# Stable transport equations for rarefied gases at high orders in the Knudsen number

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An approach is presented to derive transport equations for rarefied gases from the Boltzmann equation within higher orders of the Knudsen number. The method focuses on the order of magnitude of the moments of the phase density, and the order of accuracy of the transport equations, both measured in powers of the Knudsen number. The method is developed up to the third order, and it is shown that it yields the Euler equations at zeroth order, the Navier–Stokes–Fourier equations at first order, Grad's 13 moment equations (with omission of a nonlinear term) at second order, and a regularization of these at third order. The method is discussed in detail, and compared with the classical methods of kinetic theory, i.e., Chapman–Enskog expansion and Grad moment method. The advantages of this method above the classical approaches are discussed conclusively. An important feature of the method presented is that the equations of any order are stable, other than in the Chapman–Enskog method, where the second and third approximation–Burnett and super-Burnett equations—are unstable. © 2004 American Institute of Physics. [DOI: 10.1063/1.1782751]

### **I. INTRODUCTION**

In this paper we present a method to develop equations for the flow of rarefied gases by studying the order of magnitude of terms in the equation in powers of the Knudsen number  $\varepsilon$  (the ratio between the mean free path and a meaningful macroscopic length). This approach is based on the complete set of moment equations of the Boltzmann equations—an infinite set of equations—which is reduced to sets of only few equations, when the desired agreement with the Boltzmann equation is of the order  $O(\varepsilon^{\lambda})$ .

#### A. Background

The usual expansion procedure for the Boltzmann equation is the Chapman–Enskog method,<sup>1,2</sup> which gives the Euler equations in zeroth order and the Navier-Stokes-Fourier (NSF) equations in first order. The second and third order equations according to the Chapman–Enskog method are the Burnett<sup>3</sup> and super-Burnett equations.<sup>4</sup> While the Euler and NSF equations are accepted and widely used, the higher order Chapman-Enskog expansions suffer from instabilities<sup>5</sup> and unphysical behavior in steady state processes,<sup>6</sup> and cannot be considered to be useful tools for the description of rarefied gas flows.<sup>7</sup> Recent attempts to stabilize the Burnett equations either by adding some super-Burnett terms (augmented Burnett equations),<sup>8,9</sup> or by entropy based regularization,<sup>10,11</sup> lack a rational derivation from the Boltzmann equation,<sup>7</sup> and some results of the augmented Burnett equations are unphysical.<sup>6</sup>

The other well-known method for obtaining equations for rarefied gas flows is Grad's method of moments<sup>12–14</sup> 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,<sup>15</sup> and that the equations are not related *a priori* to the Knudsen number as a smallness parameter. The last point makes it difficult to develop criteria for the choice of moments that must be considered. While there is general agreement that larger Knudsen numbers require more moments,<sup>14</sup> there is no argument available in the present literature that links the Knudsen number to the choice of moments required.

The methods of Chapman–Enskog and Grad are completely independent of each other, since they are derived from different premises. However, 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.<sup>16,17</sup> For this, they used the method of Maxwellian iteration which is essentially equivalent to a Chapman– Enskog expansion of the moment equations.<sup>18</sup> One may conclude that the Grad equations are richer than the Burnett equations, and that the latter fail stability tests due to the omission of terms that are present in the stable Grad equations. Nevertheless, this observation does not provide a link between Grad equations and Knudsen number arguments.

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, <sup>7,19,20</sup> termed as the R13 equations. Struchtrup and Torrilhon showed that the R13 equations are linearly stable for all wavelengths and/or frequencies, show phase speeds and damping coefficients that match experiments better than those for the Navier–Stokes–Fourier equations or the original Grad 13 moments system, exhibit Knudsen bound-

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ary layers, and lead to smooth shock structures for all Mach numbers. Moreover they showed that a Chapman–Enskog expansion of their equations yields the Burnett and super-Burnett equations for Maxwell molecules.<sup>19</sup> While the properties of the R13 equations are highly desirable, their derivation by a method which stands between the methods of Grad and Chapman–Enskog did not convince all readers.

#### B. Summary of main results

In this paper we use a different way of accounting for the order of magnitude of moments, and terms in moment equations, in order to derive transport equations up to third order in the Knudsen number. This procedure yields the Euler and NSF equations in zeroth and first order, a set of equations very similar to Grad's 13 moment equations in second order, and a variation of Struchtrup and Torrilhon's R13 equations in third order. Higher order approximations (fourth order and higher) will be discussed only briefly, but it seems that the fourth order approximation is equivalent to a 26 moment system of Grad type, and the fifth order to its regularization.

Since the method is based on accounting orders in the Knudsen numbers, it provides a direct link between Grad type equations, and the Knudsen number. Moreover, it reproduces the zeroth and first order results—Euler and NSF—of the Chapman–Enskog method, but not the unstable higher order Chapman–Enskog results, that is, the Burnett and super-Burnett equations.

In other words, this method provides a common umbrella for sets of equations that up to now were thought to stem from very different arguments. Moreover, all sets of equations derived are stable for disturbances of all wavelengths and frequencies.

How close the second and third order equations agree with Grad's original equations, or the R13 equations, depends on the interaction model chosen. In this paper we shall focus on Maxwell interaction potentials and the Bhatnagar–Gross–Krook (BGK) model, where the second order equations are exactly Grad's 13 moment equations,<sup>12,13</sup> with the omission of a nonlinear term, and the third order equations are the original R13 equations, again under omission of several higher order nonlinear terms. The changes that can be expected when other interaction models are considered are only sketched, detailed accounts shall be published later. Thus, the equations derived in this paper are not entirely new, but the method to derive them is.

The first attempt to derive Grad equations by means of arguments on the Knudsen number is due to Müller *et al.*, termed as "consistent order extended thermodynamics" (COET).<sup>21</sup> These authors considered the infinite system of coupled moment equations of the BGK equation.<sup>22</sup> Our method shares some similarity with the COET method, but is distinctly different in detail. These differences will be discussed below, and in Sec. V, which will also give a more detailed discussion of our method in relation to the methods of Chapman–Enskog, Grad, and Struchtrup and Torrilhon.

#### C. Short outline of the method

As the COET method, our method is based on considering not the Boltzmann equation, but the infinite system of moment equations, and one can say that the problem of expanding the Boltzmann equation is moved from the phase space to moment space.

The method of finding the proper equations with *order of* accuracy  $\lambda_0$  in the Knudsen number consists of the following three steps.

(1) Determination of the *order of magnitude*  $\lambda$  of the moments.

(2) Construction of a moment set with minimum number of moments at order  $\lambda$ .

(3) Deletion of all terms in all equations that would lead only to contributions of orders  $\lambda > \lambda_0$  in the conservation laws for energy and momentum.

Step (1) is based on a Chapman–Enskog-like expansion where a moment  $\phi$  is expanded according to

$$\phi = \phi_0 + \varepsilon \phi_1 + \varepsilon^2 \phi_2 + \varepsilon^3 \phi_3 + \cdots,$$

and the leading order of  $\phi$  is determined by inserting this ansatz into the complete set of moment equations. A moment is said to be of leading order  $\lambda$  if  $\phi_{\beta}=0$  for all  $\beta < \lambda$ . It must be emphasized that we are interested only in the leading order of the moments, and that we shall not be interested in determining the coefficients  $\phi_{\beta}$  in the expansion. Indeed, the latter is the approach of the Chapman–Enskog method, which aims at computing the coefficients  $\phi_{\beta}$  in terms of gradients of mass density, velocity, and temperature. This first step agrees with the ideas of COET,<sup>21</sup> where, however, the authors use a Maxwell-type iteration<sup>23</sup> instead of a Chapman–Enskog expansion.

In step (2), new variables are introduced by linear combination of the moments originally chosen. The new variables are constructed such that the number of moments at a given order  $\lambda$  is minimal. This step does not only simplify the later discussion, but gives an unambiguous set of moments at order  $\lambda$ . This ensures that the final result will be independent of the initial choice of moments.

Step (3) follows from the definition of the order of accuracy  $\lambda_0$  that we chose to adopt: A set of equations is said to be accurate of order  $\lambda_0$ , when the pressure deviator  $\sigma_{ij}$  and the heat flux  $q_i$  are known within the order  $O(\varepsilon^{\lambda_0})$ .

The evaluation of this condition is based on the fact that all moment equations are strongly coupled. This implies that each term in any of the moment equations has some influence on all other equations, in particular, on the conservation laws. The influence of each term can be weighted by some power in the Knudsen number, and is related, but not equal to the order of magnitude of the moments appearing in the term. A theory of order  $\lambda_0$  will consider only those terms in all equations whose leading order of influence in the conservation laws is  $\lambda \leq \lambda_0$ . Luckily, in order to evaluate this condition, we can start with the conservation laws, and step by step, order by order, add the relevant terms that are required: We start with the  $O(\varepsilon^0)$  equations (Euler), then add the relevant terms to obtain the  $O(\varepsilon^1)$  equations (NSF), and so on. The accounting for the order of accuracy is the main difference between our method, and the COET, which assumes that *all* terms in all moment equations that are of leading order  $\lambda \leq \lambda_0$  or smaller must be retained. This is quite different, e.g., in order to compute the heat flux with third order accuracy, as is necessary in a third order theory, our method requires other moments only with second order accuracy, while others can be ignored completely. COET, on the other hand, would require higher order accuracy for these moments, and a larger number of moments. Our approach leads to smaller systems of equations for a given order, and can be performed for the full three-dimensional and time dependent equations (Ref. 21 presents the equations only for one-dimensional steady state processes).

