

## On the Domain of Hyperbolicity of the Cumulant Equations

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In this article we consider the influence of non-equilibrium values of classical variables on the eigenvalues of the advection part of the cumulant equations. Real and finite eigenvalues are a necessary condition for the cumulant equations to be hyperbolic which can be used to obtain estimates on admissible deviations from equilibrium for a model of particular order still to be valid. We find that this condition puts no constraints on velocity and shear stress values, but specific energy must be positive, normal stress must be bounded by specific energy and heat flux not be too large.

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**KEY WORDS:** Boltzmann equation; moment method; cumulant method; hyperbolic conservation laws.

Characterizing fluid flow by the ratio of mean free path and a characteristic flow length (the Knudsen number  $Kn$ ) we have two extremes: dense gases ( $Kn \ll 1$ ) where modeling by Euler or Navier–Stokes equations is valid and rarefied gases ( $Kn \gg 1$ ) for which modeling by the Boltzmann equation is necessary. Developing models for the intermediate transition regime is subject to active current research. With the emerging technology of micro-scale machinery efficient methods for simulating transition regime flows become essential as dense gas models become invalid and solution of the Boltzmann equation is too expensive. The first part of this paper gives an overview on modeling flow of a non-reacting mixture of gases by kinetic theory and how to derive approximate, mesoscopic model equations, the moment equations. The second part gives a short overview of the cumulant method, an alternative method of approximation that results

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in particularly simple equations. For these equations we consider constraints imposed on the admissible values of classical variables (e.g. velocity, specific energy, shear and normal stress and heat flux) by demanding hyperbolicity of the resulting equations.

## 1. KINETIC THEORY

We assume the fluid is composed of  $N_s$  different species, enumerated by the set  $\mathcal{N}_s$  with each species having its own set of associated properties. For a species  $s$ , these are the particle mass  $m_s$  and the laws of interaction with particles of any other species  $r$ . We let the phase space density  $f_s(t, \underline{x}, \underline{c})$  denote the density of particles of species  $s$  at time  $t$  and position  $\underline{x}$ , moving with absolute velocity  $\underline{c}$ , normalized such that

$$n_s(t, \underline{x}) = \int d\underline{c} f_s(t, \underline{x}, \underline{c}) \quad (1)$$

are the partial particle number densities of the various species (integrals are taken over the whole velocity space  $\mathcal{R}^d$ ).

The  $f_s$  have to satisfy the Boltzmann equation, which – by considering a sufficiently dilute gas (in an inertial frame) where accounting only for the effect of binary collisions is sufficient – takes the form<sup>(1)</sup>

$$\partial_t f_s + \underline{c} \cdot \partial_{\underline{x}} f_s + \underline{a}_s \cdot \partial_{\underline{c}} f_s = \sum_{r \in \mathcal{N}_s} S_{rs}[f_r, f_s], \quad s \in \mathcal{N}_s, \quad (2)$$

where  $\underline{a}_s$  is the acceleration of a  $s$ -particle due to external forces as a function of time  $t$ , particle position  $\underline{x}$  and particle velocity  $\underline{c}$ . We regard forces exerted on particles due to particle–particle interaction as internal and any other (e.g. gravity) as external. The collision operator  $S_{rs}[f_r, f_s]$  describes the change of  $f_s$  due to interaction of  $r$ - and  $s$ -particles.

Describing the evolution of mixtures of gases on a macroscopic scale we are interested in partial quantities, such as the partial pressure, density, etc. of each species. Given a phase space density  $f_s(t, \underline{x}, \underline{c})$ , the density of a partial macroscopic thermodynamic quantity  $(\overline{\Psi})_s(t, \underline{x})$  can be obtained as the mean of an associated microscopic function  $\Psi(t, \underline{x}, \underline{c})$

$$\overline{(\Psi)}_s(t, \underline{x}) = \int d\underline{c} \Psi(t, \underline{x}, \underline{c}) f_s(t, \underline{x}, \underline{c}). \quad (3)$$

Multiplying (2) with  $\Psi$  and integrating over  $\underline{c}$  we obtain<sup>(2)</sup> a balance equation for the quantity  $\Psi$  (also known as Enskog's general equation of change)

$$\partial_t \overline{(\Psi)}_s + \partial_{\underline{x}} \cdot \overline{(\underline{c} \Psi)}_s = \overline{(\partial_t \Psi + \partial_{\underline{x}} \cdot \underline{c} \Psi + \partial_{\underline{c}} \cdot \underline{a}_s \Psi)}_s + \sum_{r \in N_s} \int d\underline{c} \Psi S_{rs}, \quad (4)$$

where we made use of partial integration and the property  $f_s \rightarrow 0$  for  $\|\underline{c}\| \rightarrow \infty$  due to (1). Setting  $\Psi = \frac{1}{(2\pi)^{d/2}} e^{i\underline{\chi} \cdot \underline{c}}$  we find the associated  $\overline{(\Psi)}_s$  to be the characteristic function<sup>(3)</sup>  $\varphi_s$  with the equation of motion

$$\begin{aligned} \partial_t \varphi_s + \partial_{\underline{x}} \cdot \partial_{i\underline{\chi}} \varphi_s &= \Gamma_s + \sum_{r \in N_s} \Xi_{rs}[\varphi_r, \varphi_s], \\ \text{collision term } \Xi_{rs}[\varphi_r, \varphi_s] &= \frac{1}{(2\pi)^{d/2}} \int d\underline{c} S_{rs} e^{i\underline{\chi} \cdot \underline{c}} \\ \text{and force term } \Gamma_s[\varphi_s] &= \frac{1}{(2\pi)^{d/2}} \int d\underline{c} f_s \partial_{\underline{c}} \cdot \underline{a}_s e^{i\underline{\chi} \cdot \underline{c}}. \end{aligned} \quad (5)$$

