QUASI-EQUILIBRIUM CLOSURE HIERARCHIES FOR THE BOLTZMANN EQUATION

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Abstract

Explicit method of constructing of approximations (Triangle Entropy Method) is developed for strongly nonequilibrium problems of Boltzmann's–type kinetics, i.e. when standard moment variables are insufficient. This method enables one to treat any complicated nonlinear functionals that fit the physics of a problem (such as, for example, rates of processes) as new independent variables.

The method is applied to the problem of derivation of hydrodynamics from the Boltzmann equation. New macroscopic variables are introduced (moments of the Boltzmann collision integral, or collision moments). They are treated as independent variables rather than as infinite moment series. This approach gives the complete account of rates of scattering processes. Transport equations for scattering rates are obtained (the second hydrodynamic chain), similar to the usual moment chain (the first hydrodynamic chain). Using the triangle entropy method, three different types of the macroscopic description are considered. The first type involves only moments of distribution functions, and results coincide with those of the Grad method in the Maximum Entropy version. The second type of description involves only collision moments. Finally, the third type involves both the moments and the collision moments (the mixed description). The second and the mixed hydrodynamics are sensitive to the choice of the collision model. The second hydrodynamics is equivalent to the first hydrodynamics only for Maxwell molecules, and the mixed hydrodynamics exists for all types of collision models excluding Maxwell molecules. Various examples of the closure of the first, of the second, and of the mixed hydrodynamic chains are considered for the hard spheres model. It is shown, in particular, that the complete account of scattering processes leads to a renormalization of transport coefficients.

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Contents

1 Triangle Entropy Method

Many works are devoted to the problem of constructing approximate solutions of the Boltzmann kinetic equation, and to obtaining a closed macroscopic description. Hilbert [14], Chapman-Enskog [16] and Grad [19] methods, as well as their modifications are most commonly used for solving this problem. In the present section, which is of introductory character, we shall mean for certainty the Boltzmann kinetic equation for simple gas whose state (in the microscopic sense) is described by the one-particle distribution function $f(\mathbf{v}, \mathbf{x}, t)$ depending on the velocity vector $\mathbf{v} = \{v_k\}_{k=1}^3$, the spatial position $x = \{x_k\}_{k=1}^3$ and time t. The the Boltzmann equation describes the evolution of f and in the absence of external forces is

$$\partial_t f + v_k \partial_k f = St(f, f), \tag{1}$$

where $\partial_t \equiv \partial/\partial t$ is the time partial derivative, $\partial_k \equiv \partial/\partial x_k$ is partial derivative with respect to k-th component of $\mathbf{x}$, here summation in two repeating indices is assumed, and $St(f, f)$ is the collision integral (its concrete form is of no importance for the present, just note that it is functional-integral operator quadratic with respect to f).

The Boltzmann equation possesses two properties principal for the subsequent reasoning.

1. There are exactly five scalar functions $\psi_\alpha(\mathbf{v})$(additive collision invariants), $1, \mathbf{v}, \mathbf{v}^2$ such that for any their linear combination with coefficients depending on $\mathbf{x}, t$ and for arbitrary f ensuring existence of the integrals the following equality is true:

$$\int \sum_{\alpha=1}^{5} a_\alpha(\mathbf{x}, t) \psi_\alpha(\mathbf{v}) St(f, f) d\mathbf{v} = 0. \tag{2}$$

2. The equation (1) possesses global Lyapunov functional: the H-function,

$$H(t) \equiv H[f] = \int f(\mathbf{v}, \mathbf{x}, t) \ln f(\mathbf{v}, \mathbf{x}, t) d\mathbf{v} d\mathbf{x}, \tag{3}$$

the derivative of which by virtue of the equation (1) is non-positive under appropriate boundary conditions:

$$dH(t)/dt \leq 0 \tag{4}$$

and turns into zero in the only point of the space, corresponding to the spatially uniform Maxwell distribution function $f_0(\mathbf{v})$. The H-function is unique within the accuracy of adding to it of a moment with respect to f of arbitrary linear combination of additive collision invariants.

Grad's method [19] and its variants result in constructing of closed systems of equations for macroscopic parameters are represented by moments (or, in more general consideration, linear functionals) of the distribution function f (hence their alternative name is "moment methods"). The entropy maximum method [11] is of particular importance for the subsequent reasoning. It consists in the following. A finite set of the moments describing macroscopic state is chosen. Then, the distribution function of the quasi-equilibrium state under given values of the chosen moments is determined, i.e. the problem is solved

$$H[f] \to \min, \text{ for } \hat{M}_i[f] = M_i, \quad i = 1, \ldots, k, \tag{5}$$

where $\hat{M}_i[f]$ are linear functionals with respect to f; M_i are the corresponding values of the chosen set of k macroscopic parameters. The obtained quasi-equilibrium distribution function $f^*(\mathbf{v}, M(\mathbf{x}, t))$, $M = \{M_1, \dots, M_k\}$, parametrically depends on M_i, its dependence on space $\mathbf{x}$ and on time t being represented only by $M(\mathbf{x}, t)$. Then the obtained f^* is substituted into the Boltzmann equation (1).

As a result we have closed systems of equations with respect to $M_i(\mathbf{x}, t)$, $i = 1, \dots, k$:

$$\partial_t M_i + \hat{M}_i[\mathbf{v}_k \partial_k f^*(\mathbf{v}, M)] = \hat{M}_i[St(f^*(\mathbf{v}, M), f^*(\mathbf{v}, M))]. \tag{6}$$

The following heuristic explanation [6, 7, 11, 15] can be given to the entropy method. A state of the gas can be described by a finite set of moments on some temporal scale θ only if all the other ("fast") moments of the distribution function during some characteristic time $\tau, \tau << \theta$, relax to their values determined by the chosen set of "slow" moments, while the latter almost do not change during the time τ. In the process of the fast relaxation the H-function decreases, and in the end of this fast relaxation process a quasi-equilibrium state sets in with a distribution function being solution of the problem (5). Then "slow" moments relax to the equilibrium state by virtue of (6).

The entropy method has a number of advantages in comparison with the classical Grad method [2]. Firstly, being not necessarily restricted to any specific system of orthogonal polynomials, and leading to solving an optimization problem, it is more convenient from the technical point of view. Secondly, and what is more important, the resulting quasi-equilibrium H-function, $H^*(M) = H[f^*(\mathbf{v}, M)]$, decreases due of the moment equations (6).

Let us note one common disadvantage of all the moment methods, and, in particular, of the entropy method. Macroscopic parameters, for which these methods enable to obtain closed systems, must be moments of the distribution function. On the other hand, it is easy to find examples when the interesting macroscopic parameters are not linear functionals of the distribution function. In the case of simple gas those are the integrals of velocity polynomials with respect to the collision integral $St(f, f)$ of (1), for chemically reacting mixture those are the reaction rates and so on. If the characteristic relaxation time of such non-linear macroscopic parameters is comparable with that of the "slow" moments, then they should be included into the list of "slow" variables on the same footing.

In this paper for constructing closed systems of equations for non-linear (in a general case) macroscopic variables the triangle entropy method proposed in [8, 9, 10] is used. Let us describe the scheme of this method after the example of the equation (1).

Let a set of $\hat{M}[f] = \left\{\hat{M}_1[f], \dots, \hat{M}_k[f]\right\}$ linear, and $\hat{N}[f] = \left\{\hat{N}_1[f], \dots, \hat{N}_l[f]\right\}$ nonlinear (in a general case) macroscopic variables be chosen. Then, just as for the problem (5), the first quasi-equilibrium approximation is constructed under fixed values of the linear macroscopic parameters M:

$$H[f] \to \min \ \text{ for } \hat{M}_i[f] = M_i, \ i = 1, \dots, k, \tag{7}$$

and the resulting distribution function is $f^*(\mathbf{v}, M)$. After that, we seek the true distribution function in the form,

$$f = f^*(1 + \varphi), \tag{8}$$

where φ is a deviation from the first quasi-equilibrium approximation. In order to determine the latter, the second quasi-equilibrium approximation is constructed. Let us denote

$\Delta H[f^*, \varphi]$ as the quadratic term in the expansion of the H-function into powers of φ in the neighbourhood of the first quasi-equilibrium state f^*. The distribution function of the second quasi-equilibrium approximation is the solution to the problem,

$$\begin{aligned}&\Delta H[f^*, \varphi] \to \min \text{ for}\\ &\hat{M}[f^* \varphi] = 0, \quad i = 1, \dots, k\\ &\Delta \hat{N}_j[f^*, \varphi] = \Delta \hat{N}_j, \quad j = 1, \dots, l,\end{aligned} \tag{9}$$

where $\Delta \hat{N}_j$ are linear operators characterizing the linear with respect to φ deviation of (nonlinear) macroscopic parameters N_j from their values, $N_j^* = \hat{N}_j[f^*]$, in the first quasi-equilibrium state. The obtained distribution function,

$$f = f^*(\mathbf{v}, M)(1 + \varphi^{**}(\mathbf{v}, M, \Delta N)) \tag{10}$$

is used to construct the closed system of equations for the macroparameters M, and ΔN.

Further in this section some examples of using the triangle entropy method for chemically non-reacting gases are considered. Applications of the triangle entropy method to chemically reacting gases see in [10].

Finally, let us note that the entropy and triangle entropy methods are particular cases of elimination of rapid variables by means of the Lyapunov function (general statements and detailed analysis of this problem for Pauli equation see in [6]).

2 Linear Macroscopic parameters

Let us consider the simplest example of using the triangle entropy method, when all the macroscopic parameters both of the first and of the second quasi-equilibrium states are the moments of the distribution function.

2.1 Quasi-equilibrium projector

Let $\mu_1(\mathbf{v}), \dots, \mu_k(\mathbf{v})$ be the microscopic densities of the moments $M_1(\mathbf{x}, t), \dots, M_k(\mathbf{x}, t)$ determining the first quasi-equilibrium state,

$$M_i(\mathbf{x}, t) = \int \mu_i(\mathbf{v}) f(\mathbf{v}, \mathbf{x}, t) d\mathbf{v}, \tag{11}$$

and, let $\nu_1(\mathbf{v}), \dots, \nu_l(\mathbf{v})$ be the microscopic densities of the moments $N_1(\mathbf{x}, t), \dots, N_l(\mathbf{x}, t)$ determining together with (1) the second quasi-equilibrium state,

$$N_i(\mathbf{x}, t) = \int \nu_i(\mathbf{v}) f(\mathbf{v}, \mathbf{x}, t) d\mathbf{v}. \tag{12}$$

The choice of the set of the moments of the first and second quasi-equilibrium approximations depends on a specific problem. The only natural restriction being always imposed on the distribution function is the normalization condition. Further on we will suppose that the microscopic density $\mu_0 \equiv 1$ corresponding to that condition is always included in the list of microscopic densities of the moments of the first quasi-equilibrium state ($\mu_1 = \mu_0 = 1$). The distribution function of the first quasi-equilibrium state results from solving the optimization problem,

$$H[f]=\int f(\mathbf{v})\ln f(\mathbf{v})d\mathbf{v}\to\min \tag{13}$$

for

$$\int\mu_i(\mathbf{v})f(\mathbf{v})d\mathbf{v}=M_i, i=1,\dots,k.$$

Let us denote by $M=\{M_1,\dots,M_k\}$ the vector of moments of the first quasi-equilibrium state, and by $f^*(\mathbf{v},M)$ let us denote the solution of the problem (13).

