Technische Universität Ilmenau
Institut für Mathematik

Preprint No. M 22/03

Balanced states and closure relations: the fluid dynamic limit of kinetic models

Babovsky, Hans; Bold, Lea

April 2022

URN: urn:nbn:de:gbv:ilm1-2022200188

Impressum:

Tel.: +49 3677 69-3621
Fax: +49 3677 69-3270
https://www.tu-ilmenau.de/mathematik/

Balanced States and Closure Relations: The Fluid Dynamic Limit of Kinetic Models

Hans Babovsky and Lea Bold
Technische Universität Ilmenau
Institute for Mathematics
Weimarer Str. 25
D-98693 Ilmenau, Germany,
email: hans.babovsky@tu-ilmenau.de,
lea.bold@tu-ilmenau.de

Abstract

The paper is concerned with closure relations for moment hierarchies of gaskinetic systems in the fluid dynamic limit. We develop the concept of balanced solutions which provides a more detailed description of kinetic solutions that the classical approaches. This allows to compare different models in use like the nonlinear Boltzmann equation, its linearization, and the BGK model and their relation to the classical Navier-Stokes equations.

Key words: Gas kinetic models, moment hierarchy, closure relations, fluid dynamic limit.

MSC classification: 76P05, 82B40

1 Introduction

A common way to pass from the detailed flow description provided by the equations of rarefied gas dynamics (Boltzmann collision operator, linearized collision operator, BGK model etc.) to the reduced moment system (Euler, Navier-Stokes) is to establish the moment hierarchy and to truncate it applying appropriate closure relations. Classical ways of doing this are the assumption of local equilbrium (leading to the hyperbolic system of the Euler equations) or e.g. a formal series expansion technique as proposed by Chapman and Enskog (turning the Euler equations into the parabolic system of the Navier-Stokes equations). These fluid dynamical systems are at present widely accepted. However, there are situations which are not adequately described and need some corrections. An example is the "ghost effect" produced by in the course of a series expansion in connection with a condensation-evaporation problem of a gas mixture as described in [1].

A way to avoid the paradox described in [1] is to pass from a description centered around local equilibria (Maxwellians) to one which focusses on the tangent space of the manifold of Maxwellians. In [4] we proposed such a procedure for the condensation-evaporation problem and investigated the perturbation of the spectrum of the linearized collision operator under a moving obstacle in the flow. In the present paper, we pick up the idea of some kind of dynamics in tangent space for a single-species gas (without recourse to the condensation-evaporation problem). We derive closure relations which take the form of nonlinear first order differential terms and thus are completely different from the parabolic second order terms of the Navier-Stokes system. The results allow to interpret the differences of various kinetic models (here: nonlinear and linearized Boltzmann collision operators and the BGK relaxation operator) in the fluid dynamical limit. As particular results we point at a purely nonlinear effect of the Boltzmann collision operator which is not reflected in the Navier-Stokes approach (section 5.3), and we demonstrate that the BGK system produces systematic artificial effects which are non-local and which do not vanish in the fluid dynamical limit (section 6.1).

The idea to construct intermediate states between arbitrary density functions and Maxwellians is not new. E.g. Shakhov [9] proposed such a system which is at present used for numerical simulations [11]. A comparable intention lies behind the idea of the extended BGK model with an additional relaxation parameter to match the correct Prandtl number. However, a better understanding of the transfer to fluid dynamics is not a question of parameter matching, and the above approaches do not yield a theoretical basis and a save mathematical ground. Proposing a modified structure of kinetic solutions, the present paper claims to provide a new attempt to better understand the passage from the rarefied gas description to the macroscopic limit.

The paper is organized as follows. Section 2 gives a short review over the abovementioned kinetic models. Section 3 introduces the general (non-closed) moment system derived from gas kinetics and derives the Euler system. Section 4 reinterprets the steps of the first order Chapman-Enskog approach for the Navier-Stokes system. In this way the central point of procedure can be generalized and becomes applicable to the full nonlinear collision operator without recourse to a formal series expansion. A new concept of balanced states is introduced, which are elements of the tangent space to the manifold of the Maxwellians and which replace (resp. supplement) the first order terms of the density function as provided by the Chapman-Enskog procedure. In Section 5 we introduce the concept of traces of kinetic solutions. Traces are comparable to projections of kinetic solutions onto the tangent spaces. The differential structure of the underlying dynamics provides a powerful tool to describe distributions in the neighborhood of Maxwellians. In order to keep the underlying ideas as concise and understandable as possible, we restrict theory and numerical examples to one-species gases in simple one-dimensional steady situations. Section 6 applies the results to the heat layer problem, yields numerical simulations and comparisons and shortly discusses further fields of application. All numerical simulations of the paper are produced by applying 2D and 3D Discrete Velocity Models (DVM) to all of the above kinetic systems.

2 Kinetic Models

The most fundamental kinetic model equation for a density function $f = f(t, x, v)$ (with space variable x and velocity variable $v = (v_\xi)_{\xi=1}^d$) of a single-species gas in the $2d$-dimensional phase space $\mathbb{R}^d \times \mathbb{R}^d$ ($d = 2, 3$) is the classical Boltzmann equation

$$(\partial_t + v\nabla_x)f = \frac{1}{\epsilon} \cdot C_J f \tag{1}$$

The small parameter ϵ is related to the mean free path in the gas and in some sense measures the distance to the fluid dynamic limit $\epsilon \searrow 0$.

The *Boltzmann collision operator* $C_J f = J[f, f]$ is a bilinear operator integrating over all possible conservative two-particle collisions and thus satisfying the conservation laws

$$\langle 1, C_J f\rangle = 0 \qquad \text{(mass conservation)} \tag{2}$$

$$\langle v, C_J f\rangle = 0 \qquad \text{(momentum conservation)} \tag{3}$$

$$\langle v^2, C_J f\rangle = 0 \qquad \text{(energy conservation)} \tag{4}$$

It is ruled by the H-Theorem stating that in a space homogeneous environment all densities converge for $t \nearrow \infty$ to equilibrium functions e (these are density functions satisfying $C_J e = 0$);

all equilibrium functions are *Maxwellians*, i.e. functions of the form

$$e(v) = e[\rho, \overline{v}, T](v) = \frac{\rho}{\sqrt{2\pi T}^d} \cdot \exp\left(-|v - \overline{v}|^2/2T\right) \tag{5}$$

uniquely determined by their macroscopic moments

$$\rho = \langle 1, e\rangle \qquad \text{(density)} \tag{6}$$

$$\rho\overline{v} = \langle v, e\rangle \qquad \text{(momentum)} \tag{7}$$

$$T = \frac{1}{d\cdot\rho} \cdot \langle (v-\overline{v})^2, e\rangle \qquad \text{(temperature)} \tag{8}$$

(For an introduction to the Boltzmann equation see e.g. [6, 10].) The set of all Maxwellians is denoted by $\mathcal{E}$.

