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Scale-Induced Closure for Approximations of Kinetic Equations

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Abstract

The order-of-magnitude method proposed by Struchtrup (Phys. Fluids **16**/11, 2004, p.3921-3934) is a new closure procedure for the infinite moment hierarchy in kinetic theory of gases, taking into account the scaling of the moments. The scaling parameter is the Knudsen number Kn, which is the mean free path of a particle divided by the system size.

In this paper, we generalize the order-of-magnitude method and derive a formal theory of scale-induced closures on the level of the kinetic equation. Generally, different orders of magnitude appear through balancing the stiff production term of order $1/Kn$ with the advection part of the kinetic equation. A cascade of scales is then induced by different powers of Kn.

The new closure produces a moment distribution function that respects the scaling of a Chapman-Enskog expansion. The collision operator induces a decomposition of the non-equilibrium part of the distribution function in terms of the Knudsen number.

The first iteration of the new closure can be shown to be of second-order in Kn under moderate conditions on the collision operator, to be L^2-stable and to possess an entropy law. The derivation of higher order approximations is also possible. We illustrate the features of this approach in the framework of a 16 discrete velocities model.

1 Introduction

Kinetic theory describes the flow of gases by means of a stochastic description based on the distribution function of the particle velocities. The distribution function obeys the Boltzmann equation - an integro-differential equation that considers free streaming and collisions of the particles, see e.g., the textbook [6]. This description of gases is a detailed, complex, microscopic approach reflected in the fact that the state of the gas at a spatial point is given by a function, i.e., an infinite dimensional object. In contrast, gases in classical fluid dynamics are described by a low dimensional vector of variables, typically density, velocity and temperature in each space point.

The aim of approximation methods in kinetic theory is to reduce the high dimensional particle description rigorously to a low-dimensional continuum model. Classical approaches are given by asymptotic analysis and function approximation theory. The Chapman-Enskog expansion conducts an asymptotic analysis where the smallness parameter is the Knudsen number, see for example the textbook [7]. This expansion successfully derives the fluid dynamic laws of

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Navier-Stokes and Fourier, but fails to produce useful higher order results beyond the first order. Instead, the Burnett- and super-Burnett-equations have been shown to be unstable in [2]. Grad's moment approach uses approximation theory and represents the distribution function as series of Hermite functions, see [9, 10].. In the limit, this series is supposed to reproduce any distribution function.. Truncations of the series give rise to moment equations that approximate Boltzmann's equation. However, the approximation converges slowly and also unphysical artifacts, like subshocks, are produced, see e.g. [24].

Various attempts exist to remedy the drawbacks of the Chapman-Enskog expansion. The work [12] introduced a hyperbolic form of the Burnett equations which is stable, while in [3] it was shown that a variable transformation may be able to remove unstable terms from the second order Chapman-Enskog result. Moment equations have been popular for their mathematical structure, see [13], and also for some success in describing physical processes, see the textbook [14]. A combination of Grad's moment method and an asymptotic approach has been introduced in [19].

Recently, in [17], a new derivation of macroscopic equations was presented that was claimed to be different from both Chapman-Enskog and Grad.. This so-called *order-of-magnitude method* is based on general moment equations and follows the scale of the variables for a closure, see also the textbook [16]. The resulting equations exhibit an inherent asymptotic accuracy in the sense of Chapman-Enskog and they are stable. The method succeeded to derive generalized 13-moment-equations in [18] and also showed that the R13-equations of [19] are a correct, stable, third order accurate approximation of Boltzmann's equation. This may explain the success of the R13-equations as demonstrated in [21, 22, 23, 24]. The R13-equations even allow to construct reasonable boundary conditions, see [11, 20, 25].

In this paper, we extend the order-of-magnitude method to the level of kinetic equations. So far, this method was only applied to the full non-linear moment hierarchy with little chance to gain insight into the general mathematical idea and structure of the closure. Our aim is to develop a formal theory of the new closure and to apply it to general kinetic equations. Here, we restrict ourselves to a linear kinetic model equation and demonstrate the relation of the new method to the classical approaches of Chapman-Enskog and Grad. We prove the asymptotic accuracy of the resulting closure and show the existence of an entropy law and L^2-stability, once specific variables are chosen. Our findings clearly show how the method exploits the scaling of the distribution function and the structures that this scaling creates in the phase space. Hence, it is reasonable to call this method a *scale-induced closure*.

The paper is organized as follows: The next section briefly resumes the order-of-magnitude method as applied to the moment hierarchy in [16] and discusses the results. Sec. 3 introduces the linear kinetic model and Sec. 4 discusses the classical closure theories in their application to the model. The new scale-induced closure is derived in Sec. 5 where also the asymptotic accuracy and stability are proven. As examples of the new method, Sec. 6 discusses the generalized 13-moment-system of [18], the application of the new closure to a 16 discrete velocities scheme and an application to a more general, high dimensional "kinetic type" equation. In that setting, the classical closures are compared to the scale induced closure, and the advantage of the latter is clearly shown. The paper ends with a conclusion.

2 Struchtrup's Order-of-Magnitude Approach

In the papers [17] and [18], Struchtrup proposes an order-of-magnitude approach to derive macroscopic transport equations in kinetic gas theory based on Boltzmann's equation. We briefly summarize the results of his method which will be generalized in the later sections. For

details we refer to the original papers and the textbook [16].

The Boltzmann equation

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = \frac{1}{\varepsilon} J(f, f) \tag{1}$$

describes the evolution of the distribution function f of the particle velocities in a mon-atomic gas. The value of $f(\mathbf{x}, t, \mathbf{c})\, d\mathbf{c}$ gives the number density 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 collision operator J is an integral functional which depends quadratically on f (see, for example, [6]). We assume, that the equation is normalized in such a way that the Knudsen number, i.e., the ratio between the mean free path and a macroscopic length, appears as scaling parameter ε.

Relevant for macroscopic equations are the equilibrium moments density, momentum density and energy density

$$\varrho = m \int_{\mathbb{R}^3} f \, d\mathbf{c}, \qquad \varrho \boldsymbol{v} = m \int_{\mathbb{R}^3} \mathbf{c}\, f \, d\mathbf{c}, \qquad \frac{3}{2}\rho\theta + \frac{1}{2}\varrho v^2 = \frac{1}{2} m \int_{\mathbb{R}^3} c^2 \, f \, d\mathbf{c} \tag{2}$$

from which average velocity $\boldsymbol{v}$ and temperature θ (in energy units) are derived. Additional higher order non-equilibrium moments are defined as

$$u^s_{i_1 \cdots i_n} = m \int_{\mathbb{R}^3} C^{2s} C_{\langle i_1} \cdots C_{i_n \rangle} \, (f - f_M) \, d\mathbf{C}. \tag{3}$$

Here, f_M is the Maxwell distribution and $\mathbf{C} = \mathbf{c} - \boldsymbol{v}$ is the peculiar velocity. Indices in angular brackets denote the symmetric and trace-free part of the corresponding tensor. Evolution equations for the moments follow from integration of (1). They form an infinite hierarchy with a closure problem.

The order-of-magnitude approach closes the system of equations in three steps. As first step, a Chapman-Enskog expansion is conducted (e.g., $u^s_i = \varepsilon\, u^s_{i|1} + \varepsilon^2\, u^s_{i|2} + ...$) on the infinite hierarchy in order to assign an order of magnitude in terms of the Knudsen number to all moments. In the first expansion, only vectorial and second degree tensors with arbitrary number of traces are non-zero and we obtain

$$u^s_{i|1} = -\kappa_s\, \rho\theta^s \frac{\partial \theta}{\partial x_i}, \quad u^s_{ij|1} = -\mu_s\, \rho\theta^{s+1} \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}, \quad u^s_{i_1 \cdots i_n} = 0 \ (n > 2). \tag{4}$$

The subscript 1 denotes the first expansion, κ_s and μ_s are pure numbers. All other moments vanish to first order in ε. Obviously, heat flux $q_{i|1} = \frac{1}{2} u^1_{i|1}$ and stress tensor $\sigma_{ij|1} = u^0_{ij|1}$ are among the first order moments. The coefficients κ_s and μ_s stem from the production terms of the moment equations. For a more specific representation in terms of quantities involving the collision operator, we refer to [19].

The fact that all vectorial and 2-tensorial moments are of the same order of magnitude is used as constitutive relation in the second step of the method. Indeed, up to an error of second order in the Knudsen number, two of all these moments suffice to calculate the value of the others. As natural candidates for a basis we choose heat flux $u^1_{i|1}$ and stress tensor $u^0_{ij|1}$ and eliminate the gradient expressions in (4). The result are local constitutive equations for all higher moments accurate up to an error of second order in ε. They read

$$u^s_{i|1} = \frac{\kappa_s}{\kappa_1}\, \theta^{s-1} u^1_{i|1} \qquad (s > 1), \tag{5}$$

$$u^s_{ij|1} = \frac{\mu_s}{\mu_0} \theta^s u^0_{ij|1} \qquad (s > 0), \tag{6}$$

$$u^s_{i_1 \cdots i_n\, |1} = 0 \qquad (s > 0,\ n > 2). \tag{7}$$

In the last step of the method, these relations are inserted into the moment hierarchy and all expressions that have been shown to be of higher order in ε than two, are simply set to zero. The final equations form a closed system based on quantities and expressions with consistent order of magnitude. It is important to note, that the closure (5)/(6) depends on the collision integral through the parameters κ_s and μ_s.

The order-of-magnitude method is, in principle, capable to produce equations at any order of Knudsen number, see [16]. However, only equations up to third order have been derived, so far.

3 Linear Kinetic Model

In the following we will recast the order-of-magnitude approach into a general kinetic framework and demonstrate attractive properties of the resulting equations.

The theory is developed for a generic linear kinetic model which includes discrete velocity models with finite velocity sets $\mathcal{C} \subset \mathbb{R}^d$ as well as the continuous case $\mathcal{C} = \mathbb{R}^d$.

Definition 1 (Kinetic Model) *Starting from an open spatial domain $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$ and a velocity set $\mathcal{C} \subset \mathbb{R}^d$ we identify distribution functions $f : \mathbb{R}^+ \times \Omega \times \mathcal{C} \to \mathbb{R}$ with elements $f_{t,\mathbf{x}} : \mathcal{C} \to \mathbb{R}^+$ of a suitable Hilbert space V of real valued functions on $\mathcal{C}$. A solution of the linear kinetic model is a distribution function which satisfies*

$$\partial_t f(t,\mathbf{x},\mathbf{c}) + \mathbf{c}\cdot\nabla f(t,\mathbf{x},\mathbf{c}) + \frac{1}{\varepsilon} K f(t,\mathbf{x},\mathbf{c}) = 0, \qquad (t,\mathbf{x},\mathbf{c}) \in \mathbb{R}^+ \times \Omega \times \mathcal{C} \tag{8}$$

with Knudsen number ε and a linear collision operator $K : V \to V$, independent of $(t,\mathbf{x})$, with the following properties:

1. *K has a p-dimensional kernel ($p \in \mathbb{N}$) injectively parametrized by an equilibrium distribution*

$$M : \mathbb{R}^p \to V, \quad \rho \longmapsto M\,\rho \tag{9}$$

satisfying $K\,M = 0$. The operator M does not depend on $(t,\mathbf{x})$. The function $(M\rho)(t,\mathbf{x},\mathbf{c})$ plays the role of the Maxwellian distribution function. The components of ρ are called equilibrium parameters.

2. *There exists a surjective equilibrium operator generalizing the mapping to the equilibrium moments, which is independent of $(t,\mathbf{x})$*

$$E_0 : V \to \mathbb{R}^p, \quad f \longmapsto \rho = E_0 f \tag{10}$$

and satisfies the conservation property $E_0\,K = 0$ as well as $E_0\,M = id_{\mathbb{R}^p}$. Note that the combination $Q = ME_0$ is a projection onto the kernel of K, the so called equilibrium projection. Accordingly, $P = id - Q$ is called non-equilibrium projection. With this projections we have the decomposition $V = V_0 \oplus V_{NE}$ with the equilibrium space $V_0 = QV$ and the non-equilibrium space $V_{NE} = PV$.

3. *There exists a linear mapping $K^\dagger : V \to V$ with the properties*

$$K^\dagger Q = 0, \qquad K^\dagger K = K K^\dagger = P \tag{11}$$

The condition $E_0 M = id_{\mathbb{R}^p}$ clearly implies that E_0 inverts the action of M, or in other words, that E_0 is a pseudo-inverse of M.

Definition 2 *Let X, Y be vector spaces and $A : X \to Y$ be linear. A linear mapping $B : Y \to X$ is called a pseudo inverse of A (abbreviated as $B = A^\dagger$), provided*

$$ABA = A, \qquad BAB = B. \tag{12}$$

If X, Y are Hilbert spaces, B is called Moore-Penrose-inverse of A if in addition to (12) *the operators AB and BA are self-adjoint, i.e.*

$$(AB)^* = AB, \qquad (BA)^* = BA. \tag{13}$$

One can show that the Moore-Penrose-inverse is unique (see, for example, [8] and App. A) and, in the case of injective A and finite dimensional X, it is given by $B = (A^*A)^{-1}A^*$.

Applied to our situation with $M = A$ and $E_0 = B$, we first see that $E_0 M = id_{\mathbb{R}^p}$ implies (12) so that E_0 is indeed a pseudo-inverse of M. Moreover, the identity $E_0 M$ is self-adjoint with respect to any scalar product on $\mathbb{R}^p$ and the self-adjointness of the converse product $Q = ME_0$ is equivalent to the orthogonality of the projection Q. In particular, the Moore-Penrose-inverse $M^\dagger = (M^*M)^{-1}M^*$ can serve as equilibrium operator E_0 provided $M^\dagger K = 0$. Since

$$M^\dagger K = (M^*M)^{-1}M^*K = (M^*M)^{-1}(K^*M)^*,$$

we see that this condition is satisfied when K is self-adjoint, i.e. $K^* = K$, because $KM = 0$. This case will be of importance in section 7.

Using the properties of K and $K^\dagger$ one can show (12)

$$\begin{aligned} KK^\dagger K &= KP = K - KQ = K \\ K^\dagger K K^\dagger &= K^\dagger P = K^\dagger - K^\dagger Q = K^\dagger \end{aligned}$$

so that $K^\dagger$ is really a pseudo-inverse of K. If K is self adjoint and E_0 is chosen as Moore-Penrose-inverse of M, then Q and P are also self-adjoint. In this case, $K^\dagger$ is the Moore-Penrose-inverse of K because (13) is also satisfied.

Further properties of K and $K^\dagger$ which will be frequently used later can also directly be deduced from the basic assumptions:

$$KQ = QK = 0, \qquad KP = PK = K, \qquad K^\dagger P = PK^\dagger = K^\dagger, \qquad K^\dagger Q = QK^\dagger = 0. \tag{14}$$

In the case of the Boltzmann equation, the space V would be some weighted $\mathbf{L}^2$ space. The equilibrium parameters are $\rho = E_0 f = \int \psi f$ with $\psi = (1, \mathbf{c}, c^2)^T$ and $p = 2 + d$. Furthermore, $M\,\rho$ would be given by the Maxwell distribution $f_M(\varrho, \boldsymbol{v}, \theta; \mathbf{c})$.

The vector of equilibrium parameters ρ is a mapping

$$\rho : \Omega \times \mathbb{R}^+ \to \mathbb{R}^p. \tag{15}$$

The modelling task in kinetic theory is to find reasonable evolution equations for ρ by using a projected space with much lower dimension than V. The following theory will achieve this goal.

4 Classical Approximations

Classical asymptotic limits and approximations of kinetic equations include the Euler equations, Chapman-Enskog expansion and Grad's method. We review these results here for our model since the new approach is built upon them and shows various connections to them.

In equation (8), the limit $\varepsilon \to 0$ formally leads to $Kf = 0$ so that the distribution function is asymptotically given by an equilibrium $M\,\rho = Qf$. Any extension beyond equilibrium will be written

$$f = Qf + Pf = M\,\rho + f^{(\mathrm{NE})} \tag{16}$$

with a non-equilibrium disturbance $f^{(\mathrm{NE})}$.