The distribution function of the second quasi-equilibrium state is sought for in the form,

$$f=f^*(\mathbf{v},M)(1+\varphi). \tag{14}$$

Expanding the H-function (3) in the neighbourhood of $f^*(\mathbf{v},M)$ into powers of φ to second order, we obtain,

$$\Delta H(\mathbf{x},t)\equiv\Delta H[f^*,\varphi]=H^*(M)+\int f^*(\mathbf{v},M)\ln f^*(\mathbf{v},M)\varphi(\mathbf{v})d\mathbf{v}+ \\ +\frac{1}{2}\int f^*(\mathbf{v},M)\varphi^2(\mathbf{v})d\mathbf{v}, \tag{15}$$

where $H^*(M)=H[f^*(\mathbf{v},M)]$ is the value of the H-function in the first quasi-equilibrium state.

When searching for the second quasi-equilibrium state, it is necessary that the true values of the moments M coincide with their values in the first quasi-equilibrium state, i.e.,

$$M_i=\int\mu_i(\mathbf{v})f^*(\mathbf{v},M)(1+\varphi(\mathbf{v}))d\mathbf{v}=\int\mu_i(\mathbf{v})f^*(\mathbf{v},M)d\mathbf{v}=M_i^*, i=1,\dots,k. \tag{16}$$

In other words, the set of the uniform restrictions on φ in the problem (9),

$$\int\mu_i(\mathbf{v})f^*(\mathbf{v},M)\varphi(\mathbf{v})d\mathbf{v}=0, i=1,\dots,k, \tag{17}$$

ensures a shift (change) of the first quasi-equilibrium state only due to introducing the new moments $N_1,\dots,N_l$ in addition to M. In order to take this condition into account automatically, let us introduce the following structure of a Hilbert space:

1. Define the scalar product

$$(\psi_1,\psi_2)=\int f^*(\mathbf{v},M)\psi_1(\mathbf{v})\psi_2(\mathbf{v})d\mathbf{v}. \tag{18}$$

2. Let E_μ be the linear envelope of the set of moment densities $\{\mu_1(\mathbf{v}),\dots,\mu_k(\mathbf{v})\}$. Let us construct a basis of E_μ $\{e_1(\mathbf{v}),\dots,e_r(\mathbf{v})\}$ orthonormal in the sense of the scalar product (18):

$$(e_i,e_j)=\delta_{ij}, \tag{19}$$

$i,j=1,\dots,r;\delta_{ij}$ is the Kronecker symbol.

3. Define a projector $\hat{P}^*$ on the first quasi-equilibrium state,

$$\hat{P}^*\psi=\sum_{i=1}^{r}e_i(e_i,\psi). \tag{20}$$

The projector $\hat{P}^*$ is orthogonal: for any pair of functions ψ_1, ψ_2,

$$(\hat{P}^*\psi_1, (\hat{1} - \hat{P}^*)\psi_2) = 0, \tag{21}$$

where $\hat{1}$ is the unit operator. Then the condition (17) means that

$$\hat{P}^*\varphi = 0, \tag{22}$$

and the expression for the quadratic part of the H-function (15) takes the form,

$$\Delta H[f^*, \varphi] = H^*(M) + (\ln f^*, \varphi) + (1/2)(\varphi, \varphi). \tag{23}$$

Now, let us note that the function $\ln f^*$ is invariant with respect to action of the projector $\hat{P}^*$:

$$\hat{P}^* \ln f^* = \ln f^*. \tag{24}$$

This directly follows from the solution of the problem (13) using of the method of Lagrange multipliers:

$$f^* = \exp \sum_{i=1}^{k} \lambda_i(M)\mu_i(\mathbf{v}),$$

where $\lambda_i(M)$ are Lagrange multipliers. Thus, if the condition (22) is satisfied, then from (21) and (24) it follows that

$$(\ln f^*, \varphi) = (\hat{P}^* \ln f^*, (\hat{1} - \hat{P}^*)\varphi) = 0.$$

Condition (22) is satisfied automatically, if ΔN_i are taken as follows:

$$\Delta N_i = ((\hat{1} - \hat{P}^*)\nu_i, \varphi), i = 1, \dots, l. \tag{25}$$

Thus, the problem (9) of finding the second quasi-equilibrium state reduces to

$$\begin{aligned} \Delta H[f^*, \varphi] - H^*(M) = (1/2)(\varphi, \varphi) \to \min \text{ for} \\ ((\hat{1} - \hat{P}^*)\nu_i, \varphi) = \Delta N_i, \quad i = 1, \dots, l. \end{aligned} \tag{26}$$

Note that it is not strictly necessary to introduce the structure of the Hilbert space. Moreover that may be impossible, since the “distribution function” and the “microscopic moment densities” are, strictly speaking, elements of different (conjugate one to another) spaces, which may be not reflexive. However, in the examples considered below the mentioned difference is not manifested.

In the remainder of this section we demonstrate how the triangle entropy method is related to Grad’s moment method.

2.2 Ten-moment Grad approximation.

Let us take the five additive collision invariants as moment densities of the first quasi-equilibrium state:

$$\mu_1 = 1;\ \mu_{1+k} = v_k\,(k = 1, 2, 3);\ \mu_5 = mv^2/2, \tag{27}$$

where v_k are Cartesian components of the velocity, and m is particle's mass. Then the solution to the problem (13) is the local Maxwell distribution function $f^{(0)}(\mathbf{v},\mathbf{x},t)$:

$$f^{(0)} = n(\mathbf{x},t)\left(\frac{2\pi k_B T(\mathbf{x},t)}{m}\right)^{-3/2} \exp\left\{-\frac{m(\mathbf{v}-\mathbf{u}(\mathbf{x},t))^2}{2k_B T(\mathbf{x},t)}\right\}, \tag{28}$$

where $n(\mathbf{x},t) = \int f(\mathbf{v})d\mathbf{v}$ is local gas density, $\mathbf{u}(\mathbf{x},t) = n^{-1}(\mathbf{x},t)\int f(\mathbf{v})\mathbf{v}d\mathbf{v}$ is local flow density, $T(\mathbf{x},t) = \int f(\mathbf{v})\frac{m(\mathbf{v}-\mathbf{u}(\mathbf{x},t))^2}{3k_B n(\mathbf{x},t)}d\mathbf{v}$ is local temperature, k_B is the Boltzmann constant.

Orthonormalization of the set of moment densities (27) with the weight (28) gives

$$\begin{aligned} e_1 &= [5k_BT - m(\mathbf{v}-\mathbf{u})^2]/[(10n)^{1/2}k_BT], \\ e_{1+k} &= m^{1/2}(v_k-u_k)/(nk_BT)^{1/2}, k=1,2,3, \\ e_5 &= m(\mathbf{v}-\mathbf{u})^2/[(15n)^{1/2}k_BT]. \end{aligned} \tag{29}$$

For the moment densities of the second quasi-equilibrium state let us take,

$$\nu_{ik} = mv_iv_k,\ i,k = 1,2,3. \tag{30}$$

Then

$$(\hat{1}-\hat{P}^{(0)})\nu_{ik} = m(v_i-u_i)(v_k-u_k) - \frac{1}{3}\delta_{ik}m(\mathbf{v}-\mathbf{u})^2, \tag{31}$$

and, since $((\hat{1}-\hat{P}^{(0)})\nu_{ik},(\hat{1}-\hat{P}^{(0)})\nu_{ls}) = (\delta_{il}\delta_{ks}+\delta_{kl}\delta_{is})Pk_BT/m$, where $P = nk_BT$ is the pressure, and $\sigma_{ik} = (f,(\hat{1}-\hat{P}^{(0)})\nu_{ik})$ is the traceless part of stress tensor, then from (14), (27), (28), (31) we obtain the distribution function of the second quasi-equilibrium state in the form

$$f = f^{(0)}\left(1+\frac{\sigma_{ik}m}{2Pk_BT}\left[(v_i-u_i)(v_k-u_k)-\frac{1}{3}\delta_{ik}(\mathbf{v}-\mathbf{u})^2\right]\right) \tag{32}$$

which is precisely the distribution function of the ten-moment Grad approximation [11, 19] (let us recall that here summation in two repeated indices is assumed).

2.3 Thirteen-moment Grad approximation

In addition to (27), (30) let us extend the list of moment densities of the second quasi-equilibrium state with the functions

$$\xi_i = mv_iv^2/2,\ i=1,2,3. \tag{33}$$

The corresponding orthogonal complements to the projection on the first quasi-equilibrium state are

$$(\hat{1}-\hat{P}^{(0)})\xi_i = \frac{m}{2}(v_i-u_i)\left((\mathbf{v}-\mathbf{u})^2-\frac{5k_BT}{m}\right). \tag{34}$$

The moments corresponding to the densities $(\hat{1}-\hat{P}^{(0)})\xi_i$ are the components of the heat flux vector q_i:

$$q_i = (\varphi,(\hat{1}-\hat{P}^{(0)})\xi_i). \tag{35}$$

Since

$$((\hat{1}-\hat{P}^{(0)})\xi_i,(\hat{1}-\hat{P}^{(0)})\nu_{lk})=0$$

,

for any i,k,l, then the constraints

$$((\hat{1}-\hat{P}^{(0)})\nu_{lk},\varphi)=\sigma_{lk},((\hat{1}-\hat{P}^{(0)})\xi_i,\varphi)=q_i$$

in the problem (26) are independent, and Lagrange multipliers corresponding to ξ_i are

$$\frac{1}{5n}\left(\frac{k_BT}{m}\right)^2 q_i. \tag{36}$$

Finally, taking into account (27), (32), (34), (36), we find the distribution function of the second quasi-equilibrium state in the form

$$f=f^{(0)}\left(1+\frac{\sigma_{ik}m}{2Pk_BT}\left((v_i-u_i)(v_k-u_k)-\frac{1}{3}\delta_{ik}(\mathbf{v}-\mathbf{u})^2\right)+\right.$$
$$\left.+\frac{q_im}{Pk_BT}(v_i-u_i)\left(\frac{m(\mathbf{v}-\mathbf{u})^2}{5k_BT}-1\right)\right), \tag{37}$$

which coincides with the thirteen-moment Grad distribution function [11, 19].

Let us remark on the thirteen-moment approximation. From (37) it follows that for large enough negative values of (v_i-u_i) the thirteen-moment distribution function becomes negative. This peculiarity of the thirteen-moment approximation is due to the fact that the moment density ξ_i is odd power of v_i. In order to eliminate this difficulty, one may from the very beginning consider that in a finite volume the square of velocity of a particle does not exceed a certain value v^2_{lim}, which is finite owing to the finiteness of the total energy, and q_i is such that when changing to infinite volume $q_i\to 0, v^2_{\text{lim}}\to\infty$ and $q_i(v_i-u_i)(\mathbf{v}-\mathbf{u})^2$ is finite.

On the other hand, the solution to the optimization problem (5) does not exist (is not normalizable), if the highest-order velocity polynomial is odd, as it is for the 13-moment Grad moment system.