In the following we define by

$$\mathcal{M} \quad = \quad \mathrm{span}(1, v_\xi(\xi = 1, \ldots, d), v^2) \tag{9}$$

the space of collision invariants, and by $\mathcal{M}^\perp$ its orthogonal complement. We make use of the

(2.1) Decomposition Lemma: Given a density function f and a Maxwellian e, there exists a unique decomposition

$$f \quad = \quad eM\cdot r + f_\perp, \quad r = (r_i)_{i=0}^{d+1}, \quad f_\perp \in \mathcal{M}^\perp \tag{10}$$

with M defined as

$$M \quad = \quad (1, v_\xi(\xi = 1, \ldots, d), v^2) \tag{11}$$

The decomposition takes the special form

$$f \quad = \quad e + f_\perp \tag{12}$$

if and only if e has the same macroscopic moments as f.
($eM\cdot r$ is a short hand notation for an element in $e\mathcal{M}$, fully written as $e\cdot(r_0 + \sum_{\xi=1}^d r_\xi v_\xi + r_{d+1} v^2)$.)

Proof: r can be uniquely determined by calculating mass, momenta and temperature on both sides of (10). $\square$

Two simplified alternatives to the nonlinear Boltzmann collision operator C_J are the *linearized collision operator* C_L and the *BGK relaxation model* C_{BGK}. Both are based on the decomposition (12). Given $f = e + f_\perp$, the Boltzmann collision operator is

$$J[f,f] = J[e,e] + J[e,f_\perp] + J[f_\perp,e] + J[f_\perp,f_\perp] = J[e,f_\perp] + J[f_\perp,e] + J[f_\perp,f_\perp]$$

Dropping the term which is quadratic in $f_\perp$, we end up with the *linearization of* C_J *around* e,

$$C_L f = L_e f = L_e f_\perp \quad = \quad J[e, f_\perp] + J[f_\perp, e] \tag{13}$$

L_e transfers f exponentially in time to its equilibrium e. The well-known properties of L_e are as follows.

(2.2) The linearized collision operator: Write $L_e f =: K(e^{-1}f)$. Then
(a) $\ker(K) = (\mathrm{im}(K))^\perp = \mathcal{M}$
(b) K is self-adjoint (e.g. in a weighted L^2 space) and negative semidefinite.
(c) The restriction $K : \mathcal{M}^\perp \to \mathcal{M}^\perp$ has an inverse K^{-1}.
(d) The linear system

$$C_L \psi = \phi \cdot e \tag{14}$$

is solvable iff $\phi \cdot e \in \mathcal{M}^\perp$. In this case, the solution is

$$\psi = L_e^\dagger \phi = e K^{-1}(\phi \cdot e) \tag{15}$$

It satisfies

$$\langle \phi, \psi \rangle = \langle \phi \cdot e, K^{-1}(\phi \cdot e) \rangle < 0 \tag{16}$$

For a more thorough treatment of L_e, see e.g. [7]. For corresponding results in the case of Discrete Velocity Models see [2, 3].

The simplest kind of exponential decay of f to its equilibrium e is given by the *one-parameter BGK model*

$$C_{BGK} f \quad = \quad \lambda \cdot (e - f) \tag{17}$$

The solution of the linear system (14) in the BGK case follows immediately from calculation.

(2.3) Linear system for BGK: Suppose $\phi \cdot e \in \mathcal{M}^\perp$. The unique solution of

$$C_{BGK} \psi = \phi \cdot e \tag{18}$$

is

$$\psi = e \cdot \left(1 - \frac{1}{\lambda} \cdot \phi\right), \quad \text{with} \quad \langle \phi, \psi \rangle = -\frac{1}{\lambda} \cdot \langle \phi, \phi \cdot e \rangle < 0 \tag{19}$$

3 The moment hierarchy and the Euler system

Taking scalar products $\langle m, . \rangle$ ($m \in \mathcal{M}$) of the Boltzmann equation (1) or one of its models, and taking into account that $\langle m, Cf \rangle = 0$ for any of the above collision operators we end up with the following moment hierarchy.

(3.4) General moment system: *(In the following, $\xi, \eta \in \{1, \ldots, d\}$.)*

$$\partial_t \rho + \nabla \cdot (\rho \overline{v}) = 0 \tag{20}$$

$$\partial_t (\rho \overline{v}_\xi) + \sum_\eta \partial_\eta (\rho \overline{v}_\xi \overline{v}_\eta + p_{\xi\eta}) = 0 \tag{21}$$

$$\partial_t \left(\rho \cdot |\overline{v}|^2 + d \cdot p\right) + \sum_\xi \partial_\xi \left[\rho \overline{v}_\xi |\overline{v}|^2 + q_\xi + 2(P\overline{v})_\xi + d \cdot p \overline{v}_\xi\right] = 0 \tag{22}$$

with *pressure tensor* P, *pressure* p and *heat flux* q as defined below.

(20) to (22) is not a closed system, since it contains the *closure moments*

$$P = (p_{\xi,\nu})_{1 \le \xi,\nu \le d} = (\langle \pi_{\xi,\nu}, f \rangle)_{1 \le \xi,\nu \le d} \quad \text{(pressure tensor)} \tag{23}$$

$$q = (q_\xi)_{\xi=1}^d = (\langle \sigma_\xi, f \rangle)_{\xi=1}^d \quad \text{(heat flux)} \tag{24}$$

described by the macroscopic moments (6) to (8) and the *centered moments*

$$\pi_{\xi,\nu} = \pi_{\xi,\nu}(\overline{v}) = (v_\xi - \overline{v}_\xi)(v_\nu - \overline{v}_\nu) \quad l \le \xi, \nu \le d \tag{25}$$

$$\sigma_\xi = \sigma_\xi(\overline{v}) = \frac{1}{2}(v_\xi - \overline{v}_\xi)|v - \overline{v}|^2 \tag{26}$$

For given $e = e[\rho, \overline{v}, T]$, $\xi \ne \nu$, the function $\pi_{\xi,\nu} e \in \mathcal{M}^\perp$. For the other centered moments, the projections onto $\mathcal{M}^\perp$ are given by

$$\hat{\pi}_\xi = \pi_{\xi\xi} - \frac{1}{d} \sum_\nu \pi_{\nu\nu} \tag{27}$$

$$\hat{\sigma}_\xi = \hat{\sigma}_\xi(\overline{v}, T) = \sigma_\xi - \frac{(d+2) \cdot T}{2} \cdot (v_\xi - \overline{v}_\xi) \tag{28}$$

The *pressure* p is defined by

$$p = d^{-1} \langle |v - \overline{v}|^2, f \rangle = \rho T \tag{29}$$

The easiest way to close system (20) to (22) is to assume that f is in its local equilibrium (which is formally the case in the limit $\epsilon \searrow 0$). This gives

$$P = p \cdot I = \rho T \cdot I, \quad q = 0 \tag{30}$$

with the resulting hyperbolic moment system

(3.5) Euler equations:

$$
\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho \overline{v}) &= 0 && (31)\\
\partial_t (\rho \overline{v}) + \nabla \cdot (\rho \overline{v} \otimes \overline{v}) + \nabla(\rho T) &= 0 && (32)\\
\partial_t (\rho |\overline{v}|^2 + d \cdot \rho T) + \nabla \cdot (\rho \overline{v} |\overline{v}|^2) + (d+2) \nabla \cdot (\rho T \cdot \overline{v}) &= 0 && (33)
\end{aligned}
$$

4 Navier-Stokes equations and balanced states

A prominent role in the refinement of the Euler system play the solutions $\psi_{\xi,\nu}$ $(\xi \neq \nu)$, $\hat{\psi}_\xi$ and ψ_ξ^σ in $\mathcal{M}^\perp$ of the linear equations

$$
\begin{aligned}
C_L \psi_{\xi,\nu} &= \pi_{\xi,\nu} e && (34)\\
C_L \hat{\psi}_\xi &= \hat{\pi}_{\xi,\nu} e && (35)\\
C_L \psi_\xi^\sigma &= \hat{\sigma}_\xi e && (36)
\end{aligned}
$$

(For the solvability of the equations see (2.2)(d).)

