{(0)}(x_1;t) f_1^{(0)}(\vec{r}_1, \vec{v}_2;t)\{\phi^{(1)}(x_1;t) + \phi^{(1)}(\vec{r}_1, \vec{v}_2;t)\}, \qquad (8.1)$$

one obtains:

$$P_{\alpha\beta} = p\,\delta_{\alpha\beta} - \kappa \frac{\partial}{\partial r_{1\gamma}} u_\gamma \delta_{\alpha\beta} - 2\,\eta S_{\alpha\beta}, \qquad (8.2)$$

$$q_\alpha = -\lambda \frac{\partial}{\partial r_{1\alpha}} T, \qquad (8.3)$$

where $S_{\alpha\beta}$ is the velocities shift tensor. Explicit expressions for the transport coefficients, namely, bulk κ and shear η viscosities and thermal conductivity λ, read:

$$\kappa = \frac{4}{9} n^2 (\pi m k_B T)^{1/2} H_2, \qquad (8.4)$$

$$\eta = \frac{3}{5}\kappa + \frac{1}{2} n k_B T \left\{ 1 + \frac{8}{15}\sqrt{\pi} n H_1 \right\} b^{(0)}, \qquad (8.5)$$

$$\lambda = \frac{3k_B}{2m}\kappa + \frac{5}{4} n k_B \left(\frac{2k_B T}{m}\right)^{1/2} \left\{ 1 + \frac{4}{5}\sqrt{\pi} n H_1 \right\} a^{(1)}, \qquad (8.6)$$

where

$$b^{(0)} = -b_1^{(0)},$$

$$H_1 = \frac{\sqrt{\pi}}{2}\Lambda - \sum_{i=1}^{n^*} \sigma_{li}^3 g_2^{\rm eq}(\sigma_{li}^+) \Delta s_i e^{-\Delta s_i} \times \left\{ \frac{\sqrt{\pi}}{4} - \frac{\Delta s_i^{3/2}}{3} + \frac{1}{3} e^{\Delta s_i} \Gamma\left(\frac{5}{2}, \Delta s_i\right) \right\} + \sum_{j=1}^{m^*} \sigma_{rj}^3 g_2^{\rm eq}(\sigma_{rj}^-) \Delta s_j e^{-\Delta s_j} \times \left\{ \frac{\sqrt{\pi}}{4} - \frac{\Delta s_j^{3/2}}{3} + \frac{1}{3} e^{\Delta s_j} \Gamma\left(\frac{5}{2}, \Delta s_j\right) \right\}. \qquad (8.7)$$

Thus, the problem of transport coefficients for specific interaction potential (2.2) in our approach is solved. Finally, let us consider some limiting cases.

A. Hard spheres potential

$$\Delta\epsilon_{li} = 0, \quad \Delta s_i = 0, \quad i = 1, \ldots, n^*,$$

$$\Delta\epsilon_{rj} = 0, \quad \Delta s_j = 0, \quad j = 1, \ldots, m^*. \qquad (8.8)$$

In this case model MSPI (2.2) transfers to that for hard spheres, whereas kinetic equation (2.13) transfers to that of the SET (RET) theory. It is naturally to expect that results (8.4)–(8.6) should transfer to the well-known results of the SET theory. This assertion really takes place. With the condition (8.8) we have:

$$\Lambda \to \sigma_0^3 g_2^{\rm eq}(\sigma_0^+), \quad D_1 \to 0,$$

$$H_1 \to \frac{\sqrt{\pi}}{2}\Lambda, \quad D_2 \to 0,$$

$$H_2 \to \sigma_0^4 g_2^{\rm eq}(\sigma_0^+), \quad \Xi(0) = 0,$$

$$H_3 \to \sqrt{\pi}, \quad K_1^*(0) = 1,$$

$$\lambda^* \to \frac{1}{2}\sigma_0^2 g_2^{\rm eq}(\sigma_0^+), \quad \Gamma(3/2) = \frac{\sqrt{\pi}}{2}.$$