Approximation (32) yields $\Delta H(5)$ as follows:

$$\Delta H=H^{(0)}+n\frac{\sigma_{ik}\sigma_{ik}}{4P^2}, \tag{38}$$

while ΔH corresponding to (37) is,

$$\Delta H=H^{(0)}+n\frac{\sigma_{ik}\sigma_{ik}}{4P^2}+n\frac{q_kq_k\rho}{5P^3}, \tag{39}$$

where $\rho=mn$, and $H^{(0)}$ is the local equilibrium value of the H-function

$$H^{(0)}=\frac{5}{2}n\ln n-\frac{3}{2}n\ln P-\frac{3}{2}n\left(1+\ln\frac{2\pi}{m}\right). \tag{40}$$

These expressions coincide with the corresponding expansions of the quasi-equilibrium H-functions obtained by the entropy method, if microscopic moment densities of the first quasi-equilibrium approximation are chosen as $1, v_i$, and v_iv_j, or as $1, v_i$, v_iv_j, and v_iv^2. As it was noted in [11], they differs from the H-functions obtained by the Grad method (without the maximum entropy hypothesis), and in contrast to the latter they give proper entropy balance equations.

The transition to the closed system of equations for the moments of the first and of the second quasi-equilibrium approximations is accomplished by proceeding from the chain of the Maxwell moment equations, which is equivalent to the Boltzmann equation. Substituting f in the form of $f^{(0)}(1+\varphi)$ into equation (1), and multiplying by $\mu_i(\mathbf{v})$, and integrating over $\mathbf{v}$, we obtain

$$\begin{aligned}&\partial_t(1,\hat{P}^{(0)}\mu_i(\mathbf{v}))+\partial_t(\varphi(\mathbf{v}),\mu_i(\mathbf{v}))+\partial_k(v_k\varphi(\mathbf{v}),\mu_i(\mathbf{v}))+\\&+\partial_k(v_k,\mu_i(\mathbf{v}))=M_{\mathrm{St}}[\mu_i,\varphi].\end{aligned}\tag{41}$$

Here

$$M_{\mathrm{St}}[\mu_i,\varphi]=\int St(f^{(0)}(1+\varphi),f^{(0)}(1+\varphi))\mu_i(\mathbf{v})d\mathbf{v}$$

is a moment (corresponding to the microscopic density) $\mu_i(\mathbf{v})$ with respect to the collision integral (further we will term M_{St} the collision moment). Now, if one uses f given by equations (32), and (37), then the system (41) gives closed ten- and thirteen-moment Grad equations, respectively, whereas only linear terms in φ should be kept when calculating M_{St}.

Let us note some limitation of the truncating the chain (41) by means of the quasi-equilibrium distribution functions (32) and (37) (or for any other depending on the moments of the distribution functions only). When such closure is used, it is assumed implicitly that the collision moments in the right hand side of (41) “rapidly” relax to their values determined by “slow” (quasi-equilibrium) moments. Collision moments are, generally speaking,independent variables. This peculiarity of the chain (41), resulting from non-linear character of the Boltzmann equation, distinguishes it essentially from the other hierarchy equations of statistical mechanics (for example, from the BBGKY chain [3] which follows from the linear Liouville equation). Thus, equations (41) are not closed twice: into the left hand side of the equation for the i-th moment enters the $(i+1)$-th moment, and the right hand side contains additional variables: collision moments.

A consequent way of closure of (41) should address both sets of variables (moments and collision moments) as independent variables. The triangle entropy method enables to do this.

3 Transport Equations for Collision Moments in the Neighbourhood of Local Equilibrium. Second and Mixed Hydrodynamic Chains

In this section we derive equations of motion for the collision moments. It proves convenient to use the following form of the collision integral $St(f,f)$:

$$St(f,f)(\mathbf{v})=\int\hat{w}(\mathbf{v_1'},\mathbf{v}'|\mathbf{v},\mathbf{v_1})\left(f(\mathbf{v}')f(\mathbf{v_1'})-f(\mathbf{v})f(\mathbf{v}_1)\right)d\mathbf{v}'d\mathbf{v_1'}d\mathbf{v_1},\tag{42}$$

where $\mathbf{v}$ and $\mathbf{v}_1$ are velocities of the two colliding particles before the collision, $\mathbf{v}'$ and $\mathbf{v_1'}$ are their velocities after the collision, $\hat{w}$ is a kernel responsible for the post-collision relations $\mathbf{v}'(\mathbf{v},\mathbf{v}_1)$ and $\mathbf{v_1'}(\mathbf{v},\mathbf{v}_1)$, momentum and energy conservation laws being taken into account in $\hat{w}$ by means of corresponding δ-functions. The kernel $\hat{w}$ has the following symmetry property with respect to its arguments:

$$\hat{w}(\mathbf{v_1'},\mathbf{v}'|\mathbf{v},\mathbf{v_1}) = \hat{w}(\mathbf{v_1'},\mathbf{v}'|\mathbf{v_1},\mathbf{v}) = \hat{w}(\mathbf{v}',\mathbf{v_1'} \mid \mathbf{v_1},\mathbf{v}) = \hat{w}(\mathbf{v},\mathbf{v_1} \mid \mathbf{v}',\mathbf{v_1'}). \tag{43}$$

Let $\mu(\mathbf{v})$ be the microscopic density of a moment M. The corresponding collision moment $M_{\mathrm{St}}[f,\mu]$ is defined as follows:

$$M_{\mathrm{St}}[f,\mu] = \int St(f,f)(\mathbf{v})\mu(\mathbf{v})d\mathbf{v}. \tag{44}$$

First, we should obtain transport equations for collision moments (44), analogous to the moment transport equations. Let us restrict ourselves to the case when f can be represented in the form,

$$f = f^{(0)}(1+\varphi), \tag{45}$$

where $f^{(0)}$ is local Maxwell distribution function (28), and all the quadratic with respect to φ terms will be neglected below.

Since, by detail balance,

$$f^{(0)}(\mathbf{v})f^{(0)}(\mathbf{v}_1) = f^{(0)}(\mathbf{v}')f^{(0)}(\mathbf{v_1'}) \tag{46}$$

for all such $(\mathbf{v},\ \mathbf{v_1})$, $(\mathbf{v}',\ \mathbf{v_1'})$ which are related to each other by conservation laws, we have,

$$M_{\mathrm{St}}[f^{(0)},\mu] = 0, \ \text{ for any } \mu. \tag{47}$$

Further, by virtue of conservation laws,

$$M_{\mathrm{St}}[f,\hat{P}^{(0)}\mu] = 0, \ \text{ for any } f. \tag{48}$$

From (46)-(48) it follows,

$$\begin{gathered} M_{\mathrm{St}}[f^{(0)}(1+\varphi),\mu] = M_{\mathrm{St}}[\varphi,(\hat{1}-\hat{P}^{(0)})\mu] = \\ = -\int \hat{w}(\mathbf{v}',\mathbf{v_1'} \mid \mathbf{v},\mathbf{v_1})f^{(0)}(\mathbf{v})f^{(0)}(\mathbf{v_1})\left\{(1-\hat{P}^{(0)})\mu(\mathbf{v})\right\}d\mathbf{v}'d\mathbf{v_1'}d\mathbf{v_1}d\mathbf{v}. \end{gathered} \tag{49}$$

We used notation,

$$\{\psi(\mathbf{v})\} = \psi(\mathbf{v}) + \psi(\mathbf{v}_1) - \psi(\mathbf{v}') - \psi(\mathbf{v_1'}). \tag{50}$$

Also, it proves convenient to introduce the microscopic density of the collision moment, $\mu_{\mathrm{St}}(\mathbf{v})$:

$$\mu_{\mathrm{St}}(\mathbf{v}) = \int \hat{w}(\mathbf{v}',\mathbf{v_1'} \mid \mathbf{v},\mathbf{v}_1)f^{(0)}(\mathbf{v}_1)\left\{(1-\hat{P}^{(0)})\mu(\mathbf{v})\right\}d\mathbf{v}'d\mathbf{v_1'}d\mathbf{v}_1. \tag{51}$$

Then,

$$M_{\mathrm{St}}[\varphi,\mu] = -(\varphi,\mu_{\mathrm{St}}), \tag{52}$$

where $(\cdot,\cdot)$ is the scalar product with the distribution function $f^{(0)}$(28).

Now, we obtain transport equations for the collision moments (52). We write down the time derivative of the collision integral due to the Boltzmann equation,

$$\partial_t \mathrm{St}(f,f)(\mathbf{v}) = \ \hat{T}\mathrm{St}(f,f)(\mathbf{v}) + \ \hat{R}\mathrm{St}(f,f)(\mathbf{v}), \tag{53}$$

where

$$\begin{aligned}
\hat{T}St(f,f)(\mathbf{v}) \ &= \ \int \hat{w}(\mathbf{v}', \mathbf{v_1}' \mid \mathbf{v}, \mathbf{v_1}) \left[f(\mathbf{v}) v_{1k} \partial_k f(\mathbf{v}_1) + f(\mathbf{v}_1) v_k \partial_k f(\mathbf{v}) - \right. \\
&\left. - f(\mathbf{v}') v'_{1k} \partial_k f(\mathbf{v_1}') - f(\mathbf{v_1}') v'_k \partial_k f(\mathbf{v}') \right] d\mathbf{v}' d\mathbf{v_1}' d\mathbf{v_1} d\mathbf{v}; \qquad (54) \\
\hat{R}St(f,f)(\mathbf{v}) \ &= \ \int \hat{w}(\mathbf{v}', \mathbf{v_1}' \mid \mathbf{v}, \mathbf{v_1}) \left[St(f,f)(\mathbf{v}') f(\mathbf{v_1}') + St(f,f)(\mathbf{v_1}') f(\mathbf{v}') - \right. \\
&\left. - St(f,f)(\mathbf{v}_1) f(\mathbf{v}) - St(f,f)(\mathbf{v}) f(\mathbf{v}_1) \right] d\mathbf{v}' d\mathbf{v_1}' d\mathbf{v_1} d\mathbf{v}. \qquad (55)
\end{aligned}$$

