

DERIVATION OF 13 MOMENT EQUATIONS FOR RAREFIED GAS FLOW TO SECOND ORDER ACCURACY FOR ARBITRARY INTERACTION POTENTIALS*

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Abstract. A recent approach to derive transport equations for rarefied gases from the Boltzmann equation within higher orders of the Knudsen number [H. Struchtrup, *Phys. Fluids*, 16 (2004), pp. 3921–3934] is used to derive a set of 13 moment equations for arbitrary molecular interaction potentials. It is shown that the new set of equations is accurate to second order, while Grad's original 13 moment equations are of second order accuracy only for Maxwell molecules and Bhatnagar–Gross–Krook models.

Key words. Boltzmann equation, Chapman–Enskog expansion, Grad's moment method, regularized 13 moment equations

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1. Introduction. While it is well known that the Navier–Stokes–Fourier (NSF) equations fail to describe processes in rarefied gases for Knudsen numbers above 0.05, it is still a matter of debate how a set of meaningful macroscopic equations for larger Knudsen numbers can be derived from the Boltzmann equation.

The NSF equations are routinely derived from the Boltzmann equation by means of the Chapman–Enskog expansion [1], [2], [3], which yields the NSF equations in first order of the Knudsen number. However, the Chapman–Enskog expansions to second and third order yield the Burnett and super-Burnett equations [3], [4], which are known to be unstable in transient processes [5] and to give unphysical results in steady state problems [6]. Thus one has to conclude that the Chapman–Enskog expansion fails at higher orders. The reasons for that failure, however, remain unclear.

In recent years some authors proposed ad hoc improvements of the Burnett equations which yield stability [7], [8], [9], [10] but are somewhat difficult to justify, since they are not linked well to the Boltzmann equation; see [11], [6] for a discussion.

Another well-known method for obtaining equations for rarefied gas flows is Grad's method of moments [12], [13], which provides stable equations at any level, that is, for any set of moments considered as the basic variables of the theory. There are two major points of criticism against Grad's method, namely, that Grad's equations fail to describe smooth shock structures for Mach numbers above a critical value [14] and that the equations are not related a priori to the Knudsen number as a smallness parameter.

The failure to describe smooth shock structures is related to the fact that the Grad equations are of hyperbolic type and thus have a maximum signal velocity [14]. Only recently Struchtrup and Torrilhon introduced a regularization for Grad's 13 moment equations which is based on a Chapman–Enskog expansion around a nonequilibrium state [15], [11]; see also [16] for a similar approach. The regularized Grad equations

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produce smooth shock structures for all Mach numbers and thus overcome this particular problem.

In a series of papers Reinecke and Kremer were able to show that NSF and Burnett equations can be derived from certain sets of Grad's moment equations by means of a Maxwellian iteration [17], [18], a method that is essentially equivalent to a Chapman–Enskog expansion of the moments [19]. Struchtrup and Torrillon showed that a Chapman–Enskog expansion of the regularized 13 moment equations yields the Burnett and super-Burnett equations for Maxwell molecules [15], so that this set of equations is of third order.

The first attempt to derive Grad's equations by means of arguments on the Knudsen number is due to Müller, Reitebuch, and Weiss [20], who considered the infinite system of coupled moment equations of the Bhatnagar–Gross–Krook (BGK) equation [21]. From these they determined the order of magnitude of moments in terms of orders in powers of the Knudsen number and declared that a theory of order λ needs to consider all terms in all moment equations up to the order $\mathcal{O}(\varepsilon^\lambda)$. At first, these are the moment equations for all moments of order $\beta \leq \lambda$ under omission of higher order terms. However, these equations split into two independent subsystems, and only a smaller number of equations (and variables) remain as equations of importance [20].

In the method developed below, we do not ask for the order of terms in all moment equations but of the order of magnitude of their influence in the conservations laws, i.e., on heat flux and stress tensor. This is quite different. For example, in order to compute the heat flux with third order accuracy, as is necessary in a third order theory, other moments are needed only with second order accuracy, while others can be ignored completely. Müller, Reitebuch, and Weiss's consistent order extended thermodynamics [20], on the other hand, would require higher order accuracy for these moments and a larger number of moments. The new method was applied to the special cases of Maxwell molecules and the BGK model in [22], and it could be shown that it yields the Euler equations at zeroth order, the NSF equations at first order, Grad's 13 moment equations (with omission of a nonlinear term) at second order, and Struchtrup and Torrillon's regularization of these at third order. An important feature of the new method is that the equations at any order are stable, other than in the Chapman–Enskog method, where the second and third approximation—Burnett and super-Burnett equations—are unstable.

The restriction to Maxwell molecules, or the BGK model, leads to a comparatively simple application of the new method, and what has to be done for other models of molecular interaction was only sketched roughly in [22]. The present paper gives a detailed account of the method applied to arbitrary interaction models up to second order accuracy. It will be shown that, again, the first order approximation agrees with the NSF equations as they are derived by means of the Chapman–Enskog expansion, while the theory of second order accuracy yields a set of 13 moment equations which differ from Grad's original 13 moment equations. In particular the new equations have different numerical coefficients and some additional terms. All coefficients depend on the interaction model used. The latter feature is well known from the Burnett equations where the coefficients depend on the interaction model used as well [1], [18].

In the present paper, the method is outlined in detail, but numerical values of the coefficients are not computed. Indeed, this paper serves to set the stage for detailed calculations, since it carefully analyzes the problem for the most general setting—arbitrary interaction potentials of particles. This allows us to identify exactly what quantities—mostly coefficient matrices for moments of the collision term—must be determined for a theory of second order. Thus, the present paper presents the

necessary work that needs to be done *before* numerical values for coefficients can be computed. Detailed calculations of the numerical values of coefficients for the generalized 13 moment equations, and tests of the new equations, are planned for the future.

Accordingly, the present paper is quite technical in nature. The reader interested in more background to the new method used here is referred to [22], where the new method is discussed in detail, including careful comparisons with the classical methods of Chapman–Enskog and Grad.

The remainder of the paper is organized as follows. In section 2 the moments are defined as basic irreducible tensors, and the infinite set of moment equations is derived. The moments of the collision term of the Boltzmann equation are discussed in section 3. Their computation requires an expression for the particle distribution function in terms of the moments, and the Reinecke–Kremer–Grad method [17], [18] is suggested to determine that function. In section 4 the order of magnitude of the moments is determined, and the minimum number of moments of first order is discussed. The results are then used in section 5 to develop the proper sets of equations for zeroth to second order accuracy. The paper ends with our conclusions.

2. Basic equations.

2.1. Boltzmann equation. Our starting point is the Boltzmann equation [1], [2], which we write as

$$(2.1) \quad \frac{Df}{Dt} + C_k \frac{\partial f}{\partial x_k} = \frac{1}{\varepsilon} \mathcal{S}(f),$$

where f denotes the phase density, $C_k = c_k - v_k$ denotes the peculiar velocity with c_k as the velocity of a particle, and v_k denotes the center of mass velocity of the flow. $\frac{D}{Dt} = \frac{\partial}{\partial t} + v_k \frac{\partial}{\partial x_k}$ denotes the material time derivative.

ε is a formal smallness parameter which stands for the Knudsen number. This parameter will be used for monitoring the order of magnitude of the moments and the order of magnitude of terms within equations. At the end of all calculations, ε will be set equal to unity. In fact, if proper dimensionless quantities were introduced, the dimensionless Boltzmann equation would read as (2.1) with the Knudsen number instead of ε , and the Knudsen number could be used as the smallness parameter for the procedure below. Reinserting of the dimensions would then remove the Knudsen number—this corresponds to setting $\varepsilon = 1$ at the end of the computations. Thus the use of ε removes the necessity of introducing dimensionless quantities.

$\mathcal{S}(f)$ is the collision term that accounts for the change of f due to collisions and is given as [1], [2]

$$(2.2) \quad \mathcal{S}(f) = \int (f' f'_1 - f f_1) \sigma g \sin \Theta d\Theta d\varepsilon d\mathbf{c}_1,$$

where \mathbf{c} and \mathbf{c}_1 are the velocity vectors of two colliding particles before the collision, \mathbf{c}' and \mathbf{c}'_1 are the velocities after collision, $\mathbf{g} = \mathbf{c} - \mathbf{c}_1$ is the relative velocity and $g = |\mathbf{g}|$, σ is the collisional cross section, Θ is the collision angle, and ε is an angle that defines the direction of the collisional plane. Finally, $f' = f(\mathbf{x}, t, \mathbf{c}')$, etc.

The collision term has the following properties: (a) conservation of mass, momentum, and energy, so that

$$(2.3) \quad m \int \{1, c_i, C^2\} \mathcal{S}(f) d\mathbf{c} = 0.$$

(b) In equilibrium, the phase density is the Maxwellian,

$$(2.4) \quad \mathcal{S}(f) = 0 \implies f = f_M = \frac{\rho}{m} \sqrt{\frac{1}{2\pi\theta}}^3 \exp\left[-\frac{C^2}{2\theta}\right],$$

where ρ is the mass density, and $\theta = \frac{k}{m}T$ is the temperature in energy units, where T is the temperature, m is the particle mass, and k denotes Boltzmann's constant.

(c) The Boltzmann equation leads to a positive entropy production.

2.2. Moments. We define the general irreducible moments of the phase density as

$$(2.5) \quad u_{i_1 \dots i_n}^a = m \int C^{2a} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle} f d\mathbf{c},$$

where indices in angular brackets denote the symmetric and trace-free part of a tensor. Note that the moments $u_{i_1 \dots i_n}^a$ that are used in this paper are trace-free by definition, $u_{i_1 \dots i_n}^a = u_{\langle i_1 \dots i_n \rangle}^a$, and that this is not made explicit with brackets in order to avoid confusing notation involving several pairs of brackets. Appendix A gives a short introduction to trace-free tensors.

Some of the moments have a particular interpretation, namely,

$$u^0 = \rho, \quad u_i^0 = 0, \quad u^1 = 2\rho e = 3\rho\theta = 3p, \quad u_{ij}^0 = \sigma_{ij}, \quad u_i^1 = 2q_i.$$

Here we introduced the specific internal energy $e = \frac{3}{2}\theta$ of the ideal gas, the pressure p , the irreducible part of the pressure tensor σ_{ij} , and the heat flux q_i .

The values of the moments in equilibrium (E), when by (2.4) the phase density is a Maxwellian, are given by

$$u_{|E}^a = (2a+1)!! \rho \theta^a, \quad u_{i_1 \dots i_n |E}^a = 0, \quad n \geq 1,$$

where $(2a+1)!! = \prod_{s=1}^a (2s+1)$. The moments of the collision term of the Boltzmann equation (2.1) are defined as

$$\mathcal{P}_{i_1 \dots i_n}^a = m \int C^{2a} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle} \mathcal{S}(f) d\mathbf{c}$$

and will be discussed in section 3. Due to the conservation conditions (2.3), we have

$$(2.6) \quad \mathcal{P}^0 = \mathcal{P}_i^0 = \mathcal{P}^1 = 0.$$

2.3. Generic moment equation. Multiplication of the Boltzmann equation with $mC^{2a}C_{\langle i_1}C_{i_2}\dots C_{i_n \rangle}$ and subsequent integration over velocity space yields, after some rearrangement, the general equation for the moments (2.5),

$$(2.7) \quad \begin{aligned} & \frac{Du_{i_1 \dots i_n}^a}{Dt} + 2a u_{i_1 \dots i_n k}^{a-1} \frac{Dv_k}{Dt} + \frac{n}{2n+1} (2a+2n+1) u_{\langle i_1 \dots i_{n-1} \rangle}^a \frac{Dv_{i_n}}{Dt} + \frac{\partial u_{i_1 \dots i_n k}^a}{\partial x_k} \\ & + \frac{n}{2n+1} \frac{\partial u_{\langle i_1 \dots i_{n-1} \rangle}^{a+1}}{\partial x_{i_n}} + 2a u_{i_1 \dots i_n k l}^{a-1} \frac{\partial v_k}{\partial x_l} + 2a \frac{n+1}{2n+3} u_{\langle i_1 \dots i_n \rangle}^a \frac{\partial v_k}{\partial x_k} \\ & + 2a \frac{n}{2n+1} u_{\langle i_1 \dots i_{n-1} \rangle}^a \frac{\partial v_k}{\partial x_{i_n}} + n u_{k \langle i_1 \dots i_{n-1} \rangle}^a \frac{\partial v_{i_n}}{\partial x_k} + u_{i_1 \dots i_n}^a \frac{\partial v_k}{\partial x_k} \\ & + \frac{n(n-1)}{4n^2-1} (2a+2n+1) u_{\langle i_1 \dots i_{n-2} \rangle}^{a+1} \frac{\partial v_{i_{n-1}}}{\partial x_{i_n}} = \frac{1}{\varepsilon} \mathcal{P}_{i_1 \dots i_n}^a. \end{aligned}$$

Note that all moments are trace-free by definition, and additional trace-free tensors are made explicit by means of angular brackets. This implies that each of the terms in the above equation is trace-free and symmetric in the indices $i_1 \cdots i_n$. The derivation of the equation above requires multiple use of relation (A.2) [23]

$$C^{2a} C_{\langle i_1} C_{i_2} \cdots C_{i_n \rangle} C_k = C^{2a} C_{\langle i_1} C_{i_2} \cdots C_{i_n} C_k \rangle + \frac{n}{2n+1} C^{2a+2} C_{\langle i_1} C_{i_2} \cdots C_{i_{n-1}} \delta_{i_n \rangle k}.$$

The set of infinitely many moment equations ($a \rightarrow \infty$, $n \rightarrow \infty$) is equivalent to the Boltzmann equation. We are interested in limits of the Boltzmann equation given by orders of the Knudsen number ε , and due to this equivalence we can perform the limiting process on the moment equations, rather than on the Boltzmann equation itself.