4.1 Equilibrium Closure

The Euler equations arise if we apply the equilibrium operator E_0 to (8) and obtain

$$\partial_t \rho + E_0 \mathbf{c} \cdot \nabla M\rho + E_0 \mathbf{c} \cdot \nabla f^{(\mathrm{NE})} = 0 \tag{17}$$

The closure assumption $f^{(\mathrm{NE})} = 0$ produces the Euler equations.

4.2 Chapman-Enskog Closure

The Chapman-Enskog expansion asks for the structure of the disturbance $f^{(\mathrm{NE})} = Pf$. It is easy to find an evolution equation for this quantity by applying the non-equilibrium projection P to (8) and observing (14)

$$\partial_t f^{(\mathrm{NE})} + P\mathbf{c} \cdot \nabla f^{(\mathrm{NE})} + P\mathbf{c} \cdot \nabla M\rho + \frac{1}{\varepsilon} K\, f^{(\mathrm{NE})} = 0. \tag{18}$$

Inserting the expansion $f^{(\mathrm{NE})} = \varepsilon\, f_1^{(\mathrm{NE})} + \varepsilon^2 f_2^{(\mathrm{NE})} + \ldots$, applying $K^\dagger$ and using (11) and (14), we obtain under the condition that all coefficients $f_k^{(\mathrm{NE})}$ and their derivatives are bounded with respect to ε

$$Pf_1^{(\mathrm{NE})} + K^\dagger \mathbf{c} \cdot \nabla\, M\rho = O(\varepsilon). \tag{19}$$

In the Chapman-Enskog approach, this necessary condition on $f_1^{(\mathrm{NE})}$ is replaced by the sufficient but more strict requirement

$$f_1^{(\mathrm{NE})} = -K^\dagger \mathbf{c} \cdot \nabla\, M\rho. \tag{20}$$

Using $\varepsilon f_1^{(\mathrm{NE})}$ as approximation for $f^{(\mathrm{NE})}$ in (17), we can close the equation in a more accurate way, leading to the general Navier-Stokes-Fourier equations

$$\partial_t \rho + E_0 \mathbf{c} \cdot \nabla M\rho = \varepsilon\, E_0 (\mathbf{c} \cdot \nabla)\, K^\dagger (\mathbf{c} \cdot \nabla) M\rho. \tag{21}$$

Going one order further and using relation (20) for $f_1^{(\mathrm{NE})}$, we get from (18)

$$Kf_2^{(\mathrm{NE})} - K^\dagger \mathbf{c} \cdot \nabla M \partial_t \rho - P\mathbf{c} \cdot \nabla K^\dagger \mathbf{c} \cdot \nabla M\rho = O(\varepsilon) \tag{22}$$

which can be solved in the form

$$Pf_2^{(\mathrm{NE})} = K^\dagger K^\dagger \mathbf{c} \nabla M \partial_t \rho + K^\dagger \mathbf{c} \cdot \nabla K^\dagger \mathbf{c} \cdot \nabla M\rho + O(\varepsilon) \tag{23}$$

Again, dropping the non-equilibrium projection and the possible $O(\varepsilon)$ contribution, the necessary condition is replaced by a more strict requirement in the classical Chapman-Enskog

approach. In these so called Burnett relations for $f_2^{(\mathrm{NE})}$, the time derivatives $\partial_t \rho$ can be replaced by $-E_0 \mathbf{c} \cdot \nabla M\rho$ (Euler equations) with no loss of order. The equations then read

$$\begin{aligned} \partial_t \rho + E_0 \mathbf{c} \cdot \nabla M\rho =& \varepsilon\, E_0(\mathbf{c}\cdot\nabla)\, K^\dagger (\mathbf{c}\cdot\nabla) M\rho \\ & - \varepsilon^2 E_0(\mathbf{c}\cdot\nabla) K^\dagger(\mathbf{c}\cdot\nabla) K^\dagger(\mathbf{c}\cdot\nabla) M\rho \\ & + \varepsilon^2 E_0(\mathbf{c}\cdot\nabla) K^\dagger K^\dagger (\mathbf{c}\nabla M) E_0(\mathbf{c}\cdot\nabla) M\rho. \end{aligned} \tag{24}$$

However, (24) can be proven to be unstable in the realistic cases of the full Boltzmann collision operator, see [2]. Higher order expansions like super-Burnett equations, turn out to be unstable as well, [16]. This failure of the expansion indicates that the assumptions on the coefficients are too strict in the higher order cases. In fact, for a model problem (see [5]) one can show that less rigid assumptions help to avoid the stability breakdown.

There exist various attempts to stabilize the Burnett equations, for example [3] and [12] which can be seen as particular choices of the right hand side in (23).

4.3 Grad Closure

Grad in [9] and [10] assumes a specific form of the distribution function which we summarize as

$$f = M\,\rho + G\,\mu + \tilde{f}. \tag{25}$$

Here, the non-equilibrium part is composed of the Grad distribution $G\mu$ and a remainder $\tilde{f}$, where $G : \mathbb{R}^q \to V$ maps certain non-equilibrium parameters $\mu \in \mathbb{R}^q$ onto a distribution function. The dependencies of G on the equilibrium variables ρ are neglected in accordance with a linear theory. The range of the mapping G can be viewed as vectors of the distribution space V opening a subspace additional to the equilibrium space given by M. In the original Grad theory, this subspace is spanned by Hermite polynomials. The parameters μ are typically defined in terms of higher order moments, for example, as non-equilibrium parts of the fluxes of the equilibrium variables. More generally, we assume that $\mu = E_1 f$ with a linear mapping $E_1 : V \to \mathbb{R}^q$ which satisfies

$$E_1 G = id_{\mathbb{R}^q}, \quad E_1 M = 0, \quad E_0 G = 0. \tag{26}$$

As a consequence, $S = GE_1$ is a projection which decomposes P into two parts S and $R = P - S$, the latter one being the projection onto the remainder term.

Application of E_0 and E_1 to the equation (8) yields evolution equations for ρ and μ. We find

$$\partial_t \rho + E_0 \mathbf{c} \cdot \nabla M\rho + E_0 \mathbf{c} \cdot \nabla G\mu + E_0 \mathbf{c} \cdot \nabla \tilde{f} = 0 \tag{27}$$

and

$$\partial_t \mu + E_1 \mathbf{c} \cdot \nabla M\rho + E_1 \mathbf{c} \cdot \nabla G\mu + E_1 \mathbf{c} \cdot \nabla \tilde{f} + \frac{1}{\varepsilon} E_1 K\, G\, \mu + \frac{1}{\varepsilon} E_1 K\, \tilde{f} = 0, \tag{28}$$

where in Grad's approach $\tilde{f} = 0$ leads to a closure of the system. Grad's equations can typically be shown to be stable.

From a geometric point of view, Grad's approach amounts to a splitting of the non-equilibrium space V_{NE} into a resolved and an unresolved subspace where the resolved subspace $V_1 = \mathrm{Im}(G)$ is parametrized through an - up to conditions (26) - arbitrary choice of higher order moments E_1 (see Figure 1). Hence, the asymptotic accuracy in terms of Knudsen number remains unclear for Grad's equations.

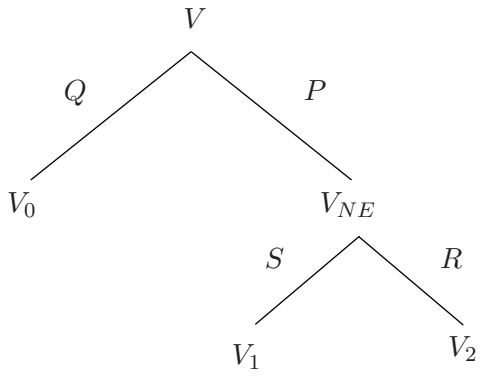

Figure 1: Splitting of the phase space into an equilibrium subspace V_0 with projection $Q = ME_0$ and the non-equilibrium remainder $V_{NE} = PV$ which is again split into the primary non-equilibrium subspace $V_1 = SV$ with Grad-projection $S = GE_1$ and the secondary non-equilibrium subspace $V_2 = RV$.

5 Scale-Induced Closure

The order-of-magnitude approach wants to derive stable moment equations which are asymptotically accurate in the sense of a Chapman-Enskog expansion. Burnett equations satisfy the accuracy condition, but are unstable. On the other hand, Grad's equations are stable but the closure is based on a distribution function which is arbitrarily reconstructed through higher moments and has no a-priori asymptotic properties.

5.1 Derivation

The Chapman-Enskog expansion implies a distribution function in the form

$$f = M\,\rho + \varepsilon\, f_1^{(\mathrm{NE})} + \varepsilon^2 f_2^{(\mathrm{NE})} + \mathcal{O}(\varepsilon^3), \tag{29}$$

while in Grad's approach, the distribution function is structured according to

$$f = M\,\rho + G\,\mu + f_R \tag{30}$$

with equilibrium part $M\rho \in V_0$, the primary non-equilibrium contribution $G\mu \in V_1$ and the secondary contribution $f_R \in V_2$ (see Figure 1).

A compatibility between the two representations (29) and (30) may be achieved if V_1 is constructed in such a way that it contains $\varepsilon f_1^{(\mathrm{NE})}$. Thus, the task is to appropriately define G and moments μ with their operator E_1 such that, apart from the basic requirements

$$E_1 G = id_{\mathbb{R}^q}, \qquad E_1 M = 0 \qquad E_0 G = 0, \tag{31}$$

also $\varepsilon f_1^{(\mathrm{NE})} = G\mu \in \mathrm{Im}(G) = V_1$ is possible. In contrast to Grad's moment approach where the distribution function is specified, for example, as Hermite series independent of the kinetic equation, the condition $\varepsilon f_1^{(\mathrm{NE})} \in V_1$ combines the phase space splitting with the structure of the kinetic equation.

Using the equilibrium projection Q, and the projections $S = GE_1$ and $R = P - S$ related to the primary and secondary non-equilibrium, we can derive equations for ρ, μ and f_R. Applying R to (8), we obtain

$$\varepsilon^2 \partial_t \hat{f}_R + R\mathbf{c}\cdot\nabla M\rho + \varepsilon R\mathbf{c}\cdot\nabla G\,\hat{\mu} + \varepsilon^2 R\mathbf{c}\cdot\nabla \hat{f}_R + RK\,G\,\hat{\mu} + \varepsilon RK\,\hat{f}_R = 0, \tag{32}$$

where we scaled the moments $\mu = \varepsilon\hat{\mu}$ and $f_R = \varepsilon^2 \hat{f}_R$. If we choose the primary non-equilibrium G such that for some suitable $\hat{\mu}$

$$G\,\mu = \varepsilon G\,\hat{\mu} = -\varepsilon K^\dagger \mathbf{c}\cdot\nabla M\rho \tag{33}$$

we automatically satisfy the following equivalent requirements

1. the first expansion coefficient $\varepsilon f_1^{(\mathrm{NE})}$ in (20) can be written in the form $G\,\mu$.
2. the evolution of the remainder f_R in (32) is governed only by quantities at least first order in ε.
3. the distribution $G\,\mu$ is given by the leading order term of the expansion of the distribution function f in powers of ε conducted on (18).

To see Item 2, we do a short calculation: using the zeroth order terms in (32) we have

$$R\mathbf{c}\cdot\nabla M\rho + RKG\hat{\mu} \overset{(33)}{=} R\left(\mathbf{c}\cdot\nabla M\rho - P\mathbf{c}\cdot\nabla M\rho\right) = 0 \tag{34}$$

since $RP = R$.

In order to derive an expression for G from (33) we will write it in the form

$$G\,\hat{\mu} = -K^\dagger\mathbf{c}\cdot M\,\nabla\rho, \tag{35}$$

where now the operator $-K^\dagger\mathbf{c}\cdot M$ acts on $p\times d$ gradients $\nabla\rho =: A \in \mathbb{R}^{p\times d}$ according to

$$-K^\dagger\mathbf{c}\cdot MA = -K^\dagger \sum_{i=1}^{p}\sum_{\alpha=1}^{d} c_\alpha M\,\mathbf{e}_i A_{i\alpha} \tag{36}$$

where $\mathbf{e}_i$ are the $\mathbb{R}^p$ unit vectors. The same convention is applied to operators with the same structure.

In the next two sections we consider two alternative paths to the specification of the operators G and E_1. In order to keep notation simple, we use μ for the scaled higher moments $\hat{\mu}$ in the following.

5.2 Constructing the Distribution

In this section we choose a moment operator $E_1 : V \to \mathbb{R}^q$ with some restrictions and determine the distribution function G from it. This point of view corresponds to constructing a closure $G\mu$ for the infinite moment hierachy by saying that $f = M\rho + G\mu$ for given moments $\mu = E_1 f$. This directly corresponds to Struchtrup's order-of-magnitude approach. Note, that the moment production terms can be computed without any further assumptions on f. This simplifies the process originally developed by Struchtrup in [18].

The projector E_1 cannot be chosen entirely arbitrarily. Since we require $E_1 G = id_{\mathbb{R}^q}$ and want to replace gradients by moments in (35) we have to choose E_1 such that the linear equation

$$\mu = E_1 G\mu = -\varepsilon E_1 K^\dagger\mathbf{c}\cdot M\nabla\rho \tag{37}$$

is essentially solvable for $\nabla\rho$. We expect that this leaves quite some freedom for the choice of E_1.

Let us make this restriction a bit more precise: In general, the operator $K^\dagger \mathbf{c} \cdot M$ has a non-trivial nullspace $\ker\left(K^\dagger \mathbf{c} \cdot M\right) \in \mathbb{R}^{p\times d}$. We define $V_1 := \mathrm{Im}(K^\dagger \mathbf{c} \cdot M)$ and choose E_1 injective on V_1, i.e. $\ker(E_1) \cap V_1 = \{0\}$, meaning that E_1 should not enlarge the kernel of $K^\dagger \mathbf{c} \cdot M$. Furthermore we require the basic relation that $E_1 M = 0$ and define q such that $E_1 : V_1 \to \mathbb{R}^q$ is surjective.

Defining the projections T_0 onto $\ker\left(K^\dagger \mathbf{c} \cdot M\right)$ and T_1 onto any subspace complementary to $\ker(K^\dagger \mathbf{c} \cdot M)$ in $\mathbb{R}^{p\times d}$, we can write $\nabla\rho = T_0\nabla\rho + T_1\nabla\rho$. We then solve

$$T_1 \nabla\rho = -\frac{1}{\varepsilon}\left(E_1 K^\dagger \mathbf{c} \cdot M\right)^\dagger \mu, \tag{38}$$

which now determines the relevant part of $\nabla\rho$ in terms of μ. The symbol † denotes any pseudoinverse, see Sec. 3. This procedure should be compared to the elimination of gradient expressions in Section 2 for the order-of-magnitude method conducted on moments.

For G we then compute

$$\begin{aligned} G\mu &= -\varepsilon K^\dagger \mathbf{c} \cdot M \left(T_0\nabla\rho + T_1\nabla\rho\right) && (39)\\ &= -\varepsilon K^\dagger \mathbf{c} \cdot M \left(T_0\nabla\rho - \frac{1}{\varepsilon}\left(E_1 K^\dagger \mathbf{c} \cdot M\right)^\dagger \mu\right) && (40)\\ &= K^\dagger \mathbf{c} \cdot M \left(E_1 K^\dagger \mathbf{c} \cdot M\right)^\dagger \mu && (41) \end{aligned}$$

and thus

$$G = K^\dagger \mathbf{c} \cdot M \left(E_1 K^\dagger \mathbf{c} \cdot M\right)^\dagger. \tag{42}$$

Lemma 1 (Scale-Induced Distribution) *Under the assumptions* $\ker(E_1) \cap V_1 = \{0\}$ *with* $V_1 = \mathrm{Im}\left(K^\dagger \mathbf{c} \cdot M\right)$ *and* $E_1 M = 0$ *for the moment projector* $E_1 : V \to \mathbb{R}^q$ *with* $q = \dim V_1$*, we have for the distribution function (42):*

1. *The construction is in accordance with the requirements* (31)*. The non-equilibrium space can be split into* $V_{NE} = V_1 \oplus V_2$*, with* $V_1 := G\mathbb{R}^q = GE_1V_{NE} = SV_{NE}$ *and* $V_2 = (P - S)V_{NE} = RV_E$*.*

2. *The construction satisfies* $\mathrm{Im}\,(G) = \mathrm{Im}\left(K^\dagger \mathbf{c} \cdot M\right) = V_1$ *in agreement with the condition (35) as well as* $\ker(G) = \{0\}$*.*

3. V_1 *constains contributions to the distribution function up to order* $\mathcal{O}(\varepsilon)$ *and* V_2 *contains all orders higher than* ε^2 *in a Chapman-Enskog expansion.*

Proof.