Using the representation,

$$\partial_k f^{(0)}(\mathbf{v}) = A_k(\mathbf{v}) f^{(0)}(\mathbf{v});$$

$$A_k(\mathbf{v}) = \partial_k \ln(nT^{-3/2}) + \frac{m}{k_B T}(v_i - u_i)\partial_k u_i + \frac{m(\mathbf{v}-\mathbf{u})^2}{2k_B T} \partial_k \ln T, \tag{56}$$

and after some simple transformations using the relation

$$\{A_k(\mathbf{v})\} = 0, \tag{57}$$

in linear with respect to φ deviation from $f^{(0)}$ (45), we obtain in (53):

$$\begin{aligned}
\hat{T}St(f,f)(\mathbf{v}) \ &= \ \partial_k \int \hat{w}(\mathbf{v}', \mathbf{v_1}' \mid \mathbf{v}, \mathbf{v_1}) f^{(0)}(\mathbf{v_1}) f^{(0)}(\mathbf{v}) \left\{ v_k \varphi(\mathbf{v}) \right\} d\mathbf{v_1}' d\mathbf{v}' d\mathbf{v_1} + \\
&+ \int \hat{w}(\mathbf{v}', \mathbf{v_1}' \mid \mathbf{v}, \mathbf{v_1}) f^{(0)}(\mathbf{v_1}) f^{(0)}(\mathbf{v}) \left\{ v_k A_k(\mathbf{v}) \right\} d\mathbf{v}' d\mathbf{v_1}' d\mathbf{v_1} + \\
&+ \int \hat{w}(\mathbf{v}', \mathbf{v_1}' \mid \mathbf{v}, \mathbf{v}_1) f^{(0)}(\mathbf{v}) f^{(0)}(\mathbf{v_1}) \left[\varphi(\mathbf{v}) A_k(\mathbf{v}_1)(v_{1k} - v_k) + \right. \\
&+ \varphi(\mathbf{v_1}) A_k(\mathbf{v})(v_k - v_{1k}) + \varphi(\mathbf{v}') A_k(\mathbf{v_1}')(v'_k - v'_{1k}) + \\
&\left. + \varphi(\mathbf{v_1}') A_k(\mathbf{v}')(v'_{1k} - v'_k) \right] d\mathbf{v_1}' d\mathbf{v}' d\mathbf{v_1}; \qquad (58) \\
\hat{R}St(f,f)(\mathbf{v}) \ &= \ \int \hat{w}(\mathbf{v}', \mathbf{v_1}' \mid \mathbf{v}, \mathbf{v_1}) f^{(0)}(\mathbf{v}) f^{(0)}(\mathbf{v_1}) \left\{ \xi(\mathbf{v}) \right\} d\mathbf{v_1}' d\mathbf{v}' d\mathbf{v_1}; \\
\xi(\mathbf{v}) \ &= \ \int \hat{w}(\mathbf{v}', \mathbf{v_1}' \mid \mathbf{v}, \mathbf{v_1}) f^{(0)}(\mathbf{v_1}) \left\{ \varphi(\mathbf{v}) \right\} d\mathbf{v}' d\mathbf{v} d\mathbf{v_1}; \qquad (59) \\
\partial_t St(f,f)(\mathbf{v}) \ &= \ -\partial_t \int \hat{w}(\mathbf{v}', \mathbf{v_1}' \mid \mathbf{v}, \mathbf{v_1}) f^{(0)}(\mathbf{v}) f^{(0)}(\mathbf{v_1}) \left\{ \varphi(\mathbf{v}) \right\} d\mathbf{v}' d\mathbf{v_1}' d\mathbf{v_1} \qquad (60)
\end{aligned}$$

Now, multiplying (58)-(60) by the microscopic moment density $\mu(\mathbf{v})$ and performing integration over $\mathbf{v}$ using the symmetry property of the kernel $\hat{w}$ (43) which follows from (43), (46),

$$\begin{aligned}
&\int \hat{w}(\mathbf{v}', \mathbf{v_1}' \mid \mathbf{v}, \mathbf{v_1}) f^{(0)}(\mathbf{v_1}) f^{(0)}(\mathbf{v}) g_1(\mathbf{v}) \left\{ g_2(\mathbf{v}) \right\} d\mathbf{v}' d\mathbf{v_1}' d\mathbf{v_1} d\mathbf{v} = \\
&\quad \int \hat{w}(\mathbf{v}', \mathbf{v_1}' \mid \mathbf{v}, \mathbf{v_1}) f^{(0)}(\mathbf{v_1}) f^{(0)}(\mathbf{v}) g_2(\mathbf{v}) \left\{ g_1(\mathbf{v}) \right\} d\mathbf{v}' d\mathbf{v_1}' d\mathbf{v_1} d\mathbf{v}, \qquad (61)
\end{aligned}$$

and is true for any two functions g_1, g_2 ensuring existence of the integrals, and also using the consequence

$$\{\varphi(\mathbf{v})\} = \left\{ (\hat{1} - \hat{P}^{(0)}) \varphi(\mathbf{v}) \right\} \tag{62}$$

of the conservation laws, it is straightforward to obtain the required transport equation for the collision moment in th linear neighbourhood of the local equilibrium:

$$
\begin{aligned}
&-\partial_t \Delta M_{\mathrm{St}}[\varphi,\mu] \equiv -\partial_t(\varphi,\mu_{\mathrm{St}}) = \\
&= (v_k A_k(\mathbf{v}), \mu_{\mathrm{St}}((\hat{1}-\hat{P}^{(0)})\mu(\mathbf{v}))) + \\
&+\partial_k(\varphi(\mathbf{v})v_k, \mu_{\mathrm{St}}((\hat{1}-\hat{P}^{(0)})\mu(\mathbf{v}))) + \int \hat{w}(\mathbf{v}',\mathbf{v_1}' \mid \mathbf{v},\mathbf{v_1}) f^{(0)}(\mathbf{v_1}) f^{(0)}(\mathbf{v}) \times \\
&\times \left\{(\hat{1}-\hat{P}^{(0)})\mu(\mathbf{v})\right\} A_k(\mathbf{v_1})(v_{1k}-v_k)\varphi(\mathbf{v}) d\mathbf{v}' d\mathbf{v_1}' d\mathbf{v_1} d\mathbf{v} + \\
&+ \left(\xi(\mathbf{v}), \mu_{\mathrm{St}}\left((\hat{1}-\hat{P}^{(0)})\mu(\mathbf{v})\right)\right). \qquad (63)
\end{aligned}
$$

The chain of equations (63) is an analogue of the hydrodynamic moment chain (41) for collision moments (further on, we will call equation (63) the second chain, and (41) - the first chain). The second chain possesses the same way of chaining as the first one: the last term in the right part of (32) $(\xi, \mu_{\mathrm{St}}((\hat{1}-\hat{P}^{(0)})\mu))$ depends on the whole totality of moments and collision moments and may be treated as a new variable. Therefore, generally speaking, we have an infinite sequence of chains of increasingly higher orders. Only in the case of a special choice of collision model - Maxwell potential $U = -\kappa r^{-4}$ - this sequence degenerates: the second and the sequent chains are equivalent to the first (see below).

Let us restrict ourselves to the first and second hydrodynamic chains. Then deviation from local equilibrium state and transition to closed macrodescription equations may be performed in three different ways for the microscopic density $\mu(\mathbf{v})$. Firstly, one can specify the moment $\hat{M}[\mu]$ and perform closure of the chain (41) by the triangle method given in sections 1,2, and leading to Grad's moment method. Secondly, one can specify collision moment $\hat{M}_{\mathrm{St}}[\mu]$ and perform closure of the second hydrodynamic chain (32). Finally, one can use simultaneously both $\hat{M}[\mu]$ and $\hat{M}_{\mathrm{St}}[\mu]$(mixed chain). Quasi-equilibrium distribution functions corresponding to the last two variants will be constructed in the following section. As collision models, hard spheres and Maxwell molecules will be considered.

4 Distribution Functions of the Second Quasi-equilibrium Approximation for Collision Moments

4.1 First five moments plus collision stress tensor

Throughout below as first quasi-equilibrium approximation local equilibrium state $f^{(0)}$(28) is chosen.

Let us choose $\nu_{ik} = mv_iv_k$(30) as the microscopic density $\mu(\mathbf{v})$ of the second quasi-equilibrium state. Let us write down the corresponding collision moment (collision stress tensor) Δ_{ik} in the form,

$$\Delta_{ik} = -(\varphi, \nu_{\mathrm{St}ik}), \qquad (64)$$

where

$$\nu_{\mathrm{St}ik}(\mathbf{v}) = m \int \hat{w}(\mathbf{v}',\mathbf{v_1}' \mid \mathbf{v_1},\mathbf{v}) f^{(0)}(\mathbf{v_1}) \times$$

$$\times \left\{ (v_i - u_i)(v_k - u_k) - \frac{1}{3}\delta_{ik}(\mathbf{v}-\mathbf{u})^2 \right\} d\mathbf{v}' d\mathbf{v_1}' d\mathbf{v_1} \qquad (65)$$

is the microscopic density of the collision moment Δ_{ik}.

Function of the second quasi-equilibrium approximation under the given collision moment (64) is determined as the solution to the problem

$$\begin{gathered} (\varphi, \varphi) \rightarrow \min \ \text{for} \\ (\varphi, \nu_{\mathrm{St}ik}) = -\Delta_{ik}. \end{gathered} \qquad (66)$$

The method of Lagrange multipliers yields

$$\begin{gathered} \varphi(\mathbf{v}) = \lambda_{ik}\nu_{\mathrm{St}ik}(\mathbf{v}), \\ \lambda_{ik}(\nu_{\mathrm{St}ik}, \nu_{\mathrm{St}ls}) = \Delta_{ls}, \end{gathered} \qquad (67)$$

where λ_{ik} are the Lagrange multipliers.

In the considered below examples of collision models (and in general, for central interaction forces of particles) $\nu_{\mathrm{St}ik}$ is of the form

$$\nu_{\mathrm{St}ik}(\mathbf{v}) = (\hat{1} - \hat{P}^{(0)})\nu_{ik}(\mathbf{v})\Phi((\mathbf{v}-\mathbf{u})^2), \qquad (68)$$

where $(\hat{1} - \hat{P}^{(0)})\nu_{ik}$ is determined only by the correlation (31), and Φ depends only on the absolute value of the peculiar velocity $(\mathbf{v}-\mathbf{u})$. Then

$$\begin{gathered} \lambda_{ik} = r\Delta_{ik}; \\ r^{-1} = (2/15)\left(\Phi^2((\mathbf{v}-\mathbf{u})^2), (\mathbf{v}-\mathbf{u})^4\right), \end{gathered} \qquad (69)$$

and the distribution function of the second quasi-equilibrium approximation for collision moments (64) is given by the expression

$$f = f^{(0)}(1 + r\Delta_{ik}\mu_{\mathrm{St}ik}). \qquad (70)$$

The form of the function $\Phi((\mathbf{v}-\mathbf{u})^2)$, and the value of the parameter r are determined by the model of particle's interaction. In the Appendix, they are obtained for hard spheres and Maxwell molecules models (see equations 129-134). The distribution function (70) is given by the following expressions:
For Maxwell molecules:

$$\begin{gathered} f = f^{(0)}\left\{1 + \mu_0^{\mathrm{M.M.}} m(2P^2k_BT)^{-1}\Delta_{ik}\left((v_i-u_i)(v_k-u_k) - \frac{1}{3}\delta_{ik}(\mathbf{v}-\mathbf{u})^2\right)\right\}, \\ \mu_0^{\mathrm{M.M.}} = \frac{k_BT\sqrt{2m}}{3\pi A_2(5)\sqrt{\kappa}}, \end{gathered} \qquad (71)$$

where $\mu_0^{\mathrm{M.M.}}$ is a viscosity coefficient obtained at first approximation of the Chapman-Enskog method (exact in this case), κ is a force constant, $A_2(5)$ is a number, $A_2(5) \approx 0.436$ (see [16], p.209);

For the hard spheres model:

$$f = f^{(0)} \left\{ 1 + \frac{2\sqrt{2}\tilde{r}m\mu_0^{\text{H.S.}}}{5P^2 k_B T} \Delta_{ik} \int_{+1}^{-1} \exp\left\{ -\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_B T} y^2 \right\} (1-y^2)(1+y^2) \times \right.$$
$$\left. \times \left(\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_B T}(1-y^2) + 2 \right) dy \left((v_i - u_i)(v_k - u_k) - \frac{1}{3}\delta_{ik}(\mathbf{v}-\mathbf{u})^2 \right) \right\},$$
$$\mu_0^{\text{H.S.}} = (5\sqrt{k_B T m})/(16\sqrt{\pi}\sigma^2), \tag{72}$$

where $\tilde{r}$ is a number represented as follows:

$$\tilde{r}^{-1} = \frac{1}{16} \int_{-1}^{+1} \int_{-1}^{+1} \alpha^{-11/2} \beta(y)\beta(z)\gamma(y)\gamma(z) \times$$
$$\times (16\alpha^2 + 28\alpha(\gamma(y) + \gamma(z)) + 63\gamma(y)\gamma(z)) dy dz, \tag{73}$$
$$\alpha = 1 + y^2 + z^2, \qquad \beta(y) = 1 + y^2, \qquad \gamma(y) = 1 - y^2.$$

Numerical value of $\tilde{r}^{-1}$ is 5.212 to the third digit accuracy.