2.4. Conservation laws. First, we consider the conservation laws, that is, those equations which, by (2.6), have a vanishing collision moment. For $a = 0$, $n = 0$ we obtain the mass balance

$$\frac{Du^0}{Dt} + u^0 \frac{\partial v_k}{\partial x_k} = 0,$$

and for $a = 1$, $n = 0$ we find the balance of internal energy as

$$\frac{Du^1}{Dt} + \frac{\partial u_k^1}{\partial x_k} + 2u_{kl}^0 \frac{\partial v_k}{\partial x_l} + \frac{5}{3} u^0 \frac{\partial v_k}{\partial x_k} = 0.$$

Note that by introducing ρ , θ , σ_{ij} , q_i and some simple manipulations these two equations can be brought into their usual textbook form:

$$(2.8) \quad \frac{D\rho}{Dt} + \rho \frac{\partial v_k}{\partial x_k} = 0,$$

$$(2.9) \quad \frac{3}{2} \rho \frac{D\theta}{Dt} + \rho \theta \frac{\partial v_k}{\partial x_k} + \frac{\partial q_k}{\partial x_k} + \sigma_{kl} \frac{\partial v_k}{\partial x_l} = 0.$$

For the choice $a = 1$, $n = 1$ we obtain the balance of momentum

$$(2.10) \quad \rho \frac{Dv_i}{Dt} + \theta \frac{\partial \rho}{\partial x_i} + \rho \frac{\partial \theta}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = 0.$$

2.5. Scalar moments. For scalar moments ($n = 0$), the general equation (2.7) reduces to

$$\frac{Du^a}{Dt} + 2au_k^{a-1} \frac{Dv_k}{Dt} + \frac{\partial u_k^a}{\partial x_k} + 2au_{kl}^{a-1} \frac{\partial v_k}{\partial x_l} + \frac{2a+3}{3} u^a \frac{\partial v_k}{\partial x_k} = \frac{1}{\varepsilon} \mathcal{P}^a.$$

Next, we introduce the difference between the scalar variables and their equilibrium values as

$$(2.11) \quad w^a = u^a - u_{|E}^a$$

and rewrite the scalar equations for these new variables, where all time derivatives of ρ , θ , v_i are replaced by means of the conservation laws. This yields

$$\begin{aligned} & \frac{Dw^a}{Dt} - \frac{2a}{3} (2a+1)!! \theta^{a-1} \frac{\partial q_k}{\partial x_k} - \frac{2a}{3} (2a+1)!! \theta^{a-1} \sigma_{kl} \frac{\partial v_k}{\partial x_l} + 2au_{kl}^{a-1} \frac{\partial v_k}{\partial x_l} \\ & - 2au_k^{a-1} \frac{\partial \theta}{\partial x_k} - 2au_k^{a-1} \theta \frac{\partial \ln \rho}{\partial x_k} - 2a \frac{u_k^{a-1}}{\rho} \frac{\partial \sigma_{kl}}{\partial x_l} + \frac{\partial u_k^a}{\partial x_k} + \frac{2a+3}{3} w^a \frac{\partial v_k}{\partial x_k} = \frac{1}{\varepsilon} \mathcal{P}^a. \end{aligned}$$

Of course, for $a = 0$ and $a = 1$, the equations are identically fulfilled, so that the above equation makes sense only for $a \geq 2$. Note that $w^0 = w^1 = 0$ and $u_i^0 = 0$.

2.6. Vector moments. For vectors, the general equation (2.7) reduces to

$$\begin{aligned} \frac{Du_i^a}{Dt} + 2au_{ik}^{a-1} \frac{Dv_k}{Dt} + \frac{2a+3}{3} u^a \frac{Dv_i}{Dt} + \frac{\partial u_{ik}^a}{\partial x_k} + \frac{1}{3} \frac{\partial u^{a+1}}{\partial x_i} + 2au_{ikl}^{a-1} \frac{\partial v_k}{\partial x_l} \\ + \frac{4a}{5} u_{\langle i}^a \frac{\partial v_{k\rangle}}{\partial x_k} + \frac{2a}{3} u_k^a \frac{\partial v_k}{\partial x_i} + u_k^a \frac{\partial v_i}{\partial x_k} + u_i^a \frac{\partial v_k}{\partial x_k} = \frac{1}{\varepsilon} \mathcal{P}_i^a. \end{aligned}$$

We introduce the quantities w^a in the vector equation and replace the time derivatives of the velocity by means of the momentum balance (2.10) to obtain

$$\begin{aligned} (2.12) \quad \frac{Du_i^a}{Dt} + \frac{a(2a+3)!!}{3} \rho \theta^a \frac{\partial \theta}{\partial x_i} - \frac{2a+3}{3} w^a \frac{\partial \theta}{\partial x_i} - 2au_{ik}^{a-1} \frac{\partial \theta}{\partial x_k} - 2au_{ik}^{a-1} \theta \frac{\partial \ln \rho}{\partial x_k} \\ - \frac{2a+3}{3} w^a \theta \frac{\partial \ln \rho}{\partial x_i} - 2a \frac{u_{ik}^{a-1}}{\rho} \frac{\partial \sigma_{kl}}{\partial x_l} - \frac{2a+3}{3} \frac{w^a}{\rho} \frac{\partial \sigma_{ik}}{\partial x_k} - \frac{(2a+3)!!}{3} \theta^a \frac{\partial \sigma_{ik}}{\partial x_k} + \frac{\partial u_{ik}^a}{\partial x_k} \\ + \frac{1}{3} \frac{\partial w^{a+1}}{\partial x_i} + 2au_{ikl}^{a-1} \frac{\partial v_k}{\partial x_l} + \frac{2a+5}{5} u_i^a \frac{\partial v_k}{\partial x_k} + \frac{2a+5}{5} u_k^a \frac{\partial v_i}{\partial x_k} + \frac{2a}{5} u_k^a \frac{\partial v_k}{\partial x_i} = \frac{1}{\varepsilon} \mathcal{P}_i^a. \end{aligned}$$

This equation is relevant for $a \geq 1$. Note that $w^1 = 0$ and $u_i^0 = 0$.

2.7. Rank-2 tensor moments. After replacing the time derivatives of velocity by (2.10), the equations for tensors of rank 2 read

$$\begin{aligned} (2.13) \quad \frac{Du_{ij}^a}{Dt} - 2a \frac{u_{ijk}^{a-1}}{\rho} \left(\frac{\partial \sigma_{kl}}{\partial x_l} + \theta \frac{\partial \rho}{\partial x_k} + \rho \frac{\partial \theta}{\partial x_k} \right) - \frac{2}{5} (2a+5) \frac{u_{\langle i}^a}{\rho} \left(\frac{\partial \sigma_{j\rangle k}}{\partial x_k} + \theta \frac{\partial \rho}{\partial x_j} + \rho \frac{\partial \theta}{\partial x_j} \right) \\ + \frac{\partial u_{ijk}^a}{\partial x_k} + \frac{2}{5} \frac{\partial u_{\langle i}^{a+1}}{\partial x_j} + 2au_{ijkl}^{a-1} \frac{\partial v_k}{\partial x_l} + \frac{6a}{7} u_{\langle ij}^a \frac{\partial v_{k\rangle}}{\partial x_k} + \frac{4a}{5} u_{k\langle i}^a \frac{\partial v_{j\rangle}}{\partial x_j} + 2u_{k\langle i}^a \frac{\partial v_{j\rangle}}{\partial x_k} \\ + u_{ij}^a \frac{\partial v_k}{\partial x_k} + \frac{2}{15} (2a+5) w^{a+1} + \frac{2}{15} (2a+5)!! \rho \theta^{a+1} \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = \frac{1}{\varepsilon} \mathcal{P}_{ij}^a. \end{aligned}$$

This equation is relevant for $a \geq 0$. Note that all terms in this equation are trace-free and symmetric in the index pair ij .

2.8. General equation. For moments of order higher than two, the general equation reads

$$\begin{aligned} \frac{Du_{i_1 \dots i_n}^a}{Dt} - 2a \frac{u_{i_1 \dots i_n k}^{a-1}}{\rho} \left(\frac{\partial \sigma_{kl}}{\partial x_l} + \theta \frac{\partial \rho}{\partial x_k} + \rho \frac{\partial \theta}{\partial x_k} \right) \\ - \frac{n}{2n+1} (2a+2n+1) \frac{u_{\langle i_1 \dots i_{n-1}}^a}{\rho} \left(\frac{\partial \sigma_{i_n\rangle k}}{\partial x_k} + \theta \frac{\partial \rho}{\partial x_{i_n}} + \rho \frac{\partial \theta}{\partial x_{i_n}} \right) + \frac{\partial u_{i_1 \dots i_n k}^a}{\partial x_k} \\ + \frac{n}{2n+1} \frac{\partial u_{\langle i_1 \dots i_{n-1}}^{a+1}}{\partial x_{i_n}} + 2au_{i_1 \dots i_n k l}^{a-1} \frac{\partial v_k}{\partial x_l} + 2a \frac{n+1}{2n+3} u_{\langle i_1 \dots i_n}^a \frac{\partial v_{k\rangle}}{\partial x_k} \\ + 2a \frac{n}{2n+1} u_{k\langle i_1 \dots i_{n-1}}^a \frac{\partial v_{j\rangle}}{\partial x_{i_n}} + nu_{k\langle i_1 \dots i_{n-1}}^a \frac{\partial v_{i_n\rangle}}{\partial x_k} + u_{i_1 \dots i_n}^a \frac{\partial v_k}{\partial x_k} \\ + \frac{n(n-1)}{4n^2-1} (2a+2n+1) u_{\langle i_1 \dots i_{n-2}}^{a+1} \frac{\partial v_{i_{n-1}\rangle}}{\partial x_{i_n}} = \frac{1}{\varepsilon} \mathcal{P}_{i_1 \dots i_n}^a. \end{aligned}$$

This equation is relevant for $a \geq 0$. Note that all terms in this equation are trace-free and symmetric in the indices $i_1 \dots i_n$.

3. Moments of the collision term. The moments of the collision term of the Boltzmann equation (2.2) are defined as

$$(3.1) \quad \mathcal{P}_{i_1 \dots i_n}^a = m \int C^{2a} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle} \mathcal{S}(f) d\mathbf{c}.$$

For the method used subsequently, it is necessary to express the $\mathcal{P}_{i_1 \dots i_n}^a$ through the moments. Since the collision term depends explicitly on the phase density, this is tantamount to having a relation between the moments and the phase density. Only in few special cases can the collisional moments be computed without explicit knowledge of the phase density. In particular, this is the case for BGK models [21] and Maxwell molecules. For these models, the method was discussed in detail in [22].

