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Original Article

Explicit fluxes and productions for large systems of the moment method based on extended thermodynamics

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The moment method of kinetic theory solves Boltzmann's equation approximately via an infinite hierarchy of transfer equations for the moments of the distribution function. Extended thermodynamics furnishes the moment method with a rational constitutive theory. Since more and more moment equations are needed to describe extreme non-equilibrium processes, there is need for an algorithmical derivation of large explicit moment equations. This paper presents detailed techniques and formulas which are needed to implement a numerical equation generator. This includes tensorial conversion formulas as well as the core equations of the constitutive theory. In the last part of the paper, the special case of a one dimensional process is discussed. In such a case, only one generic polynomial evaluation needs to be implemented, whereas the coefficients may be easily calculated a priori.

1 Introduction

In kinetic theory of gases the flow of a dilute gas is described by Boltzmann's equation (see e.g. [4])

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = S\left(f, f\right) \tag{1}$$

for the distribution function f. The value of $f\left(\mathbf{x}, t, \mathbf{c}\right) d\mathbf{c}$ gives the number of particles in $\mathbf{x}$ at time t with velocities in $[\mathbf{c}, \mathbf{c} + d\mathbf{c}]$ with $\mathbf{c}$ defined with respect to an absolute reference. The right hand side $S\left(f, f\right)$ denotes the collision operator

$$S\left(f, f\right) = \int \left(f'\, f'^1 - f\, f^1\right) \sigma g \sin\theta \, d\theta \, d\varphi \, d\mathbf{c}^1. \tag{2}$$

The moment method proposes an approximate solution method for (1). Details may be found in [6,10]. The main idea is not to solve (1) directly, but to solve for moments of the distribution function. From then on the moments serve as variables to describe the state of the gas. The moments are fields depending only on $(\mathbf{x}, t)$ and obey an infinite hierarchy of partial differential equations, called transfer equations. The restriction to a finite system leads to a closure problem which has to be resolved by an appropriate constitutive theory.

Our paper will present detailed formulas how to obtain a closed set of equations for any number and choice of moments. The general procedure is based on extended thermodynamics as described in [10,17] and moreover results of large moment systems may be found in [1,14,17] and again [10]. Many explicit systems for a fixed number of moments have been published in those works. But in the last years it became obvious that the moment method will only succeed, if large systems are taken into account which no more can be derived 'by hand'. In

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the literature, however, there is a lack of advisary of how to construct a generator of moment equations. Hence, this work will collect results, formulas and techniques from various existing publications and textbooks in order to present a general, selfcontained, pragmatic and straight forward deduction of the moment equations. The resulting formulas have been successfully implemented to calculate shock structures [1], shocktubes [2] and heat conduction [15] with very large moment systems.

The final moment systems of this paper will be equivalent to the systems proposed by Grad [6,7] by expansion of the distribution function. The non-equilibrium quantities enter the right and left hand side of the field equations linearly. Density, velocity and temperature, however, appear in a non-linear way. The productions are calculated for a Maxwell interaction potential [4].

1.1 Field equations by extended thermodynamics

Suppose we decide for a certain number N and form of moments $G^{(i)}$ given by

$$G^{(i)} = \int \varphi^{(i)}(\mathbf{c})\ f\, d\mathbf{c} \qquad i = 1, 2, ...N \tag{3}$$

with certain functions $\varphi^{(i)}$. Transfer equations for these variables are obtained by multiplying (1) successively with $\varphi^{(i)}$ and integrating with respect to $\mathbf{c}$. The resulting system is given by

$$\frac{\partial G^{(i)}}{\partial t} + \frac{\partial \mathcal{G}_k^{(i)}}{\partial x_k} = P^{(i)} \qquad i = 1, 2, ...N\ , \tag{4}$$

where the fluxes $\mathcal{G}$ and the productions P follow from

$$\mathcal{G}_k^{(i)} = \int c_k\, \varphi^{(i)}(\mathbf{c})\ f\, d\mathbf{c} \quad \text{and} \quad P^{(i)} = \int \varphi^{(i)}(\mathbf{c}) S(f, f)\ d\mathbf{c}. \tag{5}$$

Obviously, this yields a closure problem since fluxes and productions are a priori not related to the variables G. They are as unknown as the distribution function itself. The closure procedure for the moment systems used in this paper relies on the maximum entropy principle [5] which may be viewed as extended thermodynamics [10] applied to kinetic theory. Following this procedure the distribution function reveals the form

$$f^{(\max)}\left(\mathbf{c}, \Lambda_\varphi^{(i)}\right) = y \exp\left(-\sum_{i=1}^{N} \Lambda_\varphi^{(i)} \varphi^{(i)}(\mathbf{c})\right)\ , \tag{6}$$

if maximal entropy is enforced. The constant y is the inverse volume of a phase space element. The Langrian multipliers $\Lambda_\varphi^{(i)}$ follow as functions of the moments $G^{(i)}$ by inserting the distribution function (6) into the definition of the moments (3). Hence, the distribution function is given by the variables G and the relations in (5) turn into constitutive equations. Detailed background on the maximum entropy principle may be found in [10].

In the following sections the relations (3) and (6) are exploited in order to obtain explicit constitutive relations for moment equations. For the sake of explicity we are forced to linearize the expressions during the calculations. However, in Appendix A it is shown that this linearization does not influence the range of applicablity, since the result is equivalent to the general approach of Grad.

2 General setting

In this section we present various definitions and denotations of moments and their relatives. The appropriate conversion formulas will provide essential help when deducing the constitutive equations in the next sections.

2.1 Variable setup

The original moment of the distribution function is given by

$$F_{i_1 \cdots i_A} = m \int c_{i_1} \cdots c_{i_A}\, f\, d\mathbf{c}\ , \tag{7}$$

where m is the mass of the particles. The moment (7) is called *complete* and *convective*, because of the lack of traces and deviatoric indices and the inclusion of convective parts. The first two complete, convective moments are

$$\rho = F = m \int f \, d\mathbf{c} \qquad \text{and} \quad \rho v_i = F_i = m \int c_i \, f \, d\mathbf{c} \,, \tag{8}$$

i.e. the mass density ρ and momentum density ρv_i, where v_i is the center of mass velocity of the gas. By means of the the peculiar velocity $C_i = c_i - v_i$ we define complete *central* moments via

$$\rho_{i_1 \cdots i_A} = m \int C_{i_1} \cdots C_{i_A} \, f \, d\mathbf{C}. \tag{9}$$

These moments do not contain convective contributions. Especially we have $\rho_i = 0$. Some central moments are given by[1]

$$\text{internal energy density } 2\rho\varepsilon = \rho_{ii} = m \int C^2 \, f \, d\mathbf{C}, \tag{10}$$

$$\text{pressure tensor } \; p_{ij} = \rho_{ij} = m \int C_i C_j \, f \, d\mathbf{C}, \tag{11}$$

$$\text{heat flux } 2q_i = \rho_{ikk} = m \int C^2 C_i \, f \, d\mathbf{C}. \tag{12}$$

From this it follows

$$2\rho\varepsilon = 3p = 3\rho \frac{k}{m} T \tag{13}$$

a relation that marks the restriction to monatomic gases and defines the temperature T. Here, k is the Boltzmann constant.