At first glance, the reader might feel overwhelmed by the amount of equations in this paper, and their length. This, unfortunately, is unavoidable due to the complexity of the problem. The reader is invited to focus first on the structure of the proceedings, as outlined above, rather than on the details of the equations, and I hope that the presentation below puts enough emphasis on the structure to allow that. It should not be forgotten that a nonlinear three-dimensional third order theory is derived, which competes with the super-Burnett equations—the derivation of the latter is by far more complicated, and was never performed for the full nonlinear, three-dimensional case.<sup>4</sup>

The remainder of the paper is organized as follows: In Sec. II we define the moments as basic irreducible tensors, and derive the infinite set of moment equations. The moments of the collision term of the Boltzmann equation are presented for Maxwell molecules and the BGK model. In Sec. III the order of magnitude of the moments is determined, as described above. The results are then used in Sec. IV to develop the proper sets of equations for zeroth to third order accuracy. Section V contains a detailed discussion of the results, in particular, a comparison to other ideas available in the literature. The paper ends with conclusions.

#### II. BASIC EQUATIONS

#### A. Boltzmann equation

Our starting point is the Boltzmann equation<sup>1,2</sup> which we write as

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

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  $v_k$  as the center of mass velocity of the flow.  $D/Dt = (\partial/\partial t) + v_k \partial/\partial x_k$  denotes the material time derivative.

 $\varepsilon$  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,  $\varepsilon$  will be set equal to unity.

In fact, if proper dimensionless quantities were introduced, the dimensionless Boltzmann equation would read as Eq. (1) with the Knudsen number instead of  $\varepsilon$ , and the Knudsen number could be used as 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  $\varepsilon$  removes the necessity of introducing dimensionless quantities.

S(f) is the collision term that accounts for the change of *f* due to collisions, and has the following properties.<sup>1,2</sup>

(1) Conservation of mass, momentum, and energy, so that

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

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

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

where  $\rho$  is the mass density,  $\theta = (k/m)T$  is the temperature in energy units, where *T* is the temperature, *m* is the particle mass, and *k* denotes Boltzmann's constant.

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

This last point will not be discussed further within this paper.

#### **B. Moments**

We define the general irreducible moments of the phase density as

$$u_{i_1\cdots i_n}^a = m \int C^{2a} C_{\langle i_1} C_{i_2} \cdots C_{i_n} f d\mathbf{c}, \qquad (4)$$

where indices in angular brackets denote the symmetric and trace free part of a tensor, e.g.,

$$A_{\langle i \rangle} = A_i,$$

$$A_{\langle i j \rangle} = \frac{1}{2}A_{ij} + \frac{1}{2}A_{ji} - \frac{1}{3}A_{kk}\delta_{ij},$$

$$A_{\langle i j k \rangle} = A_{(ijk)} - \frac{1}{5}[A_{(irr)}\delta_{jk} + A_{(jrr)}\delta_{ik} + A_{(krr)}\delta_{ij}].$$

Here,  $A_{(iik)}$  denotes the symmetric part of the tensor  $A_{iik}$ .

Some of the moments have a particular interpretation, viz.,

$$u^{0} = \rho, \quad u_{i}^{0} = 0, \quad u^{1} = 2\rho e = 3\rho \theta = 3p,$$
  
 $u_{ij}^{0} = \sigma_{ij}, \quad u_{i}^{1} = 2q_{i}.$  (5)

Here we introduced the specific internal energy  $e = (3/2)\theta$  of the ideal gas, the pressure *p*, the irreducible part of the pressure tensor  $\sigma_{ii}$ , and the heat flux  $q_i$ .

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

$$u_{|E}^{a} = (2a+1)!!\rho\theta^{a}, \quad u_{i_{1}\cdots i_{n}|E}^{a} = 0, \quad n \ge 1,$$
(6)

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

$$\mathcal{P}^{a}_{i_{1}\cdots i_{n}} = m \int C^{2a} C_{\langle i_{1}} C_{i_{2}} \cdots C_{i_{n}\rangle} \mathcal{S}(f) d\mathbf{c}.$$
<sup>(7)</sup>

### C. Generic moment equation

Multiplication of the Boltzmann equation with  $mC^{2a}C_{\langle i_1C_{i_2}...C_{i_n}\rangle}$  and subsequent integration over velocity space yields, after some rearrangement, the general equation for the moments (4),

$$\frac{Du_{i_{1}\cdots i_{n}}^{n}}{Dt} + 2au_{i_{1}\cdots i_{n}k}^{a-1} \frac{Dv_{k}}{Dt} 
+ \frac{n}{2n+1}(2a+2n+1)u_{\langle i_{1}\cdots i_{n-1}}^{a} \frac{Dv_{i_{n}}\rangle}{Dt} + \frac{\partial u_{i_{1}\cdots i_{n}k}^{a}}{\partial x_{k}} 
+ \frac{n}{2n+1}\frac{\partial u_{\langle i_{1}\cdots i_{n-1}}^{a+1}}{\partial x_{i_{n}}\rangle} + 2au_{i_{1}\cdots i_{n}kl}^{a-1}\frac{\partial v_{k}}{\partial x_{l}} 
+ 2a\frac{n+1}{2n+3}u_{\langle i_{1}\cdots i_{n}}^{a} \frac{\partial v_{k}}{\partial x_{k}} + 2a\frac{n}{2n+1}u_{k\langle i_{1}\cdots i_{n-1}}^{a} \frac{\partial v_{k}}{\partial x_{i_{n}}\rangle} 
+ nu_{k\langle i_{1}\cdots i_{n-1}}^{a} \frac{\partial v_{i_{n}}\rangle}{\partial x_{k}} + u_{i_{1}}^{a}\cdots i_{n}\frac{\partial v_{k}}{\partial x_{k}} 
+ \frac{n(n-1)}{4n^{2}-1}(2a+2n+1)u_{\langle i_{1}\cdots i_{n-2}}^{a+1} \frac{\partial v_{i_{n-1}}}{\partial x_{i_{n}}\rangle} = \frac{1}{\varepsilon}\mathcal{P}_{i_{1}\cdots i_{n}}^{a}.$$
(8)

Note that all moments are trace free, and additional trace free tensors are made explicit by means of angular brackets. The derivation of the equation above requires multiple use of the relation<sup>24</sup>

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

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  $\varepsilon$ , and due to this equivalence we can perform the limiting process on the moment equations, rather than on the Boltzmann equation itself.

#### D. Conservation laws

First, we consider the conservation laws, that is, those equations which, by Eq. (2), have no production. 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 means of Eq. (5) these two equations can be brought into their usual textbook form

$$\frac{D\rho}{Dt} + \rho \frac{\partial v_k}{\partial x_k} = 0, \tag{9}$$

$$\frac{3}{2}\rho \frac{D\theta}{Dt} + \rho \theta \frac{\partial v_k}{\partial x_k} + \frac{\partial q_k}{\partial x_k} + \sigma_{kl} \frac{\partial v_k}{\partial x_l} = 0.$$
(10)

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

$$\rho \frac{Dv_i}{Dt} + \theta \frac{\partial \rho}{\partial x_i} + \rho \frac{\partial \theta}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = 0.$$
(11)

There are no further moment equations with vanishing production terms.

#### E. Scalar moments

For scalar moments (n=0), the general equation (8) 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

$$w^{a} = u^{a} - u^{a}_{|E} \tag{12}$$

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

$$\frac{Dw^{a}}{Dt} - \frac{2a}{3}(2a+1)!!\theta^{a-1}\frac{\partial q_{k}}{\partial x_{k}}$$
$$- \frac{2a}{3}(2a+1)!!\theta^{a-1}\sigma_{kl}\frac{\partial v_{k}}{\partial x_{l}} + 2au_{kl}^{a-1}\frac{\partial v_{k}}{\partial x_{l}} - 2au_{k}^{a-1}\frac{\partial \theta}{\partial x_{k}}$$
$$- 2au_{k}^{a-1}\theta\frac{\partial\ln\rho}{\partial x_{k}} - 2a\frac{u_{k}^{a-1}}{\rho}\frac{\partial\sigma_{kl}}{\partial x_{l}} + \frac{\partial u_{k}^{a}}{\partial x_{k}}$$
$$+ \frac{2a+3}{3}w^{a}\frac{\partial v_{k}}{\partial x_{k}} = \frac{1}{\varepsilon}\mathcal{P}^{a}.$$

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

The production term will be of the form

$$\mathcal{P}^a = -\frac{1}{\tau} \sum_b \mathcal{C}^{(0)}_{ab} \theta^{a-b} w^b,$$

where  $C_{ab}^{(0)}$  is a dimensionless matrix, and  $\tau$  is the mean free time. Mean free time and matrix  $C_{ab}^{(0)} [a, b \ge 2]$  will be discussed in Sec. II I below.