For general interaction potentials the situation is more difficult, and we suggest the Reinecke–Kremer–Grad method [17], [18]. Essentially, this method uses the Grad method to compute the phase density as a function of the moments and the microscopic velocity c_i . That phase density is then used to compute the production terms (3.1). One problem that arises here is that this method requires the restriction to a *finite* number of moments.

The ansatz for the Grad phase density reads

$$(3.2) \quad f|_G = f_M (1 + \Phi) = f_M \left[1 + \sum_n \sum_{a=0}^{A_n} \lambda_{i_1 \dots i_n}^a C^{2a} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle} \right],$$

where $\lambda_{i_1 \dots i_n}^a$ are expansion coefficients, and A_n denotes the numbers of moments of tensorial rank n that are taken into account in the approach. The A_n introduce some degree of freedom here, and we shall later give an argument on how they must be determined to ensure sufficient accuracy. For the informed reader, we mention already here that the numbers A_n correspond to the number of Sonine polynomials that is standard in the Chapman–Enskog expansion; see, e.g., [3].

The expansion coefficients follow from plugging the Grad phase density (3.2) into the definition of the moments (2.11), (2.5),

$$w^b = m \int C^{2a} (f_G - f_M) d\mathbf{c} = \rho \sum_{a=0}^{A_0} \theta^{a+b} \mathcal{B}_{ba}^{(0)} \lambda^a \quad (b = 0, \dots, A_0),$$

$$u_{j_1 \dots j_r}^b = m \int C^{2a} C_{\langle j_1} C_{j_2} \dots C_{j_r \rangle} f_G d\mathbf{c} = r! \rho \sum_{a=0}^{A_r} \theta^{a+b+r} \mathcal{B}_{ba}^{(r)} \lambda_{j_1 \dots j_r}^a \quad (b = 0, \dots, A_0),$$

where

$$\mathcal{B}_{ab}^{(r)} = \prod_{k=r+1}^{a+b+r} (2k+1) \quad (a, b \in [0, A_r]).$$

The relations between moments and the expansion coefficients are linear, and we find by inversion

$$(3.3) \quad \lambda_{j_1 \dots j_r}^a = \sum_b \left[\mathcal{B}_{ab}^{(r)} \right]^{-1} \frac{\bar{u}_{j_1 \dots j_r}^b}{r! \rho \theta^{a+b+r}} \quad \text{with} \quad \bar{u}^a = w^a, \quad \bar{u}_{i_1 \dots i_n}^a = u_{i_1 \dots i_n}^a$$

so that the Grad phase density is explicitly given. For more details on the above calculations, we refer the reader to [24].

With the Grad phase density, the collision moments are given by

$$\begin{aligned}\mathcal{P}_{i_1 \dots i_n}^a &= m \iint C^{2a} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle} \left(f'_{|G} f'_{|G,1} - f_{|G} f_{|G,1} \right) \sigma g \sin \Theta d\Theta d\varepsilon d\mathbf{c}_1 d\mathbf{c} \\ &= m \iint \left(C'^{2a} C'_{\langle i_1} C'_{i_2} \dots C'_{i_n \rangle} - C^{2a} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle} \right) f_{|G} f_{|G,1} \sigma g \sin \Theta d\Theta d\varepsilon d\mathbf{c}_1 d\mathbf{c}.\end{aligned}$$

We use $f_{|G} = f_M (1 + \Phi)$ to obtain

$$\begin{aligned}\mathcal{P}_{i_1 \dots i_n}^a &= m \iint \left(C^{2a} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle} \right) (\Phi'_1 + \Phi' - \Phi - \Phi_1 + \Phi' \Phi'_1 - \Phi \Phi_1) \\ &\quad \times f_M f_{M,1} \sigma g \sin \Theta d\Theta d\varepsilon d\mathbf{c}_1 d\mathbf{c} \\ &= m \iint \left(C'^{2a} C'_{\langle i_1} C'_{i_2} \dots C'_{i_n \rangle} - C^{2a} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle} \right) (\Phi_1 + \Phi + \Phi \Phi_1) \\ &\quad \times f_M f_{M,1} \sigma g \sin \Theta d\Theta d\varepsilon d\mathbf{c}_1 d\mathbf{c}.\end{aligned}$$

Without evaluating the integral further, we see from the equations above that $\mathcal{P}_{i_1 \dots i_n}^a$ is at most quadratic in the moments and thus must be of the general form

$$(3.4) \quad \mathcal{P}_{i_1 \dots i_n}^a = - \sum_b \mathcal{C}_{ab}^{(n)} \frac{\bar{u}_{i_1 \dots i_n}^b}{\tau \theta^{b-a}} - \sum_{r,m} \sum_{b,c} \mathcal{Y}_{a,bc}^{n,r,m} \frac{\bar{u}_{j_1 \dots j_r \langle i_1 \dots i_m}^b \bar{u}_{i_{m+1} i_{m+2} \dots i_n \rangle j_1 \dots j_r}^c}{\tau \rho \theta^{b+c+r-a}},$$

where the matrices $\mathcal{C}_{ab}^{(n)}$, $\mathcal{Y}_{a,bc}^{n,r,m}$ contain pure numbers. Above, we have introduced the mean free time τ as

$$\frac{1}{\tau} = \frac{m}{\rho} \int f_M f_{M,1} \sigma g \sin \Theta d\Theta d\varepsilon d\mathbf{c}_1 d\mathbf{c}.$$

In the present paper, we shall not compute the matrices $\mathcal{C}_{ab}^{(n)}$, $\mathcal{Y}_{a,bc}^{n,r,m}$ which depend on the particularities of the molecular interaction, as they are reflected in the collisional cross section σ . Obviously, their computation is cumbersome, and one will try to compute only those matrices that are necessary indeed. One of the goals in the following will be to give arguments in order to determine which matrices must be considered for a theory of second order. For now we shall just assume that the matrices $\mathcal{C}_{ab}^{(n)}$ are invertible, which is the case as long as the numbers A_n remain finite.

4. The order of magnitude of moments. We shall now assign orders of magnitude to the moments, and then construct new sets of moments, such that at each order of magnitude we have the minimal number of variables.

We base the discussion on a Chapman–Enskog like expansion of the moments, with ε as the smallness parameter. All moments are expanded according to

$$u_{i_1 \dots i_n}^a = \sum_{\beta=0} \varepsilon^\beta u_{i_1 \dots i_n|\beta}^a = \varepsilon^0 u_{i_1 \dots i_n|0}^a + \varepsilon^1 u_{i_1 \dots i_n|1}^a + \varepsilon^2 u_{i_1 \dots i_n|2}^a + \varepsilon^3 u_{i_1 \dots i_n|3}^a + \dots$$

and a similar series for the w^a .

We shall say that $u_{i_1 \dots i_n}^a$ is of leading order λ if $u_{i_1 \dots i_n|\beta}^a = 0$ for all $\beta < \lambda$. We emphasize that we are not interested in computing the expansion coefficients $u_{i_1 \dots i_n|\beta}^a$ but only in finding the leading order of the moments.

4.1. Zeroth and first order expansion. For the evaluation of the order of magnitude, it is important to note that the production terms are multiplied by the factor $\frac{1}{\varepsilon}$. If the above expansion is inserted into the moment equations for the non-conserved quantities, it becomes immediately clear that

$$w_{|0}^a = u_{i_1 \dots i_n|0}^a = 0$$

for all moments. This follows from balancing the factors of $\frac{1}{\varepsilon}$ on both sides of the equations—there are none of these on the left, and thus we have the above result. In other words, all quantities that are not conserved are at least of first order.

In the next step, we balance the factors of ε^0 in the equations and find

$$(4.1) \quad \begin{aligned} 0 &= - \sum_b C_{ab}^{(0)} \frac{w_{|1}^b}{\tau \theta^{b-a}}, \\ \frac{a(2a+3)!!}{3} \rho \theta^a \frac{\partial \theta}{\partial x_i} &= - \sum_b C_{ab}^{(1)} \frac{u_{i|1}^b}{\tau \theta^{b-a}}, \\ \frac{2}{15} (2a+5)!! \rho \theta^{a+1} \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} &= - \sum_b C_{ab}^{(2)} \frac{u_{ij|1}^b}{\tau \theta^{b-a}}, \\ 0 &= - \sum_b C_{ab}^{(n)} \frac{u_{i_1 \dots i_n|1}^b}{\tau \theta^{b-a}}. \end{aligned}$$

It follows that the leading order of vectors and rank-2 tensors, u_i^a and u_{ij}^a , is the first order, while the nonequilibrium parts of the scalar moments w^a and the higher moments $u_{i_1 \dots i_n}^a$ ($n \geq 3$) are at least of second order. Note that the nonlinear terms in the productions do not contribute at the zeroth and the first order.

4.2. Second order. Next, we have a look at the second order quantities. Since the vectors and rank-2 tensors are already known to be of first order in ε , we have to consider only the other moments. We make the equations for tensors of rank 3 and 4 explicit. Keeping only factors of ε^1 in the equations (note that, e.g., u_i^a is a $\mathcal{O}(\varepsilon)$ contribution) yields

$$\begin{aligned} & -\frac{2a}{3} (2a+1)!! \theta^{a-1} \frac{\partial q_k}{\partial x_k} - \frac{2a}{3} (2a+1)!! \theta^{a-1} \sigma_{kl} \frac{\partial v_k}{\partial x_l} + 2a u_{kl}^{a-1} \frac{\partial v_k}{\partial x_l} \\ & - 2a u_k^{a-1} \frac{\partial \theta}{\partial x_k} - 2a u_k^{a-1} \theta \frac{\partial \ln \rho}{\partial x_k} + \frac{\partial u_k^a}{\partial x_k} \\ & = - \sum_b C_{ab}^{(0)} \frac{w_{|2}^b}{\tau \theta^{b-a}} - \sum_{b,c} \mathcal{Y}_{a,bc}^{0,1,0} \frac{u_j^b u_j^c}{\tau \rho \theta^{b+c+1-a}} - \sum_{b,c} \mathcal{Y}_{a,bc}^{0,2,0} \frac{u_{jk}^b u_{jk}^c}{\tau \rho \theta^{b+c+2-a}} \end{aligned}$$

so that the w^a are of second order.

For the moments of rank 3 and 4, we obtain

$$\begin{aligned} & -\frac{3}{7} (2a+7) u_{\langle ij}^a \left[\theta \frac{\partial \ln \rho}{\partial x_k} + \frac{\partial \theta}{\partial x_k} \right] + \frac{3}{7} \frac{\partial u_{\langle ij}^{a+1}}{\partial x_k} + \frac{6}{35} (2a+7) u_{\langle i}^{a+1} \frac{\partial v_j}{\partial x_k} \\ & = - \sum_b C_{ab}^{(3)} \frac{u_{ijk|2}^b}{\tau \theta^{b-a}} - \sum_{b,c} \mathcal{Y}_{a,bc}^{3,0,2} \frac{u_{\langle ij}^b u_{\rangle k}^c}{\tau \rho \theta^{b+c-a}}, \end{aligned}$$

$$\frac{12}{63} (2a+9) u_{\langle ij}^{a+1} \frac{\partial v_k}{\partial x_l} = - \sum_b \mathcal{C}_{ab}^{(4)} \frac{u_{ijkl}^b}{\tau \theta^{b-a}} - \sum_{b,c} \mathcal{Y}_{a,bc}^{4,0,2} \frac{u_{\langle ij}^b u_{kl}^c \rangle}{\tau \rho \theta^{b+c-a}}$$

so that the u_{ijk}^b and the u_{ijkl}^b are also of second order. For all higher moments we find

$$0 = - \sum_b \mathcal{C}_{ab}^{(n)} \frac{u_{i_1 \dots i_n}^b}{\tau \theta^{b-a}}, \quad n \geq 5.$$

It follows that the nonequilibrium parts of the scalar moments w^a and the tensors of rank 3 and 4 are second order quantities. All higher moments are *at least* of third order. We will not go further, but it is evident that tensors of rank 5 and 6 are third order, tensors of rank 7 and 8 are fourth order, etc.