Then

$$a^{(1)} \to \frac{\frac{15}{4} n\left(1 + \frac{2}{5}\pi n \sigma_0^3 g_2^{\rm eq}(\sigma_0^+)\right)}{4\sqrt{2\pi} n^2 \sigma_0^2 g_2^{\rm eq}(\sigma_0^+)}, \qquad (8.9)$$

$$b^{(0)} \to \frac{5n\left(1 + \frac{4}{15}\pi n \sigma_0^3 g_2^{\rm eq}(\sigma_0^+)\right)}{4\sqrt{2\pi} n^2 \sigma_0^2 g_2^{\rm eq}(\sigma_0^+)} \left(\frac{m}{2k_B T}\right)^{1/2}, \qquad (8.10)$$

$$p\to nk_BT\left(1+\frac{2}{3}\pi n\sigma_0^3 g_2^{\mathrm{eq}}(\sigma_0^+)\right), \tag{8.11}$$

$$\kappa\to\frac{4}{9}n^2\sqrt{\pi mk_BT}\sigma_0^4 g_2^{\mathrm{eq}}(\sigma_0^+), \tag{8.12}$$

$$\eta\to\frac{3}{5}\kappa+\frac{5}{16}\left(\frac{mk_BT}{\pi}\right)^{1/2}\frac{1}{\sigma_0 g_2^{\mathrm{eq}}(\sigma_0^+)}\times\left(1+\frac{4}{15}\pi n\sigma_0^3 g_2^{\mathrm{eq}}(\sigma_0^+)\right)^2, \tag{8.13}$$

$$\lambda\to\frac{3k_B}{2m}\kappa+\frac{75}{64}\left(\frac{k_BT}{\pi m}\right)^{1/2}\frac{1}{\sigma_0 g_2^{\mathrm{eq}}(\sigma_0^+)}\times\left(1+\frac{2}{5}\pi n\sigma_0^3 g_2^{\mathrm{eq}}(\sigma_0^+)\right)^2. \tag{8.14}$$

Relations (8.12)–(8.14) obtained from (8.4)–(8.6) with taking into account (8.8), are identical to those from the SET (RET) theory which are obtained by means of the standard Chapman-Enskog procedure.

B. Square-well potential

$$\Delta\epsilon_{li}=0,\quad \Delta s_i=0,\quad i=1,\dots,n^*,\quad \Delta\epsilon_{r1}\neq 0,$$
$$\Delta\epsilon_{rj}=0,\quad \Delta s_j=0,\quad j=2,\dots,m^*,\quad \Delta s_1=\beta\epsilon. \tag{8.15}$$

In this case, initial MSPI (2.2) transfers into ''square-well'' one of the DRS (RDRS) theory. Defining $\sigma_{r1}=\sigma$, $\Delta s_1=\Delta s=\beta\Delta\epsilon_{r1}\equiv\beta\epsilon$, where ϵ is the square-well depth, and taking into account (8.15) one obtains:

$$\Lambda\to\sigma_0^3 g_2^{\mathrm{eq}}(\sigma_0^+)+\sigma^3 g_2(\sigma^-)\{e^{-\Delta s}-1\},$$

$$\lambda^*\to\frac{1}{2}\{\sigma_0^2 g_2^{\mathrm{eq}}(\sigma_0^+)+\sigma^2 g_2^{\mathrm{eq}}(\sigma^-)e^{-\Delta s}\Xi(\Delta s)\},$$

$$H_1\to\frac{\sqrt{\pi}}{2}\Lambda+\sigma^3 g_2^{\mathrm{eq}}(\sigma^-)\Delta s e^{-\Delta s}\times\left\{\frac{\sqrt{\pi}}{4}-\frac{1}{3}\Delta s^{3/2}+\frac{1}{3}\Delta s^{3/2}+\frac{1}{3}e^{\Delta s}\Gamma\left(\frac{5}{2},\Delta s\right)\right\},$$

$$H_2\to\sigma_0^4 g_2^{\mathrm{eq}}(\sigma_0^+)+\sigma^4 g_2^{\mathrm{eq}}(\sigma^-)e^{\Delta s}\Xi(\Delta s),$$

$$H_3\to\frac{\sqrt{\pi}}{2}+e^{\Delta s}\Gamma\left(\frac{3}{5},\Delta s\right),$$