#### F. Vector moments

For vectors, the general equation (8) reduces to

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

We introduce the quantities  $w^a$  in the vector equation, and replace the time derivatives of the velocity to obtain

$$\frac{Du_{i}^{a}}{Dt} + \frac{a(2a+3)!!}{3}\rho\theta^{a}\frac{\partial\theta}{\partial x_{i}} - \frac{2a+3}{3}w^{a}\frac{\partial\theta}{\partial x_{i}}$$

$$- 2au_{ik}^{a-1}\frac{\partial\theta}{\partial x_{k}} - 2au_{ik}^{a-1}\theta\frac{\partial\ln\rho}{\partial x_{k}} - \frac{2a+3}{3}w^{a}\theta\frac{\partial\ln\rho}{\partial x_{i}}$$

$$- 2a\frac{u_{ik}^{a-1}}{\rho}\frac{\partial\sigma_{kl}}{\partial x_{l}} - \frac{2a+3}{3}\frac{w^{a}}{\rho}\frac{\partial\sigma_{ik}}{\partial x_{k}} - \frac{(2a+3)!!}{3}\theta^{a}\frac{\partial\sigma_{ik}}{\partial x_{k}}$$

$$+ \frac{\partial u_{ik}^{a}}{\partial x_{k}} + \frac{1}{3}\frac{\partial w^{a+1}}{\partial x_{i}} + 2au_{ikl}^{a-1}\frac{\partial v_{k}}{\partial x_{l}} + \frac{2a+5}{5}u_{i}^{a}\frac{\partial v_{k}}{\partial x_{k}}$$

$$+ \frac{2a+5}{5}u_{k}^{a}\frac{\partial v_{i}}{\partial x_{k}} + \frac{2a}{5}u_{k}^{a}\frac{\partial v_{k}}{\partial x_{i}} = \frac{1}{\varepsilon}\mathcal{P}_{i}^{a}.$$
(13)

This equation is relevant for  $a \ge 1$ . Note that  $w^1 = 0$ . Here, the expression for the collision production is similar as for the scalar quantities,

$$\mathcal{P}_i^a = -\frac{1}{\tau} \sum_b \mathcal{C}_{ab}^{(1)} \theta^{a-b} u_i^b \tag{14}$$

with a dimensionless matrix  $C_{ab}^{(1)}[a,b\geq 1]$  that will be discussed in Sec. II I below.

#### G. Rank-2 tensor moments

After replacing the time derivatives of velocity by Eq. (11), the equations for tensors of rank 2 read

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

This equation is relevant for  $a \ge 0$ . Again, the expression for the collision production has the form

$$\mathcal{P}_{ij}^{a} = -\frac{1}{\tau} \sum_{b} C_{ab}^{(2)} \theta^{a-b} u_{ij}^{b}$$
(16)

with a dimensionless matrix  $C_{ab}^{(2)}[a,b \ge 0]$ .

#### H. General equation

For moments of order higher than 2, the general equation reads

$$\frac{Du_{i_{1}\cdots i_{n}}^{a}}{Dt} - 2a\frac{u_{i_{1}\cdots i_{n}k}^{a-1}}{\rho}\left(\frac{\partial\sigma_{kl}}{\partial x_{l}} + \theta\frac{\partial\rho}{\partial x_{k}} + \rho\frac{\partial\theta}{\partial x_{k}}\right) - \frac{n}{2n+1}(2a+2n+1)\frac{u_{\langle i_{1}\cdots i_{n-1}}^{a}}{\rho}\left(\frac{\partial\sigma_{i_{n}\rangle}k}{\partial x_{k}} + \theta\frac{\partial\rho}{\partial x_{i_{n}\rangle}} + \rho\frac{\partial\theta}{\partial x_{i_{n}\rangle}}\right) + \frac{\partial u_{i_{1}\cdots i_{n}k}^{a}}{\partial x_{k}} + \frac{n}{2n+1}\frac{\partial u_{\langle i_{1}\cdots i_{n-1}}^{a+1}}{\partial x_{i_{n}\rangle}} + 2au_{i_{1}\cdots i_{n}kl}^{a-1}\frac{\partial v_{k}}{\partial x_{l}} + 2a\frac{n+1}{2n+3}u_{\langle i_{1}\cdots i_{n}}^{a}\frac{\partial v_{k}}{\partial x_{k}} + 2a\frac{n}{2n+1}u_{k\langle i_{1}\cdots i_{n-1}}^{a}\frac{\partial v_{k}}{\partial x_{i_{n}\rangle}} + nu_{k\langle i_{1}\cdots i_{n-1}}^{a}\frac{\partial v_{i_{n}}}{\partial x_{k}} + u_{i_{1}\cdots i_{n}}^{a}\frac{\partial v_{k}}{\partial x_{k}} + \frac{n(n-1)}{4n^{2}-1}(2a+2n+1)u_{\langle i_{1}\cdots i_{n-1}}^{a+1}\frac{\partial v_{i_{n-1}}}{\partial x_{i_{n}\rangle}} = \frac{1}{\varepsilon}\mathcal{P}_{i_{1}\cdots i_{n}}^{a}.$$
(17)

This equation is relevant for  $a \ge 0$ . Again, the expression for the collision production is similar as for the scalar quantities,

$$\mathcal{P}^a_{i_1\cdots i_n} = -\frac{1}{\tau} \sum_b \mathcal{C}^{(n)}_{ab} \theta^{a-b} u^b_{i_1\cdots i_n}$$

with dimensionless matrices  $C_{ab}^{(n)}[a,b \ge 0]$ .

#### I. The matrices on the right-hand side

The production terms are computed from the collision term S(f) by Eq. (7) and it follows that the matrices  $C_{ab}^{(n)}$  depend on the specific form of the collision term. The

computation of the production terms requires the knowledge of the distribution function f in terms of the moments. There are only few exceptions, where the production terms can be computed without detailed knowledge of f, and these are Maxwell molecules, and BGK models.<sup>25,26</sup> In order to keep the presentation in this paper as simple as possible, we shall consider only these cases in detail, and the corresponding matrices  $C_{ab}^{(n)}$  will be presented below. Nevertheless, we shall introduce specific values for  $C_{ab}^{(n)}$  only later in our calculations, in order to give the reader some flavor of what can be expected for other models of interaction.

We shall assume that the mean free time is of the form

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$$\frac{1}{\tau} = \frac{1}{\tau_0} \rho \theta^{1-s},\tag{18}$$

where  $\tau_0$  and *s* are constants which follow from the details of the microscopic interaction (*s*=1 for Maxwell molecules, *s* =1/2 for hard spheres), but can also be considered as measurable quantities which can be obtained from viscosity data (e.g., *s*=0.8 for argon).

First we consider the matrices  $C_{ab}^{(n)}$  for the BGK model,<sup>22</sup> where

$$\mathcal{S} = -\frac{1}{\tau}(f - f_M).$$

It follows that

$$\mathcal{P}^a_{i_1\cdots i_n} = -m \int C^{2a} C_{\langle i_1} C_{i_2}\cdots C_{i_n\rangle} \frac{1}{\tau} (f - f_M) d\mathbf{q}$$
$$= -\frac{1}{\tau} (u^a_{i_1\cdots i_n} - u^a_{i_1\cdots i_n|E}).$$

With the equilibrium values (6), and the definition of the variables  $w^a$  (12), the production terms result as

$$\begin{split} \mathcal{P}^{a} &= -\frac{1}{\tau} w^{a} \Rightarrow \mathcal{C}_{ab}^{(0)} = \delta_{ab} \quad (a, b \ge 2), \\ \mathcal{P}_{i}^{a} &= -\frac{1}{\tau} u_{i}^{a} \Rightarrow \mathcal{C}_{ab}^{(1)} = \delta_{ab} \quad (a, b \ge 1), \\ \mathcal{P}_{i_{1}\cdots i_{n}}^{a} &= -\frac{1}{\tau} u_{i_{1}\cdots i_{n}}^{a} \Rightarrow \mathcal{C}_{ab}^{(n)} = \delta_{ab} \quad (n \ge 2, a, b \ge 0). \end{split}$$

For Maxwell molecules, the matrices  $C_{ab}^{(n)}$  are of lower triangular form, see Refs. 23 and 25. Here we just give those entries that we shall need later, viz.,

$$\mathcal{C}_{ab}^{(0)} = \begin{bmatrix} \frac{2}{3} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ & & \ddots & 0 \end{bmatrix} \quad (a,b \ge 2), \\
\mathcal{C}_{ab}^{(1)} = \begin{bmatrix} \frac{2}{3} & 0 & \cdots & 0 \\ -\frac{14}{3} & 1 & \ddots & \vdots \\ \vdots & & \ddots & 0 \\ \ddots & & \ddots & \ddots \end{bmatrix} \quad (a,b \ge 1), \\
\mathcal{C}_{ab}^{(2)} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ -\frac{7}{6} & \frac{7}{6} & \ddots & \vdots \\ \vdots & & \ddots & 0 \\ \vdots & & \ddots & 0 \\ \vdots & & \ddots & 0 \end{bmatrix} \quad (a,b \ge 0), \\$$

$$C_{ab}^{(3)} = \begin{bmatrix} \frac{3}{2} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ & & & 0 \\ & & & \ddots \end{bmatrix} \quad (a,b \ge 0).$$

For general interaction potentials the situation is more difficult, and will be discussed in a future paper, where we shall suggest the Reinecke-Kremer-Grad method.<sup>16,17</sup> 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 (7). This procedure adds considerable complexity, which we wish to avoid in this first paper on the method. The reader familiar with the Chapman-Enskog expansion will see that there is some analogy: the Chapman-Enskog expansion can be performed easily for Maxwell molecules and BGK model, while for other interaction potentials one has to solve integral equations by expansions in Sonine polynomials.<sup>1</sup> The Reinecke-Kremer-Grad method must be considered as the equivalent of this when one operates with moment equations instead of the Boltzmann equation.