1. We clearly have $E_1 G = E_1 K^\dagger \mathbf{c} \cdot M \left(E_1 K^\dagger \mathbf{c} \cdot M\right)^\dagger = id_{\mathbb{R}^q}$ due to the requirement $\ker(E_1) \cap V_1 = \{0\}$. The condition $E_1 M = 0$ was required for E_1 a priori. Furthermore $PG = G$ follows from $PK^\dagger = K^\dagger$ and implies that $E_0 G = E_0 PG = 0$. The splitting follows from these three requirements. For the decomposition, we observe that $G\mathbb{R}^q = V_1 \subset V_{NE}$ since $QG = ME_0G = 0$. With $E_1 M = 0$ we have that $E_1 V_0 = E_1 M E_0 V = \{0\}$ and with $E_1 R = E_1 P - E_1 S = E_1 - E_1 = 0$, we have $E_1 V_2 = E_1 RV = \{0\}$ and thus $\mathrm{Im}\, E_1 = E_1 V_1$ follows, and with this $V = V_0 \oplus V_1 \oplus V_2$.

2. Since $\ker\left(E_1 K^\dagger \mathbf{c} \cdot M\right) = \ker\left(K^\dagger \mathbf{c} \cdot M\right)$, it follows that $\mathrm{Im}\left(E_1 K^\dagger \mathbf{c} \cdot M\right)^\dagger \cap \ker\left(K^\dagger \mathbf{c} \cdot M\right) = \{0\}$, and with that $\mathrm{Im}\,(G) = \mathrm{Im}\left(K^\dagger \mathbf{c} \cdot M\right)$. It follows from the definition of q that $G\mu = 0$ implies $\mu = 0$.

3. The order of magnitude of the subspaces follows directly from the definition of $G\mu$ as in (42).

■

Herewith, the structure of the distribution function has been deduced from the kinetic equation. It strongly depends on the collision operator K and arises from the requirement of a scale separation in the non-equilibrium subspace according to an asymptotic expansion in ε.

The typical separation in the phase space of the distribution function is that into equilibrium and non-equilibrium as in (16). The order-of-magnitude method given above now shows that there exists an additional natural separation of the non-equilibrium phase space that follows from the kinetic equation itself. The first order contribution opens a subspace V_1 in non-equilibrium that can be described by a low-dimensional set of moments μ that all scale by ε. The remainder space V_2 contains all high order contributions to the distribution function when Chapman-Enskog expanded.

The result is a scale-induced closure whose distribution structure strongly depends on the collision operator K. It is characterized not by slow and fast relaxation times but instead through the scale of the contributions of the asymptotic expansions to the distribution function.

Note that this construction is extendable to higher orders, leading to a more detailed decomposition of the non-equilibrium phase space V_{NE}.

In the derivation of G the higher moments $\mu = E_1 f$ are specified only by the solvability of the system (37). This is possible, but E_1 will not be unique. This situation is equivalent to the result (4) for the order-of-magnitude method applied to the moments directly. In (4) some moments had to be chosen as basis in which the others are represented. In the calculation of this representation, gradient expressions of equilibrium variables had to be eliminated.

5.3 Constructing the Moment Operator

To some extend the approach in Sec. 5.2 above mimics the procedure used in [17] and [18] conducted on the moment equations. An alternative path to exploiting the condition (35) is to first specify the distribution G and then derive the moment operator E_1.

The easiest way to construct G in accordance with (35) is to just choose $G = K^\dagger \mathbf{c} \cdot M$. However, having condition (31) in mind, $E_1 G = id_{\mathbb{R}^q}$ cannot be fullfilled if $K^\dagger \mathbf{c} \cdot M$ is not injective. To improve our definition of G, we intoduce q linearly independent vectors which generate a complementary subspace to $\ker(K^\dagger \mathbf{c} \cdot M)$. Then we define the surjective map

$$D : \mathbb{R}^{p \times d} \to \mathbb{R}^q,\ \nabla\rho \mapsto \hat{\mu}, \tag{43}$$

such that $D(\ker(K^\dagger \mathbf{c} \cdot M)) = \{0\}$. Note that this leaves quite some freedom for the choice of D.

With D we can adjust our definition of G to

$$GD = -K^\dagger \mathbf{c} M \tag{44}$$

as an operator acting on $\nabla\rho$ according to (36), giving

$$GD\nabla\rho = -K^\dagger \mathbf{c} M \nabla\rho = -K^\dagger \mathbf{c} \cdot \nabla M\, \rho \tag{45}$$

in agreement with condition (33). Using a pseudoinverse of D the distribution G is explicitly given by

$$G = -K^\dagger \mathbf{c} M D^\dagger \tag{46}$$

as a mapping from $\mathbb{R}^q$ to V. In Sec. 5.4, we will compare (46) to (42), which was resulting from the choice of a specific operator E_1.

By construction, G is injective on the moment space $\mathbb{R}^q$ with $\operatorname{Im} G = \operatorname{Im}\left(K^\dagger \mathbf{c} M\right) = V_1 \subset V$. Hence $G : \mathbb{R}^q \to V_1$ is bijective and we can use its inverse to construct E_1 on V_1.

We remark that this definition automatically entails the condition $E_0 G = 0$: In fact, according to (14), we have $K^\dagger = PK^\dagger$ so that $G = PG$ and hence

$$E_0 G = E_0 P G = 0.$$

It remains to specify the moment mapping E_1 in such a way that the remaining conditions $E_1 M = 0$ and $E_1 G = id_{\mathbb{R}^q}$ in (31) are satisfied. While $E_1 M = 0$ fixes the behavior of E_1 on the equilibrium subspace V_0, the condition $E_1 G = id_{\mathbb{R}^q}$ shows that E_1 has to invert G on $V_1 = \operatorname{Im}(G)$. This can be summarized by saying that E_1 has to be a pseudoinverse of G whose kernel includes V_0.

The only information about the behavior of E_1 on complementary subspaces to $V_0 \oplus V_1$ is that V_2 should be the nullspace of the projection $S = GE_1$. Since G is injective, the nullspace of S is identical to the nullspace of E_1. Hence, the complete construction follows by choosing a space V_2 with the property $V_1 \oplus V_2 = V_{NE}$ and setting $E_1 = 0$ on $V_0 \oplus V_2$ and $E_1 = G^{-1}$ on V_1. Then all conditions on G and E_1 are satisfied. Summarizing, we obtain a decomposition of V into generally non-orthogonal subspaces

$$V = V_0 \oplus V_1 \oplus V_2, \qquad V_0 = QV, \quad V_{NE} = PV = V_1 \oplus V_2. \tag{47}$$

and

$$E_1 f = E_1(f_0 \oplus \varepsilon f_1^{(\mathrm{NE})} \oplus f_R) = G^{-1} \varepsilon f_1^{(\mathrm{NE})}, \qquad \text{with } f_0 \in V_0,\ \varepsilon f_1^{(\mathrm{NE})} \in V_1,\ f_R \in V_2. \tag{48}$$

If we get orthogonal sums in (47), then $S = GE_1$ is a symmetric projector. With that, additional to (31) and (48), we obtain the unique Moore-Penrose-inverse $E_1 = G^\dagger$, see Sec. 3. For a proof see App. A and [26].

In Sec. 7 we will show that the specific construction leading to $E_1 = G^\dagger$ as above produces desirable properties of the evolution equation for ρ and μ. However, if not stated otherwise, we will use a general non-orthogonal decomposition $V = V_0 \oplus V_1 \oplus V_2$.

From the construction of E_1 we can again clearly see that the order of magnitude method is based on a natural separation of the non-equilibrium phase space V_{NE} that follows from the kinetic equation itself. It should be noted that, also here, the construction of E_1 is not unique due to some arbitrariness in the choice of D and, following from this, the moment space $\mathbb{R}^q$. This situation corresponds again to the result (4) for the order-of-magnitude method applied to the moments directly. In (4) some moments had to be chosen as basis in which the others are represented.

5.4 Comparison

In Sec. 5.2 we started with the construction of a projection $E_1 : V \to \mathbb{R}^q$ with certain restrictions and computed G from it, whereas in Sec. 5.3 above, we started with the specification of $G : \mathbb{R}^q \to V$ by choosing the operator D and then determined E_1 as inverse of G. In both cases the restriction of $G\mu$ as obtained in (35) was used.

The following Lemma shows how the constructions in Sec. 5.2 and Sec. 5.3 are related.

Lemma 2 *[Relation of Different Constructions]*
Let $G\mu$ be determined through (35)*.*

1. *Consider the derivation in Sec. 5.3. If an appropriate operator D as in (43) gives rise to a distribution G as in (46) and a moment operator E_1 as in (48), then*

$$D = -E_1 K^\dagger \mathbf{c} \cdot M \quad \text{and} \quad G = K^\dagger \mathbf{c} \cdot M \left(E_1 K^\dagger \mathbf{c} \cdot M \right)^\dagger \tag{49}$$

   in agreement with the definition (42) of G in the derivation of Sec. 5.2.

2. *Consider the derivation in Sec. 5.2. If a moment operator E_1 satisfying the condition described in Sec. 5.2 gives rise to the distribution G as in (42) and additionally the projector GE_1 is symmetric, then there exists an operator $E_1^{5.3} = G^{-1}|_{V_1}$ as in* (48)*. In particular, $E_1^{5.3} = G^\dagger = E_1$ and the two approaches agree.*

Proof.

1. From (44) it follows $D = -G^\dagger K^\dagger \mathbf{c} \cdot M$ and since $K^\dagger \mathbf{c} \cdot M$ maps to V_1, we have $D = -E_1 K^\dagger \mathbf{c} \cdot M$. The second equality follows with (46).

2. $E_1^{5.3} = G^\dagger = E_1$ follows from the symmetry of S together with condition (31), stating $E_1 G = id_{\mathbb{R}^q}$.

   In the case where V is finite dimensional, we apply a standard argument using singular value decomposition. For details see App. A. If V is a generally infinite dimensional Hilbert space, we refer to Theorem 9.1.3 in [26].

■

Remark: Note that starting with $E_1^{5.2}$ as in Sec. 5.2, then, according to (42), constructing $G = K^\dagger \mathbf{c} \cdot M \left(E_1^{5.2} K^\dagger \mathbf{c} \cdot M \right)^\dagger$, and finally defining E_1 as in (48) does not necessarily yield $E_1 = E_1^{5.2}$, unless the appearing pseudo-inverses are consistently chosen, which automatically happens in the orthogonal case.

Usually, the approach in Sec. 5.3 is less practical since typically the distribution function is to be constructed after the choice of specific moments to describe the process.

This situation is equivalent to the result (4) for the order-of-magnitude method applied to the moments directly. In (4) some moments had to be chosen as basis in which the others are represented. In the calculation of this representation, gradient expressions of equilibrium variables had to be eliminated.

Finally, we want to stress that the basic idea of the construction presented here is extendable to higher orders, leading to a more detailed decomposition of the non-equilibrium phase space V_{NE}, see Sec. 8.

6 Asymptotic Order

Assuming, as in Grad's closure, $f = M\,\rho + G\,\mu$ with G and E_1 satisfying (48), we find the evolution equations

$$\partial_t \rho + E_0 \mathbf{c} \cdot \nabla M\,\rho + E_0 \mathbf{c} \cdot \nabla G\,\mu = 0 \tag{50}$$

$$\partial_t \mu + E_1 \mathbf{c} \cdot \nabla M\,\rho + E_1 \mathbf{c} \cdot \nabla G\,\mu + \frac{1}{\varepsilon} E_1 K G\,\mu = 0. \tag{51}$$

Note that in accordance with (29/30) and (33), $\mu = \varepsilon \mu_1 + \mathcal{O}(\varepsilon^2)$. We have chosen this scaling to compare (50/51) to Grad's equations (27/ 28).

We are interested in the asymptotic accuracy in terms of powers of ε of the evolution of ρ with respect to the full kinetic equation. The question is, whether the evolution for μ in (51) when expanded in ε and inserted into (50) reproduces the equations for ρ resulting from the Chapman-Enskog expansion of the full kinetic model.

6.1 Order Analysis

The following theorem completely characterizes the asymptotic behavior of the system (50)/(51).

Theorem 1 (Asymptotic Accuracy) *The system (50)/(51) with primary non-equilibrium distribution G and moment operator E_1 satisfying (48) describes an evolution of ρ that is of the following Chapman-Enskog orders:*

1) *first order in the Knudsen number ε, if the operator E_1KG is invertible on $\mathbb{R}^q$.*

2) *second order in ε, if E_1KG is invertible on $\mathbb{R}^q$, and if*

$$\widetilde{E}K^\dagger R = 0 \qquad \textit{and} \qquad \widetilde{E}K^\dagger G = \widetilde{E}G\,(E_1KG)^{-1}\,, \tag{52}$$

where $\widetilde{E} = E_0\mathbf{c}$.

Proof.

1) The kinetic model produces an evolution for ρ that is given by (24). We have to show that, up to first order, the asymptotic expansion of μ leads to the same equation. We introduce $\mu = \varepsilon\mu_1 + \varepsilon^2\mu_2$ into (51) and obtain for the first order contribution

$$E_1\mathbf{c}\cdot\nabla M\,\rho + E_1KG\,\mu_1 = 0. \tag{53}$$

We note that multiplying $E_1M = 0$ with E_0 from the right yields $E_1Q = 0$ so that $E_1P = E_1$. Using further $KK^\dagger = P$, we obtain $E_1 = E_1KK^\dagger$ and hence (53) reads

$$E_1K\left(K^\dagger\mathbf{c}\cdot\nabla M\,\rho + G\,\mu_1\right) = 0 \tag{54}$$

The expression in the bracket is contained in $V_1 = \mathrm{Im}(G) = \mathrm{Im}(K^\dagger\mathbf{c}\cdot\nabla M)$ and since $SV_1 = V_1$, we have

$$E_1KS\left(K^\dagger\mathbf{c}\cdot\nabla M\,\rho + G\,\mu_1\right) = 0. \tag{55}$$

Using the definition $S = GE_1$, the invertibility of E_1KG and the relation $E_1G = id_{\mathbb{R}^q}$, we conclude

$$\mu_1 = -E_1K^\dagger\mathbf{c}\cdot\nabla M\,\rho \tag{56}$$

and with it $G\mu_1 = -K^\dagger\mathbf{c}\cdot\nabla M\,\rho$.

Using this result, we can compute the leading order of the μ dependent expression in (50)

$$E_0\mathbf{c}\cdot\nabla G\mu = \varepsilon\,E_0(\mathbf{c}\cdot\nabla)G\mu_1 + O(\varepsilon^2) \tag{57}$$

$$= -\varepsilon\,E_0(\mathbf{c}\cdot\nabla)K^\dagger(\mathbf{c}\cdot\nabla)M\,\rho + O(\varepsilon^2) \tag{58}$$

which is precisely the first order contribution given in (21).