Distribution function of the second quasi-equilibrium approximation under fixed values of moment and collision moment corresponding to the microscopic density (30) is determined as solution of the problem

$$\begin{aligned} &(\varphi, \varphi) \to \min \quad \text{for} \\ &((\hat{1} - \hat{P}^{(0)})\nu_{ik}, \varphi) = \sigma_{ik}, \\ &(\nu_{\text{St}ik}, \varphi) = \Delta_{ik}. \end{aligned} \tag{74}$$

Taking into account the relation (68), we obtain the solution of the problem (74) in the form,

$$\varphi(\mathbf{v}) = (\lambda_{ik}\Phi((\mathbf{v}-\mathbf{u})^2) + \beta_{ik})((v_i - u_i)(v_k - u_k) - (1/3)\delta_{ik}(\mathbf{v}-\mathbf{u})^2). \tag{75}$$

Lagrange multipliers λ_{ik}, β_{ik} are determined from the system of linear equations,

$$\begin{aligned} ms^{-1}\lambda_{ik} + 2Pk_B T m^{-1}\beta_{ik} &= \sigma_{ik}, \\ mr^{-1}\lambda_{ik} + ms^{-1}\beta_{ik} &= \Delta_{ik}, \end{aligned} \tag{76}$$

where

$$s^{-1} = (2/15)(\Phi((\mathbf{v}-\mathbf{u})^2), (\mathbf{v}-\mathbf{u})^4). \tag{77}$$

If the solvability condition of the system (76) is satisfied,

$$D = m^2 s^{-2} - 2Pk_B T r^{-1} \neq 0, \tag{78}$$

then the distribution function of the second quasi-equilibrium approximation exists and takes the form

$$\begin{aligned} f \;=\; & f^{(0)} \left\{ 1 + (m^2 s^{-2} - 2Pk_B T r^{-1})^{-1} \times \right. \\ & \times [(ms^{-1}\sigma_{ik} - 2Pk_B T m^{-1}\Delta_{ik})\Phi((\mathbf{v}-\mathbf{u})^2) + \\ & \left. + (ms^{-1}\Delta_{ik} - mr^{-1}\sigma_{ik})]((v_i - u_i)(v_k - u_k) - (1/3)\delta_{ik}(\mathbf{v}-\mathbf{u})^2) \right\}. \end{aligned} \tag{79}$$

The condition (78) means independence of the set of moments σ_{ik} from the collision moments Δ_{ik}. If it is not satisfied, then the collision moments Δ_{ik} may be represented in the form of linear combinations of σ_{ik} (with coefficients depending on space and time). Then the closed by means of (70) equations of the second chain are equivalent to ten moment Grad equations, while the mixed chain does not exist. This happens only in the model of Maxwell molecules. Indeed, in this case

$$s^{-1} = 2P^2 k_B T (m^2 \mu_0^{\mathrm{M.M.}})^{-1}; D = 0.$$

The transformation changing Δ_{ik} to σ_{ik} is

$$\mu_0^{\mathrm{M.M.}} \Delta_{ik} P^{-1} = \sigma_{ik}. \tag{80}$$

For hard spheres:

$$s^{-1} = \frac{5P^2 k_B T}{4\sqrt{2}\mu_0^{\mathrm{H.S.}} m^2} \cdot \tilde{s}^{-1}, \qquad \tilde{s}^{-1} = \int_{-1}^{+1} \gamma(y)(\beta(y))^{-7/2}\left(\beta(y) + \frac{7}{4}\gamma(y)\right) dy \tag{81}$$

The numerical value of $\tilde{s}^{-1}$ is 1.115 to third digit. The condition (77) takes the form,

$$D = \frac{25}{32}\left(\frac{P^2 k_B T}{m\mu_0^{\mathrm{H.S.}}}\right)^2 (\tilde{s}^{-2} - \tilde{r}^{-1}) \neq 0. \tag{82}$$

Consequently, for the hard spheres model the distribution function of the second quasi-equilibrium approximation of the mixed chain exists and is determined by the expression

$$\begin{aligned} f \;=\; & f^{(0)}\Big\{1 + m(4Pk_B T(\tilde{s}^{-2} - \tilde{r}^{-1}))^{-1} \times \\ & \times \left[\left(\sigma_{ik}\tilde{s}^{-1} - \frac{8\sqrt{2}}{5P}\mu_0^{\mathrm{H.S.}}\Delta_{ik}\right)\int_{-1}^{+1} \exp\left(-\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_B T}y^2\right) \times \right. \\ & \times (1-y^2)(1+y^2)\left(\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_B T}(1-y^2) + 2\right) dy + \\ & \left. +2\left(\tilde{s}^{-1}\cdot\frac{8\sqrt{2}}{5P}\mu_0^{\mathrm{H.S.}}\Delta_{ik} - \tilde{r}^{-1}\sigma_{ik}\right)\right]\left((v_i - u_i)(v_k - u_k) - \frac{1}{3}\delta_{ik}(\mathbf{v}-\mathbf{u})^2\right)\Big\}. \end{aligned} \tag{83}$$

4.2 First five moments plus collision stress tensor, plus collision heat flux vector

Distribution function of the second quasi-equilibrium approximation which allows for collision heat flux vector Q is constructed in a similar way. The microscopic density $\xi_{\mathrm{St}i}$ corresponding to Q_i is

$$\xi_{\mathrm{St}i}(\mathbf{v}) = \int \hat{w}(\mathbf{v}', \mathbf{v}_1' \mid \mathbf{v}, \mathbf{v}_1) f^{(0)}(\mathbf{v}_1)\left\{(\hat{1} - \hat{P}^{(0)})\frac{v_i^2 v}{2}\right\} d\mathbf{v}' d\mathbf{v}_1' d\mathbf{v}_1. \tag{84}$$

The desired distribution functions are the solutions to the optimization problems: for the second chain it is the solution to the problem (66) with additional conditions,

$$m(\varphi, \xi_{\mathrm{St}i}) = Q_i, \tag{85}$$

for the mixed chain the distribution functions is the solution to the problem (74) with additional conditions,

$$m(\varphi, \xi_{\mathrm{St}i}) = Q_i, \tag{86}$$

$$m(\varphi, (\hat{1} - \hat{P}^{(0)})\xi_i) = q_i. \tag{87}$$

Here $\xi_i = v_i v^2/2$ (see (33)). In the Appendix $\xi_{\mathrm{St}i}$ are determined for Maxwell molecules and hard spheres (see (134)-(139)). Since

$$\begin{gathered}(\xi_{\mathrm{St}i}, \nu_{\mathrm{St}kj}) = ((\hat{1} - \hat{P}^{(0)})\xi_i, \nu_{\mathrm{St}kj}) = \\ = (\xi_{\mathrm{St}i}, (\hat{1} - \hat{P}^{(0)})\nu_{kj}) = ((\hat{1} - \hat{P}^{(0)})\xi_i, (\hat{1} - \hat{P}^{(0)})\nu_{kj}) = 0,\end{gathered} \tag{88}$$

the conditions (85) do not depend on the restrictions of the problem (66), and the conditions (87) do not depend on the restrictions of the problem (74).

Distribution function of the second quasi-equilibrium approximation of the second chain under given Δ_{ik}, Q_i is of the form,

$$f = f^{(0)}(1 + r\Delta_{ik}\nu_{\mathrm{St}ik} + \eta Q_i \xi_{\mathrm{St}i}). \tag{89}$$

The parameter η is determined by the relation

$$\eta^{-1} = (1/3)(\xi_{\mathrm{St}i}, \xi_{\mathrm{St}i}). \tag{90}$$

According to (138), for Maxwell molecules

$$\eta = \frac{9m^3(\mu_0^{\mathrm{M.M.}})^2}{10P^3(k_BT)^2}, \tag{91}$$

and the distribution function (89) is

$$\begin{gathered}f = f^{(0)}\left\{1 + \mu_0^{\mathrm{M.M.}} m(2P^2k_BT)^{-1}\Delta_{ik}((v_i - u_i)(v_k - u_k) - (1/3)\delta_{ik}(\mathbf{v} - \mathbf{u})^2) + \right. \\ \left. + \mu_0^{\mathrm{M.M.}} m(P^2k_BT)^{-1}(v_i - u_i)\left(\frac{m(\mathbf{v} - \mathbf{u})^2}{5k_BT} - 1\right)\right\}.\end{gathered} \tag{92}$$

According to the Appendix, for hard spheres

$$\eta = \tilde{\eta} \cdot \frac{64m^3(\mu_0^{\mathrm{H.S.}})^2}{125P^3(k_BT)^2}, \tag{93}$$

where η is a number equal to 16.077 to third digit accuracy.