Analytic expressions for  $\Xi_{rs}$  can be obtained for the Maxwell gas by following the idea of Bobylev,<sup>(4)</sup> as well as for the BGK approximation. After a straightforward calculation we find for the Maxwell gas

$$\Xi_{rs}^{\text{mxw}}[\varphi_r, \varphi_s] = \sqrt{\frac{2\kappa_{rs}}{\mu_{rs}}} (2\pi)^2 \int d\varepsilon \left( \varphi_r(\underline{\chi} \cdot \underline{D}_+^+) \varphi_s(\underline{\chi} \cdot \underline{D}_+^-) - \varphi_r(0) \varphi_s(\underline{\chi}) \right) \quad (6)$$

with interaction strength parameters  $\kappa_{rs}$  (where  $\kappa_{rs} = \kappa_{sr}$ ), reduced mass  $\mu_{rs} = \frac{m_r m_s}{m_r + m_s}$ , mass difference parameter  $\Delta_{rs} = \frac{m_r - m_s}{m_r + m_s}$  and

$$\underline{D}_+^+ = \left[ \frac{1 + \Delta_{rs}}{2} \underline{1} - \frac{1 - \Delta_{rs}}{2} \underline{S}^{-1} \right], \quad \underline{D}_+^- = \left[ \frac{1 - \Delta_{rs}}{2} \underline{1} + \frac{1 + \Delta_{rs}}{2} \underline{S}^{-1} \right], \quad (7)$$

where  $\underline{S}$  is such that it maps the relative pre-collision velocity to the relative post collision velocity  $\hat{\underline{c}}_{rs} = \underline{S} \cdot \underline{c}_{rs}$ . From the actual kinematics of a collision we find in 2D

$$\vartheta^{2D}(\varepsilon) = \pi \left( 1 - \frac{\varepsilon}{\sqrt{1 + \varepsilon^2}} \right) \quad \text{and} \quad \underline{S}(\varepsilon) = \begin{pmatrix} \cos \vartheta(\varepsilon) & -\sin \vartheta(\varepsilon) \\ \sin \vartheta(\varepsilon) & \cos \vartheta(\varepsilon) \end{pmatrix}. \quad (8)$$

For the BGK approximation a Fourier transform of the well-known BGK collision operator<sup>(5,6)</sup> gives

$$\Xi_{rs}^{\text{BGK}} = -\frac{n_r}{\sigma_{rs}} \left( \varphi_s - \frac{n_s}{(2\pi)^{d/2}} \exp\left(\mathbf{i}\underline{\chi} \cdot \underline{v}_r - \frac{1}{2} \varepsilon_s \|\underline{\chi}\|^2\right) \right). \quad (9)$$

By repeated differentiation of (5) with regard to  $\underline{\chi}$  and setting  $\underline{\chi}=0$  afterwards we find an infinite system of coupled, nonlinear balance equations

$$\begin{aligned} \partial_t M_s^0 + \partial_{\underline{x}} \cdot M_s^1 &= G_s^0 + \sum_r P_{rs}^0 & M_s^\alpha &= (2\pi)^{d/2} \partial_{\mathbf{i}\underline{\chi}}^\alpha \varphi_s \Big|_{\underline{\chi}=0} \\ \partial_t M_s^1 + \partial_{\underline{x}} \cdot M_s^2 &= G_s^1 + \sum_r P_{rs}^1 & & \\ & \vdots & \text{with } G_s^\alpha &= (2\pi)^{d/2} \partial_{\mathbf{i}\underline{\chi}}^\alpha \Gamma_s \Big|_{\underline{\chi}=0} \\ \partial_t M_s^\alpha + \partial_{\underline{x}} \cdot M_s^{\alpha+1} &= G_s^\alpha + \sum_r P_{rs}^\alpha & P_{rs}^\alpha &= (2\pi)^{d/2} \partial_{\mathbf{i}\underline{\chi}}^\alpha \Xi_{rs} \Big|_{\underline{\chi}=0} \\ & \vdots & & \end{aligned} \quad (10)$$

for the so-called moments  $M_s^\alpha = \overline{(\underline{c}^\alpha)_s}$ . For powers of  $\underline{c}$  or  $\partial_{\mathbf{i}\underline{\chi}}$  a scalar exponent  $\alpha$  denotes the tensorial power of order  $\alpha$ , while a multi-index will denote the appropriate element of such a tensor. Similarly, for the moments  $M_s^\alpha$ , force terms  $G_s^\alpha$  and productions  $P_{rs}^\alpha$ , a scalar superscript  $\alpha$  denotes the full tensor (of rank  $\alpha$ ) and a multi-index the corresponding element. The advection term for equation  $\alpha$  couples moments of order  $\alpha$  and  $\alpha+1$ , as the flux in one equation appears as density in the equation of next higher order and vice versa. In general we must assume that production terms may couple between any orders  $\alpha$ , but for the particular interaction models to be considered here we observe only coupling towards lower orders. Currently it appears to be not even known whether the quantities appearing in Eq. (10) are well-defined functions for *every* solution of (2). E.g. boundedness of the appearing integrals or proper differentiability of the moments are by no means obvious for non-equilibrium solutions. Anyhow, moments have been shown to be well-defined at least for the spatially homogeneous<sup>(7)</sup> and the nearly homogeneous<sup>(8)</sup> case, so it might be more generally true.