2) Balancing the next order of (51) yields

$$\partial_t \mu_1 + E_1(\mathbf{c}\cdot\nabla)G\mu_1 + E_1 K G\mu_2 = 0 \tag{59}$$

where μ_1 has to be inserted from above. The relevant term that enters the evolution of ρ reads

$$\widetilde{E}\cdot\nabla G\mu_2 = -\widetilde{E}\cdot\nabla G\left(E_1 K G\right)^{-1}\left(\partial_t\mu_1 + E_1(\mathbf{c}\cdot\nabla)G\mu_1\right) \tag{60}$$

The relation corresponding to (59) within the Chapman-Enskog expansion of the full kinetic equation can be written

$$\partial_t\left(-K^\dagger\mathbf{c}\cdot\nabla M\,\rho\right) + \mathbf{c}\cdot\nabla\left(-K^\dagger\mathbf{c}\cdot\nabla M\,\rho\right) + K f_2^{(\mathrm{NE})} = 0$$

where the expression in brackets can be replaced by $G\mu_1$ in the current context. As in Sec. 4.2, we can multiply by $K^\dagger$ and drop the non-equilibrium projection in front of $f_2^{(NE)}$, which yields

$$f_2^{(\mathrm{NE})} = -K^\dagger G\left(\partial_t\mu_1 + E_1(\mathbf{c}\cdot\nabla)G\mu_1\right) - K^\dagger R\left(\mathbf{c}\cdot\nabla\right)G\mu_1$$

which influences the evolution of ρ in the form

$$\widetilde{E}\cdot\nabla f_2^{(\mathrm{NE})} = -\widetilde{E}\cdot\nabla K^\dagger G\left(\partial_t\mu_1 + E_1(\mathbf{c}\cdot\nabla)G\mu_1\right) - \widetilde{E}\cdot K^\dagger R\left(\mathbf{c}\cdot\nabla\right)G\mu_1. \tag{61}$$

Equality with the expression obtained for μ_2 is given if

$$\widetilde{E}\cdot\nabla G\left(E_1 K G\right)^{-1} = \widetilde{E}\cdot\nabla K^\dagger G - \widetilde{E}\cdot K^\dagger R\left(\mathbf{c}\cdot\nabla\right)G. \tag{62}$$

This is guaranteed by the assumptions.

■

The theorem shows that the system resulting from the scale induced closure can be of second order, that is, of the same accuracy as the Burnett equations, and as such go beyond the first order Navier-Stokes equations. The scale induced closure combines Grad's method with the asymptotic properties of a Chapman-Enskog expansion.

Second order is given in non-trivial cases where the special conditions given in the theorem are satisfied. In general, additional expressions have to be added on the right hand side of the system stemming from higher moment equations. This can be seen in [18] where generalized 13-moment-equations are derived. Interestingly, for Maxwell-molecules the condition for direct second order is satisfied, hence the original Grad equations are of Burnett order, see [16]. For a given K, sufficient and also necessary conditions for any order can be obtained through direct comparison of the asymptotic expansion with the corresponding Chapman-Enskog expansion of (8). This is exemplified in App. B.3.

Note that the operator $\widetilde{E} = E_0\mathbf{c}$ can be interpreted as equilibrium projection of higher moments. By asking that $\widetilde{E}K^\dagger R = 0$, we demand in a weak sense that $K^\dagger$ does not map any elements of the secondary non-equilibrium V_2 to a lower order (non-)equilibrium. This is also related to condition 3) in Sec. 6.2.

6.2 Various Conditions for First and Higher Order

The conditions given in Theorem 1 are sufficient. In this section we give an overview of some more sufficient conditions for first and even higher order.

We begin with analyzing the mapping KG. To check injectivity, we note that $KG\mu = 0$ implies $G\mu \in \ker(K)$, i.e. $G\mu = M\rho$ for some $\rho \in \mathbb{R}^p$, so that condition (48) yields $\mu = E_1 M\rho = 0$. Hence, $KG\mathbb{R}^q = KV_1 = PKV_1 \subset V_{NE}$ is a q-dimensional subspace of V_{NE}. Now there are two possibilities depending on whether the intersection of KV_1 and V_2 is empty or not. Interestingly, this alternative decides about the first order accuracy condition.

Lemma 3 *The following conditions are equivalent*

$$1)\, E_1KG \text{ invertible} \qquad 2)\, V_1 = SKV_1 \qquad 3)\, KV_1 \cap V_2 = \{0\}.$$

Proof. Assuming (1), we see that $G(E_1KG)$ is injective. Since $S = GE_1$ is a projection onto V_1, we conclude that $SKV_1 = SKG\mathbb{R}^q$ is a q-dimensional subspace of V_1 and thus identical to V_1. Next, we assume (2) and $KV_1 \cap V_2 \neq \{0\}$ for a proof by contradiction. Then there exists some $f = G\mu \in V_1$ such that $0 \neq Kf \in V_2$ and hence $SKf = 0$ which shows that $SKG : \mathbb{R}^q \to V_1$ is not injective. Consequently, it cannot be surjective which contradicts the assumption (2). Finally assuming (3), we check the injectivity of E_1KG. If $\mu \in \mathbb{R}^q$ satisfies $E_1KG\mu = 0$, then also $SKG\mu = GE_1KG\mu = 0$ so that $KG\mu \in \ker(S) = V_2$. Since also $KG\mu \in KV_1$ we find $KG\mu = 0$. The injectivity of KG then yields $\mu = 0$ which finally shows (1). ■

In view of this reformulation, we should recall the construction of the operator E_1. In the construction, we had the freedom to choose V_2 and now we see that it may be beneficial to select V_2 in such a way that it intersects KV_1 only at the origin.

In order to satisfy the second order condition (52) in Thm. 1, we can choose V_1 as an invariant subspace of K, i.e.

$$KV_1 = V_1$$

which is stronger than $SKV_1 = V_1$. This is because

$$G = PG = K^\dagger KG = K^\dagger SKG = K^\dagger GE_1KG.$$

Applying the inverse of E_1KG, we find

$$G(E_1KG)^{-1} = K^\dagger G,$$

which is sufficient for the second condition in (52). If we have in addition $\widetilde{E}K^\dagger R = 0$, we get second order accuracy if V_1 is an invariant subspace of K.

Another sufficient condition for first, and in fact also higher order is given by

$$G(E_1KG)^{-1}E_1 = K^\dagger$$

which needs the invertibility of E_1KG but is a much stronger condition. In fact, one can show with asymptotic expansion that it implies $V_1 = V_{NE}$, or equivalently $V_2 = \{0\}$. Hence, we easily see that it leads to arbitrary accuracy, since higher order contributions are trivial. For our purpose, however, this case is of little interest, because the complexity of the kinetic equation is not reduced by applying the scale induced closure.

6.3 Regularization

The above construction uses the zeroth order of the evolution of the distribution $\hat{f}_R$ in (32). The first order gives additional accuracy and leads to regularized equations similar to the R13-system in [17] and [19].

Under the first order accuracy condition, the evolution of $\hat{f}_R$ in (32) reduces to

$$\varepsilon^2 \partial_t \hat{f}_R + \varepsilon^2 R\mathbf{c} \cdot \nabla \hat{f}_R + \varepsilon R\mathbf{c} \cdot \nabla G\, \hat{\mu} + \varepsilon RK\, \hat{f}_R = 0 \tag{63}$$

where zero-order terms have vanished. The first order terms in this equation are balanced by choosing

$$RK\hat{f}_R = -R\mathbf{c} \cdot \nabla G\hat{\mu} \tag{64}$$

Assuming that $(RK)^\dagger RK\hat{f}_R = \hat{f}_R$, we can write

$$\hat{f}_R = -(RK)^\dagger R\mathbf{c} \cdot G\nabla\hat{\mu}. \tag{65}$$

This gives a first contribution to the secondary non-equilibrium in (30) based on gradients of the non-equilibrium variables μ. The elaboration of this procedure is left for future work. In fact, an additional first order term has been suppressed above. This regularization procedure has been successfully conducted on the moment hierarchy for Maxwell-molecules in [17].

7 Stability

In this section we assume that

1) V is a Hilbert space with scalar product $\langle \cdot, \cdot \rangle_V$.
2) The collision operator K and the equilibrium projection Q are self-adjoint.
   Furthermore K is positive semi-definite. (66)
3) The multiplication operator $c_\alpha : V \to V$ defined by $(c_\alpha f)(\mathbf{v}) = v_\alpha f(\mathbf{v})$ is self-adjoint.
4) The projector $S = GE_1$ as constructed in Sec. 5.1 - 5.4 is self-adjoint.

The distribution M is defined in Sec. 1. After introducing symmetric positive definite operators based on the adjoints of the distributions, we will show that the equations (50)/(51) possess an entropy law and are therefore stable.

Definition 3 (Adjoint) *We denote $\langle \cdot, \cdot \rangle_{\mathbb{R}^n}$ the standard scalar product in $\mathbb{R}^n$*

1) We define the adjoint M^* of M through the Riesz representation theorem as the unique linear operator $M^* : V \to \mathbb{R}^p$ such that

$$\langle x, M^* f \rangle_{\mathbb{R}^p} = \langle Mx, f \rangle_V, \qquad \forall f \in V,\ x \in \mathbb{R}^p \tag{67}$$

2) Similarly we define $G^* : V \to \mathbb{R}^q$, such that

$$\langle y, G^* f \rangle_{\mathbb{R}^q} = \langle Gy, f \rangle_V, \qquad \forall f \in V,\ y \in \mathbb{R}^q \tag{68}$$

3) Based on the adjoints we define

$$B := M^*M : \mathbb{R}^p \to \mathbb{R}^p \text{ and } L := G^*G : \mathbb{R}^q \to \mathbb{R}^q. \tag{69}$$

The matrices B and L are symmetric, positive definite by construction. They will give rise to symmetric forms which constitute the entropy of the moment system. Again we keep notation simple, and use μ for the scaled higher moments $\hat{\mu}$ in the following. Generally the stability result does not depend on the scaling of μ.

In this orthogonal setting, the pseudoinverse $G^\dagger$ is the unique Moore-Penrose inverse. Due to injectivity of G, it can be computed as $G^\dagger = (G^*G)^{-1}G^*$. Furthermore we have through (66) 2) and 4) that indeed E_0 and E_1 are the unique Moore-Penrose inverses of M and G respectively (see Sec. 3 and 5.4).

Theorem 2 (Stability) *Let the moment system (50)/(51) be given, based on the operators M, G and E_0, E_1 defined in Sec. 3 and 5.3. Then the system features the convex entropy*

$$\eta = \frac{1}{2}\langle \rho, B\rho\rangle_{\mathbb{R}^p} + \frac{1}{2}\langle \mu, L\mu\rangle_{\mathbb{R}^q}, \qquad \rho \in \mathbb{R}^p, \quad \mu \in \mathbb{R}^q \tag{70}$$

with associated negative definite entropy production. In particular, the system is symmetric hyperbolic.

Proof.
Convexity of η: $\langle \cdot, B\cdot\rangle_{\mathbb{R}^p}$ and $\langle \cdot, L\cdot\rangle_{\mathbb{R}^q}$ define scalar products based on the symmetric, positive definite matrices from (69). The function η is therefore convex. Note that η shows similarities with the entropies in [3] and [20].
Entropy law: Multiplying (50) with $\langle \rho, B\cdot\rangle$ and (51) with $\langle \mu, L\cdot\rangle$ yields

$$\langle \rho, B\partial_t\rho\rangle_{\mathbb{R}^p} + \langle \rho, BE_0\mathbf{c}\cdot M\,\nabla\rho\rangle_{\mathbb{R}^p} + \langle \rho, BE_0\mathbf{c}\cdot G\,\nabla\mu\rangle_{\mathbb{R}^p} = 0 \tag{71a}$$

$$\langle \mu, L\partial_t\mu\rangle_{\mathbb{R}^q} + \langle \mu, LE_1\mathbf{c}\cdot M\,\nabla\rho\rangle_{\mathbb{R}^q} + \langle \mu, LE_1\mathbf{c}\cdot G\,\nabla\mu\rangle_{\mathbb{R}^q} = -\frac{1}{\varepsilon}\langle \mu, LE_1KG\,\mu\rangle_{\mathbb{R}^q} \tag{71b}$$

From the definition of B we immediately see

$$BE_0 = M^*ME_0 = M^*Q = (QM)^* = M^* \tag{72}$$

since Q is self-adjoint.

For the product LE_1 we analogously find with $(66)_4$ that

$$LE_1 = G^*GE_1 = G^*S = (SG)^* = G^*. \tag{73}$$

Plugging in these expressions yields

$$\langle \rho, B\partial_t\rho\rangle_{\mathbb{R}^p} + \langle \rho, M^*\mathbf{c}\cdot M\,\nabla\rho\rangle_{\mathbb{R}^p} + \langle \rho, M^*\mathbf{c}\cdot G\,\nabla\mu\rangle_{\mathbb{R}^p} = 0 \tag{74a}$$

$$\langle \mu, L\partial_t\mu\rangle_{\mathbb{R}^q} + \langle \mu, G^*\mathbf{c}\cdot M\,\nabla\rho\rangle_{\mathbb{R}^q} + \langle \mu, G^*\mathbf{c}\cdot G\,\nabla\mu\rangle_{\mathbb{R}^q} = -\frac{1}{\varepsilon}\langle \mu, G^*KG\,\mu\rangle_{\mathbb{R}^q} \tag{74b}$$

After adding the equations (74) and using the self-adjointness of L, B and $\mathbf{c}$, we obtain

$$\begin{aligned}
&\partial_t\left(\frac{1}{2}\langle \rho, B\rho\rangle_{\mathbb{R}^p} + \frac{1}{2}\langle \mu, L\mu\rangle_{\mathbb{R}^q}\right)\\
&+ \nabla\cdot\left(\frac{1}{2}\langle \rho, M^*\mathbf{c}M\,\rho\rangle_{\mathbb{R}^p} + \langle \rho, M^*\mathbf{c}G\,\mu\rangle_{\mathbb{R}^p} + \frac{1}{2}\langle \mu, G^*\mathbf{c}G\,\mu\rangle_{\mathbb{R}^q}\right)\\
&= -\frac{1}{\varepsilon}\langle \mu, G^*KG\,\mu\rangle_{\mathbb{R}^q}
\end{aligned} \tag{75}$$

which is an entropy law.
Negativity of entropy production: Since K is self-adjoint and positive semidefinite, we have $G^*KG = (\sqrt{K}G)^*\sqrt{K}G$. Hence, we can rewrite $\langle \mu, G^*KG\,\mu\rangle_{\mathbb{R}^q} = \langle \sqrt{K}G\mu, \sqrt{K}G\,\mu\rangle_V > 0$, since K is positive on the range of G. Therefore the entropy production is negative definite. ■

With Theorems 1 and 2 we have shown that the scale induced closure yields equations which are physically accurate in terms of a Knudsen number expansion as well as mathematically stable.

We have seen before that, in the new theory, the definition of the distribution function $G\,\mu$ depends on the structure of the collision operator. This is a natural outcome since the scale decompostion of the non-equilbrium phase space is induced by the collision operator. To find a symmetric projector GE_1, additional constraints on the choice of the variables μ follow. Hence, also the choice of variables μ is governed by K which is somewhat surprising. For the moments in (4) this results in an additional recombination of the vectors and tensors to find an appropriate basis.

8 Higher Order Scale Induced Closure

The orignial order-of-magnitude method developed by Struchtrup in [17] is a 3rd order approximation. In this section we sketch how to construct the scale induced closure including contributions of order up to ε^n in our linear case. This is just an outline and shall serve as starting point for future research. Many details remain unspecified.

Extending (30), we decompose

$$f = M\rho + \varepsilon G_1\hat{\mu}_1 + \varepsilon^2 G_2\hat{\mu}_2 + \cdots \varepsilon^n G_n\hat{\mu}_n + \varepsilon^{n+1}\hat{f}_{R_n}, \tag{76}$$

with moments $\hat{\mu}_k \in \mathbb{R}^{q_k}$. The corresponding operators E_1,...,E_n and G_1,...,G_n are required to fulfill

$$E_kG_k = id_{\mathbb{R}^{q_k}}, \quad E_kM = 0, \quad E_0G_k = 0, \quad E_iG_j = 0, \tag{77}$$

where i, j, $k = 1, ..., n$ and $i \neq j$.

With these operators, we can construct the projections $S_k = G_kE_k$, $k = 1, ..., n$ and $R_n = P - S_1 - ... - S_n$, such that our phase space is divided as in Fig. 2.