In practice the complete moments play only a minor role. Any complete tensor will be decomposed into its traces. A tensor of degree n admits $\lfloor \frac{n}{2} \rfloor$ traces, where the Gauss-brackets $\lfloor a \rfloor$ give the largest integer smaller or equal to a. For convenience we introduce the following multi-index abbreviation

$$F^s_A := F_{k_1 \cdots k_s k_1 \cdots k_s i_1 \cdots i_A} = m \int c^{2s} \, c_{i_1} \cdots c_{i_A} \, f \, d\mathbf{c}, \tag{14}$$

$$\rho^s_A := \rho_{k_1 \cdots k_s k_1 \cdots k_s i_1 \cdots i_A} = m \int C^{2s} \, C_{i_1} \cdots C_{i_A} \, f \, d\mathbf{C}. \tag{15}$$

Thus, the moment F^s_A is a tensor with s traces and A different free indices. Its original tensorial degree is given by $2s + A$. In extension of notation we also have

$$F^s_A = m \int c^{2s} \, c_A \, f \, d\mathbf{c} \tag{16}$$

for the definition of F^s_A. Correspondingly we write F^s_{A+B} for a moment with $A + B$ different free indices. A contraction of indices is written as

$$F_{A+B} F_A = F_{i_1 i_2 \cdots i_A \, j_1 j_2 \cdots j_B} F_{i_1 i_2 \cdots i_A}. \tag{17}$$

Additionally we use symmetry-brackets

$$\begin{aligned} F_{(A} \rho_{B)} &= F_{(i_1 i_2 \cdots i_A} \rho_{j_1 j_2 \cdots j_B)} \\ &= \frac{1}{\text{number of permutations}} \left(F_{i_1 i_2 \cdots i_A} \rho_{j_1 j_2 \cdots j_B} + \text{index permutations} \right). \end{aligned} \tag{18}$$

The decomposition into traces imposes a canonical structure on the set of moments which may be read off the tableau shown in Fig. 1. In the figure each box corresponds to a tensor. A row shows a complete moment which is decomposed in tensors with increasing number of traces through the columns.

As example we consider the well known 13-moment-case of Grad: It uses the boxes 1–5 as variables, i.e. the complete 0th, 1st and 2nd moment and the trace of the third moment.

[1] Throughout this paper we will assume the summation convention to hold. Double indices at tensors will be summed over 1,2,3. Moreover a squared velocity vector has to be thinked of as the square of its norm.

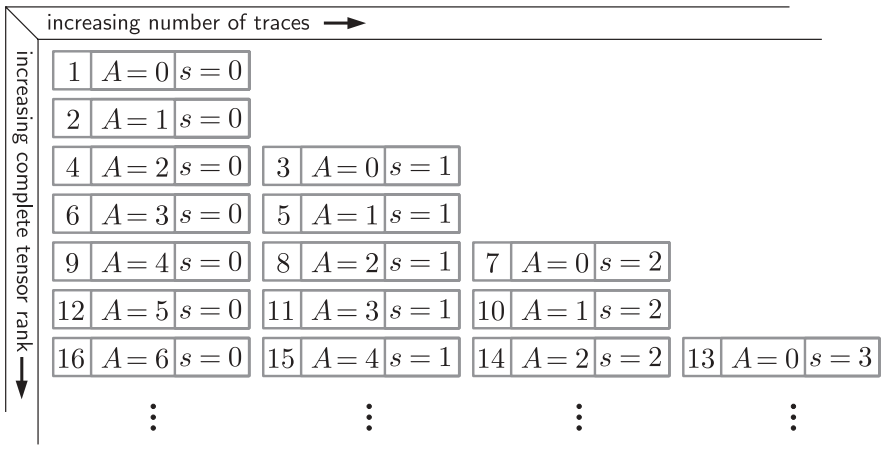

Fig. 1. Structure of the set of variables in the moment method if each moment is decomposed into its traces. Each box represents a moment with A free indices and s traces

For the conversion of convective moments in central moments and vice versa one obtains from the definitions (7) and (9)

$$F^s_A = \sum_{B=0}^{A} \sum_{s_1+s_2+s_3=s} \binom{A}{B} \binom{s}{s_1, s_2} 2^{s_3} v^{2s_2} v_{s_3} v_{(A-B} \rho^{s_1}_{B)+s_3}, \tag{19}$$

$$\rho^s_A = \sum_{B=0}^{A} \sum_{s_1+s_2+s_3=s} (-1)^{s_3+A-B} \binom{A}{B} \binom{s}{s_1, s_2} 2^{s_3} v^{2s_2} v_{s_3} v_{(A-B} F^{s_1}_{B)+s_3}. \tag{20}$$

In these formulas v_{s_3} and v_{A-B} stand for s_3, respectively $A-B$, velocity vectors with different indices and v^{2s_2} denotes the $2s_2$-power of the norm of the velocity. In the product $v_{s_3} v_{(A-B} F^{s_1}_{B)+s_3}$ the moment F will be contracted s_3-times with the velocity vector and form a symmetric tensor product with $A-B$ velocity vectors. The result is a symmetric tensor with A free indices. In the formulas (19) and (20) appear binomial and trinomial coefficients which are given by

$$\binom{n}{k} = \frac{n!}{k!\,(n-k)!}, \qquad \binom{n}{k_1, k_2} = \frac{n!}{k_1! k_2!\,(n-k_1-k_2)!}. \tag{21}$$

Each tensor, with traces or without, may be additionally decomposed into its deviatoric, i.e. traceless parts. Deviatoric indices are marked with angular brackets. We have as definition for traceless, central moments

$$\rho^s_{\langle A\rangle} := \rho_{k_1\cdots k_s k_1\cdots k_s \langle i_1\cdots i_A\rangle} = m \int C^{2s}\, C_{\langle i_1} \cdots C_{i_A\rangle}\, f\, d\mathbf{C} = m \int C^{2s}\, C_{\langle A\rangle}\, f\, d\mathbf{C}. \tag{22}$$

In this paper non-deviatoric moments are sometimes called *plain* moments for shortness. The conversion between traceless and plain parts is given by

$$\rho^s_{\langle A\rangle} = \sum_{r=0}^{\lfloor \frac{A}{2} \rfloor} a_{A,r}\, \delta_{(2r} \rho^{s+r}_{A-2r)}, \tag{23}$$

$$\rho^s_A = \sum_{r=0}^{\lfloor \frac{A}{2} \rfloor} b_{A,r}\, \delta_{(2r} \rho^{s+r}_{\langle A-2r\rangle)}. \tag{24}$$

These hold if ρ is substituted by any tensor. δ_{2r} denotes the completely symmetric delta-tensor of degree $2r$. It is defined by the symmetric product of r Kronecker symbols

$$\delta_{2r} = \delta_{(i_1 i_2} \delta_{i_3 i_4} \cdots \delta_{i_{2r-1} i_{2r})}.$$

The coefficients in (23) and (24) read

$$a_{A,r} = (-1)^r \frac{A!}{(A-2r)!r!2^r} \prod_{j=A-r}^{A-1} \frac{1}{2j+1}, \tag{25}$$

$$b_{A,r} = \frac{A!}{(A-2r)!r!2^r} \prod_{j=A-2r+1}^{A-r} \frac{1}{2j+1}. \tag{26}$$

2.2 Choice of variables

Up to now, field equations for the moments have not been mentioned. They will be obtained after moments are chosen by multiplying Boltzmann's equation (1) with the corresponding functions of the velocity $\mathbf{c}$ and integrating the resulting expression.