$$D_1\to\sigma^3 g_2^{\mathrm{eq}}(\sigma^-)\Delta s e^{-\Delta s}H_3(\Delta s),$$

$$D_2\to\sigma^2 g_2^{\mathrm{eq}}(\sigma^-)\Delta s^2 e^{-\Delta s},$$

$$\Xi(\Delta s)=e^{\Delta s}-\frac{1}{2}\Delta s-2\int_0^\infty dx\; x^2\sqrt{x^2+\Delta s},$$

$$a^{(1)}\to\frac{\frac{15}{4}n(1+\frac{2}{5}\pi n\Lambda)+\frac{3}{2}\sqrt{\pi}n^2\sigma^3 g_2^{\mathrm{eq}}(\sigma^-)\Delta s e^{-\Delta s}H_3(\Delta s)}{8\sqrt{2\pi}n^2\{\lambda^*+\frac{11}{32}\sigma^2 g_2^{\mathrm{eq}}(\sigma^-)\Delta s^2 e^{-\Delta s}\}} \tag{8.16}$$

$$b^{(0)}\to\frac{5n(1+\frac{4}{15}\pi n\Lambda)+\frac{4}{3}\sqrt{\pi}n^2\sigma^3 g_2^{\mathrm{eq}}(\sigma^-)\Delta s e^{-\Delta s}H_3(\Delta s)}{8\sqrt{2\pi}n^2\{\lambda^*+\frac{1}{12}\sigma^2 g_2^{\mathrm{eq}}(\sigma^{-1})\Delta s^2 e^{-\Delta s}\}}\times\left(\frac{m}{2k_BT}\right)^{1/2}, \tag{8.17}$$

and

$$p\to nk_BT\left(1+\frac{2}{3}\pi n\Lambda\right), \tag{8.18}$$

$$\kappa\to\frac{4}{9}n^2\sqrt{\pi mk_BT}H_3, \tag{8.19}$$

$$\eta\to\frac{3}{5}\kappa+\frac{1}{2}nk_BT\left\{1+\frac{8}{15}\sqrt{\pi}nH_1\right\}b^{(0)}, \tag{8.20}$$

$$\lambda\to\frac{3k_B}{2m}\kappa+\frac{5}{4}nk_B\left(\frac{2k_BT}{m}\right)^{1/2}\left\{1+\frac{4}{5}\sqrt{\pi}nH_1\right\}a^{(1)}. \tag{8.21}$$

Relations for transport coefficients (8.19)–(8.21) coincide with those for DRS (RDRS) theory which were obtained by means of the standard Chapman-Enskog procedure. Of course, only the first approximation in gradients of the hydrodynamic parameters is implied everywhere.

C. Smooth long-range potential

Finally let us consider briefly the case, when

$$\Delta\epsilon_{li}\to 0,\quad \Delta\sigma_{li}\to 0,\quad i=1,\dots,n^*.\quad n^*\to\infty,$$
$$\Delta\epsilon_{rj}\to 0,\quad \Delta\sigma_{rj}\to 0,\quad j=1,\dots,m^*,\quad m^*\to\infty, \tag{8.22}$$

and an additional condition for (8.22):

$$-\frac{\Delta\epsilon_{li}}{\Delta\sigma_{li}}\to\phi_t'(\sigma_{li}), \tag{8.23a}$$

$$\frac{\Delta\epsilon_{rj}}{\Delta\sigma_{rj}}\to\phi_t'(\sigma_{rj}). \tag{8.23b}$$

From the geometrical point of view, (8.22) and (8.23) correspond to the case when MSPI (2.2) is ''merged'' into some smooth long-range potential ϕ_t at $r>\sigma$. It can be shown that in this case

$$p\to nk_BT\left(1+\frac{2}{3}\pi n\sigma_0^3 g_2^{\mathrm{eq}}(\sigma_0^+)-\frac{2}{3}\pi n^2\int dr\; r^3 g_2^{\mathrm{eq}}(r)\phi_t'(r)\right). \tag{8.24}$$

Expressions for κ, η and λ are completely similar to (8.12)–(8.14) of the SET (RET) theory with the only difference in

TABLE I. Parameters for different theories and calculations for transport coefficient η. Bottom part contains square displacement of results of SET (RET), MET (BH), DRS (RDRS) theories and our theory denoted by GDRS (i.e., generalized DRS) from MD simulation. The GDRS result is the closest to MD simulation. The same parameters were used for calculation of other transport coefficients.