The distribution function (89) for hard spheres takes the form

$$\begin{aligned}f \;\; = \;\; & f^{(0)}\left\{1 + \frac{2\sqrt{2}\tilde{r}m\mu_0^{\mathrm{H.S.}}}{5P^2k_BT}\Delta_{ik}\int_{-1}^{+1}\exp\left(-\frac{m(\mathbf{v} - \mathbf{u})^2}{2k_BT}y^2\right)\beta(y)\gamma(y) \times \right. \\ & \times \left(\frac{m(\mathbf{v} - \mathbf{u})^2}{2k_BT}\gamma(y) + 2\right)dy\left((v_i - u_i)(v_k - u_k) - \frac{1}{3}\delta_{ik}(\mathbf{v} - \mathbf{u})^2\right) + \\ & + \frac{2\sqrt{2}\tilde{\eta}m^3\mu_0^{\mathrm{H.S.}}}{25P^2(k_BT)^2}Q_i\left[(v_i - u_i)\left((\mathbf{v} - \mathbf{u})^2 - \frac{5k_BT}{m}\right) \times \right.\end{aligned}$$

$$
\begin{aligned}
&\times \int_{-1}^{+1} \exp\left(-\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}y^2\right)\beta(y)\gamma(y)\left(\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}\gamma(y)+2\right)dy+\\
&+(v_i-u_i)(\mathbf{v}-\mathbf{u})^2\int_{-1}^{+1} \exp\left(-\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}y^2\right)\beta(y)\gamma(y)\times\\
&\times\left(\sigma(y)\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}+\delta(y)\right)dy\Bigg]\Bigg\}. \qquad (94)
\end{aligned}
$$

The functions $\beta(y), \gamma(y), \sigma(y)$ and $\delta(y)$ are

$$
\beta(y) = 1+y^2,\ \gamma(y) = 1-y^2,\ \sigma(y) = y^2(1-y^2),\ \delta(y) = 3y^2-1. \qquad (95)
$$

The condition of existence of the second quasi-equilibrium approximation of the mixed chain (78) should be supplemented with the requirement

$$
R = m^2\tau^{-2} - \frac{5P(k_BT)^2}{2m}\eta^{-1} \neq 0. \qquad (96)
$$

Here

$$
\tau^{-1} = \frac{1}{3}\left((\hat{1}-\hat{P}^{(0)})\frac{v_i^2 v}{2}, \xi_{\mathrm{St}_i}(\mathbf{v})\right). \qquad (97)
$$

For Maxwell molecules

$$
\tau^{-1} = (5P^2k_B^2T^2)/(3\mu_0^{\mathrm{M.M.}}m^3),
$$

and the condition (96) is not satisfied. Distribution function of the second quasi-equilibrium approximation of mixed chain does not exist. The variables Q_i are changed to q_i by the transformation

$$
3\mu_0^{\mathrm{M.M.}}Q_i = 2Pq_i. \qquad (98)
$$

For hard spheres

$$
\tau^{-1} = \tilde{\tau}^{-1}\frac{25(Pk_BT)^2}{8\sqrt{2}m^3\mu_0^{\mathrm{H.S.}}}, \qquad (99)
$$

where

$$
\begin{aligned}
\tilde{\tau}^{-1} = \frac{1}{8}\int_{-1}^{+1}&\beta^{-9/2}(y)\gamma(y)\left\{63(\gamma(y)+\sigma(y)+7\beta(y)(4-10\gamma(y)+2\delta(y)-5\sigma(y))+\right.\\
&\left.+\beta^2(y)(25\gamma(y)-10\delta(y)-40)+20\beta^3(y)\right\}dy. \qquad (100)
\end{aligned}
$$

Numerical value of $\tilde{\tau}^{-1}$ is about 4.322.

Then the condition (96) is satisfied:

$$
R \approx 66m^{-4}(Pk_BT)^4(\mu_0^{\mathrm{H.S.}})^2.
$$

Finally, under given values of $\sigma_{ik}, \Delta_{ik}, q_i$ and Q_i the distribution function of the second quasi-equilibrium approximation of the second chain for hard spheres is of the form,

$$
\begin{aligned}
f \;=\;& f^{(0)}\{1+\\
&+\frac{m}{4Pk_BT}(\tilde{s}^{-2}-\tilde{r}^{-1})^{-1}\left[\left(\tilde{s}^{-1}\sigma_{ik}-\frac{8\sqrt{2}}{5P}\mu_0^{\mathrm{H.S.}}\Delta_{ik}\right)\int_{-1}^{+1}\exp\left(-\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}y^2\right)\times\right.
\end{aligned}
$$

$$
\begin{aligned}
&\times\beta(y)\gamma(y)\left(\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}\gamma(y)+2\right)dy+2\left(\tilde{s}^{-1}\frac{8\sqrt{2}}{5P}\mu_0^{\text{H.S.}}\Delta_{ik}-\tilde{r}^{-1}\sigma_{ik}\right)\Bigg]\times\\
&\times\left((v_i-u_i)(v_k-u_k)-\frac{1}{3}\delta_{ik}(\mathbf{v}-\mathbf{u})^2\right)+\\
&+\frac{m^2}{10(Pk_BT)^2}(\tilde{\tau}^{-2}-\tilde{\eta}^{-1})^{-1}\Bigg[\left(\tilde{\tau}^{-1}q_i-\frac{4\sqrt{2}}{5P}\mu_0^{\text{H.S.}}Q_i\right)\times\\
&\Bigg((v_i-u_i)\left((\mathbf{v}-\mathbf{u})^2-\frac{5k_BT}{m}\right)\int_{-1}^{+1}\exp\left(-\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}y^2\right)\times\\
&\times\beta(y)\gamma(y)\left(\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}\gamma(y)+2\right)dy+(v_i-u_i)(\mathbf{v}-\mathbf{u})^2\times\\
&\times\int_{-1}^{+1}\exp\left(-\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}y^2\right)\beta(y)\gamma(y)\left(\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}\sigma(y)+\delta(y)\right)dy\Bigg)+\\
&+2\left(\frac{4\sqrt{2}}{5P}\mu_0^{\text{H.S.}}\tilde{\tau}^{-1}Q_i-\tilde{\eta}^{-1}q_i\right)(v_i-u_i)\left((\mathbf{v}-\mathbf{u})^2-\frac{5k_BT}{m}\right)\Bigg]\Bigg\}. \qquad (101)
\end{aligned}
$$

Thus, the expressions (71), (72), (83), (92), (94) and (101) give distribution functions of the second quasi-equilibrium approximation of the second and mixed hydrodynamic chains for Maxwell molecules and hard spheres. They are analogues of ten- and thirteen-moment Grad approximations (32), (36).

The next step is to close the second and mixed hydrodynamic chains by means of the found distribution functions.

5 Closure of the the Second and Mixed Hydrodynamic Chains

The distribution function of the second quasi-equilibrium approximation under fixed Δ_{ik} for Maxwell molecules (71) presents the simplest example of closure of the first (40) and second (63) hydrodynamic chains. With the help of it, we obtain from (40) the following transport equations for the moments of the first (local equilibrium) approximation:

$$
\begin{aligned}
&\partial_t\rho+\partial_i(u_i\rho)=0;\\
&\rho(\partial_t u_k+u_i\partial_i u_k)+\partial_k P+\partial_i(P^{-1}\mu_0^{\text{M.M.}}\Delta_{ik})=0; \qquad (102)\\
&\frac{3}{2}(\partial_t P++u_i\partial_i P)+\frac{5}{2}P\partial_i u_i+P^{-1}\mu_0^{\text{M.M.}}\Delta_{ik}\partial_i u_k=0 \qquad (103)
\end{aligned}
$$

Now, let us from the collision moment transport chain (63) find an equation for Δ_{ik} which closes the system (64). Substituting (71) into (63), we obtain after simple calculations:

$$
\begin{aligned}
&\partial_t\Delta_{ik}+\partial_s(u_s\Delta_{ik})+\Delta_{is}\partial_s u_k+\Delta_{ks}\partial_s u_i-\frac{2}{3}\delta_{ik}\Delta_{ls}\partial_s u_l+\\
&+P^2(\mu_0^{\text{M.M.}})^{-1}\left(\partial_i u_k+\partial_k u_i-\frac{2}{3}\delta_{ik}\partial_s u_s\right)+P(\mu_0^{\text{M.M.}})^{-1}\Delta_{ik}+\Delta_{ik}\partial_s u_s=0. \qquad (104)
\end{aligned}
$$

For comparison, let us give ten-moment Grad equations obtained when closing the chain (40) by the distribution functions (32):

$$
\partial_t\rho+\partial_i(u_i\rho)=0;
$$

$$\begin{gathered}\rho(\partial_t u_k + u_i\partial_i u_k) + \partial_k P + \partial_i\sigma_{ik} = 0;\\ \frac{3}{2}(\partial_t P + +u_i\partial_i P) + \frac{5}{2}P\partial_i u_i + \sigma_{ik}\partial_i u_k = 0; \qquad (105)\end{gathered}$$

$$\begin{gathered}\partial_t\sigma_{ik} + \partial_s(u_s\sigma_{ik}) + P\left(\partial_i u_k + \partial_k u_i - \frac{2}{3}\delta_{ik}\partial_s u_s\right) +\\ +\sigma_{is}\partial_s u_k + \sigma_{ks}\partial_s u_i - \frac{2}{3}\delta_{ik}\sigma_{ls}\partial_s u_l + P(\mu_0^{\text{M.M.}})^{-1}\sigma_{ik} = 0. \qquad (106)\end{gathered}$$

Using the explicit form of $\mu_0^{\text{M.M.}}$(71), it is easy to make sure that the transformation (80) maps the systems (102), (104) and (105) into one another. This is a consequence of the degeneration of the mixed hydrodynamic chain which was discussed in the end of the section 3. The systems (102), (104) and (105) are essentially equivalent. These specific properties of Maxwell molecules result from the fact that for them the microscopic densities $(\hat{1} - \hat{P}^{(0)})v_i v_k$ and $(\hat{1} - \hat{P}^{(0)})v_i v^2$ are eigen-functions of the linearized collision integral.

We now turn our attention to the case of closure of the second and of the mixed hydrodynamic chains for the hard spheres model. Substituting the distribution function (72) into (40) and (63), we obtain an analogue of the systems (102) and (104) (second chain, hard spheres):

$$\begin{gathered}\partial_t\rho + \partial_i(u_i\rho) = 0;\\ \rho(\partial_t u_k + u_i\partial_i u_k) + \partial_k P + \tilde{r}\tilde{s}^{-1}\cdot\frac{8\sqrt{2}}{5}\partial_i(\mu_0^{\text{H.S.}}P^{-1}\Delta_{ik}) = 0;\\ \frac{3}{2}(\partial_t P + u_i\partial_i P) + \frac{5}{2}P\partial_i u_i + \tilde{r}\tilde{s}^{-1}\cdot\frac{8\sqrt{2}}{5}\mu_0^{\text{H.S.}}P^{-1}\Delta_{ik}\partial_i u_k = 0;\\ \partial_t\Delta_{ik} + \partial_s(u_s\Delta_{ik}) + \tilde{r}\tilde{a}_1(\partial_s u_s)\Delta_{ik} + \frac{5\tilde{s}^{-1}P^2}{8\sqrt{2}\mu_0^{\text{H.S.}}}\left(\partial_i u_k + \partial_k u_i - \frac{2}{3}\delta_{ik}\partial_s u_s\right) +\\ +\tilde{r}(\tilde{a}_1 + \tilde{a}_2)\left(\Delta_{is}\partial_s u_k + \Delta_{ks}\partial_s u_i - \frac{2}{3}\delta_{ik}\Delta_{ls}\partial_s u_l\right) +\\ +\tilde{r}(\tilde{a}_1 + \tilde{a}_3)\left(\Delta_{is}\partial_k u_s + \Delta_{ks}\partial_i u_s - \frac{2}{3}\delta_{ik}\Delta_{ls}\partial_s u_l\right) + (P\hat{r}\tilde{a}_0/\mu_0^{\text{H.S.}})\Delta_{ik} = 0. \qquad (107)\end{gathered}$$