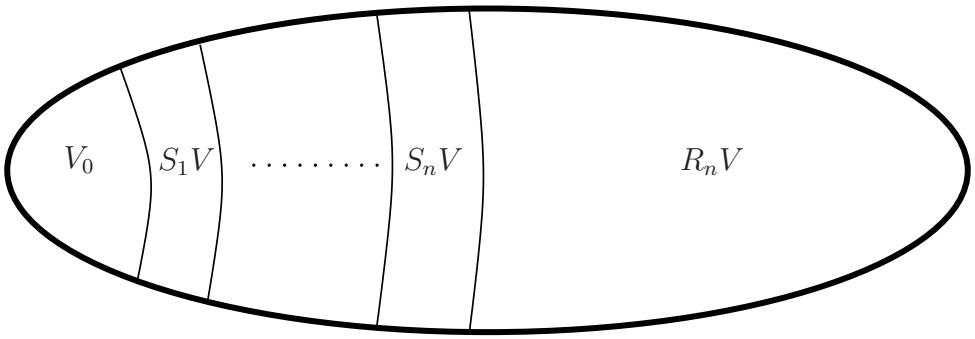

Figure 2: The phase space is subdivided into various higher non-equilibrium parts.

In accordance with the construction in Sec. 5.1, we match orders as in (32) and derive the

equations determining the $G_k\hat{\mu}_k$ as

$$\begin{aligned} G_1\hat{\mu}_1 &= -K^\dagger \mathbf{c}\cdot M\nabla\rho \\ G_2\hat{\mu}_2 &= -K^\dagger \mathbf{c}\cdot G_1\nabla\hat{\mu}_1 \\ &\vdots \\ G_n\hat{\mu}_n &= -K^\dagger \mathbf{c}\cdot G_{n-1}\nabla\hat{\mu}_{n-1} \end{aligned} \tag{78}$$

Under certain conditions on the relation between the image sets of $K^\dagger\mathbf{c}\cdot G_i$ and S_j, the operators can be constructed analogously to Sec. 5.2 and Sec. 5.3.

The equations are derived by plugging (76) into the linear kinetic equation, applying the operators E_0,...,E_n and setting $f_{R_n} = 0$. Using scaled variables $\mu_k = \varepsilon^k\hat{\mu}_k$, $k = 1, ..., n$, they read

$$\begin{aligned} \partial_t\rho + E_0\mathbf{c}\cdot\nabla M\rho + E_0\mathbf{c}\cdot\nabla G_1\mu_1 + \cdots + E_0\mathbf{c}\cdot\nabla G_n\mu_n &= 0 \\ \partial_t\mu_1 + E_1\mathbf{c}\cdot\nabla M\rho + E_1\mathbf{c}\cdot\nabla G_1\mu_1 + \cdots + E_1\mathbf{c}\cdot\nabla G_n\mu_n + \frac{1}{\varepsilon}E_1KG_1\mu_1 + \cdots + \frac{1}{\varepsilon}E_1KG_n\mu_n &= 0 \\ &\vdots \\ \partial_t\mu_n + E_n\mathbf{c}\cdot\nabla M\rho + E_n\mathbf{c}\cdot\nabla G_1\mu_1 + \cdots + E_n\mathbf{c}\cdot\nabla G_n\mu_n + \frac{1}{\varepsilon}E_nKG_1\mu_1 + \cdots + \frac{1}{\varepsilon}E_nKG_n\mu_n &= 0 \end{aligned} \tag{79}$$

8.1 Stability for the Higher Order case

The stability analysis in the higher order case uses similar arguments as in Sec. 7. We need the first 3 assumptions of (66), assumption 4) needs to be extended to all the projectors S_1,...,S_n, and the positive semi-definiteness of K will need some extension as well. The entropy becomes

$$\eta_n = \frac{1}{2}\langle\rho, B\rho\rangle_{\mathbb{R}^p} + \frac{1}{2}\langle\mu_1, L_1\mu_1\rangle_{\mathbb{R}^{q_1}} + \cdots + \frac{1}{2}\langle\mu_n, L_n\mu_n\rangle_{\mathbb{R}^{q_n}}, \qquad \rho\in\mathbb{R}^p, \quad \mu_k\in\mathbb{R}^{q_k}, \quad k = 1, ..., n, \tag{80}$$

where $L_k = G_k^*G_k$.

We proceed analogously to the proof of Thm. 2 and get the entropy flux

$$\frac{1}{2}\langle\rho, M^*\mathbf{c}M\rho\rangle_{\mathbb{R}^p} + \sum_{k=1}^n\langle\rho, M^*\mathbf{c}G_k\mu_k\rangle_{\mathbb{R}^p} + \frac{1}{2}\sum_{k=1}^n\langle\mu_k, G_k^*\mathbf{c}G_k\mu_k\rangle_{\mathbb{R}^{q_k}} + \sum_{j=1}^n\sum_{i=j+1}^n\langle\mu_j, G_j^*\mathbf{c}G_i\mu_i\rangle_{\mathbb{R}^{q_j}}. \tag{81}$$

On the right hand side of the entropy equation, we get

$$-\frac{1}{\varepsilon}\sum_{j=1}^n\sum_{k=1}^n\langle\mu_j, G_j^*KG_k\mu_k\rangle_{\mathbb{R}^{q_j}}. \tag{82}$$

Since this quantity should be negative, assumption 2) in (66) extends to negativity not only of $-K$, but of the above combination. This is satisfied, for example, if K is self adjoint and negative definite on $V_0^\perp$ and if the subspaces S_iV are K-invariant for $i = 1, ..., n$.

If all these assumptions are met, we obtain an entropy law with negative entropy production, and therefore symmetric hyperbolic and stable equations.

8.2 Order Analysis

The order analysis becomes even more technical for $n \geq 2$ than it is in Sec. 6. A general analysis is therefore beyond the scope of this work. For examples like the following 16 discrete velocities model in Sec. 9.2, the easiest way to check the order of accuracy is a direct asymptotic expansion of the equations under consideration, see App. B.3. Note however that the 16 discrete velocities models is not complex enough to serve as a good testcase for higher orders in the scale induced closure.

9 Examples

As examples for the theory described above we discuss three specific cases. One displays the generalized 13-moment-case. Then we consider a model with 16 discrete velocities and show the approximation features of the various closures. The last case demonstrates the accuracy of the closure approximations in the case of a generic linear model system.

9.1 Generalized 13-Moment-Equations

The generalized 13-moment-equations have been derived by Struchtrup in [18] by the order-of-magnitude approach described above. In the derivation a general interaction potential has been assumed and, hence, general production terms in the moment equations have been considered. The closure approximation takes into account the structure of the production terms and the resulting coefficients could be identified with classical Burnett coefficients.

The final equations for stress tensor σ_{ij} and heat flux q_i read

$$\begin{aligned}\frac{D\sigma_{ij}}{Dt} + \sigma_{ij}\frac{\partial v_k}{\partial x_k} + 2\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} + \Pr\frac{4\varpi_3}{5\varpi_2}\left(\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - \omega\, q_{\langle i}\frac{\partial \ln\theta}{\partial x_{j\rangle}}\right) \\ + \Pr\frac{4\varpi_4}{5\varpi_2}q_{\langle i}\frac{\partial \ln p}{\partial x_{j\rangle}} + \Pr\frac{4\varpi_5}{5\varpi_2}q_{\langle i}\frac{\partial \ln\theta}{\partial x_{j\rangle}} + \frac{\varpi_6}{\varpi_2}\sigma_{k\langle i}S_{j\rangle k} = -\frac{2p}{\varpi_2\mu}\left[\sigma_{ij} + 2\mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]\end{aligned} \tag{83}$$

and

$$\begin{aligned}\frac{Dq_i}{Dt} + q_k\frac{\partial v_i}{\partial x_k} + \frac{5}{3}q_i\frac{\partial v_k}{\partial x_k} - \frac{5}{2\Pr}\sigma_{ik}\frac{\partial\theta}{\partial x_k} + \frac{5\theta_3}{4\theta_2\Pr}\sigma_{ik}\frac{\partial \ln p}{\partial x_k} \\ + \frac{5\theta_4}{4\theta_2\Pr}\theta\left(\frac{\partial\sigma_{ik}}{\partial x_k} - \omega\sigma_{ik}\frac{\partial\ln\theta}{\partial x_k}\right) + \frac{15\theta_5}{4\theta_2\Pr}\sigma_{ik}\frac{\partial\theta}{\partial x_k} = -\frac{5p}{2\theta_2\Pr\mu}\left[q_i + \frac{5\mu}{2\Pr}\frac{\partial\theta}{\partial x_i}\right]\end{aligned} \tag{84}$$

where v_i is the velocity, θ is the temperature (in energy units), p is the pressure, Pr is the Prandtl number, μ viscosity and ϖ_α, θ_α are Burnett coefficients. Interestingly, for Maxwell molecules the equations reduce to the 13-moment-system of Grad which is based on a Hermite series of the distribution function. This is a mere coincidence and related to the fact that the eigenfunctions of the linearized collision operator for Maxwell molecules are Hermite functions. Hence, Grad's equations form the accurate second order system only for Maxwell molecules while the above system is the second order accurate extension to general interaction potentials. I.e., it is a stable system that reproduces the correct general Burnett relations when expanded in Knudsen number. In that sense it is also related to the regularized Burnett equations in [12].

The system demonstrates the capabilities of the described scale-induced closure procedure.

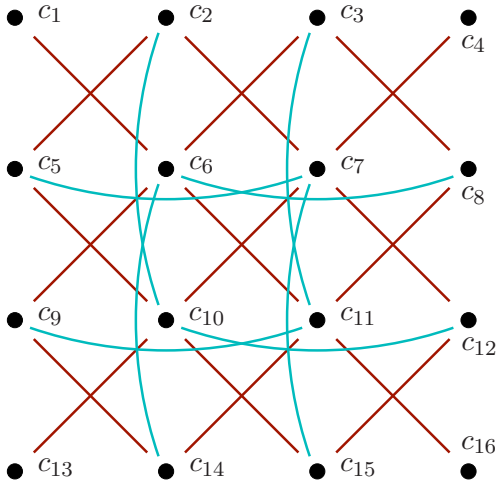

Figure 3: 2-D velocity space with interactions in the 16 discrete velocities model.

9.2 Linearized 16 Discrete Velocity Model

The following example considers a linearized 16 discrete velocities model in one space and two velocity dimensions [1]. Such models are a generalization of models initially developed in [4]. They have been more thoroughly investigated in [1].

Choosing the bilinear interactions as in Fig. 3, we obtain the kinetic equations

$$\partial_t u_i(x,t) + \sum_{j=1}^{16} V_{ij}\partial_x u_j(x,t) + \frac{1}{\varepsilon} K_i^{\text{nonlin}}[u] = 0, \tag{85}$$

with $V_{ij} = \delta_{ij} c_i^{(1)}$, $K^{\text{nonlin}} = K^{\text{diag}} + K^{\text{straight}}$ being positive semidefinite bilinear forms (see Appendix B.1, equations (114) and (115)). We linearize (85) around a constant equilibrium $f_i^0 = 1$ by the ansatz $u_i = 1 + \varepsilon f_i$ and neglect all higher order terms. This leads again to a positive semidefinite linear map $K : V \to V$. The linear equations read

$$\partial_t f_i(x,t) + \sum_{j=1}^{16} V_{ij}\partial_x f_j + \frac{1}{\varepsilon}\sum_{j=1}^{16} K_{ij} f_j = 0, \tag{86}$$

with K as in (116).
The nullspace of K defines the equilibrium moments[1]

$$\rho = \sum_{i=1}^{16} f_i, \quad \rho v_x = \sum_{i=1}^{16} c_i^{(1)} f_i, \quad \rho v_y = \sum_{i=1}^{16} c_i^{(2)} f_i, \quad e = \sum_{i=1}^{16} c_i^2 f_i. \tag{87}$$

The orthogonal complement of the nullspace of K is spanned by the arbitrarily chosen vectors r_1,...,r_{12}.

For the detailed computations leading to the form of the classical equations in the following subsections we refer to B.2. Here we only give the results.

[1]Note that left and right eigenvectors are equal since K is symmetric.

9.2.1 Euler Equations

The Euler equations (17) become

$$\partial_t \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & \frac{66}{5} & 0 & 0 \end{pmatrix} \partial_x \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{88}$$

9.2.2 Navier-Stokes-Fourier System

With the pseudoinverse of K we get the Navier Stokes Fourier equations according to (21)

$$\partial_t \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & \frac{66}{5} & 0 & 0 \end{pmatrix} \partial_x \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \end{pmatrix} = \varepsilon \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{4}{5} & 0 & 0 \\ 0 & 0 & \frac{289}{20} & 0 \\ -\frac{140}{5} & 0 & 0 & \frac{14}{5} \end{pmatrix} \partial_x^2 \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \end{pmatrix} \tag{89}$$

9.2.3 Burnett Equations

From (24), the Burnett equations turn out to be

$$\begin{aligned} \partial_t \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & \frac{66}{5} & 0 & 0 \end{pmatrix} \partial_x \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \end{pmatrix} =& \varepsilon \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{4}{5} & 0 & 0 \\ 0 & 0 & \frac{289}{20} & 0 \\ -\frac{140}{5} & 0 & 0 & \frac{14}{5} \end{pmatrix} \partial_x^2 \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \end{pmatrix} \\ & - \varepsilon^2 \begin{pmatrix} 0 & 0 & 0 & 0 \\ -\frac{19}{4} & 0 & 0 & \frac{27}{40} \\ 0 & 0 & 0 & 0 \\ 0 & \frac{1354}{125} & 0 & \frac{14}{5} \end{pmatrix} \partial_x^3 \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \end{pmatrix} \end{aligned} \tag{90}$$

9.2.4 Grad Equations

To obtain a Grad Closure, we have to choose some higher moments through the operators G and E_1, satisfying the constraints given in section 4.3. We will argue that the scale induced closure produces a set of 3 higher moments, so in order to have a fair comparison, we chose the same number for Grad.

We will choose these moments once arbitrarily and, to compare, also as fluxes of lower order equations.

Arbitrary Choice of Moments
Let arbitrarily $\mu_1 = E_1 r_1$, $\mu_2 = E_1 r_2$ and $\mu_3 = E_1 r_3$, with the again arbitrary choice of E_1 and G, as shown in App. B.2.1, fullfilling only (26), but not necessarily (33). For details of the construction of G and E_1, see App. B.2.1.

With E_1 and G, we use (27) and (28) and get the equations

$$\partial_t \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \\ \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix} + \left(\begin{array}{cccc|ccc} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 9 & -1 & 1 \\ 0 & 66/5 & 0 & 0 & 72/5 & 56/5 & -56/5 \\ \hline -30/32 & 0 & 0 & 3/32 & 9/4 & 3/4 & 3/4 \\ 5/16 & 0 & -1/20 & -1/32 & 2/5 & -6/5 & -1/5 \\ 5/8 & 0 & -1/10 & -1/16 & 4/5 & -2/5 & 3/5 \end{array}\right) \partial_x \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \\ \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix}$$
$$+\frac{1}{\varepsilon} \left(\begin{array}{cccc|ccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 4 & -7 & 7 \\ 0 & 0 & 0 & 0 & 0 & 11 & -3 \\ 0 & 0 & 0 & 0 & 2 & 1 & 7 \end{array}\right) \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \\ \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{91}$$

Kinetic Fluxes as Moments

A more natural way to construct E_1 and G for the Grad equations is to consider those variables that appear in the fluxes of the equations, see also the remark in section 4.3. From the kinetic model, we obtain heat fluxes in x and y direction, as well as the pressure tensor

$$q_x = \sum_{i=1}^{16} c_i^{(1)} c_i^2 f_i, \quad qy = \sum_{i=1}^{16} c_i^{(2)} c_i^2 f_i, \quad \sigma_{xy} = \sum_{i=1}^{16} c_i^{(1)} c_i^{(2)} f_i. \tag{92}$$

However, building E_1 and G from these vectors, we can compute that their equilibrium part is not zero, i.e. conditions (26) are not fullfilled in our model with 16 discrete velocities. The remedy is to chose the non-equilibrium projections

$$Pq_x, \quad Pq_y, \quad P\sigma_{12}. \tag{93}$$

For more details, see App. B.2.1. The resulting equations are:

$$\partial_t \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \\ \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix} + \left(\begin{array}{cccc|ccc} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 20 \\ 0 & 66/5 & 0 & 0 & 16\sqrt{34/5} & 0 & 0 \\ \hline -\sqrt{85/128} & 0 & 0 & \sqrt{1.7}/16 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2\sqrt{1.7} \\ 0 & 0 & 1/4 & 0 & 0 & 2\sqrt{1.7} & 0 \end{array}\right) \partial_x \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \\ \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix}$$
$$+\frac{1}{\varepsilon} \left(\begin{array}{cccc|ccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 25/17 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 25/17 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 9/25 \end{array}\right) \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \\ \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{94}$$

9.2.5 Scale Induced Closure

The operator $-K^\dagger \mathbf{c}\cdot M$ in (33) has a 3-dimensional image, its nullspace is $(1,0,0,10)^T$. Therefore we get 3 higher moments μ_1, μ_2 and μ_3. We choose D as parametrization of the orthogonal complement of $(1,0,0,10)^T$

$$D = \begin{pmatrix} \frac{10}{\sqrt{101}} & 0 & 0 & -\frac{1}{\sqrt{101}} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad D^\dagger = \begin{pmatrix} \frac{10}{\sqrt{101}} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -\frac{1}{\sqrt{101}} & 0 & 0 \end{pmatrix}. \tag{95}$$

Constructing E_1 as the pseudoinverse $G^\dagger$ and plugging all into (50/51), we obtain the equations

$$\partial_t \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \\ \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & -\frac{4}{5} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{289}{20} \\ 0 & \frac{66}{5} & 0 & 0 & \frac{14\sqrt{101}}{5} & 0 & 0 \\ -\frac{5600}{487\sqrt{101}} & 0 & 0 & \frac{560}{487\sqrt{101}} & 0 & \frac{608}{487\sqrt{101}} & 0 \\ 0 & -2 & 0 & 0 & \frac{19\sqrt{101}}{16} & 0 & 0 \\ 0 & 0 & -\frac{289}{841} & 0 & 0 & 0 & 0 \end{pmatrix} \partial_x \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \\ \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix}$$
$$+ \frac{1}{\varepsilon} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{560}{487} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{289}{841} \end{pmatrix} \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \\ \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{96}$$

These equations are of second order accuracy since the conditions in Thm. 1 are met. Another way of checking the accuracy is through direct asymptotic expansion of (96). This furthermore shows that the equations are not of 3rd order (see App. B.3).