One promising approach to modelling mesoscopic fluid flow is to consider finite subsets of (10) as approximations of (2) by taking only equations of order  $\alpha = 0, \dots, N_\alpha$ , where the ‘level of detail’ can be adjusted by  $N_\alpha$ . Truncation of (10) at some order  $N_\alpha$  imposes the so-called closure problem, which consists in expressing the moments  $M_s^\alpha$ , the force

terms  $G_s^\alpha$  and the productions  $P_s^\alpha$  as a function of some set of variables (traditionally the moments themselves) so that the finite subsystem is closed. This is achieved by making an ansatz – or imposing physical principles to determine a suitable ansatz – for the phase space density  $f_s$  or the characteristic function  $\varphi_s$  with some ansatz parameters. Given the functional form of the ansatz, a relation of the parameters and the moments is determined by the condition that the first  $N_\alpha$  moments of the ansatz should equal those of the ‘true’ (but unknown) solution. Solving this relation for the parameters as a function of the moments allows to express the ansatz for  $f_s$  in terms of the moments and in turn to determine  $M_s^{N_\alpha+1}$ ,  $G_s^\alpha$  and  $P_s^\alpha$  as a function of the moments so that (10) is closed.

There are various criteria proposed in the literature on how to achieve this closure. In the method proposed by Grad,<sup>(9)</sup>  $f_s$  is factored into an equilibrium and a non-equilibrium part, the latter being expanded in a series of Hermite polynomials ortho-normalized with regard to the  $(t, \underline{x})$ -local equilibrium part. Later Waldmann<sup>(10)</sup> observed that for states close to thermal equilibrium – where a linear approximation of the collision operator holds – expressing  $f_s$  as a *sum* of a (local) equilibrium and a small deviation-from-equilibrium part leads to a linear integro-differential equation for the deviation from equilibrium. Assuming a space-homogeneous gas with a solution where the deviation from equilibrium decays exponentially in time leads to an eigenvalue problem for the function describing the deviation from equilibrium. An analytical solution can be given for the special case of a Maxwell gas where an orthonormal system of eigenfunctions can be constructed as a product of Sonine polynomials and spherical harmonics when using spherical coordinates in velocity space. These correspond to irreducible homogeneous tensors when using cartesian coordinates in velocity space, which is why Waldmann considers an expansion of the deviation from equilibrium with regard to these eigentensors of the linearized collision operator.

Both the methods proposed by Grad and Waldmann allow to determine the closure exactly but it appears to be difficult to give useful expressions for the entropy density, its flux or production rate. This is the main emphasis in the framework of Extended Irreversible Thermodynamics (EIT) by Müller and Ruggeri.<sup>(11)</sup> There, a particular ansatz form is obtained by applying a local formulation of the second law of thermodynamics. The resulting functional form is the same as proposed by Levermore<sup>(12)</sup> except that he adds more restrictive constraints on the admissible parameter values. Unfortunately, closure appears to be a very hard problem, as the resulting ansatz function is an exponential of a tensor polynomial in  $\underline{c}$ . Nevertheless

entropy density and flux can be given but it appears to be difficult to give an analytic form of the entropy production, which is at the center of the modified moment method<sup>(13)</sup> proposed by Eu. There the ansatz for  $f_s$  is chosen such that the entropy production takes a simple form, making the connection of evolution of non-conserved variables and entropy production quite obvious. But again: neither is there a method for exact closure nor is it simple to give an analytic form of the entropy density. Recently Müller *et al.*<sup>(14)</sup> have proposed a “consistent order of magnitude closure” which employs the expansion proposed by Waldmann but assigns orders of magnitude to the various terms in the resulting equations by the technique of a Maxwell expansion.<sup>(15)</sup> When considering only terms up to a chosen order, they observe that the resulting equations are closed, without any further assumptions to be made.

## 2. THE CUMULANT METHOD

Except for the simplest closure by assuming local equilibrium phase space densities, none of the methods proposed to obtain ‘more detailed’ approximations of (2) by truncated moment systems (10) allows us to obtain exact equations of motion *and* analytic results for entropy density and entropy production. Further, except for the original method by Grad, we need to make the assumption of the gas being in a state close to equilibrium even for obtaining the equations of motion. In contrast, the cumulant method allows to derive the exact, fully non-linear equations of motion for the ansatz parameters. However, neither can we give analytic expressions for the entropy density and production for the cumulant method,<sup>(16–18)</sup> but its theory gives some insight in how such closures can possibly be constructed. Compared to other methods, derivation of the resulting equations of motion up to high approximation orders to be simple. Also the resulting equations are of particularly simple, quasi-linear structure compared to the often highly equations obtained by other methods.

The relation of the cumulant method to the method proposed by Grad has been touched briefly in an earlier paper.<sup>(16)</sup> We find that – at least for the one-dimensional case considered there – the low-order cumulants coincide with Grad’s expansion coefficients. For higher truncation orders  $N_\alpha$ , however, the moment equations obtained from the cumulant ansatz yield extra terms which we suspect to be responsible for the simple quasi-linear structure of the advection form of the equations of motion. Also, the eigenvariables for the linearized production terms of the Maxwell gas and their relaxation times have been determined.<sup>(17)</sup> The relation of these eigenvariables to the eigenfunctions determined by

Waldmann is clearly beyond the scope of this paper, which is concerned with the advection part of the cumulant equations only. This advection part is purely determined by the exactly defined relation between cumulants and moments but has quite some implications on the well-posedness of the equations. For the sake of simplicity we will restrict to the 2D case, but there is no difficulty in extending the method to the 3D case.