The dimensionless parameters $\tilde{a}_0, \tilde{a}_1, \tilde{a}_2$ and $\tilde{a}_3$ are determined by the quadratures

$$\begin{aligned}\tilde{a}_1 &= \frac{1}{16}\int_{-1}^{+1}\int_{-1}^{+1}\beta(y)\beta(z)\gamma^2(z)\gamma(y)\alpha^{-13/2}(y,z)\times\\ &\times\{99\gamma(y)\gamma(z)(\gamma(z)-1) + 18\alpha(y,z)(2\gamma(z)(\gamma(z)-1) +\\ &+4\gamma(y)(4\gamma(z)-3)) + 8\alpha^2(y,z)(4\gamma(z)-3)\}dydz;\\ \tilde{a}_2 &= \frac{1}{16}\int_{-1}^{+1}\int_{-1}^{+1}\beta(y)\beta(z)\gamma(y)\gamma^2(z)\alpha^{-11/2}(y,z)\{63\gamma(y)\gamma(z) +\\ &+14\alpha(y,z)(3\gamma(y) + 2\gamma(z)) + 24\alpha^2(y,z)\}dydz;\\ \tilde{a}_3 &= \frac{1}{16}\int_{-1}^{+1}\int_{-1}^{+1}\alpha^{-11/2}(y,z)\beta(y)\beta(z)\gamma(y)\gamma(z)\times\\ &\times\{63\gamma(y)\gamma(z)(\gamma(z)-1) + 14(2\gamma(z)(\gamma(z)-1) +\\ &+\gamma(y)(3\gamma(z)-2))\alpha(y,z) + 8\alpha^2(y,z)(3\gamma(z)-2)\}dydz; \qquad (108)\\ \tilde{a}_0 &\approx \frac{1}{1536\sqrt{2}}\int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1}(\psi(x,y,z))^{-13/2}\beta(x)\beta(y)\beta(z)\times\\ &\times\gamma(x)\gamma(y)\gamma(z)\{10395\gamma(x)\gamma(y)\gamma(z) + 3780\psi(x,y,z)\times\end{aligned}$$

$$\begin{aligned}&\times(\gamma(x)\gamma(y)+\gamma(x)\gamma(z)+\gamma(y)\gamma(z))+1680\psi^2(x,y,z)\times\\&\times(\gamma(x)+\gamma(y)+\gamma(z))+960\psi^3(x,y,z)\}dxdydz;\\&\psi(x,y,z)=1+x^2+y^2+z^2.\end{aligned}\tag{109}$$

Their numerical values are $\tilde{a}_1 \approx 0.36$, $\tilde{a}_2 \approx 5.59$, $\tilde{a}_3 \approx 0.38$, $\tilde{a}_0 \approx 2.92$ to second digit.

Closure of the mixed hydrodynamic chain at the functions (83) gives the following modification of the system of equations (107):

$$\begin{aligned}\partial_t\rho+\partial_i(u_i\rho)=0;\\ \rho(\partial_t u_k+u_i\partial_i u_k)+\partial_k P+\partial_i\sigma_{ik}=0;\\ \frac{3}{2}(\partial_t P+u_i\partial_i P)+\frac{5}{2}P\partial_i u_i+\sigma_{ik}\partial_i u_k=0;\\ \partial_t\sigma_{ik}+\partial_s(u_s\sigma_{ik})+P\left(\partial_i u_k+\partial_k u_i-\frac{2}{3}\delta_{ik}\partial_s u_s\right)+\\ +\sigma_{is}\partial_s u_k+\sigma_{ks}\partial_s u_i-\frac{2}{3}\delta_{ik}\sigma_{ls}\partial_s u_l+\Delta_{ik}=0;\\ \partial_t\Delta_{ik}+\partial_s(u_s\Delta_{ik})+\frac{5P^2}{\tilde{s}8\sqrt{2}\mu_0^{\text{H.S.}}}\left(\partial_i u_k+\partial_k u_i-\frac{2}{3}\delta_{ik}\partial_s u_s\right)+\\ +\frac{5P}{4\sqrt{2}\mu_0^{\text{H.S.}}(\tilde{s}^{-2}-\tilde{r}^{-1})}\left\{\frac{\tilde{a}_1}{2}(\partial_s u_s)\alpha_{ik}+\frac{1}{2}(\tilde{a}_1+\tilde{a}_2)\left(\alpha_{is}\partial_s u_k+\right.\right.\\ \left.+\alpha_{ks}\partial_s u_i-\frac{2}{3}\delta_{ik}\alpha_{ls}\partial_s u_l\right)+\frac{1}{2}(\tilde{a}_1+\tilde{a}_3)\left(\alpha_{is}\partial_k u_s+\alpha_{ks}\partial_i u_s-\frac{2}{3}\delta_{ik}\alpha_{ls}\partial_s u_l\right)+\\ +\tilde{b}_1(\partial_s u_s)\beta_{ik}+(\tilde{b}_1+\tilde{b}_2)\left(\beta_{is}\partial_s u_k+\beta_{ks}\partial_s u_i-\frac{2}{3}\delta_{ik}\beta_{ls}\partial_s u_l\right)+\\ \left.+(\tilde{b}_1+\tilde{b}_3)\left(\beta_{is}\partial_k u_s+\beta_{ks}\partial_i u_s-\frac{2}{3}\delta_{ik}\beta_{ls}\partial_s u_l\right)\right\}+\\ +\frac{5P^2}{8\sqrt{2}(\mu_0^{\text{H.S.}})^2(\tilde{s}^{-2}-\tilde{r}^{-1})}\left\{\frac{5}{8\sqrt{2}\tilde{r}}\beta_{ik}+\tilde{a}_0\alpha_{ik}\right\}=0;\end{aligned}\tag{110}$$

$$\begin{aligned}\alpha_{ik}=\tilde{s}^{-1}\sigma_{ik}-\frac{8\sqrt{2}}{5P}\cdot\mu_0^{\text{H.S.}}\Delta_{ik};\\ \beta_{ik}=\tilde{s}^{-1}\frac{8\sqrt{2}}{5P}\cdot\mu_0^{\text{H.S.}}\Delta_{ik}-\tilde{r}^{-1}\sigma_{ik}.\end{aligned}\tag{111}$$

It is clear from the analysis of distribution functions of the second quasi-equilibrium approximations of the second hydrodynamic chain that in the Grad moment method a substitution of a constant for the function $\Phi(c^2)$ is performed. Finally, let us note the simplest consequence of variability of $\Phi(c^2)$. If μ_0 is multiplied with a small parameter (Knudsen number Kn equal to the ratio of the main free path the to characteristic spatial scale of variations of hydrodynamic values), then the first with respect to Kn approximation of collision stress tensor $\Delta_{ik}^{(0)}$ has the form,

$$\Delta_{ik}^{(0)}=P\left(\partial_i u_k+\partial_k u_i-\frac{2}{3}\delta_{ik}\partial_s u\right)\tag{112}$$

for Maxwell molecules, and

$$\Delta_{ik}^{(0)}=\frac{5\tilde{r}}{8\sqrt{2}\tilde{s}\tilde{a}_0}P\left(\partial_i u_k+\partial_k u_i-\frac{2}{3}\delta_{ik}\partial_s u_s\right)\tag{113}$$

for hard spheres. Substitution of these expressions into the momentum equations results in the Navier-Stokes equations with effective viscosity coefficients μ_{eff},

$$\mu_{\text{eff}} = \mu_0^{\text{M.M.}} \tag{114}$$

for Maxwell molecules and

$$\mu_{\text{eff}} = \tilde{a}_0^{-1}\mu_0^{\text{H.S.}} \tag{115}$$

for hard spheres. When using ten-moment Grad approximation which does not distinguish Maxwell molecules and hard spheres, we obtain $\mu_{\text{eff}} = \mu_0^{\text{H.S.}}$.

6 Appendix: Calculation of distribution functions of the second quasi-equilibrium approximation of the second and mixed hydrodynamic chains for Maxwell molecules and hard spheres

Write $\nu_{\text{St}ik}$ (65) in the standard form:

$$\nu_{\text{St}ik} = \int f^{(0)} \mid \mathbf{v_1} - \mathbf{v} \mid \left\{(v_i - u_i)(v_k - u_k) - \frac{1}{3}\delta_{ik}(\mathbf{v} - \mathbf{u})^2\right\} bdbd\epsilon d\mathbf{v_1}, \tag{116}$$

where b is the impact parameter, ϵ is the angle between the plane containing the trajectory of the particle being scattered in the system of the center of mass and the plane containing the entering asymptote, the trajectory, and a certain fixed direction. It is convenient to switch to the dimensionless velocity $\mathbf{c}$:

$$c_i = \left(\frac{m}{2k_BT}\right)^{1/2}(v_i - u_i) \tag{117}$$

and to the dimensionless relative velocity $\mathbf{g}$:

$$g_i = \frac{1}{2}\left(\frac{m}{k_BT}\right)^{1/2}(v_{1i} - u_i) \tag{118}$$

After standard transformations and integration with respect to ϵ (see [16], p. 212) we obtain in (116)

$$\nu_{\text{St}ik} = \frac{3P}{m}\pi^{-1/2}\int \exp(-c_1^2)\varphi_1^{(2)}(g)\left((c_{1i} - c_i)(c_{1k} - c_k) - \frac{1}{3}\delta_{ik}(\mathbf{c}_1 - \mathbf{c})^2\right)d\mathbf{c_1} \tag{119}$$

Here

$$\varphi_1^{(2)} = \int (1 - \cos^2\chi) \mid \mathbf{v_1} - \mathbf{v} \mid b(\chi)\left|\frac{db}{d\chi}\right|d\chi, \tag{120}$$

and χ is an angle between the vectors g and g'.

The dependence of $\varphi_1^{(2)}$ on the vector g is determined by the choice of the model of particle's interaction.

For Maxwell molecules,

$$\varphi_1^{(2)} = \left(\frac{2\kappa}{m}\right)^{1/2} A_2(5), \tag{121}$$

where κ is a force constant, $A_2(5)$ is a number, $A_2(5) \approx 0.436$.

For the model of hard spheres

$$\varphi_1^{(2)} = \frac{\sqrt{2}\sigma^2}{3}\left(\frac{k_BT}{m}\right)^{1/2} \mid \mathbf{c_1} - \mathbf{c} \mid, \tag{122}$$

where σ is diameter of the sphere modelling the particle.