9.2.6 Comparison

In order to compare the results of the different closures, we look at the spatial Fourier transform $f_j(x,t) = \sum_{k\in\mathbb{Z}} e^{-ikx} \hat{f}_j^k(t)$. This transforms the gradients into factors of $-ik$. We apply the Fourier transform to (85), (88), (89), (91) and (96) and obtain ordinary differential equations with the solution

$$\partial_t \hat{f}_j^k(t) - i\sum_{j=1}^{16} V_{ij} k \hat{f}_j^k(t) + \frac{1}{\varepsilon}\sum_{j=1}^{16} K_{ij} \hat{f}_j^k(t) = 0, \qquad \hat{\mathbf{f}}^k(t) = \exp[ik\mathbf{V} - \frac{1}{\varepsilon}\mathbf{K}]\hat{\mathbf{f}}^k(0) \tag{97}$$

As initial condition we choose $\hat{f}_j^k(0) = 1$ for the wave number $k = 2\pi$ and for all $j = 1, ...16$, corresponding to Dirac peaks in the untransformed space. We show the results obtained with the various closures for the real part of the Fourier transformed mass density $\hat{\rho}^k = \sum_{j=1}^{16} \hat{f}_j^k(t)$ in Fig. 5.

For any ε, the Euler solution is oscillating without damping (no influence of the collision term). In Fig. 5, we see that the damping in Navier-Stokes dominates already after short time ($\varepsilon = 0.1$, $\varepsilon = 0.5$). Both, Euler and Navier-Stokes use 4 variables. For the Grad solution,

we have different options of chosing the closure. We compare some of these choices in Fig. 4 (r_1, r_2, r_3; r_5, r_6, r_7; projected heat fluxes and pressure tensor). Clearly, the choice of heat flux and pressure tensor projected onto the non-equilibrium space (see Sec. 9.2.4), performs best for all ε.

The Grad solution, using 7 variables, shows damping, and there is a phase shift to the kinetic solution. The scale induced closure performs better with the same number of variables for $\varepsilon = 0.01$ and $\varepsilon = 0.1$. We see hardly any difference between the scale induced closure and the kinetic equation for $\varepsilon = 0.01$, $\varepsilon = 0.1$, only at $\varepsilon = 0.5$ some deviations start to occur.

Summarizing, the choice of variables is the main point in all these methods - among the totally 16 kinetic variables, we want to choose a few linear combinations to build macroscopic variables. These should mimic the microscopic behaviour as good as possible.

Burnett equations (90) are unstable for large relaxation times $\varepsilon = 0.5$. This is due to the fact that the Burnett equations only consider a Taylor series in ε, which does not necessarily become more accurate by adding higher order terms. In the scale induced closure, we are not only taking into account higher orders but additionally an enrichment of the approximation space.

To validate our results, we also show the imaginary part of the Fourier transformed velocity in x direction, $\hat{v}_x^k = \sum_{j=1}^{16} c_j^{(1)} \hat{f}_j^k(t)$ in Fig. 6. Density and x-velocity are non-trivial quantities in the model under consideration. The energy shows to be just a scaling of the density. Usually, higher moments are more difficult to capture, however in our case, the approximations for the velocity show the same qualities as for the density.

9.3 Linear Matrix System

The second example is more abstract and illustrates the fundamental range of the new closure procedure. We consider a vector function $y : \mathbb{R}^+ \to \mathbb{R}^N$ satisfying an ordinary differential equation

$$\partial_t y + T\, y + \frac{1}{\varepsilon} K\, y = 0, \qquad y|_{t=0} = y^{(0)} \tag{98}$$

with initial conditions $y^{(0)}$. The matrix T generalizes the transport operator, while K can be viewed as collisional part. As for the kinetic model we assume that there exist vectors or matrices M and E_0 with $KM = 0$ and $E_0 K = 0$, as well as $E_0 M = id$. Equilibrium variables are given by $\rho = E_0\, y$. The whole theory derived above can be easily translated to the present case. The aim is to replace the high-dimensional system (98) by a lower dimensional system for ρ with high accuracy.

To check the approximation quality we consider a concrete example and take $N = 4$ and

$$K = \frac{1}{54} \begin{pmatrix} 45 & -3 & 21 & -21 \\ -3 & 65 & 31 & -31 \\ 21 & 31 & 53 & 1 \\ -21 & -31 & 1 & 53 \end{pmatrix} \tag{99}$$

as collision matrix. This matrix was constructed such that it exhibits the eigenvalues $\lambda_i \in \{0, 1, 1, 2\}$ and a one-dimensional kernel given by $M = (1, 1, -1, 1)^{tr}$ with $KM = 0$. In accordance with section 7, the equilibrium operator with $E_0 K = 0$ is given by $E_0 = (M^* M)^{-1} M^* = \frac{1}{4}(1, 1, -1, 1)$ and the equilibrium variable $\rho = E_0\, y$ is scalar. T is chosen to be

$$T = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{100}$$

We will solve the full system (98) with (99) and (100) numerically and compare the numerical results of various approximations like a Chapman-Enskog-type or the scale-induced closure to the full solution.

The kinetic variable ("distribution") satisfies $y = M\,\rho + y_1$ with a disturbance computed in (20)

$$y_1 = -\varepsilon\, K^\dagger T\, M\, \rho. \tag{101}$$

This leads to the equation (see (21))

$$\partial_t \rho + (E_0 T\, M)\, \rho - \varepsilon\, (E_0 T\, K^\dagger T\, M)\, \rho = 0 \tag{102}$$

in the sense of a first Chapman-Enskog expansion. Initial conditions are given by $\rho|_{t=0} = E_0 y^{(0)} = \rho^{(0)}$. For our example, it turns out that $E_0 T\, M = 0$ and $E_0 T\, K^\dagger T\, M = \frac{65}{54}$, so we find $\rho(t) = \rho^{(0)} \exp\left(-\varepsilon \frac{65}{54} t\right)$ as first approximation. According to the theory above, a better approximation is given by equations for ρ coupled to a scalar higher moment $\mu = E_1 y$ with the structure (compare (27), (28))

$$\partial_t \begin{pmatrix} \rho \\ \mu \end{pmatrix} + \underbrace{\begin{pmatrix} E_0 T\, M & E_0 T\, G \\ E_1 T\, M & E_1 T\, G \end{pmatrix}}_{A} \begin{pmatrix} \rho \\ \mu \end{pmatrix} = -\frac{1}{\varepsilon} \underbrace{\begin{pmatrix} 0 & 0 \\ 0 & E_1 K\, G \end{pmatrix}}_{B} \begin{pmatrix} \rho \\ \mu \end{pmatrix} \tag{103}$$

and particular choices for G and E_1.

Some of these choices are proposed through the Grad closure. As we have seen in the previous example, not every choice of G and E_1 just fulfilling (26) offers the same accuracy. Thus we first choose $E_1 = E_0 T$ and with it $G = (E_1 E_1^*)^{-1} E_1^*$, imitating the selection of higher moments from the kinetic equations. Luckily, conditions (26) are met, meaning that $E_0 T$ contains no equilibrium part.

Out of curiosity, we construct arbitrary vectors

$$G = \left(-\frac{1}{2}, 1, \frac{1}{14}, -\frac{3}{7}\right)^{tr}, \quad E_1 = \left(1, \frac{1}{2}, -1, -\frac{5}{2}\right) \tag{104}$$

satisfying the basic requirements $E_0 G = 0$, $E_1 M = 0$ and $E_1 G = 1$, for comparison. In Grad's approach, independent of the choice of non-equilibrium moments, the kinetic structure given through K is not fully exploit. Instead, the new scale-induced order-of-magnitude approach ($D = 1$) suggests to use

$$G = -K^\dagger T M D^\dagger, \quad E_1 = (G^* G)^{-1}\, G^* \tag{105}$$

which is adapted to the structure of the kinetic equation.

In Fig. 7 we compare the evolution of ρ as predicted from the full system (98), from the Chapman-Enskog-type result, the two Grad approaches and the order-of-magnitude equations.

The relaxation times are chosen to be $\varepsilon = 0.01$, $\varepsilon = 0.1$ and $\varepsilon = 0.5$. The CE result manages to predict a general decaying behaviour, while the random moment Grad approximation gives an initial behaviour that is qualitatively correct but fails for large times t. The Grad approximation with $E_1 = T E_0$ performs much better, however also fails in the low $\varepsilon = 0.01$ case, compared to the scale induced closure. The scale induced closure result matches the full solution in a nearly perfect way for $\varepsilon = 0.01$ and $\varepsilon = 0.1$. For $\varepsilon = 0.5$, the Grad method becomes better. We do not want to overstress this rather special example, but it indicates that the scale-induced closure may considerably improve the accuracy of lower dimensional approximations of more general equations.

For completeness we give the resulting matrices in the system (103) for the random moment Grad approach

$$A = \begin{pmatrix} 0 & -\frac{41}{28} \\ \frac{5}{4} & -\frac{81}{28} \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ 0 & \frac{55}{27} \end{pmatrix}, \tag{106}$$

the Grad approach with $E_1 = TE_0$

$$A = \begin{pmatrix} 0 & 1 \\ -\frac{3}{2} & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ 0 & \frac{113}{81} \end{pmatrix}. \tag{107}$$

and the sclae induced closure

$$A = \begin{pmatrix} 0 & \frac{65}{57} \\ -\frac{65}{54} & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ 0 & \frac{65}{57} \end{pmatrix}. \tag{108}$$

As initial condition for the full system $y^{(0)} = (1, 4, -2, 1)$ was used which corresponds to $\rho^{(0)} = 2$.

10 Conclusion

This work supplements the work of Struchtrup in [17] and [18] where an order-of-magnitude closure for moment equations in kinetic gas theory was developed. Here, we generalize this approach to the level of kinetic equations and relate it to standard methods of Chapman-Enskog and Grad. The new closure obeys a scaling of the non-equilibrium phase space that is introduced by asymptotic expansion. This scaling structures the phase space and allows to formulate a distribution function based on moments respecting the asymptotic properties of the kinetic equation. In this sense, it provides a scale-induced closure. The resulting moment equations exhibit high asymptotic accuracy in a natural way.

The theory is developed in the case of a linear kinetic model equation. The final equations can be shown to possess an entropy law and to be L^2-stable. In future work the results need to be extended to the non-linear case. This should be possible since the original method was conducted on non-linear moment equations, however the necessary mathematical tools in the non-linear setting will be more sophisticated. Our example with a linearized discrete velocity model showed that the scale induced closure is performing very well in approximating the high-dimensional kinetic evolution by low dimensional equations, giving good reasons to also use it in more general settings.

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A Appendix: Proof of Lemma 2 Part 2

We proove that $E_1 = G^\dagger$ given symmetry of $S = GE_1$ and conditions (31). Denote $N := dim(V) < \infty$.

A singular value decomposition of G yields

$$G = U \left(\begin{array}{c} \mathbf{\Sigma} \in \mathbb{R}^{q\times q} \\ \hline \mathbf{0} \in \mathbb{R}^{(N-q)\times q} \end{array} \right) W^*, \tag{109}$$

with $U \in \mathbb{R}^{N\times N}$ and $W \in \mathbb{R}^{q\times q}$ orthogonal, and $\Sigma \in \mathbb{R}^{q\times q}$ the diagonal matrix containing the non zero singular values of G. Any left inverse E_1 of G is of the form

$$E_1 = W \left(\begin{array}{c|c} \Sigma^{-1} & \mathbf{C} \in \mathbb{R}^{q\times(N-q)} \end{array} \right) U^*, \tag{110}$$

with $\mathbf{C}$ an arbitrary matrix. Now

$$GE_1 = U \left(\begin{array}{c|c} \mathbf{id} \in \mathbb{R}^{q\times q} & \mathbf{\Sigma}\cdot\mathbf{C} \\ \hline \mathbf{0}\cdot\mathbf{\Sigma}^{-1} & \mathbf{0}\cdot\mathbf{C} \end{array} \right) U^*. \tag{111}$$

This can only be symmetric if $\mathbf{C} = \mathbf{0}$, which yields the Moore-Penrose-inverse $G^\dagger$ in (110). For the case of a general Hilbertspace, we refer to Theorem 9.1.3 in [26].

B Appendix: Details for the 16 Velocities Model

For reference we give the detailed expressions for the distribution functions and the moment operator for different closures of the 16-velocity model.