The choice of variables is the crucial point in the moment method. The pure number of moments is not clear a priori, but given implicitly by the degree of non-equilibrium of the simulated process. Additionally there is a lot of freedom what structure the set of variable should have, e.g. what boxes shoud be picked from Fig. 1. Some guidelines are given by

- physicality: In [1] it is shown that not every set of variables produces a system that is Galilei invariant. A sufficient condition for Galilei invariance is to build successive sets of variables by starting with the highest trace of a new moment. The numbering of the boxes in Fig. 1 shows such a structure: The rows are numbered from the *right*.
  Only recently the order of magnitude of the moments has been investigated in [11]. Such considerations are at the beginning, but could set up general field equations of consistent orders one day.
- analytical comfort: Clearly, when considering larger systems the analytical handling should be managable. Using orthogonal polynomials in c_i allows to calculate the productions easily, see the next section. Unfortunately, the left hand side becomes quite difficult to obtain in orthogonal variables. Plain convective variables have a very easy flux/variable connection, however the right hand side is more involved.
- numerical comfort: Finally, the large systems will be solved numerically, which should be taken into account when choosing the variables. The use of central, traceless or plain variables destroys the conservative form of the equations that is often needed by highly developed numerical schemes (see e.g. [9,12]). Convective variables show some numerical instabilities in the case of very large systems. In [13] an alternative approach is presented to get rid of this instability, but that approach sacrifies the conservative form.

This paper uses convective, non-deviatoric moments F^s_A as basic variables despite of their minor disadvantages. The great advantage is the very simple form of the transfer equations, which read

$$\partial_t F^s_A + \operatorname{div} F^s_{A+1} = P^s_A. \tag{27}$$

The flux is a convective, plain moment with one additional free index. According to Fig. 1 the flux of a variable is always the variable of the box below. Hence, the closure problem appears in the last row where the corresponding fluxes are not anymore in the set of variables. The production follows from the integral over the collision operator (2) as

$$P^s_A = m \int c^{2s} c_A \, S\left(f, f\right) d\mathbf{c}. \tag{28}$$

To build up ever larger systems, we propose to fill up successively complete moments according to the numbering of Fig. 1, i.e. to include the highest trace of new complete moments first. Moreover, gaps in the figure are avoided by starting a new row only, if the preceeding row has been completed. Systems build in such a manner will be called *regular*.

For the navigation through the tableau of Fig. 1 for a regular system, several formulas turned out to be useful. The number of a variable according to the numbering in the figure is given by

$$i\left(A, s\right) = \left\lfloor \frac{A + 2\left(s+1\right)}{2} \right\rfloor \left(A + 2\left(s+1\right) - \left\lfloor \frac{A + 2\left(s+1\right)}{2} \right\rfloor \right) - s, \tag{29}$$

where s is the number of traces and A is the number of free indices. Again the Gauss-brackets denote the largest integer. To obtain the tensorial degree $T\left(i\right)$, the number of traces $s\left(i\right)$ or the number of free indices $A\left(i\right)$ for a

specific variable i, the following formulas may be used

$$T(i) = \left\lfloor \sqrt{4i-3} - 1 \right\rfloor , \tag{30}$$

$$s(i) = \left\lfloor \left(1 + \tfrac{1}{2}T(i)\right)^2 \right\rfloor - i , \tag{31}$$

$$A(i) = T(i) - 2s(i) . \tag{32}$$

The equations (31) and (32) give the inversion of (29) since we have $i(A(i), s(i)) = i$.

3 Constitutive equations

Any set of variables chosen from the tableau in Fig. 1, be it regular or irregular, may be characterized by the set of numbers,

$$\left\{ \hat{n}^{(0)}, \hat{n}^{(1)}, \hat{n}^{(2)}, \ldots \hat{n}^{(A^{(\max)})} \right\} . \tag{33}$$

The values $n^{(B)} \geq 0$ with $B = 0, 1, ...$ give the number of variables with B free indices, with $A^{(\max)}$ the largest number of free indices in the chosen system. An important advantage of restricting to regular systems is, that they are characterized by only one number because

$$A^{(\max)}(N) = \begin{cases} T(N) - 1 & i(T(N), 0) > N , \\ T(N) & \text{else} \end{cases} \tag{34}$$

$$\hat{n}^{(B)}(N) = \left\lfloor \frac{1 - B + \sqrt{4N - 2B - 2}}{2} \right\rfloor \tag{35}$$

hold for a regular system with N variables.

3.1 Fluxes

To close the system (27) we need constitutive equations that connect the fluxes in the highest equations with our variables, i.e. with convective, non-deviatoric moments. However, the constitutive theory is more simply formulated in central, deviatoric moments. But the relations for our variables will follow by conversion formulas. The structure of this procedure is shown in Fig. 2.

We aim at relations of type (A) but the theory gives relations of type (C). Thus we firstly convert the convective, plain moments via (20) and (23) to central, traceless moments. After obtaining the corresponding parts of the fluxes, these are again assembled by (24) and (19) to give the required fluxes.

In the following, only the constitutive relations of type (C) will be presented. According to Sect. 1.1 any central, tracefree moment is given by

$$\rho^s_{\langle A\rangle}\left(\hat{\lambda}^r_{\langle B\rangle}\right) = m \int C^{2s} C_{\langle A\rangle} f^{(\max)}\left(\mathbf{C}, \hat{\lambda}^r_{\langle B\rangle}\right) d\mathbf{C} \tag{36}$$

with the maximum entropy distribution function

$$f^{(\max)}\left(\mathbf{C}, \hat{\lambda}^s_{\langle A\rangle}\right) = y \exp\left(- \sum_{A=0}^{A^{(\max)}} \sum_{s=0}^{\hat{n}^{(A)}-1} \hat{\lambda}^s_{\langle A\rangle} C^{2s} C_{\langle A\rangle} \right) . \tag{37}$$

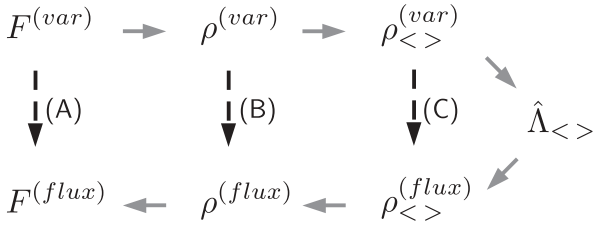

Fig. 2. Procedure to calculate the fluxes for convective, non-deviatoric moments F^s_A (type A). The constitutive theory is simpler for central, deviatoric moments (type C). Thus, for type A two conversion steps will be attached before and after