For now we shall just assume that the matrices are invertible—in particular, that will be the case for the triangular matrices of the Maxwell molecules, and the unit matrices of the BGK model. However, we shall introduce the matrices given above only towards the end of the computation, so that we can present more general results for future reference.

#### **III. 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  $\varepsilon$  as smallness parameter. All moments are expanded according to

$$u_{i_{1}\cdots i_{n}}^{a} = \sum_{\beta=0} \varepsilon^{\beta} u_{i_{1}\cdots i_{n}|\beta}^{a} = \varepsilon^{0} u_{i_{1}\cdots i_{n}|0}^{a} + \varepsilon^{1} u_{i_{1}\cdots i_{n}|1}^{a} + \varepsilon^{2} u_{i_{1}\cdots i_{n}|2}^{a} + \varepsilon^{3} u_{i_{1}\cdots i_{n}|3}^{a} + \cdots$$

$$(19)$$

and a similar series for the  $w^a$ .

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

#### A. 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  $1/\varepsilon$ . If the above expansion is inserted into the moment equations for the nonconserved quantities, it becomes immediately clear that

$$w_{|0}^{a} = u_{i_{1}\cdots i_{n}|0}^{a} = 0$$
<sup>(20)</sup>

for all moments. This follows from balancing the factors of  $1/\epsilon$  on both sides of the equations—there are none of these on the left-hand side, and thus 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  $\varepsilon^0$  in the equations, and find

$$0 = -\frac{1}{\tau} \sum_{b} C_{ab}^{(0)} \theta^{a-b} w_{|1}^{b},$$

$$\frac{a(2a+3)!!}{3} \rho \theta^{a} \frac{\partial \theta}{\partial x_{i}} = -\frac{1}{\tau} \sum_{b} C_{ab}^{(1)} \theta^{a-b} u_{i|1}^{b},$$

$$\frac{2}{15} (2a+5)!! \rho \theta^{a+1} \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} = -\frac{1}{\tau} \sum_{b} C_{ab}^{(2)} \theta^{a-b} u_{ij|1}^{b},$$

$$0 = -\frac{1}{\tau} \sum_{b} C_{ab}^{(n)} \theta^{a-b} u_{i_{1}\cdots i_{n}|1}^{b}.$$
(21)

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  $u_{i,\dots,i_n}^a$   $(n \ge 3)$  are at least of second order.

#### B. 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  $\varepsilon$ , we have to consider only the other moments. We make the equations for tensors of ranks 3 and 4 explicit. Keeping only factors of  $\varepsilon^1$  in the equations [note that, e.g.,  $u_i^a$  is a  $O(\varepsilon)$  contribution] yields

$$-\frac{2a}{3}(2a+1)!!\theta^{a-1}\frac{\partial q_k}{\partial x_k} - \frac{2a}{3}(2a+1)!!\theta^{a-1}\sigma_{kl}\frac{\partial v_k}{\partial x_l} + 2au_{kl}^{a-1}\frac{\partial v_k}{\partial x_l} - 2au_k^{a-1}\frac{\partial \theta}{\partial x_k} - 2au_k^{a-1}\theta\frac{\partial \ln \rho}{\partial x_k} + \frac{\partial u_k^a}{\partial x_k} = -\frac{1}{\tau}\sum_b C_{ab}^{(0)}\theta^{a-b}w_{|2}^b, \qquad (22)$$

$$-\frac{3}{7}(2a+7)u_{\langle ij}^{a}\left[\theta\frac{\partial\ln\rho}{\partial x_{k\rangle}}+\frac{\partial\theta}{\partial x_{k\rangle}}\right]+\frac{3}{7}\frac{\partial u_{\langle ij}^{a+1}}{\partial x_{k\rangle}}$$
$$+\frac{6}{35}(2a+7)u_{\langle i}^{a+1}\frac{\partial v_{j}}{\partial x_{k\rangle}}=-\frac{1}{\tau}\sum_{b}\mathcal{C}_{ab}^{(3)}\theta^{a-b}u_{ijk|2}^{b}\,,$$
(23)

$$\frac{12}{63}(2a+9)u_{\langle ij}^{a+1}\frac{\partial v_k}{\partial x_l} = -\frac{1}{\tau}\sum_b C_{ab}^{(4)}\theta^{a-b}u_{ijkl|2}^b,$$

$$0 = -\frac{1}{\tau} \sum_{b} \mathcal{C}_{ab}^{(n)} \theta^{a-b} u_{i_1 \cdots i_n|2}^b, \quad n \ge 5.$$

It follows that the nonequilibrium parts of the scalar moments  $w^a$ , and the tensors of ranks 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 ranks 5 and 6 are third order, tensors of ranks 7 and 8 are fourth order, etc.

#### **C.** Minimal number of moments of order $O(\varepsilon)$

From our first order result for the scalar and two-tensors, Eqs. (21), 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

$$u_{i|1}^{b} = -\sum_{a=1}^{\infty} \left[ C_{ba}^{(1)} \right]^{-1} \frac{a(2a+3)!!}{3} \frac{\tau_{0}}{\theta^{1-s-b}} \frac{\partial \theta}{\partial x_{i}}$$

$$= -\kappa_{b} \frac{\tau_{0}}{\theta^{1-s-b}} \frac{\partial \theta}{\partial x_{i}},$$

$$u_{ij|1}^{b} = -\sum_{a=0}^{\infty} \left[ C_{ba}^{(2)} \right]^{-1} \frac{2}{15} (2a+5)!! \frac{\tau_{0}}{\theta^{-s-b}} \frac{\partial v_{\langle i}}{\partial x_{j \rangle}}$$

$$= -\mu_{b} \frac{\tau_{0}}{\theta^{-s-b}} \frac{\partial v_{\langle i}}{\partial x_{j \rangle}},$$
(24)

where  $\kappa_b$  and  $\mu_b$  are pure numbers due to our assumptions on the matrices  $C_{ab}^{(n)}$ , given as

$$\kappa_b = \sum_{a=1} \left[ \mathcal{C}_{ba}^{(1)} \right]^{-1} \frac{a(2a+3)!!}{3}, \quad \mu_b = \sum_{a=0} \left[ \mathcal{C}_{ba}^{(2)} \right]^{-1} \frac{2}{15} (2a+5)!!.$$
(25)

The first few values of these coefficients are

$$\kappa_1 = 15/2, \quad \kappa_2 = 105 \quad \text{and} \quad \mu_0 = 2, \quad \mu_1 = 14, \quad (26)$$

for Maxwell molecules, and

$$\kappa_1 = 5, \quad \kappa_2 = 70 \quad \text{and} \quad \mu_0 = 2, \quad \mu_1 = 14$$
 (27)

for the BGK model.

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

$$q_{i|1} = \frac{1}{2}u_{i|1}^{1} = -\frac{1}{2}\kappa_{1}\frac{\tau_{0}}{\theta^{-s}}\frac{\partial\theta}{\partial x_{i}} = -\kappa\frac{\partial\theta}{\partial x_{i}},$$

$$\sigma_{ij|1} = u_{ij|1}^{0} = -\mu_{0}\frac{\tau_{0}}{\theta^{-s}}\frac{\partial\upsilon_{\langle i}}{\partial x_{j\rangle}} = -2\mu\frac{\partial\upsilon_{\langle i}}{\partial x_{j\rangle}},$$
(28)

where we have introduced heat conductivity and viscosity as  $\kappa$  and  $\mu$ , respectively. Thus, in first order we obtain the laws of Fourier and Navier–Stokes. Note that the computation of  $\mu$  and  $\kappa$  involves the inverses of the matrices  $C_{ab}^{(1)}, C_{ab}^{(2)}$ . For their computation for more general interaction models we refer the reader to Refs. 16 and 17.