Remembering the derivation of (10) it becomes obvious that we actually make a Taylor-expansion of  $\Psi = \frac{1}{(2\pi)^{d/2}} e^{\mathbf{i}\underline{\chi}\cdot\underline{c}}$  about  $\underline{\chi} = \underline{0}$  so that we have

$$\varphi_s = \frac{1}{(2\pi)^{d/2}} \overline{\left( \sum_{\alpha=0}^{\infty} \frac{\mathbf{i}^\alpha}{\alpha!} \underline{\chi}^\alpha \cdot \underline{c}^\alpha \right)}_s = \sum_{\alpha=0}^{\infty} \frac{\mathbf{i}^\alpha}{(2\pi)^{d/2} \alpha!} \underline{\chi}^\alpha \cdot \overline{(\underline{c}^\alpha)}_s, \quad (11)$$

with the moments  $M_s^\alpha = \overline{(\underline{c}^\alpha)}_s$  being the series coefficients and (10) are the corresponding contributions of order  $\alpha$  for a ‘Taylor expansion’ of (5). Thus we can understand the closure problem discussed above as the problem of expressing all moments  $M_s^\gamma$  with  $\gamma > N_\alpha$  as a function of the (given) moments  $M_s^\alpha$  with  $\alpha \leq N_\alpha$ . That is, series (11) is not truncated, but moments of order higher than  $N_\alpha$  have to be fully determined by the moments of lower order.

The main idea for the cumulant method is based on the argument that – being interested in ‘macroscopic’ quantities – we are also interested in changes on macroscopic (slow) time scales.<sup>(17)</sup> This allows to assume that fast relaxation processes have (almost) reached their equilibrium state and that their dynamics can be neglected if we are only interested in the slower processes. If we choose cumulants as macroscopic parameters for the description this means that we may assume equilibrium values (which are conveniently zero) for the high-order cumulants. Thus our ansatz is a polynomial approximation of the second characteristic function  $\kappa_s = \ln((2\pi)^{d/2} \varphi_s)$  so that we have

$$\varphi_s^{CM} = \frac{1}{(2\pi)^{d/2}} \exp \left( \sum_{\alpha=0}^{N_\alpha} \frac{\mathbf{i}^\alpha}{\alpha!} \underline{\chi}^\alpha \cdot \underline{C}_s^\alpha \right) \quad (12)$$

with the cumulants  $C_s^\alpha$  being the coefficients of the Taylor-expansion of  $\kappa_s$  just like the moments  $C_s^\alpha$  are the coefficients of an expansion of  $\varphi_s$ , both taken about  $\underline{\chi} = \underline{0}$ .  $N_\alpha$  denotes the arbitrary truncation number of the expansion. A closed set of equations of motion – or alternatively the relations between moments  $M_s^\alpha$ , productions  $P_s^\alpha$  and force terms  $G_s^\alpha$  and the cumulants  $C_s^\alpha$  – can be directly obtained by (10). The relation of the

moments and the cumulants has been discussed in earlier works<sup>(16,17,19)</sup> and can be obtained conveniently using computer algebra systems.<sup>(18)</sup> We obtain the following relations between the first order moments and cumulants:

$$\begin{aligned}
 M^0 &= e^{C^0}, & M^{xx} &= e^{C^0} (C^x C^x + C^{xx}), \\
 M^x &= e^{C^0} C^x, & M^{xy} &= e^{C^0} (C^x C^y + C^{xy}), \\
 M^y &= e^{C^0} C^y, & M^{yy} &= e^{C^0} (C^y C^y + C^{yy}), \\
 \\ 
 M^{xxx} &= e^{C^0} (C^x C^x C^x + 3 C^x C^{xx} + C^{xxx}), & (13) \\
 M^{xxy} &= e^{C^0} (C^x C^x C^y + 2 C^x C^{xy} + C^y C^{xx} + C^{xxy}) = M^{xyx} = M^{yxx}, \\
 M^{xyy} &= e^{C^0} (C^x C^y C^y + C^x C^{yy} + 2 C^y C^{xy} + C^{xyy}) = M^{yxy} = M^{yyx}, \\
 M^{yyy} &= e^{C^0} (C^y C^y C^y + 3 C^y C^{yy} + C^{yyy}).
 \end{aligned}$$

Equations (10) obtained this way are equations in balance form. It is clear from their definition that the moments and cumulants of order  $\alpha$  have only  $\binom{\alpha+d}{d-1}$  linearly independent components, because the product between velocity components is commutative. Denoting the tensors of the reduced, linear independent variables with a tilde, writing (10) in its reduced form and making use of the chain rule we may derive equations with the cumulants as basic fields. This is because the relation between the reduced moments and cumulants is bijective and therefore the Jacobi-matrix  $(\partial_{\tilde{C}_s} \tilde{M}_s)$  is not singular for the reduced variables and its inverse is defined. This result is a set of equations in convection (or quasi-linear) form, stated for a set of primitive variables