The function in (36) is linearly expanded

$$\rho^s_{\langle A\rangle}\left(\hat{\lambda}^r_{\langle B\rangle}\right) = \rho^s_{\langle A\rangle}\Big|_E + \sum_{B=0}^{A^{(\max)}} \sum_{r=0}^{\hat{n}^{(B)}-1} \left.\frac{\partial \rho^s_{\langle A\rangle}}{\partial \hat{\Lambda}^r_{\langle B\rangle}}\right|_E \left(\hat{\lambda}^r_{\langle B\rangle} - \hat{\lambda}^r_{\langle B\rangle}\Big|_E\right) , \tag{38}$$

where the Jacobian follows from differentiation of the distribution function (37)

$$\left.\frac{\partial \rho^s_{\langle A\rangle}}{\partial \hat{\Lambda}^r_{\langle B\rangle}}\right|_E = -m \int C^{2s} C_{\langle A\rangle} C^{2r} C_{\langle B\rangle}\ f^{(\max)}\Big|_E \, d\mathbf{C} \tag{39}$$

$$= -m \int C^{2(s+r+1)+A+B} f_M \, dC \int n_{\langle A\rangle} n_{\langle B\rangle} d\mathbf{\Omega}. \tag{40}$$

Here the velocity vector C_i has been decomposed into its absolute value C and its direction n_i. The equilibrium is given by the Maxwell distribution

$$f_M\left(C_i, \rho, T\right) = \frac{\rho/m}{\sqrt{2\pi \frac{k}{m} T}^3} \exp\left(-\frac{C^2}{2\frac{k}{m}T}\right) , \tag{41}$$

which has no dependence on the velocity direction. Thus the steradian integration in (40) separates. For the integral the relation

$$\mathcal{A}_B \int n_{\langle A\rangle} n_{\langle B\rangle} d\mathbf{\Omega} = \frac{2\pi\, A!}{\prod_{j=0}^{A}(2j+1)} \delta_{AB} \mathcal{A}_{\langle A\rangle} \tag{42}$$

holds if it is contracted with any tensor $\mathcal{A}_B$. Back to (38) we obtain

$$\rho^s_{\langle A\rangle}\left(\hat{\lambda}^r_{\langle B\rangle}\right) = \rho^s_{\langle A\rangle}\Big|_E - \rho\, A! \sum_{r=0}^{\hat{n}^{(A)}-1} \mathcal{C}^{(A)}_{sr} \left(\tfrac{k}{m}T\right)^{r+s+A} \left(\hat{\lambda}^r_{\langle A\rangle} - \hat{\lambda}^r_{\langle A\rangle}\Big|_E\right) \tag{43}$$

with the matrix elements

$$\mathcal{C}^{(A)}_{sr} = \prod_{j=A+1}^{A+r+s} (2j+1)\,. \tag{44}$$

Note that (43) holds for *any* central, traceless moment, not only for the variables of the particular system. If the Lagrangian multipliers are known, any such moment may be calculated. Of course, the moments which are part of the set of the variables need not to be calculated. Instead, they furnish (43) to calculate the Lagrangian multipliers. Equation (43) then gives for each value of A separately a linear system of equations. After inversion one obtains the equations for each A as

$$\hat{\lambda}^r_{\langle A\rangle} - \hat{\lambda}^r_{\langle A\rangle}\Big|_E = \sum_{s=0}^{\hat{n}^{(A)}-1} \frac{\left(\mathcal{C}^{(A)}_{rs}\right)^{-1}}{\rho\, A! \left(\frac{k}{m}T\right)^{r+s+A}} \left(\rho^s_{\langle A\rangle} - \rho^s_{\langle A\rangle}\Big|_E\right) \qquad r = 0, 1, ..(\hat{n}^{(A)} - 1). \tag{45}$$

Using this in (43) gives the explicit formula

$$\rho^s_{\langle A\rangle} = \rho^s_{\langle A\rangle}\Big|_E - \sum_{r=0}^{\hat{n}^{(A)}-1} \sum_{t=0}^{\hat{n}^{(A)}-1} \mathcal{C}^{(A)}_{sr} \left(\mathcal{C}^{(A)}_{rt}\right)^{-1} \left(\tfrac{k}{m}T\right)^{s-t} \left(\rho^t_{\langle A\rangle} - \rho^t_{\langle A\rangle}\Big|_E\right) \qquad \forall\, s, A \tag{46}$$

for any central, tracefree moment $\rho^s_{\langle A\rangle}$. Note, that $\mathcal{C}^{(A)}_{sr}$ is defined for any values of r and s, but $(\mathcal{C}^{(A)}_{rt})^{-1}$ is a quadratic matrix with a certain range $r, s < n^{(A)}$. Only if (46) is used to calculate moments from the set of variables, $s < n^{(A)}$ holds and the matrix product will give unity. The equilibrium values are calculated from (36) with the Maxwell distribution (41). They read

$$\rho^s_{\langle A\rangle}\Big|_E = \begin{cases} \rho \left(\frac{k}{m}T\right)^s \prod_{j=0}^{s}(2j+1) & A = 0 \\ 0 & A \neq 0 \end{cases} . \tag{47}$$

This completes (46) to give the relation (C) in Fig. 2.

3.2 Productions

Firstly, we present the results of the constitutive theory for the case that orthonormal polynomials are used. The results will be needed when calculating the production terms in the next section.

3.2.1 Orthonormal moments

Let us construct the polynomial $\psi^r_{\langle A\rangle}$ of the central velocity C_i

$$\psi^r_{\langle A\rangle}(\mathbf{C}) = \sqrt{\frac{1\cdot 3\cdot 5\cdot\ldots\cdot(2A+1)\sqrt{\pi}}{2^A\, A!}}\, S_r^{(A+\frac{1}{2})}\left(\frac{C^2}{2\frac{k}{m}T}\right)\frac{C^A}{\sqrt{2\frac{k}{m}T}^A}\, n_{\langle A\rangle}\ , \tag{48}$$

based on the generalized Laguerre (also: Sonine-) polynomials (see [10,16])

$$S_r^{(a)}(x) = \sqrt{\frac{r!}{(r+a)!}}\sum_{p=0}^{r}\frac{(-1)^p\prod_{j=p+1}^{r}(j+a)}{p!\,(r-p)!}\,x^p. \tag{49}$$

The polynomials $\psi^r_{\langle A\rangle}$ are orthonormal according to a kernel in the form of the Maxwell distribution so that

$$m\,\mathcal{A}_B\int\psi^r_{\langle A\rangle}(\mathbf{C})\,\psi^s_{\langle B\rangle}(\mathbf{C})\ f_M\,d\mathbf{C} = \rho\,\delta_{rs}\delta_{AB}\mathcal{A}_{\langle A\rangle} \tag{50}$$

for any tensor $\mathcal{A}_B$.