SET (RET)	SIGMZ0=1.047
MET (BH)	$\sigma_0(T)=\sigma_{LJ}[1.068+0.3837(k_BT/\epsilon_{LJ})]/[1.000+0.4293(k_BT/\epsilon_{LJ})]$
DRS (RDRS)	SIGMZ0=0.891, SIGMZM=1.342, EZDRS=0.929
GDRS	SIGMZ0=0.940, SIGMZM=1.960, $n_p=3$, $m_p=9$, $n^*=2$, $m^*=6$

MD	SET (RET)	MED (BH)	DRS (RDRS)	GDRS
0.0	0.01250	0.00794	0.000217	0.000206

the form for $g_2^{eq}(\sigma_0^+)$. In SET (RET), $g_2^{eq}(\sigma_0^+)$ is a binary equilibrium correlation function of hard spheres on contact, whereas here it is the binary equilibrium correlation function of a system with the interaction potential of the hard spheres type plus a long ''tail'' $\phi_t, r>\sigma_0$. Thus, one obtains the final relations for p (8.24) and κ, η, and λ of the KMFT theory [19].

IX. NUMERICAL CALCULATIONS

First of all, let us remember that in the theory under consideration we deal with the multistep potential of interaction (2.2). If we have any information about real (smooth, of course) potential of interaction, we should deal with a large number of definition parameters. However, when interaction potential is known, the number of independent master parameters is greatly reduced. That is the necessary condition, because a model interaction potential should approximate the real potential more or less correctly. The first question appearing here is how to represent an initial smooth interaction potential by a multistep one. Let us consider one possible way of definition in which all distances between walls of the same kind are equal, i.e.: $\Delta\sigma_{li}=\text{const}$, $i=1,\ldots,n^*$, $\Delta\sigma_{rj}=\text{const}$, $j=1,\ldots,m^*$. Then, to define the model interaction potential one needs to set the position of the hard sphere wall σ_0, the position of the most removed attractive wall σ_{max} ($\sigma_{max}=\sigma_{r_{m^*}}$), the number of short lengths dividing repulsive area $[\sigma_0,\sigma_{mean}]$ n_p, and the number of short lengths dividing attractive area $[\sigma_{mean},\sigma_{max}]$ m_p, where σ_{mean} is the minimum position of a real interaction potential. Now MSPI is built. Numbers of repulsive n^* and attractive m^* walls are uniquely determined via numbers of dividing lengths n_p and m_p. In this representation of a real interaction potential by

TABLE II. Transport coefficients κ, η, and λ calculated within different theories.

Bulk viscosity κ (10^{-4} Pa sec)				
ρ, g/cm^3	SET	MET	DRS	GDRS
1.4327	0.33387	0.26739	0.43672	0.43371
1.4180	0.32270	0.25654	0.40946	0.40538
1.2777	0.22253	0.17126	0.25314	0.24708
1.1621	0.16222	0.12277	0.17466	0.16928
0.8017	0.05092	0.03919	0.05914	0.05653
Shear viscosity η (10^{-3} Pa sec)				
ρ, g/cm^3	SET	MET	DRS	GDRS
0.2970	0.27460	0.22428	028794	0.28953
0.2620	0.26633	0.21627	0.27144	0.27189
0.1734	0.19113	0.15248	0.17491	0.17248
0.1255	0.14577	0.11622	0.12627	0.12383
0.5790	0.06014	0.05210	0.05134	0.05087
Thermal conductivity λ [W/(m K)]				
T, K	SET	MET	DRS	GDRS
83.90	0.22107	0.18186	0.17078	0.16850
86.50	0.21468	0.17566	0.16187	0.15877
104.50	0.15622	0.12602	0.10790	0.10325
119.56	0.12080	0.09763	0.08029	0.07603
147.10	0.05254	0.04608	0.03484	0.03309