$$\begin{aligned}
 \partial_t \tilde{C}_s + \underline{\underline{A}}_s \cdot \partial_x \tilde{C}_s &= \tilde{E}_s + \sum_{r \in \mathcal{N}_s} \tilde{B}_{rs} \\
 \text{with convection tensor } \underline{\underline{A}}_s &= \left( \partial_{\tilde{C}_s} \tilde{M}_s \right)^{-1} \cdot \left( \partial_{\tilde{C}_s} \tilde{F}_s \right), & (14) \\
 \text{production terms } \tilde{B}_{rs} &= \left( \partial_{\tilde{C}_s} \tilde{M}_s \right)^{-1} \cdot \tilde{P}_{rs} \\
 \text{and force term } \tilde{E}_s &= \left( \partial_{\tilde{C}_s} \tilde{M}_s \right)^{-1} \cdot \tilde{G}_s,
 \end{aligned}$$

which takes a particularly simple form, namely  $\tilde{E}_s = (0 \quad \underline{a}_s \quad 0 \quad 0 \quad \dots)^T$ . The convection tensor  $\underline{\underline{A}}_s$  is sparsely populated and has a particularly simple structure, as can be seen from the  $x$ -component of  $\underline{\underline{A}}_s$ . For the 2D case ( $d=2$ ) we have



$$\left[ \underline{A}_s \right]_x = \begin{pmatrix}
 C_s^x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 \hline
 C_s^{xx} & C_s^x & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
 C_s^{xy} & 0 & C_s^x & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
 \hline
 C_s^{xxx} & 2C_s^{xx} & 0 & C_s^x & 0 & 0 & 1 & 0 & 0 & 0 \\
 C_s^{xxy} & C_s^{xy} & C_s^{xx} & 0 & C_s^x & 0 & 0 & 1 & 0 & 0 \\
 C_s^{xyy} & 0 & 2C_s^{xy} & 0 & 0 & C_s^x & 0 & 0 & 1 & 0 \\
 \hline
 C_s^{xxxx} & 3C_s^{xxx} & 0 & 3C_s^{xx} & 0 & 0 & C_s^x & 0 & 0 & 0 \\
 C_s^{xxxxy} & 2C_s^{xxy} & C_s^{xxx} & C_s^{xy} & 2C_s^{xx} & 0 & 0 & C_s^x & 0 & 0 \\
 C_s^{xxyy} & C_s^{xyy} & 2C_s^{xxy} & 0 & 2C_s^{xy} & C_s^{xx} & 0 & 0 & C_s^x & 0 \\
 C_s^{xyyy} & 0 & 3C_s^{xyy} & 0 & 0 & 3C_s^{xy} & 0 & 0 & 0 & C_s^x \\
 \hline
 & \ddots & & \ddots & & & \ddots & & & \ddots
 \end{pmatrix}. \quad (15)$$

Remember that multi-index superscripts refer to the actual cumulant tensor components. In contrast to some other moment closures, the equations for some approximation order  $N_\alpha$  appear to be fully contained in the set of equations of next higher order. E.g. for closures that result in a phase space density of the form  $e^{p(c)}$ , dependance of the coefficients of the polynomial on the moments changes with the order of truncation.<sup>(11)</sup> Further, the full nonlinear equations can be obtained, without the need to assume states close to equilibrium. If one makes this assumption, however, the production terms may be linearized and a system of eigenvariables and their relaxation times can be determined (see ref. 17 and below). We expect a one-to-one correspondence of this eigensystem to the eigenfunctions proposed by Waldmann. Thus it should be possible to construct a “consistent order of magnitude” closure similar to ref. 14 by rewriting (14) in terms of the eigenvariables and starting a Maxwell iteration, the first step of which already clarifies the relation of (14) to the Navier–Stokes equations.<sup>(17)</sup> By taking the limit  $N_\alpha \rightarrow \infty$  Eq. (14) may be considered an infinite system just as (10). For a truncation of finite order  $N_\alpha$ , however, the bottom left block in (15) vanishes. Figure 1 shows the spectrum of  $\underline{A}_s(\tilde{C})$  as a function of the approximation order  $N_\alpha$ . This spectrum has been obtained by inserting the equilibrium values<sup>(16)</sup> for the cumulants in (15) and determining the eigenvalues of the resulting matrix numerically using Mathematica.<sup>(20)</sup> As for EIT,<sup>(11)</sup> the eigenvalue spectrum for a given order  $N_\alpha$  contains all eigenvalue spectra for approximations of lower order. Further

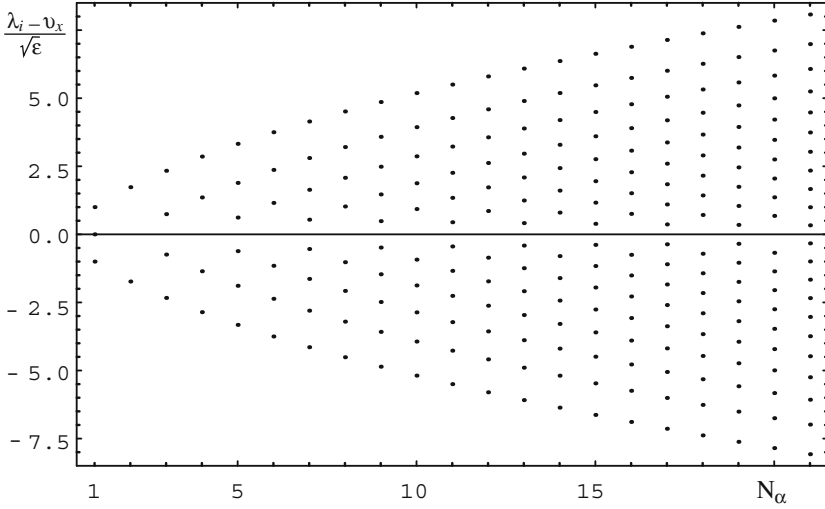


Fig. 1. Eigenspectrum of  $\underline{A}_s(\tilde{C})$  in equilibrium as it depends on the approximation order  $N_\alpha$ . For each order, only the newly appearing spectral values are plotted. We observe a finite maximum magnitude, growing monotonically with  $N_\alpha$ .