Orthonormal moments are defined by

$$g^s_{\langle A\rangle} = m\int\psi^r_{\langle A\rangle}(\mathbf{C})\ f^{(\max)}d\mathbf{C} \tag{51}$$

with the maximum entropy distribution function

$$f^{(\max)}\left(\mathbf{C},\mu^s_{\langle A\rangle}\right) = y\,\exp\left(-\sum_{A=0}^{A^{(\max)}}\sum_{s=0}^{\hat{n}^{(A)}-1}\mu^s_{\langle A\rangle}\psi^s_{\langle A\rangle}(\mathbf{C})\right). \tag{52}$$

Note that for a regular system the $g^s_{\langle A\rangle}$ follow from linear combinations of the variables $\rho^s_{\langle A\rangle}$ in a one-to-one manner

$$g^s_{\langle A\rangle}\quad\longleftrightarrow\quad\rho^s_{\langle A\rangle}. \tag{53}$$

If one follows the procedure of the preceeding section the equation analogous to (43) finally reads

$$g^s_{\langle A\rangle} - g^s_{\langle A\rangle}\Big|_E = \rho\left(\mu^s_{\langle A\rangle} - \mu^s_{\langle A\rangle}\Big|_E\right). \tag{54}$$

Hence, it follows that the orthonormal moments outside a particular set of variables take their equilibrium value which is zero due to the orthogonality

$$g^r_{\langle B\rangle} = 0\qquad r\geq\hat{n}^{(B)},\ B > A^{(\max)}. \tag{55}$$

Since the orthonormal moments are equivalent to the central, traceless moments, the relations in (55) follow equivalently by linear combinations of (46). The constitutive relations (55) are quite simple. Unfortunately, it is considerably more complicated to derive transfer equations for orthonormal moments, since the polynomials (48) depend on the temperature and the velocity (via C_i).

3.2.2 Explicit productions

The productions required are given by (28). Before these productions are calculated, let us look at the case of generic variables to uncover the structure.

The productions are functions of the Lagrange multipliers

$$P^{(i)}\left(\Lambda_\varphi^{(j)}\right) = m\int \varphi^{(i)}(\mathbf{c})\, S\left(f^{(\max)}, f^{(\max)}\right) d\mathbf{c} \tag{56}$$

by means of the distribution function

$$f^{(\max)}\left(\mathbf{c}, \Lambda_\varphi^{(i)}\right) = y\, \exp\left(-\sum_{i=1}^{N} \Lambda_\varphi^{(i)} \varphi^{(i)}(\mathbf{c})\right). \tag{57}$$

As in the case of the fluxes, Equation (56) is linearly expanded. We obtain

$$P^{(i)}\left(\Lambda_\varphi^{(j)}\right) = P^{(i)}\Big|_E + \left.\frac{\partial P^{(i)}}{\partial \Lambda_\varphi^{(j)}}\right|_E \left(\Lambda_\varphi^{(j)} - \Lambda_\varphi^{(j)}\Big|_E\right) \tag{58}$$

with the Jacobian given by

$$\left.\frac{\partial P^{(i)}}{\partial \Lambda_\varphi^{(j)}}\right|_E = m\int \varphi^{(i)}(\mathbf{c}) \left.\frac{\partial S\left(f^{(\max)}, f^{(\max)}\right)}{\partial \Lambda_\varphi^{(j)}}\right|_E d\mathbf{c} \tag{59}$$

$$= m\int \varphi^{(i)}(\mathbf{c})\, \mathcal{I}\left(\varphi^{(i)}(\mathbf{c})\right) f_M\, d\mathbf{c}. \tag{60}$$

Here $\mathcal{I}(\phi)$ is the derivative of the collision operator, i.e., the linearized operator

$$\mathcal{I}(\phi) = \int f_M^1 \left(\phi' + \phi'^1 - \phi - \phi^1\right) \sigma\, g\, \sin\theta\, d\theta\, d\varphi\, d\mathbf{c}^1. \tag{61}$$

From (60) follows that the calculation of the productions becomes most easy if the functions $\varphi^{(i)}$ are eigenfunctions of the linear operator.

In the case of Maxwell molecules, the eigenfunctions of the linear operator have been calculated in [16]. They are given by the orthonormal polynomials $\psi^s_{\langle A\rangle}$ defined in (48) so that

$$\mathcal{I}\left(\psi^s_{\langle A\rangle}\right) = -\zeta^s_A \psi^s_{\langle A\rangle} \tag{62}$$

with eigenvalues ζ^s_A. According to [8,16] the eigenvalues are proportional to the density of the gas and are given by

$$\zeta^s_A = \frac{\rho}{m} \sum_{k=0}^{\lfloor \frac{A}{2}\rfloor} \sum_{n=1}^{\lfloor \frac{s+A-k}{2}\rfloor} \frac{\prod_{j=0}^{A-k-1}(2j+1)}{(-4)^{n-1}(-2)^k (A-2k)!k!} d(s+A-k, n)\, I_n \tag{63}$$

$$\text{with } d(k,n) = (k-n-1)!\frac{k^2-2nk+k}{(k-2n+1)!n!}. \tag{64}$$

Here the integrals I_n read

$$I_n = \sqrt{\tfrac{\kappa}{m}}\pi\sqrt{2}\int_0^{\frac{\pi}{4}} \frac{\sin^{2n}\left(2\sqrt{\cos(2\tau)}\, K\left(\sin^2(\tau)\right)\right)}{\sin^2(2\tau)} d\tau\,, \tag{65}$$

where $K(s)$ is the complete elliptic integral of the first kind. The constant κ in (65) is the factor of the Maxwell interaction potential $\Phi(r) = \frac{\kappa}{4} r^{-4}$.

We start with calculating the productions at first in the case of orthonormal moments, i.e.

$$\tilde{P}^s_{\langle A\rangle} = m\int \psi^s_{\langle A\rangle}(\mathbf{C})\, S(f,f)\, d\mathbf{C}. \tag{66}$$

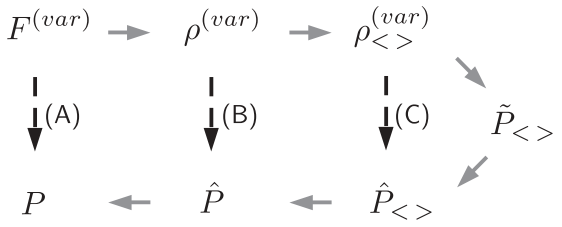

Fig. 3. Procedure to calculate the production terms for convective, non-deviatoric moments. Similar to the case of the fluxes, the calculation is simpler for the variables $\rho^s_{\langle A\rangle}$ and conversion steps need to be performed