A convenient way to derive the Navier-Stokes system is the Chapman Enskog expansion of first order [8]. Here we plug the ansatz

$$f = f_0 + \epsilon f_1$$

into the Boltzmann equation (1) and compare the terms of equal power of ϵ. For ϵ^{-1} we find

$$C_J[f_0] = 0$$

and thus $f_0 = e \in \mathcal{E}$. Power ϵ^1 yields

$$(\partial_t + v \cdot \nabla_x) e = C_L f_1 \qquad (37)$$

For its solution we perform the decomposition (12) for (37). While the part related to the Maxwellian e is integrated into the moment system, the part acting on $\mathcal{M}^\perp$ reads

$$((\partial_t + v \cdot \nabla_x) e)_\perp = C_L f_1 \qquad (38)$$

with

$$
\begin{aligned}
((\partial_t + v \cdot \nabla_x) e)_\perp &= (v \cdot \nabla_x e)_\perp \\
&= \rho \cdot \sum_\xi \sum_\nu \partial_\xi \overline{v}_\nu \left(v_\xi \partial_{\overline{v}_\nu} e[1, \overline{v}, T] \right)_\perp + \rho \cdot \sum_\xi \left(v_\xi \partial_T e[1, \overline{v}, T] \cdot \partial_\xi T \right)_\perp \\
&= \frac{\rho}{T} \cdot \sum_\xi \sum_\nu \partial_\xi \overline{v}_\nu \cdot \pi_{\xi,\nu} e + \frac{\rho}{T^2} \cdot \sum_\xi \partial_\xi T \cdot \hat{\sigma}_\xi e && (39)
\end{aligned}
$$

The solution of (38) is

$$f_1^{NS} \;=\; \frac{1}{T}\cdot\sum_\xi\left[\sum_{\nu\neq\xi}\partial_\xi\overline{v}_\nu\cdot\psi_{\xi\nu}+\partial_\xi\overline{v}_\xi\cdot\hat{\psi}_\xi\right]\cdot e+\frac{\epsilon}{2T^2}\cdot\sum_\xi\partial_\xi T\cdot\psi_\xi^\sigma\cdot e \tag{40}$$

From this we derive the *Navier-Stokes correction* to the Euler equations by calculating the moment system (3.4) for the function $f = e + \epsilon f^{(1)}$. Taking into account the inequalities (16), we find the correction terms to the closure moments of the Euler system,

$$p_{\xi,\xi}^{NS} \;=\; -\epsilon\cdot\mu^{(1)}\cdot\frac{d}{d-1}\cdot\frac{1}{T}\cdot\left(\partial_\xi\overline{v}_\xi-\frac{1}{d}\nabla\cdot\overline{v}\right) \tag{41}$$

$$p_{\xi,\nu}^{NS} \;=\; -\epsilon\mu^{(2)}\cdot\frac{1}{T}\cdot(\partial_\xi\overline{v}_\nu+\partial_\nu\overline{v}_\xi) \qquad (\xi\neq\nu) \tag{42}$$

$$q_\xi^{NS} \;=\; -\epsilon\cdot\lambda\cdot\frac{1}{2T^2}\cdot\partial_\xi T \tag{43}$$

with the positive viscosity resp. heat coefficients

$$\mu^{(1)} \;=\; -\langle\hat{\pi}_\xi,\hat{\psi}_\xi\rangle \tag{44}$$

$$\mu^{(2)} \;=\; -\langle\pi_{\xi,\nu},\psi_{\xi,\nu}\rangle \tag{45}$$

$$\lambda \;=\; -\langle\hat{\sigma}_\xi,\psi_\xi^\sigma\rangle \tag{46}$$

thus introducing parabolic smoothing terms into the hyperbolic system.

All the above results are classical and need no further explanation. Here, we find a way to reinterpret the Chapman Enskog results and to generalize them, without making use of the series expansion.

(4.6) Lemma: Let $e = e(t_0, x_0)$ be a fixed Maxwellian and $s = s(t_0, x_0) = v\cdot\nabla_x e$ the corresponding flow term. The expansion of first order $f^{(0)} + \epsilon\cdot f^{(1)}$ of Chapman-Enskog is the unique asymptotic solution ($\tau \nearrow \infty$) of the time-homogeneous initial value problem (IVP)

$$\partial_\tau f+\epsilon\cdot s_\perp \;=\; L_e f, \quad f(t_0)=e$$

Proof: Decompose f uniquely into the form

$$f(\tau) \;=\; f_\|(\tau)+f_\perp(\tau), \quad f_\|(\tau)\in e\cdot\mathcal{M}, \quad f_\perp\in\mathcal{M}^\perp$$

Since $f_\|(\tau)\in\ker(L_e)$ and $s_\perp\in\mathcal{M}^\perp$, we find

$$f_\|(\tau) \;=\; e$$

and $f_\perp(\tau)$ solution of the IVP in $\mathcal{M}^\perp$,

$$\partial_\tau f_\perp + \epsilon \cdot s_\perp \;=\; L_e f_\perp, \quad f_\perp(t_0) = 0$$

From the invertibility and negative definiteness of $C_L : \mathcal{M}^\perp \to \mathcal{M}^\perp$ we conclude thet the asymptotic solution

$$f_\perp^\infty = \lim_{\tau \nearrow \infty} f_\perp(\tau)$$

exists and satisfies

$$\epsilon \cdot s_\perp \;=\; L_e f_\perp^\infty$$

Thus $f_\perp^\infty = \epsilon \cdot f^{(1)}$. □

The Chapman Enskog procedure as sketched above may be seen as a special case of the following three-step procedure for the calculation of closure relations.

(4.7) Scheme for closure relations: *(1)* Let (t_0, x_0) and $f = f(t_0, x_0)$ be given and fixed. Calculate a reduced description $\mathbf{f}$ of f containing all information concerning the relevant moments.

(2) For an appropriate approximation $\mathbf{C}$ of the Boltzmann collision operator solve the IVP

$$\partial_\tau g + \epsilon \cdot (v \cdot \nabla_x \mathbf{f})_\perp \;=\; \mathbf{C} g, \quad g(0) = \mathbf{f} \tag{47}$$

(iii) Determine $g^\infty = \lim_{\tau \nearrow \infty} g(\tau)$ and calculate from this the closure relations for f.

In the Chapman-Enskog case, $\mathbf{f} = e$ and $\mathbf{C} = C_L$. In section 5 we are going to develop the concept of *traces*, in which $\mathbf{f}$ is a perturbation of e, and $\mathbf{C}$ is a reduced version of the full Boltzmann collision operator for $\mathbf{f}$.

We can derive (47) directly from the kinetic equation (1) (or model hereof): Introduce a microscopic time scale $\tau = (t - t_0)/\epsilon$ and solve the kinetic system. In lowest order in ϵ, we freeze the source term $(v \cdot \nabla_x \mathbf{f})_\perp$ at $\tau = 0$ and solve the system for $\tau \nearrow \infty$. In the following we call the distributions g^∞ *balanced states*, since they balance the trend to equilibrium given by the collision operator with the perturbing effects produced by the streaming term.