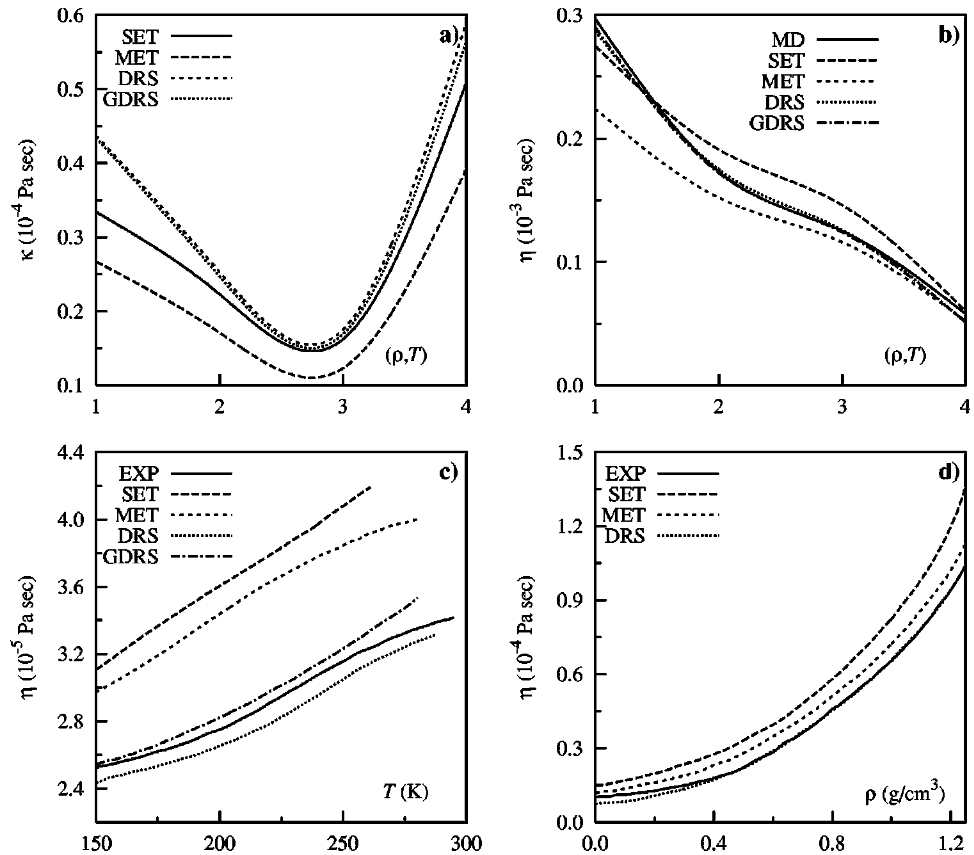

FIG. 3. Transport coefficients for argon. (a) bulk viscosity κ along the liquid-vapor curve. x-axis is in units of $\rho(\mathrm{g/cm^3})$, namely: 1.4327, 1.4180, 1.1621, and 0.8017 for 1, 2, 3, and 4, respectively. (b) shear viscosity η. x-axis is in units of $[\rho(\mathrm{g/cm^3}), T(\mathrm{K})]$, namely: $\rho_1 = 1.43$, $T_1 = 83.9$, $\rho_2 = 1.28$, $T_2 = 104.5$, $\rho_3 = 1.16$, $T_3 = 119.56$, and $\rho_4 = 0.802$, $T_4 = 147.1$. (c) $\eta = \eta(T)$ at $\rho = \rho_{\mathrm{cr}}$; (d) $\eta = \eta(\rho)$ at $T = 139.7$ K. Experimental data plotted in (c) and (d) are taken from [28].

MSPI, one realizes original entwining of model potential around the real one.

The second question is the problem of optimal dividing, i.e., how to define the parameters σ_0, $\sigma_{\max}$, n_p, m_p so that fair results are obtained already in the first approximation. We tried to solve this problem numerically.