From (58) and (60) we obtain by substituting $(\varphi^{(i)}, \Lambda^{(j)}_\varphi)$ with $(\psi^s_{\langle A\rangle}, \mu^r_{\langle B\rangle})$

$$\tilde{P}^s_{\langle A\rangle}\left(\mu^r_{\langle B\rangle}\right) = m\int \psi^s_{\langle A\rangle}(\mathbf{C})\,\mathcal{I}\left(\psi^r_{\langle B\rangle}(\mathbf{C})\right) f_M\, d\mathbf{C}\,\left(\mu^r_{\langle B\rangle} - \mu^r_{\langle B\rangle}\Big|_E\right) \tag{67}$$

$$= -\zeta^s_A\,\rho\left(\mu^s_{\langle A\rangle} - \mu^s_{\langle A\rangle}\Big|_E\right) \tag{68}$$

$$= -\zeta^s_A\left(g^s_{\langle A\rangle} - g^s_{\langle A\rangle}\Big|_E\right), \tag{69}$$

where the result (54) has been used. The orthonormal moments are linear combinations of the central, traceless moments and the conversion may be read off (48) directly. We have

$$g^s_{\langle A\rangle} = \tilde{a}^s_A \sum_{r=0}^{s} \mathcal{M}^{(A)}_{sr} \frac{1}{\left(\frac{k}{m}T\right)^r}\rho^r_{\langle A\rangle} \tag{70}$$

with a lower triangular matrix

$$\mathcal{M}^{(A)}_{sr} = \begin{cases} \frac{(-1)^r}{r!(r-p)!2^s}\prod_{j=A+r+1}^{A+s}(2j+1) & r\le s \\ 0 & \text{else}\end{cases} \tag{71}$$

and a constant

$$\tilde{a}^s_A = \frac{\sqrt{2}}{\left(2\frac{k}{m}T\right)^{\frac{A}{2}}}\sqrt{\frac{1\cdot3\cdot5\cdot\ldots(2A+1)\sqrt{\pi}\,s!}{A!(s+A+\frac{1}{2})!}}. \tag{72}$$

Analogously, the productions of the orthonormal moments $\tilde{P}^s_{\langle A\rangle}$ given by (66) may be represented as linear combination of the productions for central, tracefree moments $\hat{P}^r_{\langle A\rangle}$ given by

$$\hat{P}^s_{\langle A\rangle} = m\int C^{2s}C_{\langle A\rangle}S(f,f)\,d\mathbf{C}. \tag{73}$$

The conversion formula is the same as in (70) when $(g^s_{\langle A\rangle}, \rho^r_{\langle A\rangle})$ are substituted by $(\tilde{P}^s_{\langle A\rangle}, \hat{P}^s_{\langle A\rangle})$. Equation (69) thus reads

$$\sum_{r=0}^{s}\mathcal{M}^{(A)}_{sr}\frac{1}{\left(\frac{k}{m}T\right)^r}\hat{P}^r_{\langle A\rangle} = -\sum_{r=0}^{s}\zeta^s_A\mathcal{M}^{(A)}_{sr}\frac{1}{\left(\frac{k}{m}T\right)^r}\rho^r_{\langle A\rangle}, \tag{74}$$

and we obtain

$$\hat{P}^t_{\langle A\rangle} = -\sum_{s=0}^{t}\sum_{r=0}^{s}\left(\mathcal{M}^{(A)}_{ts}\right)^{-1}\zeta^s_A\mathcal{M}^{(A)}_{sr}\left(\frac{k}{m}T\right)^{t-r}\rho^r_{\langle A\rangle}. \tag{75}$$

The inverse of $\mathcal{M}^{(A)}_{sr}$ may be calculated explicitly

$$\left(\mathcal{M}^{(A)}_{ts}\right)^{-1} = \begin{cases}\frac{(-2)^s t!}{(t-s)!}\prod_{j=A+s+1}^{A+t}(2j+1) & s\le t \\ 0 & \text{else}\end{cases}. \tag{76}$$

The situation is now similar to that in the begining of Sect. 3.1.

According to Fig. 3, Equation (75) gives a relation of type (C) but for convective, plain moments a relation of type (A) is needed. Such relation is easy to build, since the conversion formulas (19)/(20) and (23)/(24) hold for the different productions as well, if $(F^s_A, \rho^s_A, \rho^s_{\langle A\rangle})$ are substituted by $(P^s_A, \hat{P}^s_A, \hat{P}^s_{\langle A\rangle})$. Thus one obtains the central, traceless moments by using (20) and (23) and afterwards assembling the central, deviatoric productions via (24) and (19).

4 Explicit equations in one dimension

Any system of moment equations may now be calculated from the 6 equations (19)/(20) and (23)/(24) for the conversion as well as (46) and (75) for the fluxes and the productions. Of course, the implementation in 2 or 3 dimensions is still not trivial due to the tensorial products. In one dimension these complications are skipped.

We define for the single one-dimensional component of a central, traceless moment with A free indices and s traces

$$\rho^s_{\langle A\rangle} := \rho_{i_1 i_1 i_2 i_2 \cdots i_s i_s \underbrace{\langle 111\cdots 1\rangle}_{A \text{ times}}}\,, \tag{77}$$

where A is no longer a multiindex. Similar definitions hold for F^s_A and ρ^s_A. Note that setting all indices to 1 in a *non-deviatoric* tensor yields not the only independent component in one dimensional processes. Nevertheless, if all traces of that tensor are considered, like in a regular system, nothing is missing.

Since the velocity reads $v_i \equiv (v,0,0)$ in a one dimensional process, the equations (19) and (20) reduce to

$$F^s_A = \sum_{B=0}^{A} \sum_{s_1+s_2+s_3=s} \binom{A}{B} \binom{s}{s_1,s_2} 2^{s_3} v^{2s_2+s_3+A-B} \rho^{s_1}_{B+s_3}, \tag{78}$$

$$\rho^s_A = \sum_{B=0}^{A} \sum_{s_1+s_2+s_3=s} (-1)^{s_3+A-B} \binom{A}{B} \binom{s}{s_1,s_2} 2^{s_3} v^{2s_2+s_3+A-B} F^{s_1}_{B+s_3}. \tag{79}$$

Similarly, we obtain instead of (23) and (24)

$$\rho^s_{\langle A\rangle} = \sum_{r=0}^{\lfloor \frac{A}{2} \rfloor} a_{A,r}\, \rho^{s+r}_{A-2r} \quad \text{and} \quad \rho^s_A = \sum_{r=0}^{\lfloor \frac{A}{2} \rfloor} b_{A,r}\, \rho^{s+r}_{\langle A-2r\rangle} \tag{80}$$

for the one dimensional components. The transfer equations (27) read in one dimension

$$\partial_t F^s_A + \partial_x F^s_{A+1} = P^s_A \tag{81}$$

and may be written in the canonical form

$$\partial_t u_i + \partial_x f_i(\mathbf{u}) = P_i(\mathbf{u}) \qquad i = 1,2,\ldots N \tag{82}$$

where we have defined $u_i := F^{s(i)}_{A(i)}$ for the variables. The fluxes are given by $f_i(\mathbf{u}) = u_{i(A(i)+1,s(i))}$ with use of the formulas (29), (31) and (32). For most i the flux is simply another variable. Only if $i(A(i)+1, s(i)) > N$ constitutive equations will be needed.