It follows from Eqs. (24) and (28) 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 two-tensor moments, it is now straightforward to introduce new moments  $w_i^a, w_{ij}^a$  that are of second order only,

$$w_i^a = u_i^a - \frac{2\kappa_a}{\kappa_1} \theta^{a-1} q_i \quad (a \ge 2) \quad \text{and}$$

$$w_{ij}^a = u_{ij}^a - \frac{\mu_a}{\mu_0} \theta^a \sigma_{ij} \quad (a \ge 1)$$
(29)

so that

$$w_{i}^{a} = m \int \left( C^{2a-2} - \frac{2\kappa_{a}}{\kappa_{1}} \theta^{a-1} \right) C^{2} C_{i} f d\mathbf{c} \quad (a \ge 2),$$

$$w_{ij}^{a} = m \int \left( C^{2a-2} - \frac{\mu_{a}}{\mu_{0}} \theta^{a} \right) C_{\langle i} C_{j \rangle} f d\mathbf{c} \quad (a \ge 1).$$
(30)

This means that we can formulate a set of moments, where only  $\sigma_{ij}$  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 that 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.

# IV. THE TRANSPORT EQUATIONS WITH $\lambda th$ ORDER ACCURACY

In the preceding section we have established the order of magnitude of the various moments up to  $O(\varepsilon^2)$ . Now we ask what equations we need in order to describe a flow process in a rarefied ideal gas with an accuracy of  $O(\varepsilon^{\lambda})$ . We emphasize that our interpretation differs from the interpretation of Müller *et al.* in Ref. 21, who postulate that a theory of order  $O(\varepsilon^{\lambda})$  requires all terms with orders less or equal to  $\lambda$ .

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

## A. The conservation laws and the definition of $\lambda$ th order accuracy

We start the argument by repeating the conservation laws for mass, momentum, and energy, Eqs. (9), (11), and (10), which read, when we assign the factor  $\varepsilon$  to the first order quantities  $\sigma_{ij}$  and  $q_i$ ,

$$\frac{D\rho}{Dt} + \rho \frac{\partial v_k}{\partial x_k} = 0,$$

$$\frac{3}{2}\rho \frac{D\theta}{Dt} + \rho \theta \frac{\partial v_k}{\partial x_k} + \varepsilon \left[ \frac{\partial q_k}{\partial x_k} + \sigma_{kl} \frac{\partial v_k}{\partial x_l} \right] = 0,$$

$$\rho \frac{Dv_i}{Dt} + \rho \frac{\partial \theta}{\partial x_i} + \theta \frac{\partial \rho}{\partial x_i} + \varepsilon \frac{\partial \sigma_{ik}}{\partial x_k} = 0.$$
(31)

These equations are not a closed set of equations for  $\rho$ ,  $v_i$ ,  $\theta$ , but contain pressure deviator  $\sigma_{ij}$  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  $\lambda$ th order accuracy, when both,  $\sigma_{ii}$  and  $q_i$ , are known within the order  $O(\varepsilon^{\lambda})$ .

The equations of order  $O(\varepsilon^0)$  result from Eqs. (20) by setting  $\sigma_{ij}=q_i=0$ , that is, by ignoring the terms with the factor  $\varepsilon$  in the balance laws. This yields the Euler equations for ideal gases,

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

$$\rho \frac{Dv_i}{Dt} + \theta \frac{\partial \rho}{\partial x_i} + \rho \frac{\partial \theta}{\partial x_i} = 0.$$
(32)

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

#### B. Equations for pressure deviator and heat flux

We consider Eq. (15) with a=0 where we introduce the moments (29) and obtain, after assigning the proper order of magnitude to the various terms,

$$\varepsilon \left[ \frac{D\sigma_{ij}}{Dt} + \frac{4}{5} \frac{\partial q_{\langle i}}{\partial x_{j \rangle}} + 2\sigma_{k \langle i} \frac{\partial v_{j \rangle}}{\partial x_{k}} + \sigma_{ij} \frac{\partial v_{k}}{\partial x_{k}} + \frac{1}{\tau} \sum_{b=1} C_{0b}^{(2)} \theta^{-b} w_{ij}^{b} \right] + \varepsilon^{2} \frac{\partial u_{ijk}^{0}}{\partial x_{k}} = -\rho \theta \left[ \frac{\sigma_{ij}}{\mu} + 2 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right].$$
(33)

Here we have used that

$$\sum_{b=0}^{\infty} C_{0b}^{(2)} \mu_b = \sum_{a,b=0}^{\infty} C_{0b}^{(2)} [C_{ba}^{(2)}]^{-1} \frac{2}{15} (2a+5)!!$$
$$= \sum_{a=0}^{\infty} \delta_{0a} \frac{2}{15} (2a+5)!! = 2$$

and

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

where  $\mu$  is the viscosity. The last two equations follow directly from Eqs. (25) and (28).

The underlined term of order  $O(\varepsilon)$ ,  $(1/\tau)\Sigma_{b=1}C_{0b}^{(2)}\theta^{-b}w_{ij}^{b}$ , appears only when the matrix  $C_{ab}^{(2)}$  is not of triangular form. We shall ignore this term for what follows, in order to re-

move some additional complexity from the argument, that is, we shall restrict ourselves to triangular matrices  $C_{ab}^{(n)}$  from now on.

The equation for the heat flux results from setting a=1 in (13) where we introduce the second order moments (29), and assign the proper order of magnitude to obtain (remember that  $w^1=0$ ),

$$\varepsilon \left[ \frac{Dq_i}{Dt} + \left(\frac{1}{2}\frac{\mu_1}{\mu_0} - 1\right)\sigma_{ik}\frac{\partial\theta}{\partial x_k} - \sigma_{ik}\theta\frac{\partial\ln\rho}{\partial x_k} + \left(\frac{1}{2}\frac{\mu_1}{\mu_0} - \frac{5}{2}\right)\theta\frac{\partial\sigma_{ik}}{\partial x_k} \right. \\ \left. + \frac{7}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i} + \frac{1}{2}\frac{1}{\tau}\sum_{b=2}C^{(1)}_{1b}\theta^{1-b}w_i^b \right] \\ \left. + \varepsilon^2 \left[\frac{1}{2}\frac{\partial w_{ij}^1}{\partial x_k} + \frac{1}{6}\frac{\partial w^2}{\partial x_i} + u_{ikl}^0\frac{\partial v_k}{\partial x_l} - \frac{\sigma_{ik}}{\rho}\frac{\partial\sigma_{kl}}{\partial x_l}\right] \right] \\ \left. = -\frac{5}{2}\rho\theta \left[\frac{q_i}{\kappa} + \frac{\partial\theta}{\partial x_i}\right].$$
(34)

Here we have used that

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

and

$$\frac{1}{\tau\kappa_1} = \frac{1}{\tau_0\kappa_1}\rho\theta^{1-s} = \frac{1}{2}\frac{1}{\kappa}\rho\theta$$

where  $\kappa$  is the heat conductivity. The last two equations follow directly from Eqs. (25) and (28).

The underlined term of order  $O(\varepsilon)$ ,  $(1/2) \times (1/\tau) \Sigma_{b=2} C_{1b}^{(1)} \theta^{1-b} w_i^b$ , appears only when the matrix  $C_{ab}^{(1)}$  is not of triangular form. This term corresponds to the similar one in the equation for  $\sigma_{ij}$ , and will be ignored for most of the paper as well.

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

# C. First order accuracy: Navier–Stokes–Fourier equations

We recall that our goal is to provide the equations for pressure deviator  $\sigma_{ij}$  and heat flux  $q_i$  with an accuracy of a given order. If we are satisfied with first order accuracy, we need to consider only the leading terms in Eqs. (33) and (34), which yield the laws of Navier–Stokes–Fourier,

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

where viscosity  $\mu$  and heat conductivity  $\kappa$  are given by Eqs. (25) and (28).

The equations of first order accuracy obtained here coincide with the first order Chapman–Enskog expansion. As will become clear in the following section, the higher order equations deviate from those obtained by the Chapman– Enskog method, that is, from the Burnett and super-Burnett equations. This is welcome, since the higher order Chapman–Enskog expansion yields unstable equations, and cannot be used.

# D. Second order accuracy: Grad's 13 moment theory (slightly linearized)

In the next order, we have to consider all terms in Eqs. (33) and (34) which have the factors  $\varepsilon^1$  and  $\varepsilon^0$  to obtain (after setting the formal parameter  $\varepsilon = 1$ )

$$\frac{D\sigma_{ij}}{Dt} + \frac{4}{5} \frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i} \frac{\partial v_{j\rangle}}{\partial x_k} + \sigma_{ij} \frac{\partial v_k}{\partial x_k} + 2\rho \theta \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\frac{\rho \theta}{\mu} \sigma_{ij},$$
(35)

$$\frac{Dq_i}{Dt} + \left(\frac{1}{2}\frac{\mu_1}{\mu_0} - 1\right)\sigma_{ik}\frac{\partial\theta}{\partial x_k} - \sigma_{ik}\theta\frac{\partial\ln\rho}{\partial x_k} + \left(\frac{1}{2}\frac{\mu_1}{\mu_0} - \frac{5}{2}\right)\theta\frac{\partial\sigma_{ik}}{\partial x_k} + \frac{7}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i} + \frac{5}{2}\rho\theta\frac{\partial\theta}{\partial x_i} = -\frac{5}{2}\frac{\rho\theta}{\kappa}q_i.$$
(36)

Together with the conservation laws (31) these equations form a closed set of 13 equations for the 13 variables  $\rho$ ,  $v_i$ , T,  $\sigma_{ij}$ ,  $q_i$  which are the variables that Grad considered in his famous 13 moment theory.<sup>12,13</sup> And indeed, the only difference to Grad's equations is that we had to drop the term  $-(\sigma_{ik}/\rho)(\partial\sigma_{kl}/\partial x_l)$  in the equation for heat flux since it is of order  $O(\varepsilon^2)$ , and we have the general expression  $\mu_1/\mu_0$ . For the BGK model and Maxwell molecules, we find from Eqs. (27) and (26) that  $\mu_1/\mu_0=7$  which yields  $[(1/2)(\mu_1/\mu_0)$  $-1]=\frac{5}{2}$ ,  $[(1/2)(\mu_1/\mu_0)-\frac{5}{2}]=1$ , which are just the coefficients in Grad's original equations.