B.1 Matrices

The velocities are ordered by

$$\begin{array}{cccc} c_1 = (-3,3), & c_2 = (-1,3), & c_3 = (1,3), & c_4 = (3,3), \\ c_5 = (-3,1), & c_6 = (-1,1), & c_7 = (1,1), & c_8 = (3,1), \\ c_9 = (-3,-1), & c_{10} = (-1,-1), & c_{11} = (1,-1), & c_{12} = (3,-1), \\ c_{13} = (-3,-3), & c_{14} = (-1,-3), & c_{15} = (1,-3), & c_{16} = (3,-3). \end{array} \tag{112}$$

which gives

$$V = \mathrm{Diag}\,(-3,-1,1,3,-3,-1,1,3,-3,-1,1,3,-3,-1,1,3) \tag{113}$$

for the advection operator. The diagonal interactions are defined by

$$K^{\mathrm{diag}}[u] = -\begin{pmatrix} u_2u_5 - u_1u_6 \\ u_1u_6 + u_3u_6 - u_2u_5 - u_2u_7 \\ u_2u_7 + u_4u_7 - u_3u_6 - u_3u_8 \\ u_3u_8 - u_4u_7 \\ u_1u_6 + u_6u_9 - u_2u_5 - u_5u_{10} \\ u_2u_5 + u_2u_7 + u_5u_{10} + u_7u_{10} - u_1u_6 - u_3u_6 - u_6u_9 - u_6u_{11} \\ u_3u_6 + u_3u_8 + u_6u_{11} + u_8u_{11} - u_2u_7 - u_4u_7 - u_7u_{10} - u_7u_{12} \\ u_4u_7 + u_7u_{12} - u_3u_8 - u_8u_{11} \\ u_5u_{10} + u_{10}u_{13} - u_6u_9 - u_9u_{14} \\ u_6u_9 + u_6u_{11} + u_9u_{14} + u_{11}u_{14} - u_5u_{10} - u_7u_{10} - u_{10}u_{13} - u_{10}u_{15} \\ u_7u_{10} + u_7u_{12} + u_{10}u_{15} + u_{12}u_{15} - u_6u_{11} - u_8u_{11} - u_{11}u_{14} - u_{11}u_{16} \\ u_8u_{11} + u_{11}u_{16} - u_7u_{12} - u_{12}u_{15} \\ u_9u_{14} - u_{10}u_{13} \\ u_{10}u_{13} + u_{10}u_{15} - u_9u_{14} - u_{11}u_{14} \\ u_{11}u_{14} + u_{11}u_{16} - u_{10}u_{15} - u_{12}u_{15} \\ u_{12}u_{15} - u_{11}u_{16} \end{pmatrix} \tag{114}$$

and the straight interactions are taken to be

$$K^{\mathrm{straight}}[u] = -\begin{pmatrix} 0 \\ u_5u_7 - u_2u_{10} \\ u_6u_8 - u_3u_{11} \\ 0 \\ -(u_5u_7 - u_2u_{10}) \\ -(u_6u_8 - u_3u_{11}) - (u_6u_{14} - u_9u_{11}) \\ -(u_5u_7 - u_2u_{10}) - (u_7u_{15} - u_{10}u_{12}) \\ -(u_6u_8 - u_3u_{11}) \\ u_6u_{14} - u_9u_{11} \\ u_5u_7 - u_2u_{10} + u_7u_{15} - u_{10}u_{12} \\ u_6u_8 - u_3u_{11} - (u_9u_{11} - u_6u_{14}) \\ u_7u_{15} - u_{10}u_{12} \\ 0 \\ u_9u_{11} - u_6u_{14} \\ u_{10}u_{12} - u_7u_{15} \\ 0 \end{pmatrix} \tag{115}$$

Fig. 3 displays the interactions in the velocity grid. The linearized collision operator becomes

$$K = -\begin{pmatrix}
-1 & 1 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -3 & 1 & 0 & 0 & 2 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & -3 & 1 & 0 & 0 & 2 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & -3 & 2 & -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 2 & 0 & 0 & 2 & -6 & 2 & -1 & 0 & 2 & 1 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 2 & -1 & -1 & 2 & -6 & 2 & 0 & 1 & 2 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1 & 0 & -1 & 2 & -3 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -3 & 2 & -1 & 0 & 1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 2 & 1 & 0 & 2 & -6 & 2 & -1 & -1 & 2 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 1 & 2 & 0 & -1 & 2 & -6 & 2 & 0 & 0 & 2 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 2 & -3 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 2 & 0 & 0 & 1 & -3 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 2 & 0 & 0 & 1 & -3 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 1 & -1
\end{pmatrix} \tag{116}$$

which is a symmetric positive definite matrix in $\mathbb{R}^{16\times 16}$.

B.2 Construction of the Operators for the Classical Closures:

The orthogonal complement of $\ker(K)$ is spanned by vectors r_1,...,r_{12}. The matrix M_0 consisting of equilibrium and r_1,...,r_{12} (see also (87)) gives an equivalent formulation of (86) in terms of moments

$$\partial_t M_0 f(x,t) + M_0 V M_0^{-1} \partial_x M_0 f + \frac{1}{\varepsilon} M_0 K M_0^{-1} M_0 f = 0. \tag{117}$$

The complete moment operator M_0 can be computed to be

$$M_0 = \left(\begin{array}{c} M_0^{(1)} \\ \hline M_0^{(2,1)} \;\big|\; id \end{array}\right) \in \mathbb{R}^{16\times 16} \tag{118}$$

with submatrices

$$M_0^{(1)} = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-3 & -1 & 1 & 3 & -3 & -1 & 1 & 3 & -3 & -1 & 1 & 3 & -3 & -1 & 1 & 3 \\
3 & 3 & 3 & 3 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -3 & -3 & -3 & -3 \\
18 & 10 & 10 & 18 & 10 & 2 & 2 & 10 & 10 & 2 & 2 & 10 & 18 & 10 & 10 & 18 \\
-1 & 3 & -3 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} \tag{119}$$

and

$$M_0^{(2,1)} = \begin{pmatrix}
1 & 1 & 0 & 0 & 1 & 1 & 0 & -1 & 0 & 0 & -1 \\
-1 & 0 & 3 & 2 & 1 & 2 & 5 & 6 & 5 & 6 & 9 \\
0 & -1 & -3 & -1 & -1 & -2 & -4 & -3 & -3 & -4 & -6 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & -1 & -1 & -2 & -2 & -2 & -2 & -3 & -3 & -3 & -3
\end{pmatrix}^T \tag{120}$$

and $id \in \mathbb{R}^{11\times 11}$. In the complete moment representation the production term then becomes

$$M_0 K M_0^{-1} = -\left(\begin{array}{c|cccccccccccc} \mathbf{0}\in\mathbb{R}^{4\times 4} & \multicolumn{12}{c}{\mathbf{0}\in\mathbb{R}^{4\times 12}} \\ \hline & -4 & 7 & -7 & 1 & 0 & -3 & 3 & 0 & 0 & 0 & 0 & 0 \\ & 0 & -11 & 3 & -1 & -1 & 3 & 1 & 0 & 0 & -1 & 0 & 0 \\ & -2 & -1 & -7 & 2 & -1 & 1 & 3 & 0 & 0 & 0 & -1 & 0 \\ & -2 & 3 & -3 & -3 & -1 & -3 & 3 & 1 & 0 & 0 & 0 & 0 \\ & -1 & 0 & 0 & 0 & -5 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ \mathbf{0}\in\mathbb{R}^{12\times 4} & -1 & -1 & 1 & 0 & 0 & -7 & 3 & -1 & -1 & 2 & 0 & 0 \\ & -2 & 0 & 0 & 0 & -3 & 0 & -4 & 2 & 0 & 0 & 2 & -1 \\ & -4 & 6 & -6 & 1 & -2 & -6 & 6 & -3 & 0 & 0 & 0 & 1 \\ & -3 & 7 & -3 & 0 & -2 & -7 & 3 & 0 & -1 & 1 & 0 & 0 \\ & -3 & 3 & -3 & 0 & -3 & -3 & 3 & 0 & 1 & -3 & 1 & 0 \\ & -4 & 6 & -6 & 0 & -3 & -6 & 6 & 0 & 0 & 1 & -3 & 1 \\ & -6 & 13 & -9 & 0 & -3 & -9 & 5 & 1 & 0 & 0 & 1 & -1 \end{array}\right) \tag{121}$$

We now are using M_0 to construct the operators for the various closures.. The equilibrium distribution $M\rho$ is parametrised by the four equilibrium moments only

$$M\rho = M_0^{-1}\left(\begin{array}{c|c|c} id\in\mathbb{R}^{4\times 4} & \mathbf{0}\in\mathbb{R}^{4\times 12} \end{array}\right)^T \rho = \left(\tfrac{1}{80}\tilde{M}\right)^T \rho \tag{122}$$

with

$$\tilde{M} = \begin{pmatrix} -\frac{3}{2} & 5 & 5 & -\frac{3}{2} & 5 & \frac{7}{2} & \frac{7}{2} & 5 & 5 & \frac{7}{2} & \frac{7}{2} & 5 & -\frac{3}{2} & 5 & 5 & -\frac{3}{2} \\ -3 & -1 & 1 & 3 & -3 & -1 & 1 & 3 & -3 & -1 & 1 & 3 & -3 & -1 & 1 & 3 \\ 3 & 3 & 3 & 3 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -3 & -3 & -3 & -3 \\ \frac{5}{4} & 0 & 0 & \frac{5}{4} & 0 & -\frac{5}{4} & -\frac{5}{4} & 0 & 0 & -\frac{5}{4} & -\frac{5}{4} & 0 & \frac{5}{4} & 0 & 0 & \frac{5}{4} \end{pmatrix} \tag{123}$$

Correspondingly, we construct the equilibrium operator as

$$E_0 f = \left(\begin{array}{c|c|c} id\in\mathbb{R}^{4\times 4} & \mathbf{0}\in\mathbb{R}^{4\times 12} \end{array}\right) M_0 f, \tag{124}$$

This operator turns out to be

$$E_0 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -3 & -1 & 1 & 3 & -3 & -1 & 1 & 3 & -3 & -1 & 1 & 3 & -3 & -1 & 1 & 3 \\ 3 & 3 & 3 & 3 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -3 & -3 & -3 & -3 \\ 18 & 10 & 10 & 18 & 10 & 2 & 2 & 10 & 10 & 2 & 2 & 10 & 18 & 10 & 10 & 18 \end{pmatrix}. \tag{125}$$

B.2.1 Grad

Arbitrary Moments

For the higher moments in Grad's closure, we arbitrarily chose $\mu_1 = E_1 r_1$, $\mu_2 = E_1 r_2$ and $\mu_3 = E_1 r_3$, with the again arbitrary choices of G and E_1 as

$$G = M_0^{-1}\left(\begin{array}{c|c|c|c} \mathbf{0}\in\mathbb{R}^{3\times 4} & id\in\mathbb{R}^{3\times 3} & \mathbf{0}\in\mathbb{R}^{3\times 9} \end{array}\right)^T = M_0^{-1}\left(\tfrac{1}{80}\tilde{G}\right)^T \tag{126}$$

with

$$\tilde{G} = \begin{pmatrix} -15 & -11 & -17 & 47 & 1 & 5 & -1 & -17 & 7 & 11 & 5 & -11 & 3 & 7 & 1 & -15 \\ -1 & -9 & -7 & 5 & -9 & 63 & -15 & -3 & -7 & -15 & -13 & -1 & 5 & -3 & -1 & 11 \\ 5 & -7 & -9 & -1 & -3 & -15 & 63 & -9 & -1 & -13 & -15 & -7 & 11 & -1 & -3 & 5 \end{pmatrix} \tag{127}$$

and

$$E_1 = \left(\begin{array}{c|c|c} \mathbf{0} \in \mathbb{R}^{3\times 4} & id \in \mathbb{R}^{3\times 3} & \mathbf{0} \in \mathbb{R}^{3\times 9} \end{array} \right) M_0 \tag{128}$$

$$= \begin{pmatrix} \text{-1} & 3 & \text{-3} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \text{-1} & 0 & 0 & \text{-1} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & \text{-1} & 0 & \text{-1} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{129}$$

As mentioned in 9.2.4, these operators fullfill the requirements (26), but not necessarily (33).

Kinetic Fluxes as Moments
The additional moments can be directly computed as

$$\begin{array}{rcl} q_x & = & \left(\text{-54} \quad \text{-10} \quad 10 \quad 54 \quad \text{-30} \quad \text{-2} \quad 2 \quad 30 \quad \text{-30} \quad \text{-2} \quad 2 \quad 30 \quad \text{-54} \quad \text{-10} \quad 10 \quad 54 \right) \\ q_y & = & \left(54 \quad 30 \quad 30 \quad 54 \quad 10 \quad 2 \quad 2 \quad 10 \quad \text{-10} \quad \text{-2} \quad \text{-2} \quad \text{-10} \quad \text{-54} \quad \text{-30} \quad \text{-30} \quad \text{-54} \right) \\ \sigma_{xy} & = & \left(\text{-9} \quad \text{-3} \quad 3 \quad 9 \quad \text{-3} \quad \text{-1} \quad 1 \quad 3 \quad 3 \quad 1 \quad \text{-1} \quad \text{-3} \quad 9 \quad 3 \quad \text{-3} \quad \text{-9} \right) \end{array}$$

To fullfill the conditions (26), we project these moment vectors to the non-equilibrium phase space by applying $P = (id - ME_0)$. The resulting vectors are then normalized and form the lines of E_1.

Correspondingly we chose $G = E_1^T$, and construct the equations according to (27) and (28).

B.3 Direct Asymptotic Expansion

The conditions for 2nd order in Thm. 1 are met in the case of the 16 discrete velocities model. Nontheless, in this section we show how to directly do the asymptotic expansion of (50/51) in ε.

Let us abbreviate (50) and (51) as

$$\partial_t \begin{pmatrix} \rho \\ \mu \end{pmatrix} + \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \rho \\ \mu \end{pmatrix} + \frac{1}{\varepsilon} \begin{pmatrix} 0 & 0 \\ 0 & E \end{pmatrix} \begin{pmatrix} \rho \\ \mu \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{130}$$

with $A = E_0\mathbf{c}\cdot\nabla M$, $B = E_0\mathbf{c}\cdot\nabla G$, $C = E_1\mathbf{c}\cdot\nabla M$, $D = E_1\mathbf{c}\cdot\nabla G$, $E = E_1KG$.

Inserting the expansion $\mu = \varepsilon\mu_1 + \varepsilon^2\mu_2$ into (130) yields

$$\begin{aligned} \partial_t\rho + A\rho + B\left(\varepsilon\mu_1 + \varepsilon^2\mu_2\right) &= 0 \\ \partial_t\left(\varepsilon\mu_1 + \varepsilon^2\mu_2\right) + C\rho + D\left(\varepsilon\mu_1 + \varepsilon^2\mu_2\right) + \frac{1}{\varepsilon}E\left(\varepsilon\mu_1 + \varepsilon^2\mu_2\right) &= 0 \end{aligned} \tag{131}$$

and short calculations reveal that

$$\begin{aligned} &\mu_1 = -E^{-1}C\rho, \\ &\mu_2 = -E^{-1}D\mu_1 - E^{-1}\partial_t\mu_1 = E^{-1}DE^{-1}C\rho + E^{-1}E^{-1}C\partial_t\rho \overset{\text{Euler}}{=} E^{-1}DE^{-1}C\rho - E^{-1}E^{-1}CA\rho. \end{aligned} \tag{132}$$

Plugging this into (131) yields

$$\partial_t\rho + A\rho = \varepsilon BE^{-1}C\rho + \varepsilon^2 B\left(-E^{-1}DE^{-1}C\rho + E^{-1}E^{-1}CA\rho\right), \tag{133}$$

or, by using the definitions of A,...,E:

$$\begin{aligned}\partial_t\rho + E_0\mathbf{c}\cdot\nabla M\rho = \quad & \varepsilon E_0\mathbf{c}\cdot\nabla G\left(E_1KG\right)^{-1}E_1\mathbf{c}\cdot\nabla M\rho \\ & -\varepsilon^2 E_0\mathbf{c}\cdot\nabla G\left(E_1KG\right)^{-1}E_1\mathbf{c}\cdot\nabla G\left(E_1KG\right)^{-1}E_1\mathbf{c}\cdot\nabla M\rho \\ & +\varepsilon^2 E_0\mathbf{c}\cdot\nabla G\left(E_1KG\right)^{-1}\left(E_1KG\right)^{-1}E_1\mathbf{c}\cdot\nabla ME_0\mathbf{c}\cdot\nabla M\rho.\end{aligned} \tag{134}$$

This compares to the asymptotic expansion of the original kinetic equations, as given in (24)

$$\begin{aligned}\partial_t\rho + E_0\mathbf{c}\cdot\nabla M\rho = & -\varepsilon E_0(\mathbf{c}\cdot\nabla)K^\dagger(\mathbf{c}\cdot\nabla)M\rho \\ & -\varepsilon^2 E_0(\mathbf{c}\cdot\nabla)K^\dagger(\mathbf{c}\cdot\nabla)K^\dagger(\mathbf{c}\cdot\nabla)M\rho \\ & +\varepsilon^2 E_0(\mathbf{c}\cdot\nabla)K^\dagger K^\dagger(\mathbf{c}\nabla M)E_0(\mathbf{c}\cdot\nabla)M\rho.\end{aligned} \tag{135}$$

Using now the special structure of the 16-discrete velocities model (112), we can compute the coefficient matrices for first and second order, and get:

$$\begin{aligned}\partial_t\rho + E_0VM\partial_x\rho = \quad & \varepsilon E_0VG\left(E_1KG\right)^{-1}E_1VM\partial_x^2\rho \\ & -\varepsilon^2 E_0VG\left(E_1KG\right)^{-1}E_1VG\left(E_1KG\right)^{-1}E_1VM\partial_x^3\rho \\ & +\varepsilon^2 E_0VG\left(E_1KG\right)^{-1}\left(E_1KG\right)^{-1}E_1VME_0VM\partial_x^3\rho\end{aligned} \tag{136}$$

Computing the products shows equivalence with the Chapman-Enskog expansion of the original kinetic equations. Furthermore one can compute that this equivalence breaks down for third order (super-Burnett).