4.3. Minimal number of moments of order $\mathcal{O}(\varepsilon)$. From our first order result for the scalar and 2-tensors, (4.1), we see that the first order terms $u_{i|1}^b$ and $u_{ij|1}^b$ are related to the gradients of temperature and velocity, respectively, and thus they are linearly dependent. We obtain

$$(4.2) \quad u_{i|1}^b = -\kappa_b \tau \rho \theta^b \frac{\partial \theta}{\partial x_i}, \quad u_{ij|1}^b = -\mu_b \tau \rho \theta^{1+b} \frac{\partial v_{\langle i}}{\partial x_{j \rangle}},$$

where κ_b and μ_b are pure numbers, given by

$$(4.3) \quad \kappa_b = \sum_{a=1} \left[\mathcal{C}_{ba}^{(1)} \right]^{-1} \frac{a(2a+3)!!}{3}, \quad \mu_b = \sum_{a=0} \left[\mathcal{C}_{ba}^{(2)} \right]^{-1} \frac{2}{15} (2a+5)!!.$$

The first few values of these coefficients for Maxwell molecules (MM) and the BGK model are [22]

$$(4.4) \quad \text{MM: } \kappa_1 = 15/2, \quad \kappa_2 = 105, \quad \text{and} \quad \mu_0 = 2, \quad \mu_1 = 14,$$

$$(4.5) \quad \text{BGK: } \kappa_1 = 5, \quad \kappa_2 = 70, \quad \text{and} \quad \mu_0 = 2, \quad \mu_1 = 14.$$

In particular, the pressure deviator and heat flux are given to first order as

$$(4.6) \quad q_{i|1} = \frac{1}{2} u_{i|1}^1 = -\frac{1}{2} \kappa_1 \tau \rho \theta \frac{\partial \theta}{\partial x_i} = -\kappa \frac{\partial \theta}{\partial x_i},$$

$$\sigma_{ij|1} = u_{ij|1}^0 = -\mu_0 \tau \rho \theta \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} = -2\mu \frac{\partial v_{\langle i}}{\partial x_{j \rangle}},$$

where we have introduced heat conductivity and viscosity as κ and μ , respectively. Thus, in first order we obtain the laws of Fourier and Navier–Stokes. Note that the computation of μ and κ involves the inverses of the matrices $\mathcal{C}_{ab}^{(1)}$, $\mathcal{C}_{ab}^{(2)}$.

It follows from (4.2), (4.6) that we can write

$$u_{i|1}^b = \frac{2\kappa_b}{\kappa_1} \theta^{b-1} q_{i|1}, \quad u_{ij|1}^b = \frac{\mu_b}{\mu_0} \theta^b \sigma_{ij|1}.$$

While these equations relate the first order contributions of the vector and 2-tensor moments, it is straightforward to introduce new moments w_i^a, w_{ij}^a that are of second order only,

$$(4.7) \quad w_i^a = u_i^a - \frac{2\kappa_a}{\kappa_1} \theta^{a-1} q_i \quad (a \geq 2) \quad \text{and} \quad w_{ij}^a = u_{ij}^a - \frac{\mu_a}{\mu_0} \theta^a \sigma_{ij} \quad (a \geq 1)$$

so that

$$w_i^a = m \int \left(C^{2a-2} - \frac{2\kappa_a}{\kappa_1} \theta^{a-1} \right) C^2 C_i f d\mathbf{c} \quad (a \geq 2),$$

$$w_{ij}^a = m \int \left(C^{2a-2} - \frac{\mu_a}{\mu_0} \theta^a \right) C_{\langle i} C_{j \rangle} f d\mathbf{c} \quad (a \geq 1).$$

This means that we can formulate a set of moments, where only σ_{ij} and q_i are of first order, while all other moments are at least of second order (excluding the conserved moments, of course).

It is in principle possible to go to higher order with this: the second order terms of w_i^a (say), when expanded, will be linearly dependent, and again one can use this to obtain a minimal set of moments of second order, while the remaining ones can be constructed to be of third order, etc. This is not necessary for the levels of accuracy that are important in this paper, and so we shall not pursue this idea further.

5. The transport equations with second order accuracy. In the previous section we have established the order of magnitude of the various moments up to $\mathcal{O}(\varepsilon^2)$. Now we ask what equations we need in order to describe a flow process in a rarefied ideal gas with an accuracy of $\mathcal{O}(\varepsilon^\lambda)$.

In this section, we shall use the smallness parameter ε in a slightly different manner, namely, as an indicator for the leading order of a quantity. Thus, in any equation we shall replace $u_{i_1 \dots i_n}^a$ by $\varepsilon^\beta u_{i_1 \dots i_n}^a$ when β denotes the leading order of $u_{i_1 \dots i_n}^a$. This will allow for a proper bookkeeping of the order of magnitude of all terms in an equation.

5.1. The conservation laws and the definition of λ th order accuracy.

We start the argument by repeating the conservation laws for mass, momentum, and energy, (2.8), (2.10), (2.9), which read, when we assign the factor ε to the first order quantities σ_{ij} and q_i ,

$$(5.1) \quad \begin{aligned} \frac{D\rho}{Dt} + \rho \frac{\partial v_k}{\partial x_k} &= 0, \\ \frac{3}{2} \rho \frac{D\theta}{Dt} + \rho \theta \frac{\partial v_k}{\partial x_k} + \varepsilon \left[\frac{\partial q_k}{\partial x_k} + \sigma_{kl} \frac{\partial v_k}{\partial x_l} \right] &= 0, \\ \rho \frac{Dv_i}{Dt} + \rho \frac{\partial \theta}{\partial x_i} + \theta \frac{\partial \rho}{\partial x_i} + \varepsilon \left[\frac{\partial \sigma_{ik}}{\partial x_k} \right] &= 0. \end{aligned}$$

These equations are not a closed set of equations for ρ, v_i, T , but they contain pressure deviator σ_{ij} and heat flux q_i as additional quantities, and equations for these are required to obtain a closed set of equations.

We shall speak of a theory of λ th order accuracy when both σ_{ij} and q_i are known within the order $\mathcal{O}(\varepsilon^\lambda)$.

The equations of order $\mathcal{O}(\varepsilon^0)$ result from (5.1) by setting $\sigma_{ij} = q_i = 0$, that is, by ignoring the terms with the factor ε in the balance laws. This yields the Euler equations for ideal gases,

$$\frac{D\rho}{Dt} + \rho \frac{\partial v_k}{\partial x_k} = 0, \quad \frac{3}{2} \rho \frac{D\theta}{Dt} + \rho \theta \frac{\partial v_k}{\partial x_k} = 0, \quad \rho \frac{Dv_i}{Dt} + \theta \frac{\partial \rho}{\partial x_i} + \rho \frac{\partial \theta}{\partial x_i} = 0.$$

For higher order accuracy, i.e., first order and higher, we shall need the moment equations for the pressure deviator and heat flux.

5.2. Collision moments for vectors and tensors. For these, we have to consider the production terms for vectors and 2-tensors up to first order in ε . For vectors, we obtain from (3.4) by setting $n = 1$ and making the first two terms of the r -summation explicit

$$\begin{aligned} \frac{1}{\varepsilon} \mathcal{P}_i^a &= -\frac{1}{\varepsilon} \sum_b \mathcal{C}_{ab}^{(1)} \frac{\varepsilon u_i^b}{\tau \theta^{b-a}} - \frac{1}{\varepsilon} \sum_{b,c} \mathcal{Y}_{a,bc}^{1,0,1} \frac{\varepsilon u_i^b \varepsilon^2 w^c}{\tau \rho \theta^{b+c-a}} \\ &\quad - \frac{1}{\varepsilon} \sum_{b,c} \mathcal{Y}_{a,bc}^{1,1,1} \frac{\varepsilon u_{ij}^b \varepsilon u_j^c}{\tau \rho \theta^{b+c+1-a}} - \frac{1}{\varepsilon} \sum_{r=2} \sum_{b,c} \mathcal{Y}_{a,bc}^{1,r,1} \frac{\varepsilon^{2r-1} \bar{u}_{ij_1 \dots j_r}^b \bar{u}_{j_1 \dots j_r}^c}{\tau \rho \theta^{b+c+r-a}}. \end{aligned}$$

We shall only be interested in terms up to order $\mathcal{O}(\varepsilon)$, where the above equation reduces to

$$\frac{1}{\varepsilon} \mathcal{P}_i^a = -\sum_b \mathcal{C}_{ab}^{(1)} \frac{2\kappa_b}{\kappa_1} \frac{q_i}{\tau \theta^{1-a}} - \varepsilon \left[\sum_b \mathcal{C}_{ab}^{(1)} \frac{w_i^b}{\tau \theta^{b-a}} + \sum_{b,c} \mathcal{Y}_{a,bc}^{1,1,1} \frac{2\mu_b \kappa_c}{\mu_0 \kappa_1} \frac{\sigma_{ij} q_j}{\tau \rho \theta^{2-a}} \right].$$

For 2-tensors, we obtain in the same manner

$$\begin{aligned} \frac{1}{\varepsilon} \mathcal{P}_{ik}^a &= -\sum_b \mathcal{C}_{ab}^{(2)} \frac{\mu_b}{\mu_0} \frac{\sigma_{ik}}{\tau \theta^{-a}} \\ &\quad - \varepsilon \left[\sum_b \mathcal{C}_{ab}^{(2)} \frac{w_{ik}^b}{\tau \theta^{b-a}} + \sum_{b,c} \mathcal{Y}_{a,bc}^{2,0,1} \frac{4\kappa_b \kappa_c}{\kappa_1 \kappa_1} \frac{q_{\langle i} q_{k \rangle}}{\tau \rho \theta^{2-a}} + \sum_{b,c} \mathcal{Y}_{a,bc}^{2,1,1} \frac{\mu_b \mu_c}{\mu_0 \mu_0} \frac{\sigma_{j \langle i} \sigma_{k \rangle j}}{\tau \rho \theta^{1-a}} \right]. \end{aligned}$$

5.3. Equations for the pressure deviator and heat flux. We consider (2.14) with $a = 0$, where we introduce the moments (4.7) and obtain, after assigning the proper order of magnitude to the various terms,

$$\begin{aligned} (5.2) \quad \varepsilon \left[\frac{D\sigma_{ij}}{Dt} + \frac{4}{5} \frac{\partial q_{\langle i}}{\partial x_{j \rangle}} + 2\sigma_{k \langle i} \frac{\partial v_{j \rangle}}{\partial x_k} + \sigma_{ij} \frac{\partial v_k}{\partial x_k} + \sum_b \mathcal{C}_{0b}^{(2)} \frac{w_{ik}^b}{\tau \theta^b} + \sum_{b,c} \mathcal{Y}_{0,bc}^{2,0,1} \frac{4\kappa_b \kappa_c}{\kappa_1 \kappa_1} \frac{q_{\langle i} q_{k \rangle}}{\tau \rho \theta^2} \right. \\ \left. + \sum_{b,c} \mathcal{Y}_{0,bc}^{2,1,1} \frac{\mu_b \mu_c}{\mu_0 \mu_0} \frac{\sigma_{j \langle i} \sigma_{k \rangle j}}{\tau \rho \theta} \right] + \varepsilon^2 \left[\frac{\partial u_{ijk}^0}{\partial x_k} + \dots \right] = -\rho \theta \left[\frac{\sigma_{ij}}{\mu} + 2 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right]. \end{aligned}$$

Here we have used that

$$\sum_{b=0} \mathcal{C}_{0b}^{(2)} \mu_b = \sum_{a,b=0} \mathcal{C}_{0b}^{(2)} \left[\mathcal{C}_{ba}^{(2)} \right]^{-1} \frac{2}{15} (2a+5)!! = \sum_{a=0} \delta_{0a} \frac{2}{15} (2a+5)!! = 2$$

and

$$\frac{1}{\tau \mu_0} = \frac{\rho \theta}{2\mu},$$

where μ is the viscosity. The last two equations follow directly from (4.3) and (4.6).