Thus, with the omission of the second order term,  $-(\sigma_{ik}/\rho)(\partial\sigma_{kl}/\partial x_l)$ , Grad's 13 moment equations are the proper equations of second order accuracy for the description of rarefied gas flows for Maxwell molecules, or the BGK model.

Application of the Chapman–Enskog method to the Boltzmann equation suggests that the second order equations are the Burnett equations.<sup>1,3</sup> However, it is well known by now that these are unstable,<sup>5</sup> and lead to unphysical results. It is also known that the Burnett equations can be derived by performing a Chapman–Enskog expansion on the 13 moment equations, and thus are contained within these.<sup>16–18</sup>

Grad's 13 moment equations are known to be stable, and that alone should be a reason to prefer them. However, they exhibit subshocks for Mach numbers above 1.65, which are unphysical.<sup>12,15</sup> It is quite difficult to assign a smallness parameter to shocks, and one must conclude that the failure of describing smooth shocks is an indicator for the limit of applicability of the equations. Note, however, that the computation of shock structures with the Burnett or super-Burnett equations is difficult as well, due to their unstable character.<sup>7,27</sup>

The next order of our expansion yields a natural regularization for Grad's 13 moment equations.

### E. Third order accuracy: Regularized 13 moment equations of Struchtrup and Torrilhon (slightly linearized)

To obtain the pressure deviator and the heat flux with third order accuracy, we have to consider also the  $O(\varepsilon^2)$ terms in Eqs. (33) and (34) so that the equations for  $\sigma_{ij}$  and  $q_i$  read (after setting  $\varepsilon = 1$ )

$$\frac{D\sigma_{ij}}{Dt} + \frac{4}{5} \frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i} \frac{\partial v_{j\rangle}}{\partial x_{k}} + \sigma_{ij} \frac{\partial v_{k}}{\partial x_{k}} + \frac{\partial u_{ijk}^{0}}{\partial x_{k}}$$

$$= -\rho \theta \left[ \frac{\sigma_{ij}}{\mu} + 2 \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \right], \qquad (37)$$

$$\frac{Dq_i}{Dt} + \left(\frac{1}{2}\frac{\mu_1}{\mu_0} - 1\right)\sigma_{ik}\frac{\partial\theta}{\partial x_k} - \sigma_{ik}\theta\frac{\partial\ln\rho}{\partial x_k} + \left(\frac{1}{2}\frac{\mu_1}{\mu_0} - \frac{5}{2}\right)\theta\frac{\partial\sigma_{ik}}{\partial x_k} \\
+ \frac{7}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i} + \frac{1}{2}\frac{\partial w_{ij}^1}{\partial x_k} + \frac{1}{6}\frac{\partial w^2}{\partial x_i} + u_{ikl}^0\frac{\partial v_k}{\partial x_l} \\
- \frac{\sigma_{ik}}{\rho}\frac{\partial\sigma_{kl}}{\partial x_l} = -\frac{5}{2}\rho\theta\left[\frac{q_i}{\kappa} + \frac{\partial\theta}{\partial x_i}\right].$$
(38)

In addition to the 13 variables, these equations contain the quantities  $u_{ijk}^0$ ,  $w_{ij}^1$ ,  $w^2$ , and in order to obtain a closed set of equations, we have to provide additional equations for these. As we have seen in Sec. III, the leading order of magnitude of  $u_{ijk}^0$ ,  $w_{ij}^1$ ,  $w^2$  is  $O(\varepsilon^2)$ , and if we restrict ourselves to second order accuracy in their computation, we compute pressure deviator  $\sigma_{ij}$  and heat flux  $q_i$  within *third order* accuracy. If we compute  $u_{ijk}^0$ ,  $w_{ij}^1$ ,  $w^1$  up to third order accuracy, we shall have fourth order accuracy in  $\sigma_{ij}$  and  $q_i$ , and so on.

In this section we are only interested in the leading order terms, so that we obtain the proper third order theory. The relevant equation for  $w^2$  at  $O(\varepsilon^2)$  is Eq. (22) with a=2 where we have to consider Eqs. (29) again, so that

$$\left(\frac{2\kappa_2}{\kappa_1} - 20\right)\theta\frac{\partial q_k}{\partial x_k} + \left(4\frac{\mu_1}{\mu_0} - 20\right)\theta\sigma_{kl}\frac{\partial v_k}{\partial x_l} + \left(2\frac{\kappa_2}{\kappa_1} - 8\right)q_k\frac{\partial\theta}{\partial x_k} - 8q_k\theta\frac{\partial\ln\rho}{\partial x_k} = -\frac{1}{\tau}C_{22}^{(0)}w^2.$$
(39)

The second order equation for  $u_{iik}^0$  is Eq. (23) for a=0,

$$\frac{3}{7}\frac{\mu_{1}}{\mu_{0}}\theta\frac{\partial\sigma_{\langle ij}}{\partial x_{k\rangle}} - 3\sigma_{\langle ij} \theta\frac{\partial\ln\rho}{\partial x_{k\rangle}} + \frac{12}{5}q_{\langle i}\frac{\partial v_{j}}{\partial x_{k\rangle}} + 3\left(\frac{1}{7}\frac{\mu_{1}}{\mu_{0}} - 1\right)\sigma_{\langle ij}\frac{\partial\theta}{\partial x_{k\rangle}} = -\frac{1}{\tau}\mathcal{C}_{00}^{(3)}u_{ijk}^{0}.$$
(40)

The equation for  $w_{ij}^1$  results from Eq. (15) with a=1, after replacing  $u_{ij}^1$  by  $w_{ij}^1$  by means of (29), and subsequent elimination of the time derivatives of  $\sigma_{ij}$  and  $\theta$  by means of their respective balance laws. Keeping only the leading order terms yields after some algebra

$$\frac{4}{5}\left(\frac{\kappa_{2}}{\kappa_{1}}-\frac{\mu_{1}}{\mu_{0}}\right)\theta\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + \frac{4}{5}\left(\frac{\kappa_{2}}{\kappa_{1}}-7\right)q_{\langle i}\frac{\partial\theta}{\partial x_{j\rangle}} - \frac{28}{5}\theta q_{\langle i}\frac{\partial\ln\rho}{\partial x_{j\rangle}} \\
+ 14\rho\theta^{2}\left(1-\frac{1}{7}\frac{\mu_{1}}{\mu_{0}}\right)\left(\frac{\sigma_{ij}}{2\mu}+\frac{\partial\upsilon_{\langle i}}{\partial x_{j\rangle}}\right) \\
+ \frac{4}{7}\frac{\mu_{1}}{\mu_{0}}\theta\left(\sigma_{k\langle i}\frac{\partial\upsilon_{j\rangle}}{\partial x_{k}}+\sigma_{k\langle i}\frac{\partial\upsilon_{k}}{\partial x_{j\rangle}}-\frac{2}{3}\sigma_{ij}\frac{\partial\upsilon_{k}}{\partial x_{k}}\right) = -\frac{1}{\tau}C_{11}^{(2)}w_{ij}^{1}.$$
(41)

The last three equations yield the proper closure of Eqs. (37) and (38) with third order accuracy, when all matrices  $C_{ab}^{(n)}$  are of triangular form. Below we shall make the coefficients explicit for Maxwell molecules and the BGK model.