5 Traces in tangent space

5.1 Traces

The definitions of the linearized collision operator and of the BGK model as well as the results of the Chapman Enskog procedure suggest to focus on decompositions of f of the form (12) rather than (10). In this case, the central element e contains all macroscopic moments, but no contribution to the closure moments. In view of scheme (4.7) we propose an alternative approach. For simplicity we restrict in the following to spatially one-dimensional problems (with space variable x) and with bulk velocities $\overline{v} = (\overline{v}_x, 0)^T$ resp. $\overline{v} = (\overline{v}_x, 0, 0)^T$.

Given a triple $[\overline{\rho}, \overline{v}_x, \overline{T}]$ with corresponding Maxwellian $\overline{e} = e[\overline{\rho}, \overline{v}_x, \overline{T}]$, we define the *tangent space* $\mathcal{T}[\overline{e}]$ of $\mathcal{E}$ in $\overline{e}$ as the set of all elements in

$$\mathcal{E}\mathcal{M} = \bigcup_{e \in \mathcal{E}} e \cdot \mathcal{M} \tag{48}$$

with the same macroscopic moments $[\overline{\rho}, \overline{v}_x, \overline{T}]$ as $\overline{e}$. It is a two-dimensional manifold in $\mathcal{E}\mathcal{M}$ with elements

$$\mathbf{f}(\gamma^{(1)}, \gamma^{(2)}) = \hat{e} + \gamma^{(1)} \cdot \hat{e}^{(1)} + \gamma^{(2)} \cdot \hat{e}^{(2)} \quad \text{with} \tag{49}$$

$$\hat{e} = e[\overline{\rho}, \hat{v}_x, \hat{T}] \tag{50}$$

$$\hat{e}^{(1)} = \frac{1}{\hat{T}} \cdot (v_x - \hat{v}_x) \cdot \hat{e} \tag{51}$$

$$\hat{e}^{(2)} = \frac{1}{2\hat{T}^2} \cdot \left(|v - \hat{v}|^2 - d \cdot \hat{T}\right) \cdot \hat{e} \tag{52}$$

$(\gamma^{(1)}, \gamma^{(2)})$ and $(\hat{v}_x, \hat{T})$ are connected to $(\overline{v}_x, \overline{T})$ via

$$\hat{v}_x = \overline{v}_x - \gamma^{(1)} \tag{53}$$

$$\hat{T} = \overline{T} + \frac{1}{d} \cdot \left((\gamma^{(1)})^2 - \gamma^{(2)}\right) \tag{54}$$

which can be verified easily by calculating the moments of (49). The union of tangent spaces is denoted as

$$\mathcal{T}\mathcal{E} = \bigcup_{e \in \mathcal{M}} \mathcal{T}[e] \tag{55}$$

In the following, the parameter $\gamma^{(2)}$ is not relevant in the case of the full Boltzmann collision operator. Thus we set $\gamma^{(2)} = 0$, $\gamma^{(1)} := \gamma$ and define as the *trace* of $\overline{e}$ in $\mathcal{T}\mathcal{E}$ the mapping

$$\gamma \to \mathbf{f}(\gamma) = \hat{e} + \gamma \cdot \hat{e}^{(1)} \tag{56}$$

By definition, $\mathbf{f}(\gamma)$ has the same macroscopic moments as $\overline{e}$, however it contributes to the closure moments as follows.

(5.8) Closure relations for the trace: The closure moments of the trace elements (in relation to the macroscopic moments $\overline{v}_x$, $\overline{T}$ of $\mathbf{f}(\gamma)$) are

$$\langle \hat{\pi}_x(\overline{v}), \mathbf{f}(\gamma) \rangle = -\frac{d-1}{d} \cdot \rho\gamma^2 \tag{57}$$

$$\langle \hat{\sigma}_x(\overline{v}, \overline{T}), \mathbf{f}(\gamma) \rangle = -\rho\gamma^3 \tag{58}$$

Proof: These formulas follow from

$$\langle \hat{\pi}_x(\overline{v}), \mathbf{f}(\gamma)\rangle = \frac{d-1}{d} \cdot \rho \cdot \left((\hat{v}_x - \overline{v}_x)^2 + 2\gamma \cdot (\hat{v}_x - \overline{v}_x)\right) = -\frac{d-1}{d} \cdot \rho \cdot (\hat{v}_x - \overline{v}_x)^2$$

and

$$\langle \hat{\sigma}_x(\overline{v}, \overline{T}), \mathbf{f}(\gamma)\rangle = -\rho \cdot \frac{\hat{v}_x - \overline{v}_x}{2} \cdot \left(\frac{d-2}{d}(\hat{v}_x - \overline{v}_x)^2 + (d+2) \cdot (\hat{T} - \overline{T})\right) \qquad \square$$

Given $\mathbf{f}(\gamma)$, we denote as $e(\gamma) =: e[\overline{\rho}, \hat{v}_x, \hat{T}]$, $\hat{\pi}_x(\gamma)$ and $\hat{\sigma}_x(\gamma)$ the Maxwellian and the centered closure moments corresponding to the parameters $\hat{v}_x = \overline{v}_x - \gamma$ and $\hat{T} = \overline{T} + \gamma^2/d$. For given γ, the normed vectors $\mathbf{n}_\pi$ and $\mathbf{n}_\sigma$ point into the directions of these closure moments in the sense of

$$\hat{\pi}_x(\gamma) \cdot \hat{e}(\gamma) = \|\hat{\pi}_x(\gamma)\hat{e}(\gamma)\| \cdot \mathbf{n}_\pi \tag{59}$$

$$\hat{\sigma}_x(\gamma) \cdot \hat{e}(\gamma) = \|\hat{\sigma}_x(\gamma)\hat{e}(\gamma)\| \cdot \mathbf{n}_\sigma \tag{60}$$

Furthermore the *local tangent plane* is defined as the affine linear space

$$\mathbf{f}(\gamma) + \mathrm{span}(\mathbf{n}_\pi, \mathbf{n}_\sigma) \tag{61}$$

Given $\mathbf{z} = \|z\| \cdot \mathbf{n_z} \in \mathrm{span}(\mathbf{n}_\pi, \mathbf{n}_\sigma)$, the angle $\phi_\mathbf{z}$ defined by

$$\mathbf{n_z} = \cos(\phi_\mathbf{z}) \cdot \mathbf{n}_\pi + \sin(\phi_\mathbf{z}) \cdot \mathbf{n}_\sigma \tag{62}$$

describes the position of $\mathbf{f}(\gamma) + \mathbf{z}$ in the local tangent plane.

We collect some results concerning the local structure of $\mathbf{f}(\gamma)$ which can be proved by straightforward calculations.