we observe finite but monotonically growing maximum and minimum eigenvalues. These advection tensor eigenvalues can be related to the (finite) speeds of propagation of weak discontinuities and should be real (so that (14) is hyperbolic). Consistent with EIT, growth of the maximal magnitude of the eigenvalues slows down with increasing truncation order. These eigenvalues corresponding to the highest characteristic speeds evaluated in equilibrium play an important role in modeling shock structures, as for shock speeds beyond that value unphysical sub-shocks appear in the solutions of the approximate equations.<sup>(21,22)</sup> This finding implies that many moments or cumulants have to be considered for fast shocks and might be considered a drawback of the cumulant method and moment methods in general.

The production terms  $\tilde{B}_{rs}^\alpha(\tilde{C}_r, \tilde{C}_s)$ , calculated from (6) or (9) by (10) and (14), are in general highly nonlinear functions of the cumulants  $\tilde{C}_r^\alpha$  and  $\tilde{C}_s^\alpha$ . However, for states close to equilibrium we may linearize the production terms. First we rewrite the productions in terms of the cumulants as  $\tilde{B}_{rs} = \tilde{B}_{rs}(\tilde{C}_s + \tilde{C}_{rs}, \tilde{C}_s)$  with the ‘relative cumulants’  $C_{rs}^\alpha = C_r^\alpha - C_s^\alpha$  and  $C_{rs}^0 = 0$ . With a Taylor-expansion up to first order about the equilibrium values  $\tilde{C}^{\text{eq}}$  we have  $\tilde{B}_{rs}^{\text{lin}} = \tilde{B}_s \cdot \Delta \tilde{C}_s + \tilde{B}_{rs} \cdot \Delta \tilde{C}_{rs}$  with  $\tilde{B}_s = (\partial_{\tilde{C}_s} \tilde{B}_{rs})^{\text{eq}}$ ,  $\tilde{B}_{rs} = (\partial_{\tilde{C}_{rs}} \tilde{B}_{rs})^{\text{eq}}$  and  $\Delta \tilde{C} = \tilde{C} - \tilde{C}^{\text{eq}}$ . Both  $\tilde{B}_s$  and  $\tilde{B}_{rs}$  are block-diagonal for the Maxwell model. This allows not only to give an

analytic solution for a pure, space homogeneous gas by calculating the eigensystem of  $\underline{\underline{B}}_s^{(18)}$  but also to establish the relation to the classical thermodynamic variables density  $n$ , specific energy  $\varepsilon$ , velocity  $\underline{v}$ , shear stress  $\underline{\underline{\sigma}}_{\equiv}$  and normal stress  $\sigma_{\circ}$  as well as heat flux  $\underline{j}$  as

$$\begin{aligned} n &= e^{C^0}, & \varepsilon &= \frac{1}{2}(C^{xx} + C^{yy}), \\ \underline{v} &= \begin{pmatrix} C^x \\ C^y \end{pmatrix}, & \underline{j} &= \frac{1}{2} \begin{pmatrix} C^{xxx} + C^{xyy} \\ C^{yyy} + C^{xxy} \end{pmatrix}, \\ \underline{\underline{\sigma}} &= \frac{1}{2} \begin{pmatrix} C^{xx} - C^{yy} & 2C^{xy} \\ 2C^{xy} & C^{yy} - C^{xx} \end{pmatrix} = \begin{pmatrix} \sigma_{\circ} & \sigma_{\equiv} \\ \sigma_{\equiv} & -\sigma_{\circ} \end{pmatrix}. \end{aligned} \tag{16}$$

Although other models have not yet been investigated, we would reasonably expect these relations to hold for other interaction models, as the particular type interaction has more an influence on the transport coefficients (eigenvalues) than on the qualitative behaviour of the low order terms in (11), which are directly related to the low order cumulants (see (13)).

Solving (16) for the (low-order) cumulants, and inserting these into (15), we can give the dependence of the convection tensor on the classical variables (16). As for Fig. 1 we have determined the eigenvalue spectrum by calculating the convection tensor for a given order  $N_{\alpha}$  and determined the eigenvalue spectrum using Mathematica. Figures 2–5 show the

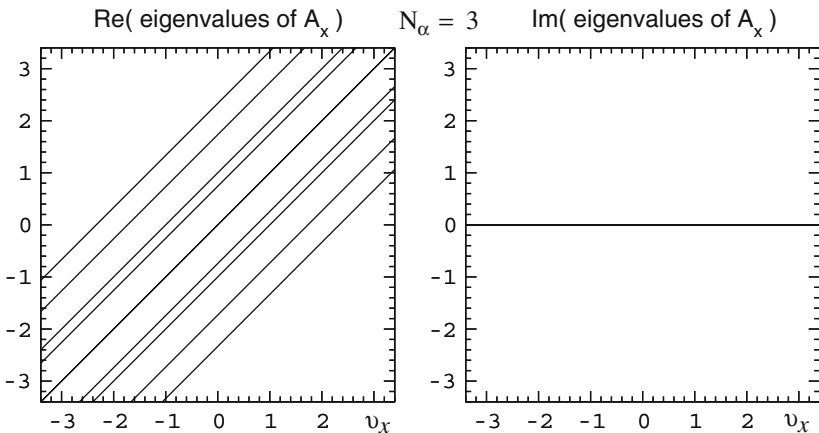


Fig. 2. Eigenspectrum of the  $x$ -component of  $\underline{A}_x$  as a function of the  $v_x$  component of velocity. We observe that a non-zero value of  $v_x$  just shifts the whole spectrum. This is due to the (expected) Galilei invariance of (14).