The corresponding equation for the heat flux results from setting $a = 1$ in (2.12), where we introduce the second order moments (4.7) and assign the proper order of

magnitude to obtain (remember that $w^1 = 0$)

$$(5.3) \quad \varepsilon \left[\frac{Dq_i}{Dt} + \left[\frac{1}{2} \frac{\mu_1}{\mu_0} - 1 \right] \sigma_{ik} \frac{\partial \theta}{\partial x_k} - \sigma_{ik} \theta \frac{\partial \ln \rho}{\partial x_k} + \left[\frac{1}{2} \frac{\mu_1}{\mu_0} - \frac{5}{2} \right] \theta \frac{\partial \sigma_{ik}}{\partial x_k} \right. \\ \left. + \frac{7}{5} q_i \frac{\partial v_k}{\partial x_k} + \frac{7}{5} q_k \frac{\partial v_i}{\partial x_k} + \frac{2}{5} q_k \frac{\partial v_k}{\partial x_i} + \frac{1}{2} \sum_b C_{1b}^{(1)} \frac{w_i^b}{\tau \theta^{b-1}} + \sum_{b,c} \mathcal{Y}_{1,bc}^{1,1,1} \frac{\mu_b \kappa_c}{\mu_0 \kappa_1} \frac{\sigma_{ij} q_j}{\tau \rho \theta} \right] \\ + \varepsilon^2 \left[\frac{1}{2} \frac{\partial w_{ij}^1}{\partial x_k} + \frac{1}{6} \frac{\partial w^2}{\partial x_i} + u_{ikl}^0 \frac{\partial v_k}{\partial x_l} - \frac{\sigma_{ik}}{\rho} \frac{\partial \sigma_{kl}}{\partial x_l} + \dots \right] = -\frac{5}{2} \rho \theta \left[\frac{q_i}{\kappa} + \frac{\partial \theta}{\partial x_i} \right].$$

Here we have used that

$$\sum_{b=1} C_{1b}^{(1)} \kappa_b = \sum_{a,b=1} C_{1b}^{(1)} \left[C_{ba}^{(1)} \right]^{-1} \frac{a(2a+3)!!}{3} = \sum_{a=1} \delta_{1a} \frac{a(2a+3)!!}{3} = \frac{5!!}{3} = 5$$

and

$$\frac{1}{\tau \kappa_1} = \frac{1}{2} \frac{1}{\kappa} \rho \theta,$$

where κ is the heat conductivity. The last two equations follow directly from (4.3) and (4.6).

We close this section by pointing out that μ and κ are $\mathcal{O}(\varepsilon)$, as are σ_{ij} and q_i , so that their respective ratios $\frac{\sigma_{ij}}{\mu}$, $\frac{q_i}{\kappa}$ are $\mathcal{O}(\varepsilon^0)$. Also τ is $\mathcal{O}(\varepsilon)$ and w_i^b, w_{ij}^b are $\mathcal{O}(\varepsilon^2)$ so that their respective ratio is $\mathcal{O}(\varepsilon)$.

5.4. First order accuracy: NSF equations. We recall that our goal is to provide the equations for pressure deviator σ_{ij} and heat flux q_i within an accuracy of a given order. If we are satisfied with first order accuracy, we need to consider only the leading terms in (5.2), (5.3)—those of $\mathcal{O}(\varepsilon^0)$ —which yields the laws of Navier–Stokes and Fourier,

$$\sigma_{ij} = -2\mu \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}, \quad q_i = -\kappa \frac{\partial \theta}{\partial x_i},$$

where viscosity μ and heat conductivity κ are given by (4.3), (4.6).

The equations of first order accuracy obtained here coincide with the first order Chapman–Enskog expansion; see [17], where viscosity and heat conductivity are computed in accordance with the above formulae.

It is worthwhile to have a look at the corresponding phase density. At this order, the only relevant moments are the vectors and 2-tensors, so that the phase density (3.2), (3.3) reduces to

$$f|_G = f_M \left[1 + \sum_{a,b=0}^{A_1} \left[\mathcal{B}_{ab}^{(1)} \right]^{-1} \frac{u_i^b}{\rho \theta^{a+b+1}} C^{2a} C_i + \sum_{a,b=0}^{A_2} \left[\mathcal{B}_{ab}^{(2)} \right]^{-1} \frac{u_{ij}^b}{2\rho \theta^{a+b+2}} C^{2a} C_{\langle i} C_{j\rangle} \right].$$

But to first order we have from (4.2), (4.6)

$$u_{i|1}^b = -2\kappa \frac{\kappa_b}{\kappa_1} \theta^b \frac{\partial \ln \theta}{\partial x_i}, \quad u_{ij|1}^b = -2\mu \frac{\mu_b}{\mu_0} \theta^b \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}$$

so that we can write the distribution function for the NSF case as

$$f_{|NSF} = f_M \left\{ 1 - \frac{2\kappa}{\rho\theta^{1/2}} \left[\sum_{a,b=0}^{A_1} [\mathcal{B}_{ab}^{(1)}]^{-1} \frac{\kappa_b C^{2a}}{\kappa_1 \theta^a} \right] \frac{C_i}{\sqrt{\theta}} \frac{\partial \ln \theta}{\partial x_i} \right. \\ \left. - \frac{\mu}{\rho\theta} \left[\sum_{a,b=0}^{A_2} [\mathcal{B}_{ab}^{(2)}]^{-1} \frac{\mu_b C^{2a}}{\mu_0 \theta^a} \right] \frac{C_{\langle i} C_{j \rangle}}{\theta} \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right\}.$$

The terms in square brackets are polynomials in $\xi^2 = C^2/\theta$ and can be rewritten in terms of Sonine polynomials; see, e.g., [25]. Thus, it is evident that the present method yields the same phase density as the classical first order Chapman–Enskog method.

Heat conductivity κ and viscosity μ are given by

$$\kappa = \tau\rho\theta \sum_{a=1}^{A_1} [\mathcal{C}_{1a}^{(1)}]^{-1} \frac{a(2a+3)!!}{6}, \quad \mu = \tau\rho\theta \sum_{a=0}^{A_2} [\mathcal{C}_{0a}^{(2)}]^{-1} \frac{(2a+5)!!}{15}$$

and thus depend on the numbers A_1, A_2 of moments that are considered. This gives a good criterion for the determination of these numbers: increasing A_1, A_2 gives successive approximations for κ, μ , and these will converge to the accurate value if A_1, A_2 go to infinity. One will choose these numbers such that an increase by one will lead only to a sufficiently small change in the values for κ, μ . This, of course, corresponds to the growing accuracy when higher order Sonine polynomials are taken into account in the Chapman–Enskog method [1].

Indeed, Reinecke and Kremer computed κ, μ essentially in this manner [17] and showed that a fourth order correction is already very accurate. Moreover, they showed that their values for κ, μ to order $A = A_1 = A_2$ agree with the corresponding values of the A th degree of approximation in Sonine polynomials, as given, e.g., in [1].

The difference between our approach and the one of Reinecke and Kremer lies in the fact that Reinecke and Kremer chose the moments to base their approach on intuitively (they consider w^a, u_i^a , and u_{ij}^a), while we reduced the full moment system ($w^a, u_{i_1 \dots i_n}^a$) by discussion of the order of magnitude of moments and the order of accuracy of equations. In particular, this makes clear that at first order the scalar moments w^a need not be considered. Moreover, Reinecke and Kremer perform a Maxwell iteration on the full moment equations, a method which essentially is equivalent to the Chapman–Enskog expansion of the moments [19]. For a second order theory, they perform the second order Maxwell iteration in [18], which yields the Burnett equations, just as in the standard Chapman–Enskog expansion. These, as is well known, are unstable [5] and therefore should not be used. Our approach does not yield the Burnett equations at second order, as will become clear in the next section.

5.5. Second order accuracy: 13 moment theory. In the next order, we have to consider all terms in (5.2), (5.3) which have the factors ε^1 and ε^0 to obtain

$$(5.4) \quad \frac{D\sigma_{ij}}{Dt} + \frac{4}{5} \frac{\partial q_{\langle i}}{\partial x_{j \rangle}} + 2\sigma_{k\langle i} \frac{\partial v_{j \rangle}}{\partial x_k} + \sigma_{ij} \frac{\partial v_k}{\partial x_k} \\ + \sum_b \mathcal{C}_{0b}^{(2)} \frac{w_{ik}^b}{\tau\theta^b} + \sum_{b,c} \mathcal{Y}_{0,bc}^{2,0,1} \frac{4\kappa_b \kappa_c}{\kappa_1 \kappa_1} \frac{q_{\langle i} q_{k \rangle}}{\tau\rho\theta^2} + \sum_{b,c} \mathcal{Y}_{0,bc}^{2,1,1} \frac{\mu_b \mu_c}{\mu_0 \mu_0} \frac{\sigma_{j\langle i} \sigma_{k \rangle j}}{\tau\rho\theta} \\ = -\rho\theta \left[\frac{\sigma_{ij}}{\mu} + 2 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right],$$

$$(5.5) \quad \frac{Dq_i}{Dt} + \left[\frac{1}{2} \frac{\mu_1}{\mu_0} - 1 \right] \sigma_{ik} \frac{\partial \theta}{\partial x_k} - \theta \sigma_{ik} \frac{\partial \ln \rho}{\partial x_k} + \left[\frac{1}{2} \frac{\mu_1}{\mu_0} - \frac{5}{2} \right] \theta \frac{\partial \sigma_{ik}}{\partial x_k} \\ + \frac{7}{5} q_i \frac{\partial v_k}{\partial x_k} + \frac{7}{5} q_k \frac{\partial v_i}{\partial x_k} + \frac{2}{5} q_k \frac{\partial v_k}{\partial x_i} + \underbrace{\sum_b \mathcal{C}_{1b}^{(1)} \frac{w_i^b}{2\tau\theta^{b-1}} + \sum_{b,c} \mathcal{Y}_{1,bc}^{1,1,1} \frac{\mu_b \kappa_c}{\mu_0 \kappa_1} \frac{\sigma_{ij} q_j}{\tau \rho \theta}}_{= -\frac{5}{2} \rho \theta \left[\frac{q_i}{\kappa} + \frac{\partial \theta}{\partial x_i} \right]}.$$

Before we proceed, we compare the above set with Grad's famous 13 moment theory [12], [13]. In Grad's equations, those terms in (5.4), (5.5) that are underlined do not appear. Moreover, our equations contain the general expression $\frac{\mu_1}{\mu_0}$ which depends on the interaction potential (through $\mathcal{C}_{ab}^{(2)}$), while in Grad's equations this value is set to $\frac{\mu_1}{\mu_0} = 7$. Finally, Grad's equations contain a term $-\frac{\sigma_{ik}}{\rho} \frac{\partial \sigma_{kl}}{\partial x_l}$ in the equation for heat flux, which does not appear here, since it is of order $\mathcal{O}(\varepsilon^2)$.

It was already shown in [22] that $\frac{\mu_1}{\mu_0} = 7$ for the BGK model and Maxwell molecules, where (4.5), (4.4) hold. In addition, the underlined terms do not appear for Maxwell molecules or for the BGK model. Thus, with the omission of the second order term, $-\frac{\sigma_{ik}}{\rho} \frac{\partial \sigma_{kl}}{\partial x_l}$, Grad's 13 moment equations are the proper equations of second order accuracy for the description of rarefied gas flows for Maxwell molecules and the BGK model *only*.

For other interaction models, however, the above equations must be used in order to give second order agreement with the Boltzmann equation. Together with the conservation laws (5.1), equations (5.4), (5.5) form a set of 13 equations for the 13 variables $\rho, \theta, v_i, \sigma_{ij}, q_i$. This system is not closed, since it contains the moments w_i^a, w_{ij}^a as well, and additional equations are required for these quantities. The w_i^a, w_{ij}^a are of order $\mathcal{O}(\varepsilon^2)$, and for the theory of second order accuracy that we are considering here, it will be sufficient to know only the leading terms for these quantities. The calculations and results for this can be found in Appendices B and C; see (B.1), (C.2).