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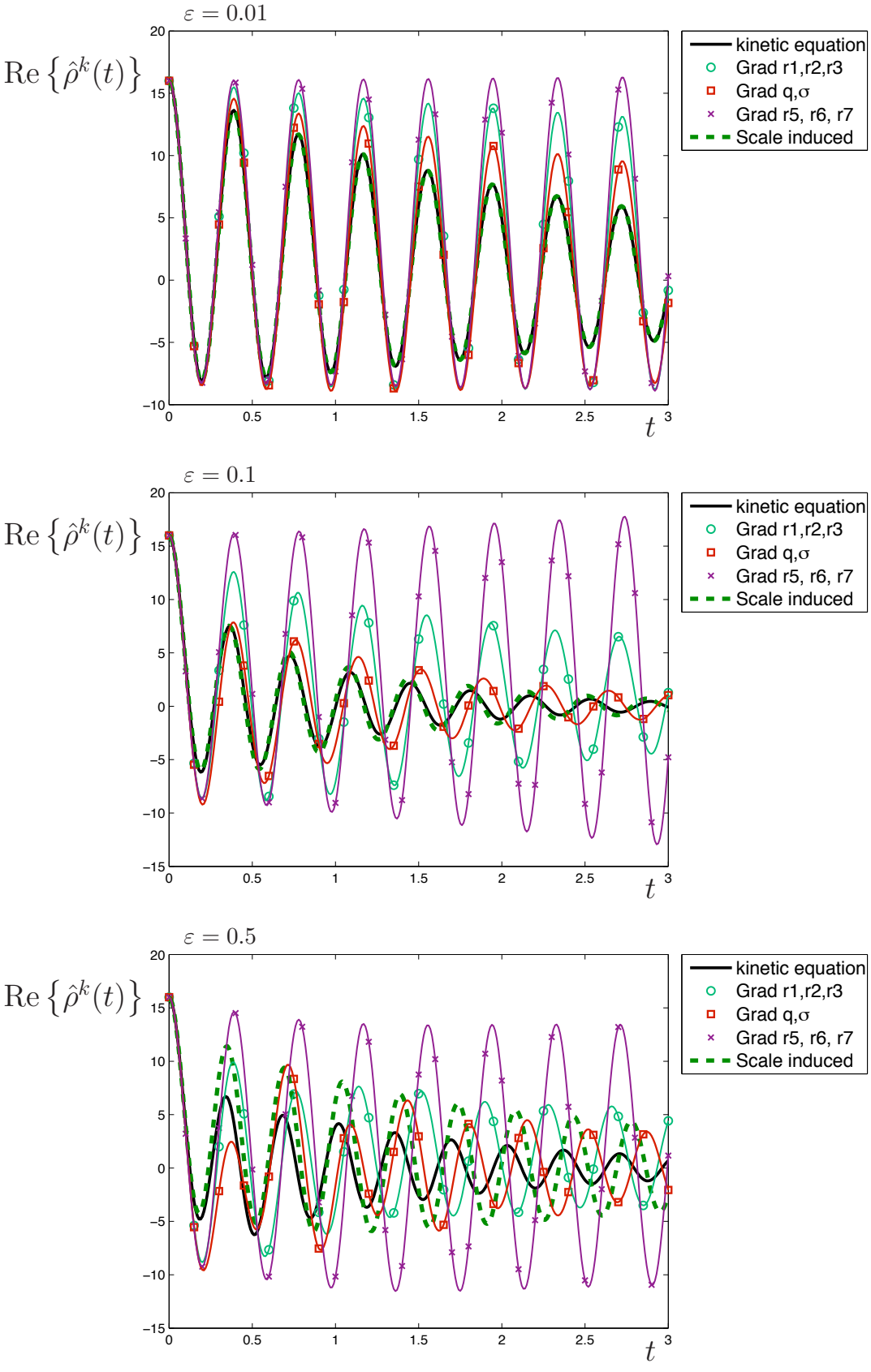

Figure 4: Various Grad closures for Fourier coefficient $k = 2\pi$ at $\varepsilon = 0.01$ (top), $\varepsilon = 0.1$ (middle) and $\varepsilon = 0.5$ (bottom).

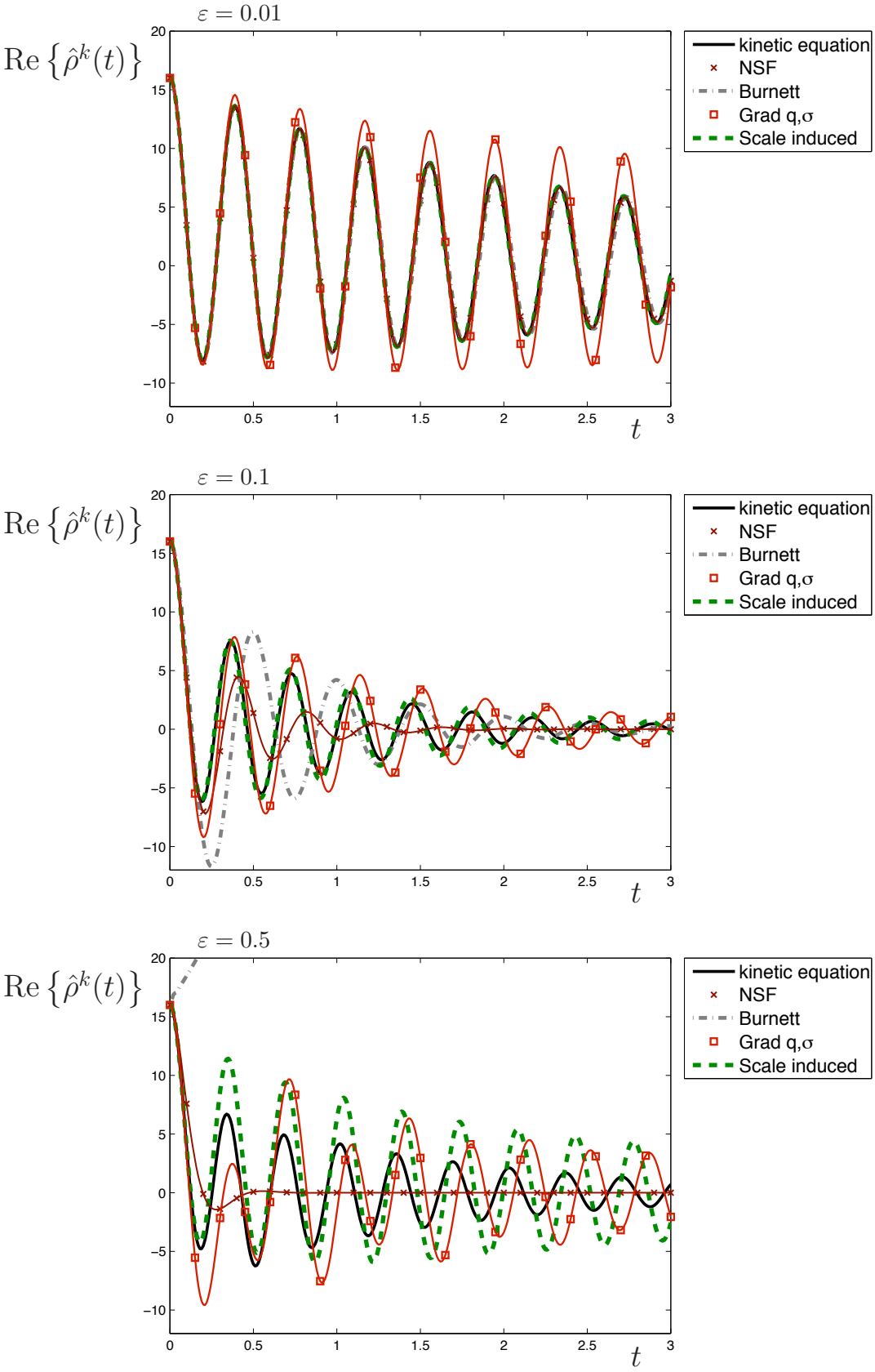

Figure 5: The different Closures for Fourier coefficient $k = 2\pi$ at $\varepsilon = 0.01$ (top), $\varepsilon = 0.1$ (middle) and $\varepsilon = 0.5$ (bottom).

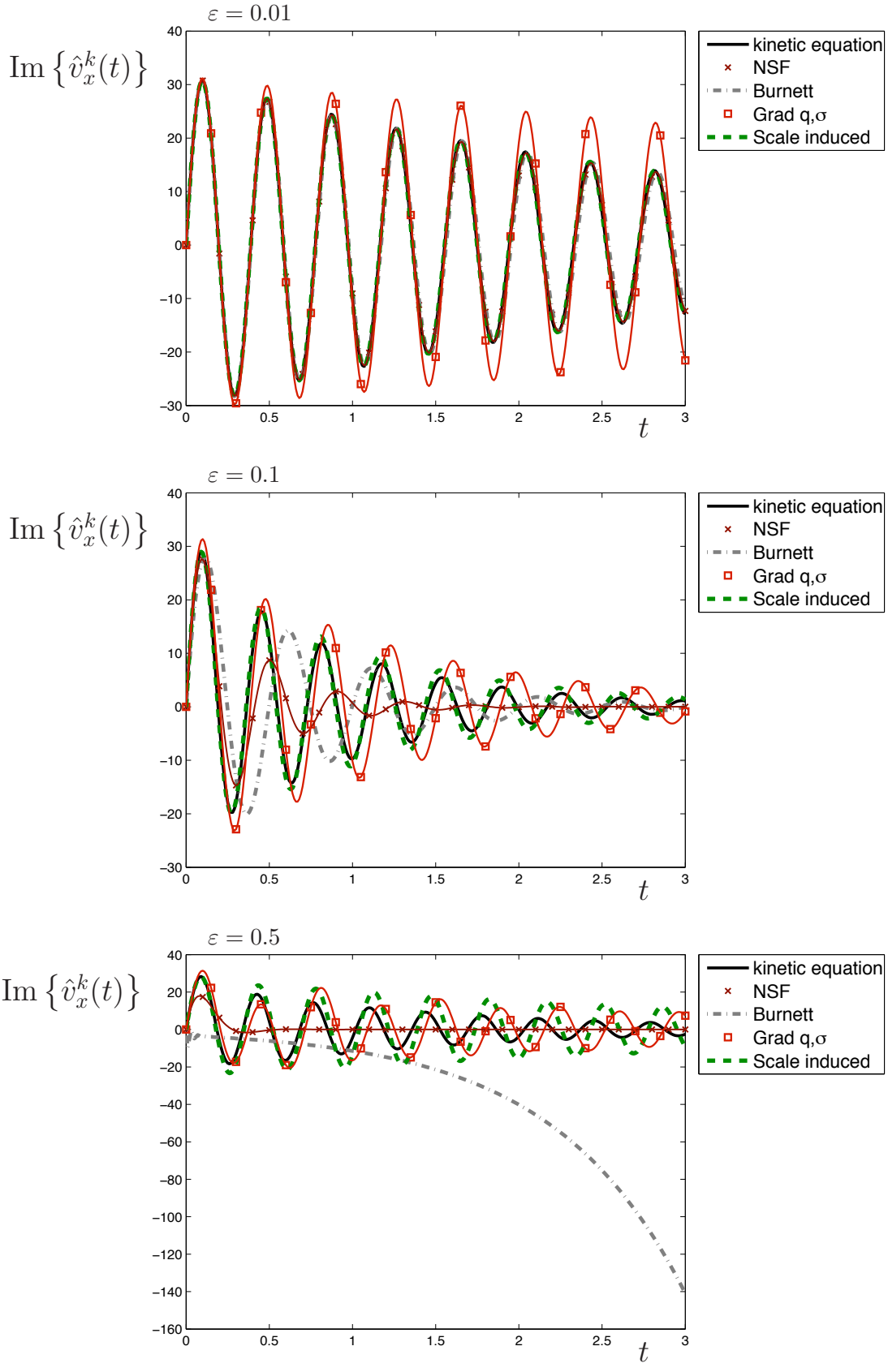

Figure 6: The different Closures for Fourier coefficient $k = 2\pi$ at $\varepsilon = 0.01$ (top), $\varepsilon = 0.1$ (middle) and $\varepsilon = 0.5$ (bottom).

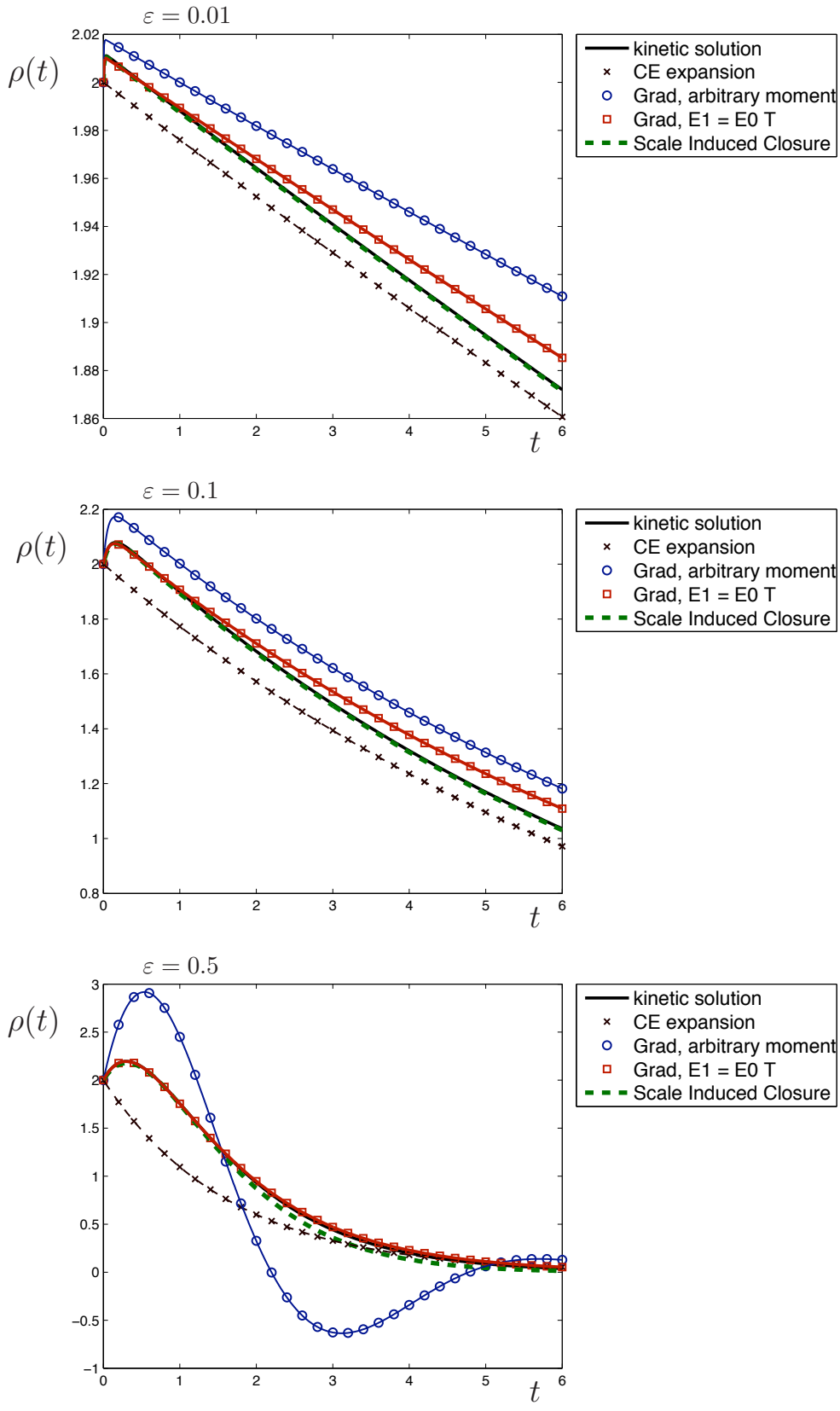

Figure 7: Solution of the full matrix system (98) and various lower dimensional approximations at $\varepsilon = 0.01$ (top), $\varepsilon = 0.1$ (middle) and $\varepsilon = 0.5$ (bottom).

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