(5.9) Differential structure of the trace : (a) $\mathbf{f}$ is differentiable with derivative

$$\partial_\gamma \mathbf{f} = \|\partial_\gamma \mathbf{f}\| \cdot \mathbf{n}_{\partial \mathbf{f}} = -\frac{\gamma}{\hat{T}^2} \cdot \|\hat{\pi}_x(\gamma) \cdot \hat{e}(\gamma)\| \cdot \mathbf{n}_\pi + \frac{2\gamma^2}{d \cdot \hat{T}^3} \cdot \|\hat{\sigma}(\gamma) \cdot \hat{e}(\gamma)\| \cdot \mathbf{n}_\sigma \tag{63}$$

(b) The leading order approximation of $\mathbf{f}(\gamma)$ for $|\gamma| \ll 1$ in the local tangent plane ($\gamma = 0$) is

$$\mathbf{f}(\gamma) = \overline{e} \cdot \left(1 - \frac{\gamma^2}{2 \cdot \overline{T}^2} \cdot \hat{\pi}_x(0) + \frac{2\gamma^3}{3d \cdot \overline{T}^3} \cdot \hat{\sigma}_x(0, \overline{T})\right) \tag{64}$$

(c) For $|\gamma| \ll 1$,

$$\tan(\phi_{\partial \mathbf{f}}(\gamma)) = -\frac{2\gamma}{d \cdot \hat{T}} \cdot \frac{\|\hat{\sigma}_x \hat{e}\|}{\|\hat{\pi}_x \hat{e}\|} =: -C_{\partial \mathbf{f}} \cdot \gamma + \mathcal{O}(\gamma^2) \tag{65}$$

$$\phi_{\partial \mathbf{f}} = \begin{cases} -C_{\partial \mathbf{f}} \cdot \gamma + \mathcal{O}(\gamma^2) & \text{for} \quad \gamma < 0 \\ \pi - C_{\partial \mathbf{f}} \cdot \gamma + \mathcal{O}(\gamma^2) & \text{for} \quad \gamma > 0 \end{cases} \tag{66}$$

Thus at $\gamma = 0$ the curve $\mathbf{f}(\gamma)$ is not differentiable in the sense of regular parametrizations.

Proof: (a) follows from straightforward calculations (using the definition (55) of $\mathbf{f}(\gamma)$ and formulas (52), (53)) which yield

$$\partial_\gamma \hat{e} = \left(-\frac{\gamma}{\hat{T}} - \frac{v_x - \hat{v}_x}{\hat{T}} + \frac{\gamma}{d \cdot \hat{T}^2} \cdot (v - \hat{v})^2 \right) \cdot \hat{e} \tag{67}$$

and

$$\partial_\gamma \left(\gamma \cdot \frac{v_x - \hat{v}_x}{\hat{T}} \right) = \frac{\gamma}{\hat{T}} + \left(\frac{1}{\hat{T}} - \frac{2\gamma^2}{d \cdot \hat{T}^2} \right) \cdot (v_x - \hat{v}_x) \tag{68}$$

(b) is obtained by integrating (62) and using $\mathbf{f}(0) = \overline{e}$ and $\partial_\gamma \mathbf{f}(0) = 0$. □

For the derivation of closure moments for the nonlinear collision operator it is useful to follow *the trace of* C_J along $\mathbf{f}(\gamma)$ which is defined as the projection of C_J given by

$$\begin{aligned} \mathbf{C}_J\mathbf{f}(\gamma) &= \langle C_J \mathbf{f}(\gamma), \mathbf{n}_{\partial \mathbf{f}} \rangle \cdot \mathbf{n}_{\partial \mathbf{f}} \\ &= \cos(\phi_{\partial \mathbf{f}}) \langle C_J \mathbf{f}(\gamma), \mathbf{n}_\pi \rangle \cdot \mathbf{n}_{\partial \mathbf{f}} + \sin(\phi_{\partial \mathbf{f}}) \cdot \langle C_J \mathbf{f}(\gamma), \mathbf{n}_\sigma \rangle \cdot \mathbf{n}_{\partial \mathbf{f}} \end{aligned} \tag{69}$$

(5.10) Trace of the nonlinear operator: (a) With

$$a^J_{\pi,\pi} = -\langle J[\hat{e}^{(1)}, \hat{e}^{(1)}], \mathbf{n}_\pi \rangle \tag{70}$$

the trace of C_J takes the form

$$\mathbf{C}_J\mathbf{f}(\gamma) = \operatorname{sign}(\gamma) \cdot \cos(\phi_{\partial \mathbf{f}}) \cdot \gamma^2 \cdot a^J_{\pi,\pi} \cdot \mathbf{n}_{\partial \mathbf{f}} \tag{71}$$

(b) Under the approximations of (5.9)(b),(c) for small γ,

$$\mathbf{C}_J\mathbf{f}(\gamma) = -\gamma^2 a^J_{\pi,\pi} \cdot \mathbf{n}_\pi + \mathcal{O}(\gamma^3)$$

The solution $\mathbf{f}(\gamma(t))$ of the homogeneous trace Boltzmann equation

$$\partial_t \mathbf{f}(\gamma(t)) = \mathbf{C}_J \mathbf{f}(\gamma(t)) \tag{72}$$

is in lowest order given by

$$\partial_t \gamma = -\lambda_{nl}\gamma, \quad \lambda_{nl} = a^J_{\pi,\pi} \cdot \overline{T}^2 \cdot \|\hat{\pi}_x \overline{e}\|^{-1} \tag{73}$$

Proof: (a) From the definition (55) of $\mathbf{f}(\gamma)$ and the fact that $\hat{e}^{(1)} \in \ker(L_{\hat{e}})$ follows

$$C_J \mathbf{f}(\gamma) = \gamma^2 \cdot J[\hat{e}^{(1)}, \hat{e}^{(1)}]$$

In a coordinate system centered around $\hat{v}$, $J[\hat{e}^{(1)}, \hat{e}^{(1)}]$ is an even function with respect to $\hat{v}_x$. Thus

$$\langle \hat{\sigma}_x(\gamma), J[\hat{e}^{(1)}, \hat{e}^{(1)}] \rangle = \langle \mathbf{n}_\sigma, J[\hat{e}^{(1)}, \hat{e}^{(1)}] \rangle = 0$$

(b) follows from inserting the approximations (5.9)(b),(c). $\square$

In our context, the most significant difference between the nonlinear collision operator on the one side, and the linearized and the BGK operator (shortly termed as *"relaxation operators"*) on the other side is that

$$C_J\mathbf{f}(\gamma) = \frac{\gamma^2}{\hat{T}^2} \cdot J[(v_x - \hat{v}_x) \cdot \hat{e}, (v_x - \hat{v}_x) \cdot \hat{e}] \tag{74}$$

is centered around $\hat{e}$ (with the asymptotics $\overline{e}$ "unvisible"), while the Maxwellian $\overline{e}$ appears in the definition of the relaxation operators and marks it as their asymptotic end point. For the same reason we find closed formulas for the solutions of the homogenous equations in the relaxation case,

$$f(t) = \overline{e} + \exp(tL_{\overline{e}}) \cdot (f_0 - \overline{e}) \quad \text{(linearized equation)} \tag{75}$$

$$f(t) = \overline{e} + \exp(-\lambda t) \cdot (f_0 - \overline{e}) \quad \text{(BGK equation)} \tag{76}$$

while the solution of the homogeneous nonlinear equation can be given only in differential form.

5.2 Relaxation problems

Consider the initial value problem

$$\partial_t f = Cf, \quad f(0) = f_0 = \hat{e} + \epsilon \cdot \phi$$

with C one of the collision operators discussed above. Depending on ϕ, there exists a unique Maxwellian $\overline{e}$ with the same macroscopic moments as f_0, which is the asymptotic state of the solution for $t \nearrow \infty$. In the relaxation case we have exponential decay to $\overline{e}$, see (75), (76). The dynamics of the nonlinear solution is more detailed, depending on the form of ϕ.