The final equations for the pressure deviator and heat flux read

$$(5.6) \quad \frac{D\sigma_{ij}}{Dt} + \psi_1 \frac{\partial q_{\langle i}}{\partial x_{j \rangle}} + (2 + \psi_2) \sigma_{k \langle i} \frac{\partial v_{j \rangle}}{\partial x_k} + \psi_2 \sigma_{k \langle i} \frac{\partial v_k}{\partial x_{j \rangle}} + \left(1 - \frac{2}{3} \psi_2 \right) \sigma_{ij} \frac{\partial v_k}{\partial x_k} \\ - \psi_3 q_{\langle i} \frac{\partial \ln \rho}{\partial x_{j \rangle}} - \psi_4 q_{\langle i} \frac{\partial \ln \theta}{\partial x_{j \rangle}} + \psi_5 \frac{q_{\langle i} q_{k \rangle}}{\mu \theta} + \psi_6 \frac{\sigma_{j \langle i} \sigma_{k \rangle j}}{\mu} = -\psi_7 \rho \theta \left[\frac{\sigma_{ij}}{\mu} + 2 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right],$$

$$(5.7) \quad \frac{Dq_i}{Dt} + \chi_1 \sigma_{ik} \frac{\partial \theta}{\partial x_k} - \chi_2 \theta \sigma_{ik} \frac{\partial \ln \rho}{\partial x_k} + \chi_3 \theta \frac{\partial \sigma_{ik}}{\partial x_k} + \frac{5}{3} \left(1 - \frac{2}{5} \chi_4 \right) q_i \frac{\partial v_k}{\partial x_k} \\ + (1 + \chi_4) q_k \frac{\partial v_i}{\partial x_k} + \chi_4 q_k \frac{\partial v_k}{\partial x_i} + \chi_5 \frac{\sigma_{ij} q_j}{\mu} = -\chi_6 \rho \theta \left[\frac{\mu_0}{\kappa_1} \frac{q_i}{\mu} + \frac{\partial \theta}{\partial x_i} \right].$$

In the above equations, the coefficients ψ_i and χ_i are pure numbers that must be computed according to

$$(5.8) \quad \psi_1 = \frac{4}{5} \left[1 - \sum_{d,a} \mathcal{C}_{0d}^{(2)} \mathcal{E}_{da}^{-1} \left[1 - \frac{\kappa_{a+1} \mu_0}{\kappa_1 \mu_a} \right] \right], \\ \psi_2 = \sum_{d,a} \mathcal{C}_{0d}^{(2)} \mathcal{E}_{da}^{-1} \frac{4a}{7},$$

$$\begin{aligned}\psi_3 &= \frac{4}{5} \sum_{d,a} \mathcal{C}_{0d}^{(2)} \mathcal{E}_{da}^{-1} (2a+5) \frac{\kappa_a \mu_0}{\kappa_1 \mu_a}, \\ \psi_4 &= \frac{4}{5} \sum_{d,a} \mathcal{C}_{0d}^{(2)} \mathcal{E}_{da}^{-1} \left[(2a+5) \frac{\kappa_a \mu_0}{\kappa_1 \mu_a} - a \frac{\kappa_{a+1} \mu_0}{\kappa_1 \mu_a} \right], \\ \psi_5 &= \frac{\mu_0}{2} \left[\sum_{b,c} \frac{4\kappa_b \kappa_c}{\kappa_1 \kappa_1} \mathcal{Y}_{0,bc}^{2,0,1} + \sum_{d,a} \mathcal{C}_{0d}^{(2)} \mathcal{E}_{da}^{-1} \sum_{b,c} \frac{4\kappa_b \kappa_c}{\kappa_1 \kappa_1} \left[\frac{\mu_0}{\mu_a} \mathcal{Y}_{a,bc}^{2,0,1} - \mathcal{Y}_{0,bc}^{2,0,1} \right] \right], \\ \psi_6 &= \frac{\mu_0}{2} \left[\sum_{b,c} \mathcal{Y}_{0,bc}^{2,1,1} \frac{\mu_b \mu_c}{\mu_0 \mu_0} + \sum_{d,a} \mathcal{C}_{0d}^{(2)} \mathcal{E}_{da}^{-1} \sum_{b,c} \frac{\mu_b \mu_c}{\mu_0 \mu_0} \left[\frac{\mu_0}{\mu_a} \mathcal{Y}_{a,bc}^{2,1,1} - \mathcal{Y}_{0,bc}^{2,1,1} \right] \right], \\ \psi_7 &= 1 - \sum_{d,a} \mathcal{C}_{0d}^{(2)} \mathcal{E}_{da}^{-1} \left[1 - \frac{\mu_0 (2a+5)!!}{\mu_a 15} \right]\end{aligned}$$

and

$$\begin{aligned}(5.9) \quad \chi_1 &= \frac{1}{2} \frac{\mu_1}{\mu_0} - 1 - \sum_{d,a} \mathcal{C}_{1d}^{(1)} \mathcal{D}_{da}^{-1} \left[\frac{1}{2} \frac{\mu_1}{\mu_0} - 1 - a \frac{\kappa_1}{\kappa_a} \left[\frac{1}{2} \frac{\mu_a}{\mu_0} - \frac{\mu_{a-1}}{\mu_0} \right] \right], \\ \chi_2 &= 1 - \sum_{d,a} \mathcal{C}_{1d}^{(1)} \mathcal{D}_{da}^{-1} \left[1 - a \frac{\kappa_1 \mu_{a-1}}{\kappa_a \mu_0} \right], \\ \chi_3 &= \frac{1}{2} \frac{\mu_1}{\mu_0} - \frac{5}{2} - \sum_{d,a} \mathcal{C}_{1d}^{(1)} \mathcal{D}_{da}^{-1} \left[\frac{1}{2} \frac{\mu_1}{\mu_0} - \frac{5}{2} - \frac{\kappa_1}{\kappa_a} \left[\frac{1}{2} \frac{\mu_a}{\mu_0} - \frac{(2a+3)!!}{6} \right] \right], \\ \chi_4 &= \frac{2}{5} - \sum_{d,a} \mathcal{C}_{1d}^{(1)} \mathcal{D}_{da}^{-1} \left[\frac{2}{5} - \frac{2a}{5} \right], \\ \chi_5 &= \frac{\mu_0}{2} \left[\sum_{b,c} \mathcal{Y}_{1,bc}^{1,1,1} \frac{\mu_b \kappa_c}{\mu_0 \kappa_1} + \sum_{d,a} \mathcal{C}_{1d}^{(1)} \mathcal{D}_{da}^{-1} \sum_{b,c} \frac{\mu_b \kappa_c}{\mu_0 \kappa_1} \left[\frac{\kappa_1}{\kappa_a} \mathcal{Y}_{a,bc}^{1,1,1} - \mathcal{Y}_{1,bc}^{1,1,1} \right] \right], \\ \chi_6 &= \frac{5}{2} - \sum_{d,a} \mathcal{C}_{1d}^{(1)} \mathcal{D}_{da}^{-1} \left[\frac{5}{2} - \frac{a(2a+3)!!}{6} \frac{\kappa_1}{\kappa_a} \right].\end{aligned}$$

The coefficients κ_b, μ_b are given by

$$(5.10) \quad \kappa_b = \sum_{a=1} \left[\mathcal{C}_{ba}^{(1)} \right]^{-1} \frac{a(2a+3)!!}{3}, \quad \mu_b = \sum_{a=0} \left[\mathcal{C}_{ba}^{(2)} \right]^{-1} \frac{2}{15} (2a+5)!!,$$

and we have introduced the matrices

$$(5.11) \quad \mathcal{D}_{ab} = \left[\mathcal{C}_{1b}^{(1)} - \mathcal{C}_{ab}^{(1)} \frac{\kappa_1}{\kappa_a} \right], \quad \mathcal{E}_{ab} = \left[\mathcal{C}_{0b}^{(2)} - \frac{\mu_0}{\mu_a} \mathcal{C}_{ab}^{(2)} \right].$$

Equations (5.6)–(5.11) give the complete set of equations for σ_{ij} and q_i . Thus, we have reduced the problem to the computation of the matrices

$$\mathcal{C}_{ad}^{(2)}, \quad \mathcal{Y}_{a,bc}^{2,0,1}, \quad \mathcal{Y}_{a,bc}^{2,1,1}, \quad \mathcal{C}_{ad}^{(1)}, \quad \mathcal{Y}_{a,bc}^{1,1,1}.$$

These follow by using the reduced Grad function (3.2)

$$f_{|G} = f_M (1 + \Phi) = f_M \left[1 + \sum_{a=0}^{A_1} \lambda_i^a C^{2a} C_i + \sum_{a=0}^{A_2} \lambda_{kl}^a C^{2a} C_{(k} C_{l)} \right]$$

to compute the collision moments $\mathcal{P}_i^a, \mathcal{P}_{ij}^a$ as outlined in section 3. We consider that to be a separate task that will be discussed in a future paper. The numbers A_1, A_2 must be chosen such that their further increase does not change the values of the coefficients ψ_α, χ_α considerably.

For Maxwell molecules and the BGK model, the coefficients have the values

$$\begin{aligned} \psi_1 &= \frac{4}{5}, & \psi_2 &= \psi_3 = \psi_4 = \psi_5 = \psi_6 = 0, & \psi_7 &= 1, \\ \chi_1 &= \frac{5}{2}, & \chi_2 &= 1, & \chi_3 &= 1, & \chi_4 &= \frac{2}{5}, & \chi_5 &= 0, & \chi_6 &= \frac{5}{2}. \end{aligned}$$

Furthermore, $\frac{\kappa_1}{\mu_0} = \frac{15}{4}$ for Maxwell molecules, and $\frac{\kappa_1}{\mu_0} = \frac{5}{2}$ for the BGK model. This choice of coefficients results in the original Grad's 13 moment equations [12], [13].

6. Conclusions. From the treatment above, it follows that the conservation laws (5.1) together with the balance laws (5.6), (5.7) form the proper transport equations for rarefied monatomic gases with second order accuracy in the Knudsen number. The coefficients in the balance equations (5.6), (5.7) depend on the microscopic interaction potential between the gas atoms, and, as was shown already in [22], the well-known 13 moment equations of Grad are of second order accuracy only for Maxwell molecules and the BGK model. Indeed, a similar behavior is observed in the Chapman–Enskog method where Burnett coefficients depend on the interaction potential.

Both the Chapman–Enskog method and the method used here become simplest when Maxwell molecules or the BGK model are considered. In [22] we were able to use our method to derive field equations up to third order accuracy, which agree with the regularization of Grad's 13 moment equations proposed before by Struchtrup and Torrilhon by means of a different argument [15], [11]. Going to third order for arbitrary interaction models will be more cumbersome by far. In particular, the third order theory will include full balance laws for the minimum number of vectors w_i^a and tensors w_{ij}^a that are of second order, and thus the number of variables will be higher than 13.

In the case of Maxwell molecules, it is well known that Grad's 13 moment equations are stable with respect to spatial and temporal disturbances, while the Burnett equations are unstable. This points to problems within the Chapman–Enskog method which proposes the Burnett equations as those equations that have second order accuracy. Our new method, however, proposes the 13 moment equations and thus stable equations.

Whether the 13 moment equations for arbitrary interaction potentials that were derived above are unconditionally stable or not remains to be seen. This can only be tested in the future, after the coefficients are computed. This task is planned for the future, and corresponding results will be presented elsewhere.

Appendix A. Symmetric and trace-free tensors.