4.1 Polynomial representation

A detailed inspection of the equations (46) and (47) as well as (78)/(79) shows that the temperature and the velocity only appear with positive integer exponents in the constitutive equations. Moreover the constitutive equations will be linear with respect to the variables u_j with $j \geq 4$ and with respect to the density ρ, if u_2 and u_3 are replaced by the velocity and the temperature. For this reason, the constitutive equations for the system (81) have the representation

$$u_i = \rho\, \varphi^{(i)}_1(v,\theta) + \sum_{j=4}^{N} \varphi^{(i)}_j(v,\theta)\, u_j \qquad i > N\,, \tag{83}$$

where $\varphi^{(i)}_j$ are polynomials in the variables v and θ with

$$\theta := \frac{k}{m} T. \tag{84}$$

The structure of these polynomials $\varphi^{(i)}_j$ follows from dimensional arguments: A variable u_j has the dimension of density$\times$(velocity)$^{T(j)}$, where the tensorial degree $T(j)$ is given by (30). Hence, the polynomial $\varphi^{(i)}_j$ has

the dimension (velocity)$^{(T(i)-T(j))}$. The variables v and θ have dimensions of velocity and velocity squared, respectively. The polynomials are thus given by

$$\varphi_j^{(i)}(v,\theta) = \sum_{k=0}^{\lfloor \frac{m}{2} \rfloor} \kappa_{j,k}^{(i)} \, \theta^k \, v^{m-2k} \quad \text{with } m = T(i) - T(j), \tag{85}$$

i.e., as homogeneous in the variables θ and (v^2). The problem of finding the constitutive equations is now condensed to finding the coefficients $\kappa_{j,k}^{(i)}$ in (85). It is quite simple to program a computer-algebra-system such that (46) is combined with the appropriate conversion formulas and the coefficients are extracted. An implemetation based on Mathematica® is available from the authors [3].

The same argument as above holds for the productions. We have the polynomial representation

$$P_i = \rho \, \bar{\varphi}_1^{(i)}(v,\theta) + \sum_{j=4}^{N} \bar{\varphi}_j^{(i)}(v,\theta) \; u_j \qquad i > N \tag{86}$$

with the polynomials $\bar{\varphi}_j^{(i)}$ given by

$$\bar{\varphi}_j^{(i)}(v,\theta) = \sum_{k=0}^{\lfloor \frac{m}{2} \rfloor} \bar{\kappa}_{j,k}^{(i)} \, \theta^k \, v^{m-2k} \quad \text{with } m = T(i) - T(j). \tag{87}$$

It remains to give the equations which relates the ordinary variables density, velocity and temperature to the variables u_i. These read

$$\rho = u_1 \, , \tag{88}$$

$$v = \frac{u_2}{u_1} \, , \tag{89}$$

$$\theta = \frac{u_3 - u_2^2}{3u_1}. \tag{90}$$

4.2 Example

To conclude this paper we shall give an example of a system of moment equations written in the form (82) with explicit fluxes and productions. As number of variables we choose (rather arbitrary) $N = 8$, i.e. we take the first four rows of Fig. 1 completely and additionally two traces of the fifth row. The resulting one-dimensional system reads

$$\begin{aligned}
&\partial_t u_1 + \partial_x u_2 = 0 \, , \\
&\partial_t u_2 + \partial_x u_4 = 0 \, , \\
&\partial_t u_4 + \partial_x u_6 = P_4(\mathbf{u}) \, , \qquad \partial_t u_3 + \partial_x u_5 = 0 \, , \\
&\partial_t u_6 + \partial_x \tilde{u}_9(\mathbf{u}) = P_6(\mathbf{u}) \, , \quad \partial_t u_5 + \partial_x u_8 = P_5(\mathbf{u}) \, , \\
&\qquad\qquad\qquad\quad \partial_t u_8 + \partial_x \tilde{u}_{11}(\mathbf{u}) = P_8(\mathbf{u}) \, , \quad \partial_t u_7 + \partial_x \tilde{u}_{10}(\mathbf{u}) = P_7(\mathbf{u}) \, .
\end{aligned} \tag{91}$$

In writing (91) we repeat the structure of Fig. 1. In the system appear five production terms P_4 through P_8 and three unknown fluxes, $\tilde{u}_9$ through $\tilde{u}_{11}$. The first three productions vanish due to the conservation of mass, momentum and energy. The fluxes and productions are given by (83)/(85) and (86)/(87), respectively. The coefficients of the polynomials are given in Table 1 for the fluxes.

Table 1. Coefficients for the polynomials (83)/(85) to calculate the unknown fluxes of the regular system consisting of 8 one dimensional equations (91)

j	$\kappa^{(9)}_{j,0}$	$\kappa^{(9)}_{j,1}$	$\kappa^{(9)}_{j,2}$	$\kappa^{(10)}_{j,0}$	$\kappa^{(10)}_{j,1}$	$\kappa^{(10)}_{j,2}$	$\kappa^{(11)}_{j,0}$	$\kappa^{(11)}_{j,1}$	$\kappa^{(11)}_{j,2}$
1	$\frac{48}{35}$	$\frac{72}{35}$	0	-2	20	-42	$-\frac{9}{35}$	$\frac{984}{35}$	-9
4	$-\frac{72}{35}$	0	0	8	-28	0	$\frac{171}{35}$	-33	0
5	$-\frac{48}{35}$	0	0	-6	14	0	$-\frac{201}{35}$	3	0
6	$\frac{16}{7}$	0	0	-4	0	0	$-\frac{17}{7}$	9	0
7	$-\frac{3}{35}$	0	0	1	0	0	$-\frac{6}{35}$	0	0
8	$\frac{6}{7}$	0	0	4	0	0	$\frac{33}{7}$	0	0

Table 2. Coefficients for the polynomials (83)/(85) to calculate the right hand sides of the regular moment system consisting of 8 one dimensional equations (91). Each entry has to be multiplied by $\rho\,\alpha$, see (97)

j	$\bar\kappa^{(4)}_{j,0}$	$\bar\kappa^{(4)}_{j,1}$	$\bar\kappa^{(4)}_{j,2}$	$\bar\kappa^{(5)}_{j,0}$	$\bar\kappa^{(5)}_{j,1}$	$\bar\kappa^{(5)}_{j,2}$	$\bar\kappa^{(6)}_{j,0}$	$\bar\kappa^{(6)}_{j,1}$	$\bar\kappa^{(6)}_{j,2}$	$\bar\kappa^{(7)}_{j,0}$	$\bar\kappa^{(7)}_{j,1}$	$\bar\kappa^{(7)}_{j,2}$	$\bar\kappa^{(8)}_{j,0}$	$\bar\kappa^{(8)}_{j,1}$	$\bar\kappa^{(8)}_{j,2}$
1	1	1	0	$\frac{4}{3}$	4	0	$\frac{1}{2}$	$\frac{3}{2}$	0	2	8	10	$\frac{5}{6}$	$\frac{7}{3}$	$\frac{13}{6}$
4	-1	0	0	$-\frac{2}{3}$	0	0	$\frac{1}{2}$	0	0	$-\frac{4}{3}$	0	0	$-\frac{1}{2}$	$\frac{7}{6}$	0
5	0	0	0	$-\frac{2}{3}$	0	0	$\frac{1}{2}$	0	0	0	0	0	$\frac{4}{3}$	0	0
6	0	0	0	0	0	0	$-\frac{3}{2}$	0	0	0	0	0	$-\frac{2}{3}$	0	0
7	0	0	0	0	0	0	0	0	0	$-\frac{2}{3}$	0	0	$\frac{1}{6}$	0	0
8	0	0	0	0	0	0	0	0	0	0	0	0	$-\frac{7}{6}$	0	0