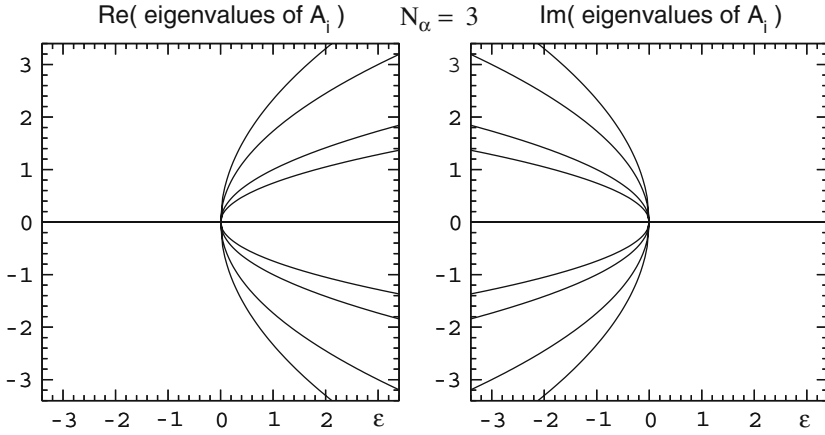


Fig. 3. Eigenvalues of  $[\underline{A}_s]_x$  and  $[\underline{A}_s]_y$  vs. specific energy  $\varepsilon$ . The specific energy must be positive for the spectrum to be real and not degenerate. This matches the well-known thermodynamic constraint of positive temperature.

dependence of the eigenvalue spectrum of (15) on the classical variables (16). For all cumulants and eigenvalues except the one varied equilibrium values have been assumed. We find that demanding real eigenvalues for all components of  $\underline{A}_s$  impose different possible constraints on the domain of allowed eigenvariable values. The first case is that no constraints are imposed, as is the case for  $v_x$  and  $v_y$ . In Fig. 2 we see that an arbitrary velocity just produces a shift of the eigenvalue spectrum of  $\underline{A}_s$ , as we would expect from a set of equations with Galileian invariance. The same situation is observed for  $\sigma_{\rightleftharpoons}$ , which does not influence the spectrum at all. That (14) obeys Galileian invariance can also easily be seen from the particular form of (15): for  $[\underline{A}_s]_x$  and every order  $\alpha$ , the main diagonal part holds just  $C_x$  which is actually the mean velocity  $v_x$ . So a given mean velocity  $v_x$  just shifts the spectrum of  $[\underline{A}_s]_x$ . The second case is observed for  $\varepsilon$ , shown in Fig. 3, where the spectra for both the  $x$  and  $y$  component impose a lower bound on  $\varepsilon$ , independent of  $N_\alpha$ . The third case is seen in Figs. 4 and 5 which impose boundedness of  $\sigma_\circ$ ,  $j_x$  and  $j_y$  but for two different reasons: for  $\sigma_\circ$ , the  $x$  and  $y$  component of  $\underline{A}_s$  impose either an upper or a lower bound which are the same for any  $N_\alpha$ . For  $j$ , however, one  $\underline{A}_s$  component imposes both upper and lower bounds and the other component of  $\underline{A}_s$  does not impose any bounds. For dependence of the eigenvalue spectrum of  $\underline{A}_s$  on the heat flux we observe the paradoxical situation that the interval of allowed  $j_x$ -values for (14) to be hyperbolic becomes smaller