A.1. Symmetry. A tensor $S_{i_1 i_2 \dots i_n}$ of rank n is called symmetric if for each pair of indices i_j, i_k

$$S_{i_1 i_2 \dots i_j \dots i_k \dots i_n} = S_{i_1 i_2 \dots i_k \dots i_j \dots i_n}.$$

A nonsymmetric tensor $A_{i_1 i_2 \dots i_n}$ can be symmetrized by the rule

$$A_{(i_1 i_2 \dots i_n)} = \frac{1}{n!} (A_{i_1 i_2 \dots i_{n-1} i_n} + A_{i_1 i_2 \dots i_n i_{n-1}} + \dots \text{all permutations of indices}).$$

Here, the indices in round brackets denote the symmetric part of the tensor. For example, for a 2-tensor, one finds the symmetric part as

$$A_{\langle ij \rangle} = \frac{1}{2} (A_{ij} + A_{ji}).$$

A.2. Trace-free tensors. A tensor $S_{i_1 i_2 \dots i_n}$ of rank n is called trace-free (or irreducible) if for each pair of indices i_j, i_k

$$(A.1) \quad S_{i_1 i_2 \dots i_j \dots i_k \dots i_n} \delta_{i_j i_k} = 0.$$

The trace-free part of a symmetric tensor $A_{i_1 i_2 \dots i_n}$ can be obtained according to the rule [23]

$$A_{\langle i_1 i_2 \dots i_n \rangle} = \sum_{k=0}^{\left\lfloor \frac{n}{2} \right\rfloor} a_{nk} \delta_{(i_1 i_2 \dots i_{2k-1} i_{2k} A_{i_{2k+1} \dots i_n) j_1 \dots j_k j_1 \dots j_k},$$

where

$$a_{nk} = (-1)^k \frac{n! (2n - 2k - 1)!!}{(n - 2k)! (2n - 1)!! (2k)!!},$$

$$\left\lfloor \frac{n}{2} \right\rfloor = \begin{cases} \frac{n}{2}, & n \text{ even,} \\ \frac{n-1}{2}, & n \text{ odd,} \end{cases}$$

$$n!! = n(n-2) \cdots (2 \text{ or } 1) = \prod_{j=0}^{\left\lfloor \frac{n-1}{2} \right\rfloor} (n - 2j).$$

We emphasize that in the above equations, $A_{i_1 i_2 \dots i_n}$ is symmetric, which is not made explicit by means of round brackets in order to avoid overly complicated notation. For actual computations, it is more convenient to use

$$\begin{aligned} A_{\langle i_1 i_2 \dots i_n \rangle} &= A_{i_1 i_2 \dots i_n} + \alpha_{n_1} (\delta_{i_1 i_2} A_{i_3 \dots i_n k k} + \text{permutations}) \\ &\quad + \alpha_{n_2} (\delta_{i_1 i_2} \delta_{i_3 i_4} A_{i_5 \dots i_n k k l l} + \text{permutations}) \\ &\quad + \dots, \end{aligned}$$

where only those permutations must be considered that are really different, i.e., that cannot be related by means of symmetry properties. Then the coefficients are given as

$$\alpha_{n_k} = \frac{(-1)^k}{\prod_{j=0}^{k-1} (2n - 2j - 1)}.$$

Simple examples are

$$\begin{aligned} A_{\langle i \rangle} &= A_i, \\ A_{\langle ij \rangle} &= A_{(ij)} - \frac{1}{3} A_{kk} \delta_{ij}, \\ A_{\langle ijk \rangle} &= A_{(ijk)} - \frac{1}{5} (A_{(ill)} \delta_{jk} + A_{(jll)} \delta_{ik} + A_{(kll)} \delta_{ij}). \end{aligned}$$

As an instructive example, let us consider the gradient of a symmetric 2-tensor, $\frac{\partial A_{ij}}{\partial x_k}$. Its symmetric part is given by

$$\frac{\partial A_{\langle ij}}{\partial x_k \rangle} = \frac{1}{3} \left(\frac{\partial A_{ij}}{\partial x_k} + \frac{\partial A_{ik}}{\partial x_j} + \frac{\partial A_{jk}}{\partial x_i} \right),$$

and its trace-free and symmetric part is

$$\begin{aligned} \frac{\partial A_{\langle ij}}{\partial x_k \rangle} &= \frac{1}{3} \left(\frac{\partial A_{ij}}{\partial x_k} + \frac{\partial A_{ik}}{\partial x_j} + \frac{\partial A_{jk}}{\partial x_i} \right) \\ &\quad - \frac{1}{15} \left[\left(\frac{\partial A_{ir}}{\partial x_r} + \frac{\partial A_{ir}}{\partial x_r} + \frac{\partial A_{rr}}{\partial x_i} \right) \delta_{jk} + \left(\frac{\partial A_{jr}}{\partial x_r} + \frac{\partial A_{jr}}{\partial x_r} + \frac{\partial A_{rr}}{\partial x_j} \right) \delta_{ik} \right. \\ &\quad \left. + \left(\frac{\partial A_{kr}}{\partial x_r} + \frac{\partial A_{kr}}{\partial x_r} + \frac{\partial A_{rr}}{\partial x_k} \right) \delta_{ij} \right]. \end{aligned}$$

Obviously, the bracket notation allows for a highly condensed notation.

Note that the moments $u_{i_1 \dots i_n}^a$ that are used in this paper are trace-free by definition, $u_{i_1 \dots i_n}^a = u_{\langle i_1 \dots i_n \rangle}^a$; and this is not made explicit with brackets. This avoids confusing notation involving several pairs of brackets. As an example, we consider the gradient of u_{ij} made symmetric and trace-free only in two of its three indices:

$$\frac{\partial u_{i \langle j}}{\partial x_k \rangle} = \frac{1}{2} \frac{\partial u_{\langle ij}}{\partial x_k} + \frac{1}{2} \frac{\partial u_{\langle ik}}{\partial x_j} - \frac{1}{3} \frac{\partial u_{\langle ir}}{\partial x_r} \delta_{jk}.$$

For this quantity we would have to write $\frac{\partial u_{\langle i \langle j \rangle}}{\partial x_k \rangle}$ if we were to make the trace-free properties of the moments explicit.

The trace-free part of the unit matrix δ_{ij} vanishes, $\delta_{\langle ij \rangle} = 0$, and this implies $A_{\langle i_1 i_2 \dots i_n \rangle} \delta_{jk} = 0$.

A.3. Spherical harmonics. Trace-free linear combinations of unit vectors $n_{\langle i_1 \dots i_n \rangle}$ are related to spherical harmonics [25]. Here, the vectors n_i are unit vectors in spherical coordinates,

$$n_i = \{ \sin \vartheta \sin \varphi, \sin \vartheta \cos \varphi, \cos \vartheta \}_i.$$

Spherical harmonics form an orthogonal set of functions, in the sense that integration over the solid angle $d\Omega = \sin \vartheta d\vartheta d\varphi$ yields

$$\int n_{\langle i_1 \dots i_n \rangle} n_{\langle j_1 \dots j_m \rangle} d\Omega = \begin{cases} 0, & n \neq m, \\ \frac{4\pi}{\prod_{j=0}^n (2j+1)} \delta_{\langle i_1 \dots i_n \rangle \langle j_1 \dots j_n \rangle}, & n = m, \end{cases}$$

where $\delta_{k_1 \dots k_l}$ is a generalized unit tensor defined as

$$\delta_{k_1 \dots k_l} = \delta_{k_1 k_2} \cdots \delta_{k_{l-1} k_l} + \cdots + \left(\frac{l!}{(\frac{l}{2})! 2^{\frac{l}{2}}} \text{ elements} \right).$$

An important relation following from this definition is that the product of the above integral with a tensor $A_{i_1 i_2 \dots i_n}$ yields

$$A_{i_1 i_2 \dots i_n} \int n_{\langle i_1 \dots i_n \rangle} n_{\langle j_1 \dots j_m \rangle} d\Omega = \begin{cases} 0, & n \neq m, \\ \frac{4\pi n!}{\prod_{j=0}^n (2j+1)} A_{\langle j_1 \dots j_n \rangle}, & n = m. \end{cases}$$

Another important relation is

$$(A.2) \quad n_{\langle i_1 \dots n_{i_n} \rangle} n_k = n_{\langle i_1 \dots n_{i_n} n_k \rangle} + \frac{n}{2n+1} n_{\langle i_1 \dots n_{i_{n-1}} \rangle} \delta_{i_n k}.$$

By introducing the direction vector of the microscopic velocity as $n_i = C_i/C$, the moments (2.5) can be written as

$$u_{i_1 \dots i_n}^a = m \int C^{2a+n+2} n_{\langle i_1 n_{i_2} \dots n_{i_n} \rangle} f dC d\Omega.$$

This indicates that our definition of moments refers to an expansion of the phase density in spherical harmonics $n_{\langle i_1 n_{i_2} \dots n_{i_n} \rangle}$ and polynomials in the absolute value of the microscopic velocity C .

Appendix B. Moment equations for w_i^a . We consider the moment equation for w_i^a , (2.12). After introducing the w_i^a, w_{ij}^a by means of (4.7), replacing the time derivative of θ by means of the energy balance (5.1)₂, and cancelling terms of $\mathcal{O}(\varepsilon^2)$ and higher, we obtain after division by $\frac{2\kappa_a}{\kappa_1} \theta^{a-1}$

$$\begin{aligned} \frac{Dq_i}{Dt} + \frac{a}{2} \frac{\kappa_1}{\kappa_a} \left[\frac{\mu_a - 2\mu_{a-1}}{\mu_0} \right] \sigma_{ik} \frac{\partial \theta}{\partial x_k} - a \frac{\kappa_1 \mu_{a-1}}{\kappa_a \mu_0} \theta \sigma_{ik} \frac{\partial \ln \rho}{\partial x_k} \\ + \frac{\kappa_1}{2\kappa_a} \left[\frac{\mu_a}{\mu_0} - \frac{(2a+3)!!}{3} \right] \theta \frac{\partial \sigma_{ik}}{\partial x_k} + \left[\frac{25-4a}{15} q_i \frac{\partial v_k}{\partial x_k} + \frac{2a+5}{5} q_k \frac{\partial v_i}{\partial x_k} + \frac{2a}{5} q_k \frac{\partial v_k}{\partial x_i} \right] \\ + \frac{1}{2\tau} \sum_b \mathcal{C}_{ab}^{(1)} \frac{\kappa_1}{\kappa_a} \frac{w_i^b}{\theta^{b-1}} + \frac{1}{\tau} \sum_{b,c} \mathcal{Y}_{a,bc}^{1,1,1} \frac{\mu_b \kappa_c}{\mu_0 \kappa_a} \frac{\sigma_{ij} q_j}{\rho \theta} = - \frac{a(2a+3)!!}{6} \frac{\kappa_1}{\kappa_a} \rho \theta \left[\frac{\partial \theta}{\partial x_i} + \frac{q_i}{\kappa} \right]. \end{aligned}$$

From this equation, we subtract the balance of the heat flux (5.5) to obtain

$$\begin{aligned} \frac{1}{2} \sum_b \left[\mathcal{C}_{1b}^{(1)} - \mathcal{C}_{ab}^{(1)} \frac{\kappa_1}{\kappa_a} \right] \frac{w_i^b}{\tau \theta^{b-1}} = \left[1 + \frac{a}{2} \frac{\kappa_1}{\kappa_a} \frac{\mu_a - 2\mu_{a-1}}{\mu_0} - \frac{1}{2} \frac{\mu_1}{\mu_0} \right] \sigma_{ik} \frac{\partial \theta}{\partial x_k} \\ + \left[1 - a \frac{\kappa_1 \mu_{a-1}}{\kappa_a \mu_0} \right] \theta \sigma_{ik} \frac{\partial \ln \rho}{\partial x_k} + \left[\frac{5}{2} + \frac{\kappa_1}{2\kappa_a} \left[\frac{\mu_a}{\mu_0} - \frac{(2a+3)!!}{3} \right] - \frac{1}{2} \frac{\mu_1}{\mu_0} \right] \theta \frac{\partial \sigma_{ik}}{\partial x_k} \\ + \frac{4-4a}{15} q_i \frac{\partial v_k}{\partial x_k} + \frac{2a-2}{5} q_k \frac{\partial v_i}{\partial x_k} + \frac{2a-2}{5} q_k \frac{\partial v_k}{\partial x_i} \\ + \sum_{b,c} \left[\mathcal{Y}_{a,bc}^{1,1,1} \frac{\mu_b \kappa_c}{\mu_0 \kappa_a} - \mathcal{Y}_{1,bc}^{1,1,1} \frac{\mu_b \kappa_c}{\mu_0 \kappa_1} \right] \frac{\sigma_{ij} q_j}{\tau \rho \theta} - \rho \theta \left[\frac{q_i}{\kappa} + \frac{\partial \theta}{\partial x_i} \right] \left[\frac{5}{2} - \frac{a(2a+3)!!}{6} \frac{\kappa_1}{\kappa_a} \right]. \end{aligned}$$