As example consider the flux of the equation for u_7 which is given by $\tilde u_{10}$. In this case the tensor degrees are $T(10) = 5$ and $T(j = 1, 4, 5, 6, 7, 8) = 0, 2, 3, 3, 4, 4$. Consequently, one calculates for the flux

$$\begin{aligned}
\tilde u_{10}(\mathbf{u}) &= \rho\,\varphi^{(10)}_1(v,\theta) + \sum_{j=4}^{8} \varphi^{(10)}_j(v,\theta)\; u_j \\
&= \rho\left(\kappa^{(10)}_{1,0}\,v^5 + \kappa^{(10)}_{1,1}\,\theta\,v^3 + \kappa^{(10)}_{1,2}\,\theta^2\,v\right) + u_4\left(\kappa^{(10)}_{4,0}\,v^3 + \kappa^{(10)}_{4,1}\,\theta\,v\right) + \\
&\quad u_5\left(\kappa^{(10)}_{5,0}\,v^2 + \kappa^{(10)}_{5,1}\,\theta\right) + u_6\,\kappa^{(10)}_{6,0}\,v^2 + u_7\,\kappa^{(10)}_{7,0}\,v + u_8\,\kappa^{(10)}_{8,0}\,v \\
&= \rho\left(-2\,v^5 + 20\,\theta\,v^3 - 42\,\theta^2\,v\right) + u_4\left(8\,v^3 - 28\,\theta\,v\right) + \\
&\quad u_5\left(-6\,v^2 + 14\,\theta\right) - u_6\,4\,v^2 + u_7\,v + u_8\,4\,v.
\end{aligned} \tag{92}$$

The analogous equations for the remaining unknown fluxes are

$$\tilde u_9(\mathbf{u}) = \rho\left(\frac{48}{35}\,v^4 + \frac{72}{35}\,\theta\,v^2\right) - \frac{72}{35}v^2\,u_4 - \frac{48}{35}v^2\,u_5 + \frac{16}{7}v\,u_6 - \frac{3}{35}u_7 + \frac{6}{7}u_8, \tag{93}$$

$$\begin{aligned}
\tilde u_{11}(\mathbf{u}) &= \rho\left(-\frac{9}{35}\,v^5 + \frac{984}{35}\,\theta\,v^3 - 9\,\theta^2\,v\right) + u_4\left(\frac{171}{35}\,v^3 - 33\,\theta\,v\right) + \\
&\quad u_5\left(-\frac{201}{35}\,v^2 + 3\,\theta\right) + u_6\left(-\frac{17}{7}\,v^2 + 9\,\theta\right) - \frac{6}{35}v\,u_7 + \frac{33}{7}v\,u_8.
\end{aligned} \tag{94}$$

For the productions the eigenvalues of the linear collision operator are obtained from (63)

$$\zeta^0_0 = \zeta^0_1 = \zeta^1_0 = 0\,, \tag{95}$$

$$\zeta^0_2 = \rho\,\alpha\,,\;\; \zeta^1_1 = \frac{2}{3}\rho\,\alpha\,,\;\; \zeta^0_3 = \frac{3}{2}\rho\,\alpha\,,\;\; \zeta^2_0 = \frac{2}{3}\rho\,\alpha\,,\;\; \zeta^1_2 = \frac{7}{6}\rho\,\alpha\,. \tag{96}$$

In this case of a rather small system all eigenvalues are rational multiples of $\rho\,\alpha$ where the constant α is given by

$$\alpha = \frac{3}{m}I_1 = \frac{4.11104191}{m}\sqrt{\frac{\kappa}{m}}\,. \tag{97}$$

It follows that all coefficients in (87) for the productions are proportional to $\rho\,\alpha$. This factor is suppressed in Table 2, where the coefficients for the productions are shown. The explicit equations may be deduced from the table in the same way like in the case of the fluxes above.

From this example it becomes clear that once the coefficients $\kappa^{(i)}_{j,k}$ and $\bar{\kappa}^{(i)}_{j,k}$ are supplied by a computer-algebra-system any regular system of moment equations may be implemented in a numerical code by just programming the polynomials (83)/(85) and (86)/(87).

A Grad's method

In the preceding sections the constitutive relations for the fluxes have been obtained by linearisation of maximum entropy relations. In this appendix we show that this linearization is merely a matter of formalism with absolutely no restriction to the physical applicablity of the constitutive relations. This follows by comparison with the original approach of Grad [6,7].

Grad relies on the expansion of the distribution function with respect to Hilbert polynomials $H_i(\mathbf{c})$. He writes

$$f(\mathbf{c},\mathbf{x},t) = \sum_{i=1}^{\infty} a_i(\mathbf{x},t)\, H_i(\mathbf{c})\, f^{(M)}(\mathbf{c}), \tag{98}$$

with certain coefficients $a_i(\mathbf{x},t)$. As Grad states himself, due to basic theorems from functional analysis it is very reasonable assuming this expansion to hold for *any* integrable distribution function. Thus any non-equilibrium process may be described via (98). As approximation Grad uses a finite sum in (98), viz.

$$f(\mathbf{c},\mathbf{x},t) = \sum_{i=1}^{N} a_i(\mathbf{x},t)\, H_i(\mathbf{c})\, f^{(M)}(\mathbf{c}) \ , \tag{99}$$

$$a_i = 0 \quad \text{for } i > N \tag{100}$$

and deduces partial differential equations for the coefficients a_i $(i \le N)$ from Boltzmann's equation.

The coefficients a_i are easily calculated. The Hilbert polynomials written in radial part and spherical harmonics are given by the polynomials $\psi^s_{\langle A\rangle}$ in (48). Due to orthogonality we obtain

$$g^s_{\langle A\rangle} = m \int \psi^r_{\langle A\rangle}(\mathbf{C})\ f\, d\mathbf{C} \tag{101}$$

$$= m \int \psi^r_{\langle A\rangle}(\mathbf{C}) \sum_{B=0}^{A^{(\max)}} \sum_{s=0}^{\hat{n}^{(B)}-1} a^s_{\langle B\rangle} \psi^s_{\langle B\rangle}(\mathbf{C})\, f^{(M)}(\mathbf{c})\ d\mathbf{C} \tag{102}$$

$$= \rho\, a^s_{\langle B\rangle}, \tag{103}$$

i.e., the coefficients are given by the orthonormal moments. Hence Grad's constitutive relations (99)/(100) are *equivalent* to our relations (55) and (46). Correspondingly the range of applicablity of (55) and (46) is the same as for Grad's expansion. More precisely, transfer equations with fluxes modeled by (46) perfectly approximate the left hand side of Boltzmann's equation for sufficiently large numbers of variables. The linearization in (38) must be considered as pure formalism.

Note, that in the original approach of Grad the production terms should follow exactly from the collision operator as quadratic terms. Those relations are very complicated to obtain for large systems. In this paper we rely on the framework of formal linearization and obtain production terms which are linear in non-equilibrium quantities.

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