Suppose

$$\phi = \hat{e} \cdot m + \phi_\perp, \quad m \in \mathcal{M}, \quad \phi_\perp \in \mathcal{M}^\perp \tag{77}$$

Then

$$J[f_0, f_0] = J[\hat{e}, \hat{e}] + \epsilon \cdot (J[\hat{e}, m\hat{e}] + J[m\hat{e}, \hat{e}]) + \epsilon \cdot (J[\hat{e}, \phi_\perp] + J[\phi_\perp, \hat{e}]) + \mathcal{O}(\epsilon^2) \tag{78}$$

with

$$
\begin{aligned}
J[\hat{e},\hat{e}] &= 0 && (79)\\
J[\hat{e},m\hat{e}] + J[m\hat{e},\hat{e}] &= L_{\hat{e}} m\hat{e} = 0 && (80)\\
J[\hat{e},\phi_\perp] + J[\phi_\perp,\hat{e}] &= L_{\hat{e}}\phi_\perp && (81)
\end{aligned}
$$

For the short time behaviour we may neglect the $\mathcal{O}(\epsilon^2)$-terms. Thus the initialization phase (*initial layer*) is dominated by the exponential relaxation of $\phi_\perp$ to the "wrong" equilibrium $\hat{e}$. After this follows a dynamics in $\mathcal{TE}$ which runs on a slower time scale and in which the initial function $\hat{e}(1+\epsilon m)$ approaches its new equilibrium $\overline{e}$. The difference between fast exponential decay for the linearized model and of the slower approach to equilibrium for the nonlinear system can be easily verified e.g. running simulations with Discrete Velocity Models. Figs. 1 (a), (b) represent on a semilogarithmic scale the relaxation rates for randomly perturbed initial conditions in the cases (a), $\phi \in \mathcal{M}^\perp$, and case (b), $\phi \in \hat{e}\cdot\mathcal{M}$. Case (a) exhibits exponential decay, with rates within a narrow band. This situation can be reasonably well imitated with a BGK model (straight line). Case (b) is more complex and we may divide the evolution into three phases. Phase I represents the relaxation of the perturbation $(1+\epsilon\phi)\hat{e}$ to $\hat{e}$, phase II (*"convex phase"*) the transition from $(1+\epsilon\mathbf{m})\hat{e}$ to $\overline{e}$, and phase III the exponential relaxation to $\overline{e}$. In the special case $\hat{e}\cdot m = \hat{e}^{(1)}$ (51), phase II marks the transition of the trace element $\mathbf{f}(\epsilon)$ to $\mathbf{f}(0) = \overline{e}$. The slope of phase III is given by the parameter λ_{nl} of (73) which describes the effect of the purely nonlinear part of the operator. The BGK model is not capable to cover this situation and we have to decide whether to match to the initial Maxwellian or the final Maxwellian, depending on whether we want to simulate the short-time or the long-time behaviour.

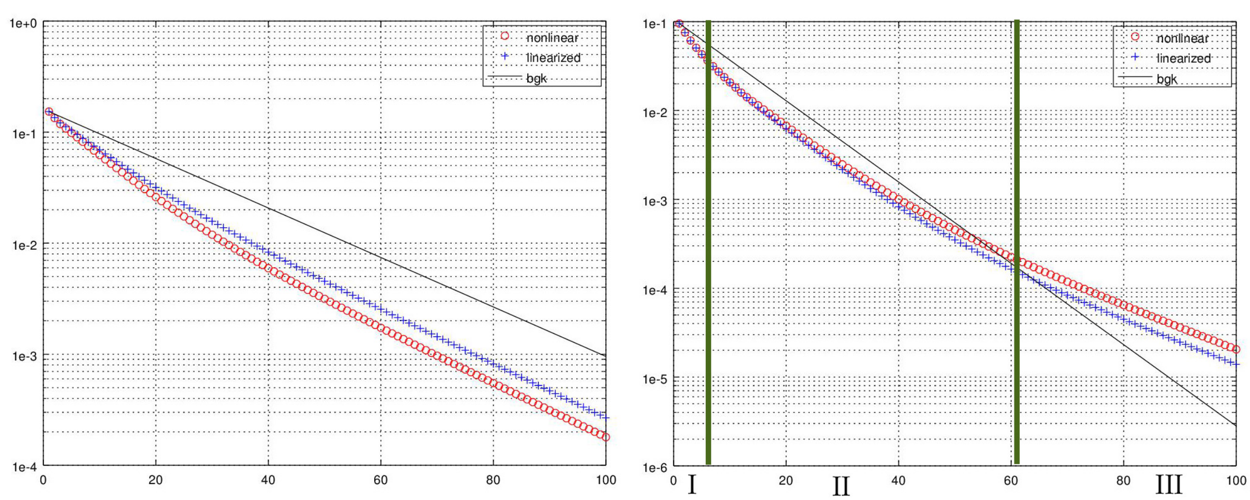

FIGURE 1: Relaxation of random initial perturbation. (a) $m = 0$, **(b)** $\phi_\perp = 0$.

5.3 Relaxation with source, balanced states

In view of scheme (4.7) to be solved for the closure relations let's have a look on solutions of the IVP with source,

$$\partial_t f + \epsilon s \;=\; Cf, \quad f(0) = \overline{e}, \quad s = \hat{\sigma}_x \cdot \overline{e} \tag{82}$$

and in particular their asymptotic states $f^{(\infty)}$ for $t \nearrow \infty$ (*balanced states*). For the relaxation systems we easily find

$$\begin{aligned}
f_{BGK}(t) \;&=\; \overline{e} + (f(0) - \overline{e}) \cdot \exp(-\lambda t) - \epsilon\lambda^{-1} \cdot s \cdot (1 - \exp(-\lambda t)) \\
&\qquad \nearrow f^{\infty}_{BGK} = \overline{e} - \epsilon\lambda^{-1} \cdot s \\
f_L(t) \;&=\; \overline{e} + \exp(tL_{\overline{e}})(f(0) - \overline{e}) + \epsilon \cdot (1 - \exp(tL_{\overline{e}}))\psi^{\sigma}_x \\
&\qquad \nearrow f^{\infty}_L = \overline{e} + \epsilon\psi^{\sigma}_x \qquad (\psi^{\sigma}_x \text{ solution of } L_{\overline{e}}\psi^{\sigma}_x = \hat{\sigma}_x \cdot \overline{e}, \text{ see } (36))
\end{aligned}$$

Both solutions satisfy the orthogonality relation

$$\langle f^{\infty}, \hat{\pi}_x \rangle \;=\; 0$$

This is no surprise, since the source is even with respect to v_x, and L maps even into even functions, while $\hat{\sigma}_x$ is odd. So it is remarkable to observe that orthogonality is not given for the nonlinear solution, as can be seen in Fig. 2. This discrepancy between linear and nonlinear case was observed (to our knowledge for the first time) in [5]. To understand this phenomenon, it helps to look at trace solutions. We easily see that $\gamma = 0$ is a balanced solution to the trace version of (82). However, it is not stable in the sense of dynamical systems, and there is another solution. Necessary and sufficient for balancing solutions is the orthogonality relation

$$\langle s - \mathbf{Cf}(\gamma) \rangle \quad \perp \quad \partial_\gamma \mathbf{f}(\gamma) \tag{83}$$

resp.