For both, Maxwell molecules and the BGK model, we have  $\mu_1/\mu_2=7$  and  $\kappa_2/\kappa_1=14$  and can use the matrices of Sec. III so that the above equations for Maxwell molecules reduce to

$$w^{2} = -12\tau \left[ \theta \frac{\partial q_{k}}{\partial x_{k}} + \theta \sigma_{kl} \frac{\partial v_{k}}{\partial x_{l}} + \frac{5}{2} q_{k} \frac{\partial \theta}{\partial x_{k}} - q_{k} \theta \frac{\partial \ln \rho}{\partial x_{k}} \right],$$
$$u^{0}_{ijk} = -2\tau \left[ \theta \frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} - \sigma_{\langle ij} \theta \frac{\partial \ln \rho}{\partial x_{k\rangle}} + \frac{4}{5} q_{\langle i} \frac{\partial v_{j}}{\partial x_{k\rangle}} \right], \qquad (42)$$

$$w_{ij}^{1} = -\frac{24}{5} \tau \left[ \theta \frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + q_{\langle i} \frac{\partial \theta}{\partial x_{j\rangle}} - \theta q_{\langle i} \frac{\partial \ln \rho}{\partial x_{j\rangle}} \right] + \frac{5}{7} \theta \left( \sigma_{k\langle i} \frac{\partial v_{j\rangle}}{\partial x_{k}} + \sigma_{k\langle i} \frac{\partial v_{k}}{\partial x_{j\rangle}} - \frac{2}{3} \sigma_{ij} \frac{\partial v_{k}}{\partial x_{k}} \right) \right].$$

These are just the regularized 13 moment equations of Struchtrup and Torrilhon,<sup>19</sup> with the omission of some terms which are nonlinear in  $\sigma_{ij}$  and  $q_k$ . These nonlinear terms are not present here, since they add terms of third order to  $u_{ijk}^0$ ,  $w_{ij}^1$ ,  $w^1$ , which are ignored in our third order theory. However, these terms would be present in a fourth order theory, together with additional contributions from other moments.

For the BGK model the equations bear different factors,

$$w^2 = -8\tau[\cdots], \quad u^0_{ijk} = -3\tau[\cdots], \quad w^1_{ij} = -\frac{28}{5}\tau[\cdots],$$

where the square brackets stand for their counterparts in (42).

The R13 equations were discussed in great detail in Refs. 7 and 19 where it is shown that they contain the Burnett and super-Burnett equations, are linearly stable for all wavelengths and/or frequencies, show phase speeds and damping coefficients that match experiments better than those for the Navier–Stokes–Fourier equations or the original Grad 13 moments system, exhibit Knudsen boundary layers, and lead to smooth shock structures for all Mach numbers.

In short, the R13 equations form a new and meaningful system of equations for the description of rarefied gas flows with third order accuracy.

### V. DISCUSSION

### A. Higher order accuracy

We shall not go further with developing the equations at higher order accuracy. However, it is clear that the next level of accuracy—fourth order—will contain full balance laws for  $u_{ijk}^0$ ,  $w_{ij}^1$ ,  $w^2$ , that is, equations of the form  $(\partial \phi / \partial t)$ +[space derivatives]= $-(1/\tau)\phi$ . The resulting equations should then be equivalent to a Grad moment system with 26 moments, as it can be found, e.g., in Ref. 14. The next order—the fifth—should then be the regularization of the 26 moment system, similar as the third order is the regularization of the second order 13 moment case.

In this context, we would like to mention that the (first order) NSF equations are the regularization of the (zeroth order) Euler equations. Altogether, the following picture emerges: Equations at even order (zeroth, second, fourth, ...) are of the Grad moment type, and hyperbolic, while equations at odd orders (first, third, ...) form the regularization of these hyperbolic equations. Hyperbolic equations of Grad moment type lead to shocks or subshocks when the inflow velocity into the shock exceeds the largest characteristic velocity of the system,<sup>14,15</sup> and these shocks are an artefact of the theory, and cannot be observed in experiments. The regularization of the hyperbolic equations (= the odd order approximations) smoothens these shocks, as was shown for the R13 equations in Ref. 7, and yields smooth shock structures at any Mach number.

The complexity of the method increases substantially when we are not dealing with the BGK model, or Maxwell molecules. Then, the second order equations (35) and (36) contain the additional terms

$$\frac{1}{\tau} \sum_{b=1} \mathcal{C}^{(2)}_{0b} \theta^{-b} w^{b}_{ij}, \quad \frac{1}{2} \frac{1}{\tau} \sum_{b=2} \mathcal{C}^{(1)}_{1b} \theta^{1-b} w^{b}_{i}$$

and, for a second order closure, we have to provide the  $w_{ij}^b$ ,  $w_i^b$  within their leading order  $O(\varepsilon^2)$ . They will have a form similar to Eq. (42). For the third order, full balance equations for the  $w_{ij}^b$ ,  $w_i^b$  are required. For this, it will be necessary to construct new variables  $\tilde{w}_{ij}^b$ ,  $\tilde{w}_i^b$  such that a minimum number of these is of second order, similar to the procedure outlined in Sec. III C.

#### B. Comparison with Chapman–Enskog method

The most pressing question on the method introduced in this paper is probably, where the differences are to the Chapman–Enskog method, and why our method gives stable and meaningful equations at each level of approximation, while the Chapman–Enskog method does not.

The Chapman–Enskog expansion aims at finding the coefficients in the expansion (19) expressed solely through gradients (of any order) of its basic variables, mass density  $\rho$ , temperature  $\theta$ , and velocity  $v_i$ . This is done by an iterative procedure, where the result of order *n* is used to compute the expressions at order n+1.

Our method considers all moments as quantities in their own right, without aiming at expressions for the expansion coefficients. In particular, no iteration process occurs, so that the higher order contributions are independent of the lower order ones. Here, we mention recent work by Spiegel and Thiffeault who use their own variant of an iterative expansion to compute transport equations up to second order of the Knudsen number.<sup>28</sup> While they argue that their method is different from, and better than, the Chapman–Enskog method, they nevertheless obtain unstable equations at second order. One might conclude that the independence of our higher order contributions of the lower ones is related to the stability of our equations (which is proven up to order 3, and expected at any order).

The Chapman–Enskog method provides terms up to a definite order, while the equations that we found above contain higher order terms in the sense of the Chapman–Enskog expansion. This can be seen nicely in Ref. 29, where the authors perform a Chapman–Enskog expansion to infinite order of the linearized Grad equations (our second order set). It seems that these higher order terms (in the Chapman–Enskog sense) in our equations are responsible for the stabilization, and the better agreement with experiments, when compared to the higher order Chapman–Enskog expansions, i.e., the Burnett and super-Burnett equations. Some discussion of this can also be found in Refs. 7 and 19.

When this answer seems to be vague, the reason will be that no definite statement on why the higher order Chapman– Enskog expansions lead to unstable equations is available in the first place.

The Chapman–Enskog expansion can be performed on third order equations, i.e., the R13 equations [(37), (38), and (42)], by setting

$$\sigma_{ij} = \sigma_{ij}^{(0)} + \varepsilon \sigma_{ij}^{(1)} + \varepsilon^2 \sigma_{ij}^{(2)} + \varepsilon^3 \sigma_{ij}^{(3)} + \cdots$$
$$q_i = q_i^{(0)} + \varepsilon q_i^{(1)} + \varepsilon^2 q_i^{(2)} + \varepsilon^3 q_i^{(3)} + \cdots$$

and then computing the expansion coefficients  $\sigma_{ij}^{(\beta)}$ ,  $q_i^{(\beta)}$  in terms of gradients of  $\rho$ ,  $v_i$ ,  $\theta$ . As was shown in Ref. 19 for the linear, three-dimensional case, and in Ref. 7 for the non-linear, one-dimensional case, the resulting equations are the Burnett equations at second order, and the super-Burnett equations at third order of the expansion. Evidently, the R13 equations are a more complete set of equations at third order.

To conclude, we summarize the advantages of our method against the Chapman–Enskog method which are as follows: stable equations at any order, better agreement with experiments, and a simpler derivation of the equations.

#### C. Comparison with the Grad method

Let us discuss the main differences between our method, and Grad's method.  $^{\rm 12-14}$ 

In the Grad method one assumes some set of moments not necessarily 13—as basic variables, and then writes the moment equations for these. These equations do not form a closed set of equations *a priori*, since they contain some higher moments that must be related to the chosen set of variables. Since all moments are defined as integrals of the phase density, this problem is solved by construction of a phase density  $f_G$  which depends explicitly on the chosen set of variables, and the microscopic velocity  $C_i$  ( $f_G$  is a poly-

nomial in  $C_i$  times the local Maxwellian). The Grad phase density  $f_G$  allows then to compute expressions for *all* moments in terms of the variables, and the system of equations for the variables is closed.

There is no statement on which sets of moments one should use, but experience shows that more moments lead to better results—many examples of this can be found in Ref. 14, see also Ref. 30. Nevertheless, the 13 moment case is the preferred one, since all variables involved have a clear physical interpretation.

In short, the main feature of the Grad method is that it provides a certain phase density, and allows only states that can be described by such a function. With Karlin *et al.*,<sup>20</sup> we can say that the Grad method assumes a nonequilibrium manifold, and forces the gas to stay on that manifold. There is no argument from physics on why the gas should be restricted to that nonequilibrium manifold, although attempts are available, which involve entropy maximization methods.<sup>14</sup>

The problem is centered in the question why a certain set of moments should be just enough to describe the gas properly—after all, the gas is not aware of our choice of variables.