Numerical computations of transport coefficients were carried out for argon with the Lennard-Jones potential

$$\phi_{\mathrm{real}} \simeq \phi_{\mathrm{LJ}} = 4\epsilon_{\mathrm{LJ}}\left[\left(\frac{\sigma_{\mathrm{LJ}}}{r}\right)^{12} - \left(\frac{\sigma_{\mathrm{LJ}}}{r}\right)^{6}\right], \tag{9.1}$$

where $\sigma_{\mathrm{LJ}} = 3.405$ Å, $\epsilon_{\mathrm{LJ}}/k_B = 119.8$ K.

The starting point in the numerical analysis of transport coefficients of our theory are relations (8.4)–(8.6) with additional equation for binary equilibrium correlation function g_2^{eq} of a system with potential in a form of multistep function. In our calculation we used for g_2^{eq} the following approximation:

$$g_2^{\mathrm{eq}}(r) = g_2^{(0)}(r)\exp\{-\beta\phi(r)\}, \tag{9.2a}$$

$$\phi(r) \equiv \varphi(r), \tag{9.2b}$$

where $g_2^{(0)}(r)$ is the binary equilibrium correlation function of hard spheres of diameter σ_0. Its analytical expression is well known [27].

First, one calculates the transport coefficients along the gas-liquid saturation curve. There were five points of calculation ($\rho_i = m n_i$, T_i, $i = 1, \ldots, 5$) along the curve of saturation for which such a transport coefficient as the shear viscosity η is known from the MD simulation [19]. MSPI parameters n_p, m_p, SIGMZ0 $= \sigma_0/\sigma_{\mathrm{LJ}}$, SIGMZM $= \sigma_{\max}/\sigma_0$ were defined from the minimum of square displacement of the theory from corresponding MD results. Parameters of the DRS (RDRS) theory were defined in much the same way: SIGMZ0 $= \sigma_0/\sigma_{\mathrm{LJ}}$, SIGMZM $= \sigma/\sigma_0$, EDRS $= \epsilon/\epsilon_{\mathrm{LJ}}$, as well as for SET (RET) theory: SIGMZ0 $= \sigma_0/\sigma_{\mathrm{LJ}}$. Table I shows the results. Table II shows all results of calculation of transport coefficients by different theories. Their comparison with experimental data and MD simulations are presented in Figs. 3 and 4. It is clearly seen that GDRS results practically coincide with the experimental data in a wide range of densities and temperatures.

X. CONCLUDING REMARKS

Let us discuss areas of application of kinetic equation (2.13). We should remember conditions of general derivation of this equation within the frame of Bogolubov-Zubarev approach [29,30]. The specific demand to the geometry of a potential and to the density of a system is that the mean free path l_f should be greatly smaller than a minimal clearance between the walls $\Delta\sigma$. Hence, one should expect that larger distance between walls and higher density give smaller error