$$\langle s, \mathbf{n}_{\partial \mathbf{f}} \rangle \;=\; \langle \mathbf{C}_J \mathbf{f}(\gamma), \mathbf{n}_\pi \rangle \tag{84}$$

which in leading order leads to

$$\epsilon \cdot \|\partial_\gamma \mathbf{f}(\gamma)\|^{-1} \cdot \frac{2\gamma^2}{d \cdot \overline{T}^3} \cdot \|\hat{\sigma}_x \overline{e}\|^2 \;=\; \gamma^2 \cdot a^J_{\pi,\pi} \tag{85}$$

With $\|\partial_\gamma \mathbf{f}\| = \mathcal{O}(\gamma)$ we finally end up with

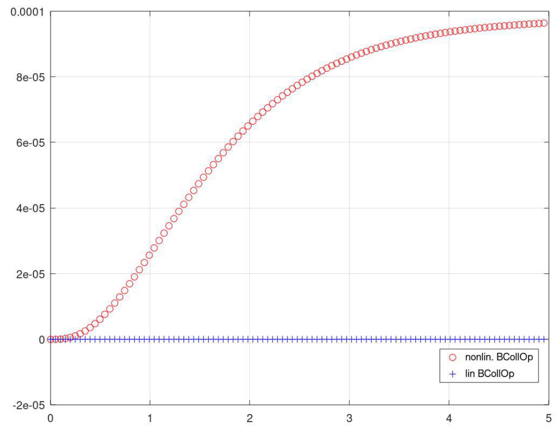

FIGURE 2: Evolution of scalar product $\langle \hat{\pi}_x, f(t) \rangle$ of IVP (82), nonlinear and linearized Boltzmann collision operator.

(5.11) Balanced state (*Relaxation with source*): Under the smallness assumptions for γ of (5.9) and with an appropriate constant $C_\sigma > 0$, the leading order term of the stable solution is given by

$$\gamma_{bs} = \epsilon \cdot C_\sigma \tag{86}$$

The solution $\mathbf{f}(\gamma_{bs})$ has an additonal contribution to the pressure tensor of the order $\mathcal{O}(\epsilon^2)$ as given in (57).

This example is an indicator that the concept of traces is relevant for the investigation of the structure of kinetic solutions in the context of closure relations. We can generalize the above principle to other sources and kinetic models.

(5.12) Balancing condition: Suppose given a source ϵs and a collision operator Cf with traces

$$\epsilon \cdot \mathbf{s}(\gamma) \;=\; \epsilon \cdot s_\pi \cdot \mathbf{n}_\pi + \epsilon \cdot s_\sigma \cdot \mathbf{n}_\sigma \tag{87}$$

$$\mathbf{Cf}(\gamma) \;=\; c_\pi \cdot \mathbf{n}_\pi + c_\sigma \cdot \mathbf{n}_\sigma \tag{88}$$

γ marks a balanced state if and only if the *orthogonality condition*

$$\epsilon \cdot \mathbf{s} - \mathbf{Cf} \quad \perp \quad \partial_\gamma \mathbf{f} = d_\pi \cdot \mathbf{n}_\pi + d_\sigma \cdot \mathbf{n}_\sigma \tag{89}$$

is satisfied which is equivalent to the *balancing condition*

$$(\epsilon \cdot s_\pi - c_\pi) \cdot d_\pi \;=\; -(\epsilon \cdot s_\sigma - c_\sigma) \cdot d_\sigma \tag{90}$$

6 Applications

6.1 Heat layers with zero flow

We consider the steady flow between two totally reflecting walls at different temperatures $T_0 = T(x = -1) > T_1 = T(x = 1)$ with a temperature difference $\Delta T = T_0 - T_1 > 0$. Since $\overline{v} = 0$, the moment equations read

$$\partial_x p_{xx} = 0 \quad (91)$$

$$\partial_x q_x = 0 \quad (92)$$

The closure moments for the solution are determined from the asymptotic solution f_{corr} for the model at hand of

$$\partial_x f_{corr} + \frac{\epsilon}{2T^2} \cdot \hat{\sigma}_x = Cf \quad (93)$$

In the *Navier-Stokes* description, f_{corr} contains no contribution to $\hat{\pi}_x$, and from equations (41)...(43) we find the heat layer solution

$$p_{xx} = p = \rho \cdot T = const \quad (94)$$

$$\lambda(T) \cdot \partial_x(T^{-1}) = const \quad (95)$$

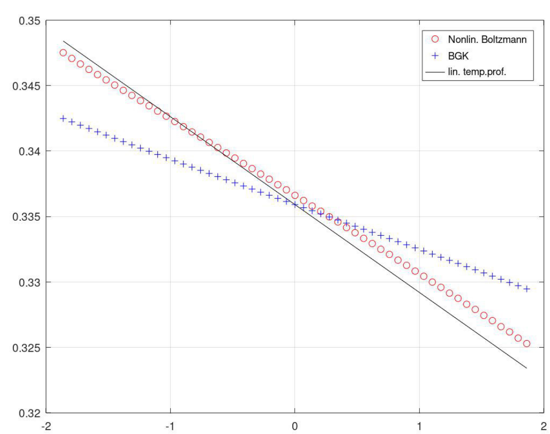

FIGURE 3: Heat layer for nonlinear collision operator and BGK model. Temperature profiles.

Comparing the temperature profiles of numerical simulations for the nonlinear and the BGK system (Fig. 3) we find that the BGK profile is considerably flatter than that of the nonlinear case. (The solid line present the linear profile between the wall temperatures.) An explanation for this is given by comparing the closure moments $\langle \hat{\pi}_x, f_{corr} \rangle$ for both models (Fig. 4(a)). From (3.11) we expect a small almost constant contribution (maybe weakly dependent on the temperature) in the nonlinear case. Zooming into Fig. 4(a) confirms this (Fig. 4(b)). However, for BGK we find a distinct, almost constant gradient over the whole field of calculation. An explanation for this is again provided by the trace description which allows to draw a rough picture pointing out the differences between nonlinear collision operator and BGK model.

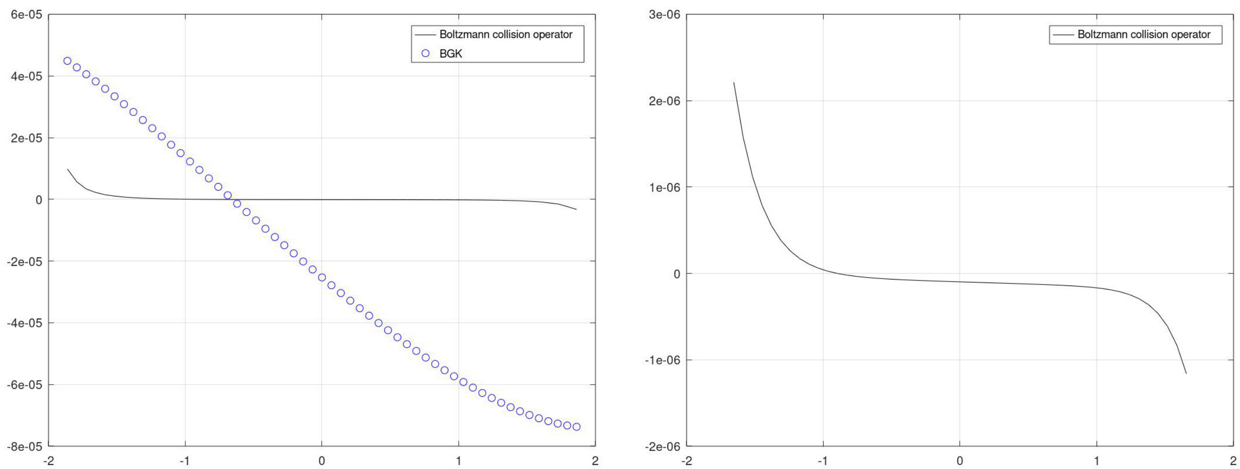

FIGURE 4: Pressure closure moment for heat layer.
(a) Nonlinear collision and BGK operators, (b) zoom into nonlinear operator.