The above equation is meaningful for $a \geq 2$ only. The w_i^b follow from inversion of the matrix

$$\mathcal{D}_{ab} = \left[\mathcal{C}_{1b}^{(1)} - \mathcal{C}_{ab}^{(1)} \frac{\kappa_1}{\kappa_a} \right]$$

as

$$(B.1) \quad \frac{w_i^d}{2\tau \theta^{d-1}} = \sum_a \mathcal{D}_{da}^{-1} \left[1 - \frac{1}{2} \frac{\mu_1}{\mu_0} + \frac{a}{2} \frac{\kappa_1}{\kappa_a} \frac{\mu_a - 2\mu_{a-1}}{\mu_0} \right] \sigma_{ik} \frac{\partial \theta}{\partial x_k} \\ + \sum_a \mathcal{D}_{da}^{-1} \left[1 - a \frac{\kappa_1 \mu_{a-1}}{\kappa_a \mu_0} \right] \theta \sigma_{ik} \frac{\partial \ln \rho}{\partial x_k}$$

$$\begin{aligned}
& + \sum_a \mathcal{D}_{da}^{-1} \left[\frac{5}{2} - \frac{1}{2} \frac{\mu_1}{\mu_0} + \frac{\kappa_1}{2\kappa_a} \left[\frac{\mu_a}{\mu_0} - \frac{(2a+3)!!}{3} \right] \right] \theta \frac{\partial \sigma_{ik}}{\partial x_k} \\
& + \sum_a \mathcal{D}_{da}^{-1} \left[\frac{4-4a}{15} q_i \frac{\partial v_k}{\partial x_k} + \frac{2a-2}{5} q_k \frac{\partial v_i}{\partial x_k} + \frac{2a-2}{5} q_k \frac{\partial v_k}{\partial x_i} \right] \\
& + \sum_a \mathcal{D}_{da}^{-1} \sum_{b,c} \left[\mathcal{Y}_{a,bc}^{1,1,1} \frac{\mu_b \kappa_c}{\mu_0 \kappa_a} - \mathcal{Y}_{1,bc}^{1,1,1} \frac{\mu_b \kappa_c}{\mu_0 \kappa_1} \right] \frac{\sigma_{ij} q_j}{\tau \rho \theta} \\
& - \sum_a \mathcal{D}_{da}^{-1} \left[\frac{5}{2} - \frac{a(2a+3)!!}{6} \frac{\kappa_1}{\kappa_a} \right] \rho \theta \left[\frac{q_i}{\kappa} + \frac{\partial \theta}{\partial x_i} \right].
\end{aligned}$$

Appendix C. Moment equations for w_{ij}^a . We consider the equation for the 2-tensors u_{ij}^a , (2.14). After introducing the w_i^a, w_{ij}^a by means of (4.7), replacing the time derivative of θ by means of the energy balance (5.1)₂, and cancelling terms of $\mathcal{O}(\varepsilon^2)$ and higher, we obtain after division by $\frac{\mu_a \theta^a}{\mu_0}$

$$\begin{aligned}
\frac{D\sigma_{ij}}{Dt} + \frac{4}{5} \frac{\kappa_{a+1}\mu_0}{\kappa_1\mu_a} \frac{\partial q_{\langle i}}{\partial x_j \rangle} + \frac{6a}{7} \sigma_{\langle ij} \frac{\partial v_k \rangle}{\partial x_k} + \frac{4a}{5} \sigma_{k\langle i} \frac{\partial v_k \rangle}{\partial x_j \rangle} - \frac{2}{3} a \sigma_{ij} \frac{\partial v_k}{\partial x_k} + 2\sigma_{k\langle i} \frac{\partial v_j \rangle}{\partial x_k} + \sigma_{ij} \frac{\partial v_k}{\partial x_k} \\
- \frac{4}{5} (2a+5) \frac{\kappa_a \mu_0}{\kappa_1 \mu_a} q_{\langle i} \frac{\partial \ln \rho}{\partial x_j \rangle} - \frac{4}{5} \left[(2a+5) \frac{\kappa_a \mu_0}{\kappa_1 \mu_a} - a \frac{\kappa_{a+1} \mu_0}{\kappa_1 \mu_a} \right] q_{\langle i} \frac{\partial \ln \theta}{\partial x_j \rangle} \\
+ \frac{\mu_0}{\mu_a \theta^a} \frac{1}{\tau} \sum_b \mathcal{C}_{ab}^{(2)} \theta^{a-b} w_{ik}^b + \sum_{b,c} \mathcal{Y}_{a,bc}^{2,0,1} \frac{4\kappa_b \kappa_c \mu_0}{\kappa_1 \kappa_1 \mu_a} \frac{q_{\langle i} q_k \rangle}{\tau \rho \theta^2} + \sum_{b,c} \mathcal{Y}_{a,bc}^{2,1,1} \frac{\mu_b \mu_c}{\mu_0 \mu_a} \frac{\sigma_{j\langle i} \sigma_k \rangle j}{\tau \rho \theta} \\
= - \frac{\mu_0 (2a+5)!!}{\mu_a 15} \rho \theta \left[\frac{\sigma_{ik}}{\mu} + 2 \frac{\partial v_{\langle i}}{\partial x_j \rangle} \right].
\end{aligned}$$

We also have

$$\begin{aligned}
\sigma_{\langle ij} \frac{\partial v_k \rangle}{\partial x_k} &= \frac{1}{3} \sigma_{ij} \frac{\partial v_k}{\partial x_k} + \frac{2}{3} \sigma_{k\langle i} \frac{\partial v_j \rangle}{\partial x_k} - \frac{4}{15} \sigma_{r\langle i} \frac{\partial v_r \rangle}{\partial x_j \rangle}, \\
\frac{6a}{7} \sigma_{\langle ij} \frac{\partial v_k \rangle}{\partial x_k} + \frac{4a}{5} \sigma_{k\langle i} \frac{\partial v_k \rangle}{\partial x_j \rangle} - \frac{2}{3} a \sigma_{ij} \frac{\partial v_k}{\partial x_k} &= \frac{4a}{7} \left(\sigma_{k\langle i} \frac{\partial v_j \rangle}{\partial x_k} + \sigma_{k\langle i} \frac{\partial v_k \rangle}{\partial x_j \rangle} - \frac{2}{3} \sigma_{ij} \frac{\partial v_k}{\partial x_k} \right).
\end{aligned}$$

From this, we subtract the balance for the pressure deviator (5.4) to obtain, after some rearrangements,

$$\begin{aligned}
\sum_b \left[\mathcal{C}_{0b}^{(2)} - \frac{\mu_0}{\mu_a} \mathcal{C}_{ab}^{(2)} \right] \frac{w_{ik}^b}{\tau \theta^b} &= \frac{4}{5} \left[\frac{\kappa_{a+1} \mu_0}{\kappa_1 \mu_a} - 1 \right] \frac{\partial q_{\langle i}}{\partial x_j \rangle} \\
& + \frac{4a}{7} \left(\sigma_{k\langle i} \frac{\partial v_j \rangle}{\partial x_k} + \sigma_{k\langle i} \frac{\partial v_k \rangle}{\partial x_j \rangle} - \frac{2}{3} \sigma_{ij} \frac{\partial v_k}{\partial x_k} \right) \\
& - \frac{4}{5} (2a+5) \frac{\kappa_a \mu_0}{\kappa_1 \mu_a} q_{\langle i} \frac{\partial \ln \rho}{\partial x_j \rangle} - \frac{4}{5} \left[(2a+5) \frac{\kappa_a \mu_0}{\kappa_1 \mu_a} - a \frac{\kappa_{a+1} \mu_0}{\kappa_1 \mu_a} \right] q_{\langle i} \frac{\partial \ln \theta}{\partial x_j \rangle} \\
& + \sum_{b,c} \left[\mathcal{Y}_{a,bc}^{2,0,1} \frac{4\kappa_b \kappa_c \mu_0}{\kappa_1 \kappa_1 \mu_a} - \mathcal{Y}_{0,bc}^{2,0,1} \frac{4\kappa_b \kappa_c}{\kappa_1 \kappa_1} \right] \frac{q_{\langle i} q_k \rangle}{\tau \rho \theta^2} \\
& + \sum_{b,c} \left[\mathcal{Y}_{a,bc}^{2,1,1} \frac{\mu_b \mu_c}{\mu_0 \mu_a} - \mathcal{Y}_{0,bc}^{2,1,1} \frac{\mu_b \mu_c}{\mu_0 \mu_0} \right] \frac{\sigma_{j\langle i} \sigma_k \rangle j}{\tau \rho \theta} - \left[1 - \frac{\mu_0 (2a+5)!!}{\mu_a 15} \right] \rho \theta \left[\frac{\sigma_{ij}}{\mu} + 2 \frac{\partial v_{\langle i}}{\partial x_j \rangle} \right].
\end{aligned}$$

The w_{ij}^b follow from inversion of the matrix

$$\mathcal{E}_{ab} = \left[\mathcal{C}_{0b}^{(2)} - \frac{\mu_0}{\mu_a} \mathcal{C}_{ab}^{(2)} \right]$$

as

$$\begin{aligned} (C.1) \quad \frac{w_{ik}^d}{\tau\theta^d} &= \sum_a \mathcal{E}_{da}^{-1} \frac{4}{5} \left[\frac{\kappa_{a+1}\mu_0}{\kappa_1\mu_a} - 1 \right] \frac{\partial q_{\langle i}}{\partial x_{j \rangle}} + \sum_a \mathcal{E}_{da}^{-1} \frac{4a}{7} \left(\sigma_{k\langle i} \frac{\partial v_{j \rangle}}{\partial x_k} + \sigma_{k\langle i} \frac{\partial v_k}{\partial x_{j \rangle}} - \frac{2}{3} \sigma_{ij} \frac{\partial v_k}{\partial x_k} \right) \\ &- \sum_a \mathcal{E}_{da}^{-1} \frac{4}{5} (2a+5) \frac{\kappa_a\mu_0}{\kappa_1\mu_a} q_{\langle i} \frac{\partial \ln \rho}{\partial x_{j \rangle}} - \sum_a \mathcal{E}_{da}^{-1} \frac{4}{5} \left[(2a+5) \frac{\kappa_a\mu_0}{\kappa_1\mu_a} - a \frac{\kappa_{a+1}\mu_0}{\kappa_1\mu_a} \right] q_{\langle i} \frac{\partial \ln \theta}{\partial x_{j \rangle}} \\ &+ \sum_a \mathcal{E}_{da}^{-1} \sum_{b,c} \left[\mathcal{Y}_{a,bc}^{2,0,1} \frac{4\kappa_b\kappa_c\mu_0}{\kappa_1\kappa_1\mu_a} - \mathcal{Y}_{0,bc}^{2,0,1} \frac{4\kappa_b\kappa_c}{\kappa_1\kappa_1} \right] \frac{q_{\langle i} q_{k \rangle}}{\tau\rho\theta^2} \\ &+ \sum_a \mathcal{E}_{da}^{-1} \sum_{b,c} \left[\mathcal{Y}_{a,bc}^{2,1,1} \frac{\mu_b\mu_c}{\mu_0\mu_a} - \mathcal{Y}_{0,bc}^{2,1,1} \frac{\mu_b\mu_c}{\mu_0\mu_0} \right] \frac{\sigma_{j\langle i} \sigma_{k \rangle j}}{\tau\rho\theta} \\ &- \sum_a \mathcal{E}_{da}^{-1} \left[1 - \frac{\mu_0}{\mu_a} \frac{(2a+5)!!}{15} \right] \rho\theta \left[\frac{\sigma_{ij}}{\mu} + 2 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right]. \end{aligned}$$

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