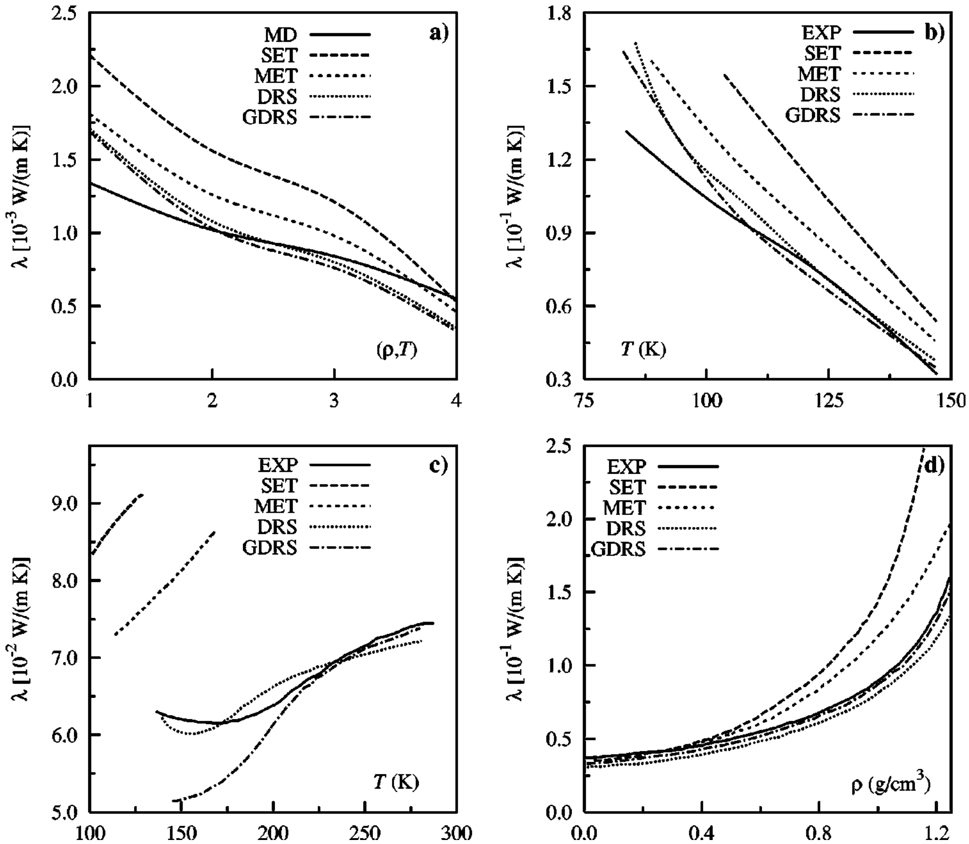

FIG. 4. Thermal conductivity λ of argon. (a) MD simulations and different theories calculations in the same points as in Fig. 3(b). (b) $\lambda=\lambda(T)$ at $\rho=2\rho_{\rm cr}$, different theories are compared with experimental data. (c) $\lambda=\lambda(T)$ at $\rho=2\rho_{\rm cr}$; (d) $\lambda=\lambda(\rho)$ at $T=298$ K. All experimental data plotted in this figure are taken from [28].

in the kinetic equation. This error is introduced by the limiting condition for interaction time $|\tau|\rightarrow+0$ [30]. On the other hand, next to the theory error there is an error caused by a deviation of the multistep potential of interaction from a real one. Real potential is smooth and the error is smaller when the clearance between walls is smaller. In the limit (8.22) this error is the smallest. One can observe that these two types of errors have opposite tendencies. So, to apply the obtained kinetic equation to systems with real smooth interparticle interaction potential in view of a geometry of MSPI one should find a compromise solution. First of all, MSPI should approximate real potential, better of worse. At the same time the condition $l_f \ll \Delta\sigma$ must be obeyed. This raises the question of optimal dividing of a real potential of interaction into a multistep one. Density decreasing makes impossible to obtain the Boltzmann analog from the considered equation in the limit $n\rightarrow 0$. Let us evaluate numerically. Suppose σ_0 is the position of a hard sphere, $\Delta\sigma$ is the minimal distance between walls, $\sigma_{\rm max}\simeq 2\sigma_0$ is the location of the most removed attractive wall. It is well known from the theory of rarefied gases [1,31] that the mean free path $l_f \approx 1/\sqrt{2}\pi n\sigma_{\rm max}^2$. In dense gases it decreases in the first approximation by $g_2^{\rm eq}(\sigma_0^+)$ times where $g_2^{\rm eq}(\sigma_0^+)$ is the contact value of binary equilibrium correlation function [23]. Thus, $l_f \approx 1/4\sqrt{2}\pi n\sigma_0^2 g_2^{\rm eq}(\sigma_0^+)$. Introducing the dimensionless density $\Delta=\frac{1}{6}\pi n\sigma_0^3$, one obtains:

$$\frac{\Delta\sigma}{\sigma_0} \gg \frac{1}{24\sqrt{2}\pi\Delta g_2^{\rm eq}(\sigma_0^+)}=\gamma. \qquad (10.1)$$

For $\Delta=0.25$ and $g_2^{\rm eq}(\sigma_0^+)\simeq 2.5$ one obtains $\gamma\approx 1/25$. As far as initial preconditions of the theory are not obeyed, then in the limit (8.22) the theory error is maximal. However, kinetic equation transfers then into the equation of the kinetic mean-field theory [19].

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