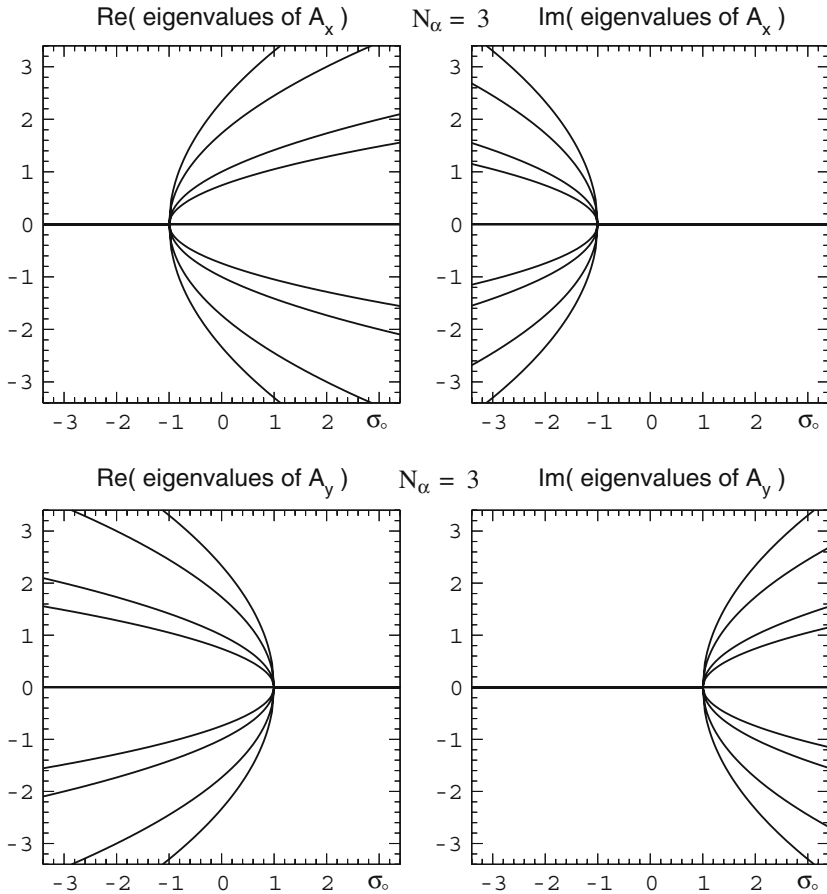


Fig. 4. Eigenspectrum of both the  $x$ - and  $y$ -component of  $\underline{A}_s$  as a function of the normal stress  $\sigma_o$ . We have assumed  $\varepsilon = 1$  and equilibrium values ( $\underline{=0}$ ) for any other eigenvariable (except  $\sigma_o$  of course). Additional variation of  $\varepsilon$  shows that in fact the  $x$ -component spectrum imposes a lower bound  $-\varepsilon$ , while the  $y$ -component spectrum imposes an upper bound  $+\varepsilon$ , so admissible heat flux values are  $\sigma_o \in (-\varepsilon, +\varepsilon)$ . There is no dependence of the spectra on the shear stress  $\sigma_{\rightleftharpoons}$ .

with increasing  $N_\alpha$ . Whether the allowed intervall remains finite or converges to the empty set for  $N_\alpha \rightarrow \infty$  remains an open question. We note that this might not be the case in real flow situations, where other cumulants may have non-equilibrium values, thereby possibly compensating this effect.

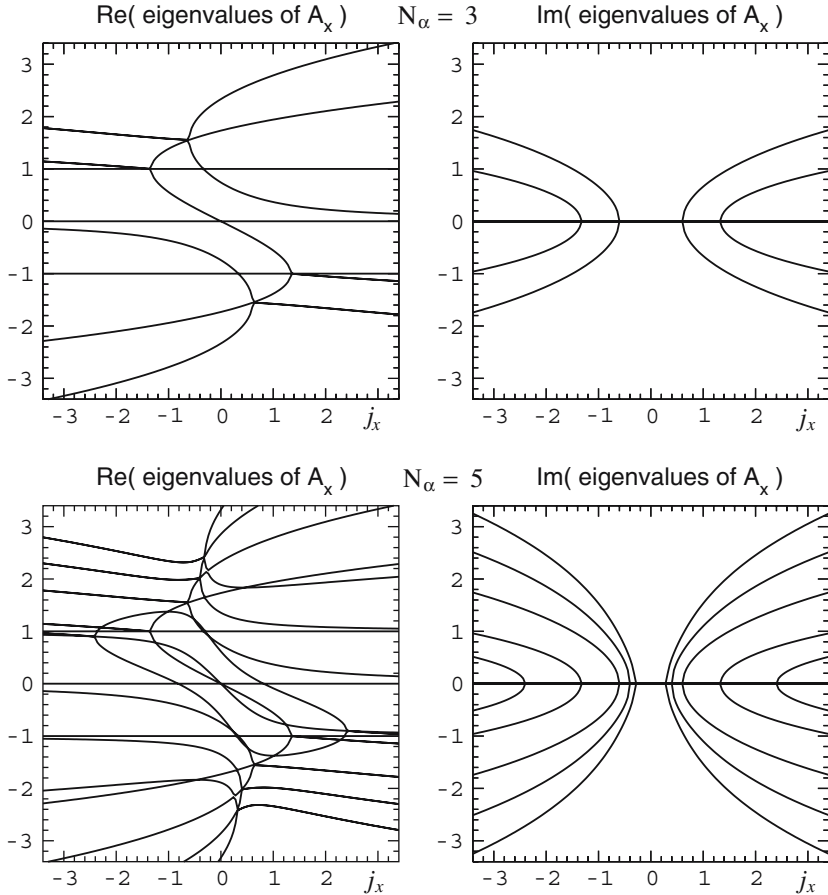


Fig. 5. Eigenspectrum of  $[A_5]_x$  as function of heat flux  $j_x$  for two different approximation orders  $N_\alpha$ . As in Fig. 4, we assume equilibrium values for all other eigenvariables. We observe that  $|j_x|$  must be smaller than some bound  $j_{\max}$ , but paradoxically  $j_{\max}$  becomes smaller with increasing  $N_\alpha$ . It remains unclear whether  $j_{\max}$  converges to zero or a finite value for  $N_\alpha \rightarrow \infty$  or if this effect disappears in a ‘true’ non-equilibrium situation where other high order variables may have non-zero values.

### 3. SUMMARY

In this paper we have first given an overview how mesoscopic models can be derived from kinetic theory. The cumulant method is one particular method of deriving a true hierarchy of such mesoscopic model equations where linear combinations of the low order cumulants can be related to classical variables. Hyperbolicity of the resulting equations is a

desirable feature, as it ensures finite propagation speeds for weak discontinuities. Non-negativity of the advection tensor components of the resulting equations is a necessary condition for hyperbolicity and can be used to find estimates for bounds on admissible values for the classical variables and thus on the domain of hyperbolicity for the cumulants. We find three kinds of constraints put on the values of the classical variables: none at all (velocity, shear stress), a lower, zero bound (specific energy) or both lower and upper bound heat flux, normal stress).

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