Only for the simplest system of Grad type, the Euler equations, is an entropy based argument valid: the Boltzmann collision term forces the gas towards the local Maxwellian, which forms the equilibrium manifold of the Boltzmann equation, and maximizes entropy. There is no intermediate nonequilibrium manifold for the Boltzmann collision term to which the gas would relax before reaching the final—Maxwellian—equilibrium. Intermediate equilibria are possible, however, in more complex systems where processes with distinct mean free times occur, e.g., in the phonon gas.<sup>31</sup>

Extended thermodynamics<sup>14</sup> has a strong relationship to the Grad method, and similar arguments can be applied.

The method presented in this paper is quite different from the Grad method, although the equations obtained bear a strong similarity to Grad's 13 moment set, and the R13 equations. More significant are the differences: In this paper, we have used a thorough analysis of the orders of magnitude of moments, and the order of accuracy of the moment equations. The moments that appear in the equations of chosen order follow from that analysis. Moreover, the Grad phase density  $f_G$  was not required to obtain closed sets of equations.

Compared to our second order equations (36) and (37), the Grad equations for 13 moments contain the term  $-(\sigma_{ik}/\rho)(\partial\sigma_{kl}/\partial x_l)$  in the heat flux equation. This term is of second order, but contributes to third order in the heat flux. Accordingly, this term appears in our third order equations (37) and (38), but there are additional third order terms that must be accounted for, viz.,  $\partial u_{ijk}^0/\partial x_k$  in the equation for  $\sigma_{ij}$ , and  $(1/2)(\partial w_{ij}^1/\partial x_k) + (1/6)(\partial w^2/\partial x_i) + u_{ikl}^0(\partial v_k/\partial x_l)$  in the equation for  $q_i$ . Accordingly, the original Grad 13 equations stand in between the orders of magnitude, since they contain some (in fact only one), but not all terms of third order.

# D. Comparison with the original derivation of the R13 equations

Some relaxation of the strong requirements of the Grad method can be found in approximations which allow states also in the vicinity of the (assumed) nonequilibrium manifold. Most prominently this idea is pursued by Karlin and Gorban, e.g., see Refs. 20 and 29, and the references therein, and just recently by Struchtrup and Torrilhon, whose regularized 13 moment equations (R13) allow for deviations from Grad's 13 moment manifold.<sup>7,19</sup> In fact, their derivation of the R13 equations can be described as a first order Chapman-Enskog expansion centered in Grad's 13 moment phase density, and not in the Maxwellian as in the standard Chapman-Enskog expansion. For this, the Grad equations for 26 moments are computed, and then run through a Chapman-Enskog-like expansion in the Knudsen number, where only the equations for higher moments (denoted as  $m_{ijk} = u_{ijk}^0, R_{ij} = w_{ij}^1, \Delta = w^2$ ) are expanded, while the equations for pressure deviator  $\sigma_{ij}$  and heat flux  $q_i$  are not expanded. Thus, the method of Struchtrup and Torrilhon takes the Grad method for granted, and just derives a regularization by ignoring certain terms that are of higher order in the Knudsen number.

In the present paper, however, the R13 equations resulted from accounting for orders of magnitude and accuracy.

Indeed, by means of our order of magnitude argument we found Eqs. (42), while the original R13 equations can be written  $as^{19}$ 

$$w_{|R13}^{2} = -12\tau \left[ \cdots - \frac{1}{\varrho} q_{j} \frac{\partial \sigma_{jk}}{\partial x_{k}} \right],$$

$$u_{ijk|R13}^{0} = -2\tau \left[ \cdots - \frac{\sigma_{\langle ij}}{\varrho} \frac{\partial \sigma_{k\rangle l}}{\partial x_{l}} \right],$$

$$w_{ij|R13}^{1} = -\frac{24}{5}\tau \left[ \cdots - \frac{1}{\rho} q_{\langle i} \frac{\partial \sigma_{j\rangle k}}{\partial x_{k}} - \frac{5}{6} \frac{\sigma_{ij}}{\varrho} \frac{\partial q_{k}}{\partial x_{k}} - \frac{5}{6} \frac{\sigma_{ij}}{\varrho} \frac{\partial q_{k}}{\partial x_{k}} - \frac{5}{6} \frac{\sigma_{ij}}{\varrho} \sigma_{kl} \frac{\partial v_{k}}{\partial x_{l}} \right],$$

where the dots indicate the same terms as in (42), so that only those terms are explicitly shown above that are added in the original R13 equations. A short glance suffices to see that these additions are of third order, which means they contribute to the fourth order in  $\sigma_{ij}$  and  $q_i$ . However, a careful analysis of the full fourth order would reveal that these are not the only fourth order terms, so that the original R13 equations stand in between third and fourth order, just as the original Grad equations stand in between second and third order.

# E. Consistent order extended thermodynamics (COET)

As we said earlier, the present order of magnitude approach owes its fundament to the ideas of Müller *et al.*, presented in Ref. 21. These authors recognized that the order of

magnitude of moments (in a Chapman–Enskog sense) can be used as the building block for a consistent hierarchy of equations in the orders of the Knudsen number.

The ideas presented in this paper differ from COET mainly in the definition of the order of accuracy of the set of equations. COET assumes that all terms in all moment equations up to the order  $O(\varepsilon^{\lambda})$  must be taken into account for a theory that aims to be accurate at  $\lambda$ th order.

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.

In our method, 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. As became clear, a third order accuracy in the equations does not require to provide balance laws for all moments that have third order contributions. Rather it is sufficient to have  $\sigma_{ij}$  and  $q_i$  up to third order, and the moments  $u_{ijk}^0$ ,  $w_{ij}^1$ ,  $w^1$  to only second order.

Müller *et al.*, however, due to their different philosophy, require the moments  $u_{ijk}^0$ ,  $w_{ij}^1$ ,  $w^1$  to third order accuracy, and need additional moments up to third order, as becomes clear from Eq. (5.7) in Ref. 21. Accordingly, their number of variables is higher for the third order than in our theory.

In our interpretation of the order of accuracy of equations, the third order COET will have higher than third order accuracy (but might stand in between orders of magnitude, similar to original Grad 13 and original R13 equations).

Müller *et al.* state that their method is independent of the phase density. This is right only as long as they use Maxwell molecules or the BGK model to describe collisions. The same is true for our approach, and we have made clear that other interaction models will require a relation between phase density and models, in order to compute the production terms  $P_{i_1\cdots i_n}^a$ , Eq. (7).

#### **VI. CONCLUSIONS**

In the present paper we have introduced a method to develop transport equations for rarefied gases up to a given order of the Knudsen number. We performed the method to find the zeroth to third order approximations which turn out to be the Euler and Navier–Stokes equations, the slightly linearized Grad 13 moment equations, and the slightly linearized R13 equations of Struchtrup and Torrilhon, respectively.

All these sets of equations are known to be stable, and to give meaningful results in accordance with experiments (within the limits of their applicability). For this paper we do not present any solution of these equations, and we refer the interested reader to the cited literature.

Our method competes with the classical methods of kinetic theory, the methods of Chapman–Enskog and Grad, and we have given arguments why our method should be preferred over both.

The main advantage over the Chapman–Enskog expansion is that the higher order equations are stable, and yield meaningful results, while the higher order Chapman–Enskog expansions (i.e., the Burnett and Super-Burnett equations) yield unstable equations and do not contribute to a better description of rarefied gases. Moreover, the development of higher order Chapman–Enskog expansions is forbiddingly complicated, while the method presented here allows a relatively easy development. We also repeat that the (second order) Burnett equations and the (third order) super-Burnett equations can be derived from our second and third order equations by a Chapman–Enskog expansion, so that the equations are more general.

The main advantage of this method above the Grad method is that no doubt remains which variables one has to consider when a certain order of accuracy should be achieved, and that it avoids the use of nonequilibrium manifolds that have no backing within the physics and mathematics of the Boltzmann equation.

In particular, we have applied our method to Maxwell molecules and the BGK model, and have only briefly mentioned how the method could be extended to other collision models. The derivation of the proper second order system for arbitrary interaction terms—a set of 13 equations for  $\rho$ ,  $v_i$ ,  $\theta$ ,  $\sigma_{ij}$ ,  $q_i$ —is the natural next step.

The equations of second and higher order need to be furnished with (jump and slip) boundary conditions in order to become useful tools for simulation of rarefied gas flows, and we continue to work on how these can be derived from the boundary conditions for the Boltzmann equation.

The method developed in this paper gives a complicated, but nevertheless straightforward method to develop stable transport equations up to a certain order in the Knudsen number from the Boltzmann equation, or any other microscopic transport equation that contains a suitable smallness parameter. Thus, the method can be applied not only to BGK model and Maxwell molecules, but to general interaction models for particles, as well as to radiative transfer, electron transport in solids, etc. The application to general interaction potentials for the Boltzmann equation was carried out already, and a paper is to appear.<sup>32</sup>

Moreover, our method gives a common background for equations that so far were considered to be of completely different origin, namely, the Navier–Stokes–Fourier equations, and Grad's 13 moment equations (as well as the R13 equations). At the same time the method discards the Burnett equations, which are still widely discussed despite their well known instabilities. Indeed, these do not appear, and instead the stable Grad13 and R13 equations are emerging as the transport equations of second and third order.

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