Substituting (121) and (122) into (119), we transform the latter to the form: for Maxwell molecules

$$\nu_{\mathrm{St}ik} = \frac{3P}{4m}\left(\frac{2\kappa}{\pi m}\right)^{1/2} A_2(5)\exp(-c^2)\left(\frac{\partial}{\partial c_i}\frac{\partial}{\partial c_k} - \frac{1}{3}\delta_{ik}\frac{\partial}{\partial c_s}\frac{\partial}{\partial c_s}\right)T^{\mathrm{M.M.}}(c^2),$$
$$T^{\mathrm{M.M.}}(c^2) = \int \exp(-x^2 - 2x_kc_k)d\mathbf{x}; \tag{123}$$

for hard spheres

$$\nu_{\mathrm{St}ik} = \frac{P\sigma^2}{2\sqrt{2}m}\left(\frac{k_BT}{\pi m}\right)^{1/2}\exp(-c^2)\left(\frac{\partial}{\partial c_i}\right)\frac{\partial}{\partial c_k} - \frac{1}{3}\delta_{ik}\frac{\partial}{\partial c_s}\frac{\partial}{\partial c_s}T^{\mathrm{H.S.}}(c^2),$$
$$T^{\mathrm{H.S.}}(c^2) = \int \mid \mathbf{x} \mid \exp(-x^2 - 2x_kc_k)d\mathbf{x}. \tag{124}$$

It is an easy matter to perform integration in (123), the integral is equal to $\pi^{3/2}e^{c^2}$. Therefore for Maxwell molecules,

$$\nu_{\mathrm{St}ik} = \frac{3}{2}n\pi\left(\frac{2\kappa}{m}\right)^{1/2} A_2(5)\left((v_i - u_i)(v_k - u_k) - \frac{1}{3}\delta_{ik}(\mathbf{v} - \mathbf{u})^2\right). \tag{125}$$

The integral $T^{\mathrm{H.S.}}$ in (124) can be transformed as follows:

$$T^{\mathrm{H.S.}}(c^2) = 2\pi + \pi\int_{-1}^{+1}\exp(c^2(1 - y^2))c^2(1 + y^2)dy. \tag{126}$$

Then for the model of hard spheres,

$$\nu_{\mathrm{St}ik} = \sqrt{2\pi}n\sigma^2\left(\frac{k_BT}{m}\right)^{3/2}\left(c_ic_k - \frac{1}{3}\delta_{ik}c^2\right)\times$$
$$\times\int_{-1}^{+1}\exp(-c^2y^2)(1 + y^2)(1 - y^2)(c^2(1 - y^2) + 2)dy. \tag{127}$$

Let us note a useful relationship:

$$d^nT^{\mathrm{H.S.}}/d(c^2)^n = \pi\int_{-1}^{+1}\exp(c^2(1 - y^2))\times$$
$$\times(1 + y^2)(1 - y^2)^{n-1}(c^2(1 - y^2) + n)dy, n \geq 1. \tag{128}$$

Use the expressions for the viscosity coefficient μ_0 which are obtained in the first approximation of the Chapman-Enskog method:
for Maxwell molecules,

$$\mu_0^{\text{M.M.}} = \left(\frac{2m}{\kappa}\right)^{1/2} \frac{k_BT}{3\pi A_2(5)}; \tag{129}$$

for hard spheres,

$$\mu_0^{\text{H.S.}} = \frac{5(k_BTm)^{1/2}}{16\pi^{1/2}\sigma^2}. \tag{130}$$

Transformation of (125), (127) to the form of (68) gives the following functions $\Phi((\mathbf{v}-\mathbf{u})^2)$:
for Maxwell molecules,

$$\Phi = P/\mu_0^{\text{M.M.}}; \tag{131}$$

for hard spheres

$$\Phi = \frac{5P}{16\sqrt{2}\mu_0^{\text{H.S.}}} \int_{-1}^{+1} \exp\left(-\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}y^2\right) \times$$
$$\times(1+y^2)(1-y^2)\left(\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}(1-y^2)+2\right)dy. \tag{132}$$

The parameter r from (69) is:
for Maxwell molecules:

$$r = \left(m\mu_0^{\text{M.M.}}\right)^2/(2P^3k_BT); \tag{133}$$

for hard spheres:

$$r = \tilde{r}\frac{64\left(m\mu_0^{\text{M.M.}}\right)^2}{25P^3k_BT}. \tag{134}$$

The dimensionless parameter $\tilde{r}$ is analytically represented as follows:

$$\tilde{r}^{-1} = \frac{1}{16}\int_{-1}^{+1}\int_{-1}^{+1} \alpha^{-11/2}\beta(y)\beta(z)\gamma(y)\gamma(z) \times$$
$$\times(16\alpha^2 + 28\alpha(\gamma(y)+\gamma(z)) + 63\gamma(y)\gamma(z))dydz. \tag{135}$$

Here and below the following notations are used:

$$\beta(y) = 1+y^2, \qquad \gamma(y) = 1-y^2, \qquad \alpha = 1+y^2+z^2. \tag{136}$$

Numerical value of $\tilde{r}^{-1}$ is 5.212 to third digit.

The parameter (77) is:
for Maxwell molecules

$$s^{-1} = (2P^2k_BT)/\left(m^2\mu_0^{\text{M.M.}}\right); \tag{137}$$

for hard spheres

$$s^{-1} = \tilde{s}^{-1} \frac{5\sqrt{2}P^2 k_B T}{8m^2 \mu_0^{\mathrm{H.S.}}}. \tag{138}$$

The dimensionless parameter $\tilde{s}^{-1}$ is of the form

$$\tilde{s}^{-1} = \int_{-1}^{+1} \gamma(y)\beta^{-7/2}(y) \left(\beta(y) + \frac{7}{4}\gamma(y)\right) dy. \tag{139}$$

Numerical value of $\tilde{s}^{-1}$ is 1.115 to third digit.

The collision moment density (84) is of the form,

$$\xi_{\mathrm{St}i} = \sqrt{2}\left(\frac{k_B T}{m}\right)^{3/2} \int f^{(0)}(\mathbf{v}_1) \mid \mathbf{v_1} - \mathbf{v} \mid \left\{c_i\left(c^2 - \frac{5}{2}\right)\right\} bdbd\epsilon d\mathbf{v_1}. \tag{140}$$

Standard transformation of the expression $\{c_i(c^2 - 5/2)\}$ and integration with respect to ϵ change (140) to the form,

$$\xi_{\mathrm{St}i} = \frac{P}{\sqrt{2\pi}m} \int \exp(-c_1^2)\varphi_1^{(2)}(3(c_1^2 - c^2)(c_{1i} - c_i) - (\mathbf{c}_1 - \mathbf{c})^2(c_{1i} + c_i))d\mathbf{c_1} \tag{141}$$

Further, using the expressions (121) and (122) for $\varphi_1^{(2)}$, we obtain:
for Maxwell molecules:

$$\xi_{\mathrm{St}i} = \frac{P}{m^2}\left(\frac{\kappa k_B T}{\pi}\right)^{1/2} A_2(5)\exp\left(-c^2\right)\hat{D}_i T^{\mathrm{M.M.}}(c^2); \tag{142}$$

for hard spheres:

$$\xi_{\mathrm{St}i} = \frac{P k_B T \sigma^2}{\sqrt{\pi}m^2} \exp(-c^2)\hat{D}_i T^{\mathrm{H.S.}}(c^2). \tag{143}$$

The operator $\hat{D}_i$ is of the form

$$\frac{1}{4}\frac{\partial}{\partial c_i}\frac{\partial}{\partial c_s}\frac{\partial}{\partial c_s} + \frac{3}{2}c_s\frac{\partial}{\partial c_s}\frac{\partial}{\partial c_i} - \frac{1}{2}c_i\frac{\partial}{\partial c_s}\frac{\partial}{\partial c_s}. \tag{144}$$

The operator $\hat{D}_i$ acts on the function $\psi(c^2)$ as follows:

$$\frac{d^2\psi}{d(c^2)^2}2c_i\left(c^2 - \frac{5}{2}\right) + c_i c^2\left(\frac{d^2\psi}{d(c^2)^2} - \frac{d^3\psi}{d(c^2)^3}\right). \tag{145}$$

From (142), (143) we obtain:
for Maxwell molecules:

$$\xi_{\mathrm{St}i} = \frac{P}{3\mu_0^{\mathrm{M.M.}}}(v_i - u_i)\left((\mathbf{v} - \mathbf{u})^2 - \frac{5k_B T}{m}\right); \tag{146}$$

for hard spheres:

$$\begin{aligned}\xi_{\mathrm{St}i} = \frac{5P}{16\sqrt{2}\mu_0^{\mathrm{H.S.}}}\Bigg\{&(v_i-u_i)\left((\mathbf{v}-\mathbf{u})^2-\frac{5k_BT}{m}\right)\times\\ &\times\int_{-1}^{+1}\exp\left(-\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}y^2\right)\beta(y)\gamma(y)\left(\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}\gamma(y)+2\right)dy+\\ &+(v_i-u_i)(\mathbf{v}-\mathbf{u})^2\int_{-1}^{+1}\exp\left(-\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}y^2\right)\beta(y)\gamma(y)\left(\sigma(y)\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}+\delta(y)\right)dy\Bigg\}\end{aligned}\tag{147}$$

The functions $\sigma(y), \delta(y)$ are of the form

$$\sigma(y) = y^2(1-y^2), \qquad \delta(y) = 3y^2-1. \tag{148}$$

The parameter η from (90) is:
for Maxwell molecules:

$$\eta = \frac{9m^3\left(\mu_0^{\mathrm{M.M.}}\right)^2}{10P^3(k_BT)^2}; \tag{149}$$

for hard spheres:

$$\eta = \tilde{\eta}\frac{64m^3\left(\mu_0^{\mathrm{H.S.}}\right)^2}{125P^3(k_BT)^2}. \tag{150}$$

The dimensionless parameter $\tilde{\eta}$ is of the form

$$\begin{aligned}\tilde{\eta}^{-1} = \int_{-1}^{+1}\int_{-1}^{+1}\beta(y)\beta(z)\gamma(y)\gamma(z)\alpha^{-13/2}\Bigg\{&\frac{639}{32}(\gamma(y)\gamma(z)+\sigma(y)\sigma(z)+\\ &+\sigma(y)\gamma(z)+\sigma(z)\gamma(y))+\frac{63}{16}\alpha(2\gamma(y)+2\gamma(z)-5\gamma(y)\gamma(z)+\\ &+2(\sigma(y)+\sigma(z))+\gamma(z)\delta(y)+\gamma(y)\delta(z)+\sigma(y)\delta(z)+\sigma(z)\delta(y))+\\ &+\frac{7}{8}\alpha^2(4-10\gamma(y)-10\gamma(z))+\frac{25}{4}\gamma(y)\gamma(z)+2\delta(y)+\\ &+2\delta(z)-5\sigma(y)-5\sigma(z)-\frac{5}{2}(\gamma(z)\delta(y)+\gamma(y)\delta(z)+\delta(y)\delta(z))+\\ &+\frac{1}{4}\alpha^3\left(-20+\frac{25}{4}(\gamma(y)+\gamma(z))-5(\delta(y)+\delta(z))\right)+\frac{5}{2}\alpha^4\Bigg\}\,dydz.\end{aligned}\tag{151}$$

Numerical value of $\tilde{\eta}^{-1}$ is 0.622 to second digit.

Finally, from (146), (147) we obtain τ^{-1}(97):
for Maxwell molecules

$$\tau^{-1} = \frac{5(Pk_BT)^2}{3\mu_0^{\mathrm{M.M.}}m^3}; \tag{152}$$

for hard spheres

$$\begin{aligned}\tau^{-1} &= \tilde{\tau}^{-1}\frac{25P^2(k_BT)^2}{8\sqrt{2}m^3\mu_0^{\mathrm{H.S.}}},\\ \tilde{\tau}^{-1} &= \frac{1}{8}\int_{-1}^{+1}\beta^{-9/2}(y)\gamma(y)\{63(\gamma(y)+\sigma(y))+\\ &+7\beta(y)(4-10\gamma(y)+2\delta(y)-5\sigma(y))+20\beta^3(y)+\\ &+\beta^2(y)(25\gamma(y)-10\delta(y)-40)\}dy \approx 4.322.\end{aligned}\tag{153}$$

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