For sake of simplicity we construct a model close to the situation at hand with a source term given by

$$s \;=\; \epsilon \cdot v_x \partial_x \mathbf{f}(\gamma(x)) \tag{96}$$

The right hand side consists of two main components – the x-derivative of γ leading to the term $\epsilon v_x \partial_x \gamma \cdot \partial_\gamma \mathbf{f}$, and the second component containing the $\overline{T}$-derivative of the Maxwellian $\overline{e}$. In regions of the x-domain with small γ, s is well-described by the model source term in trace formulation

$$\mathbf{s}_{mod} \;=\; \epsilon \cdot \frac{\partial_x \gamma}{\overline{T}} \cdot \|\hat{\pi}\overline{e}\| \cdot \mathbf{n}_\pi + \epsilon \cdot \frac{\partial_x \overline{T}}{\overline{T}^2} \cdot \|\hat{\sigma}\overline{e}\| \cdot \mathbf{n}_\sigma \tag{97}$$

For the comparison of balanced states we start with the *nonlinear collision operator*. Inserting the components $c_\pi = -\gamma^2 \cdot a^J_{\pi,\pi}$ and $c_\sigma = 0$ (71), the balancing condition (90) yields

$$\left(\epsilon \cdot \frac{\partial_x \gamma}{\overline{T}} \cdot \|\hat{\pi}\overline{e}\| + \gamma^2 \cdot a^J_{\pi,\pi}\right) \cdot \frac{\gamma}{\overline{T}^2} \cdot \|\hat{\pi}\overline{e}\| \;=\; \epsilon \cdot \frac{\partial_x \overline{T}}{\overline{T}^2} \cdot \|\hat{\sigma}\overline{e}\|^2 \cdot \frac{2\gamma^2}{d \cdot \overline{T}^3}$$

Assuming $\partial_x \gamma = 0$, we end up with the nontrivial balanced solution of (5.11).

In the *BGK case*, we pass over to the tangent plane around $\overline{e}$ and write

$$\mathbf{f}(\gamma) \;=\; \overline{e} + \Delta_\pi \cdot \mathbf{n}_\pi + \Delta_\sigma \cdot \mathbf{n}_\sigma \tag{98}$$

The trace of the BGK operator is then given by $c_\pi = -\lambda \cdot \Delta_\pi$ and $c_\sigma = -\lambda \cdot \Delta_\sigma$. The balancing condition reads

$$\left(\epsilon \cdot \frac{\partial_x \gamma}{\overline{T}} \cdot \|\hat{\pi}\overline{e}\| + \lambda \cdot \Delta_\pi\right) \cdot \frac{\gamma}{\overline{T}^2} \cdot \|\hat{\pi}\overline{e}\| \quad = \quad \left(\epsilon \cdot \frac{\partial_x \overline{T}}{\overline{T}^2} \cdot \|\hat{\sigma}\overline{e}\| + \lambda \cdot \Delta_\sigma\right) \cdot \frac{2\gamma^2}{d \cdot \overline{T}^3} \cdot \|\hat{\sigma}\overline{e}\|$$

For x-values with small $\gamma(x)$, we may neglect the Δ-terms (which are at least of order $\mathcal{O}(\gamma^2)$, see (34)), and find an approximate solution by

$$\partial_x(\gamma^2) \quad = \quad \gamma^2 \cdot \frac{2\partial_x \overline{T}}{d \cdot \overline{T}^2} \cdot \frac{\|\hat{\sigma}\overline{e}\|^2}{\|\hat{\pi}\overline{e}\|^2} \tag{99}$$

This represents an exponentially decaying layer in $-\partial_x \overline{T}$-direction for γ^2 (and with this for the closure moment $\hat{\pi}\overline{e}$, see (31)) which is not a kinetic boundary layer, since it is of macroscopic thickness (i.e. no ϵ-dependence). The related profile presented in Fig. 4(a) is the superposition of two layers, one from the left and one from the right of the computational domain. Compared to the nonlinear collision operator this presents an artificial effect, which is neither local nor small and which does not vanish in any limit of small parameters.

6.2 Further applications

We have proposed a new framework for closure relations for the nonlinear Boltzmann collision operator which is fundamentally different from that of the Navier Stokes equations, since it leads to nonlinear first order differential correction terms (in contrast to the diffusive second order terms of the Chapman Enskog approach). The field of possible relevant applications is large. First of all it is near at hand to extend the results of 6.1 to the case of a partially transmitting wall. Here, we may think of a trace ansatz at the wall of the form

$$\mathbf{f}(x=0) = \alpha^{(1)} \cdot \hat{e} + \alpha^{(2)} \cdot \left(1 + \gamma \cdot \frac{v_x - \hat{v}_x}{\hat{T}}\right) \cdot \hat{e} \qquad (\hat{v}_x(0) < 0) \tag{100}$$

where $\alpha^{(1)}$ represents the transmitted and $\alpha^{(2)}$ the reflected part. Applying the same ideas as above we can follow the trace in the interior of the flow. In the same spirit we can extend the trace formulation to the evaporation condensation problem for a gas mixture which was treated in [4] and which was the starting point of the present paper. This point will be addressed in a future paper.

Another type of application is the effect of the traces on the emergence of certain flow instabilities. In the present paper we did not consider the situation of shear stresses. In this case one may expect some pattern formation which becomes visible in the trace formulation and which could destabilize the flow. This opens a wide interesting field of research which in parts will be treated in subsequent papers.

Acknowledgement

This work has been supported by the German Research Foundation (DFG).

References

[1] K. Aoki, S. Takata, and S. Taguchi. Vapor flows with evaporation and condensation in the continuum limit: effect of a trace of noncondensable gas. *Eur. Journ. Mech. B/Fluids*, 22:51–71, 2003.

[2] H. Babovsky. A numerical model for the Boltzmann equation with applications to micro flows. *Comput. Math. Appl.*, 58:791–804, 2009.

[3] H. Babovsky. Discrete kinetic models in the fluid dynamic limit. *Computers and Mathematics with Applications*, 67:256–271, 2014.

[4] H. Babovsky. Macroscopic limit for an evaporation-condensation problem. *European Journal of Mechanics B/Fluids*, 63:106–112, 2017.

[5] L. Bold. *Diskrete Geschwindigkeitsmodelle und ihr Bezug zu den Navier-Stokes-Gleichungen.* Master thesis, Institute for Mathematics, TU Ilmenau, 2022.

[6] C. Cercignani. *The Boltzmann equation and its applications.* Springer, New York, 1988.

[7] C. Cercignani, R. Illner and M. Pulvirenti. *The Mathematical Theory of Dilute Gases.* Springer, New York, 1994.

[8] S. Chapman and T. G. Cowling. *The Mathematical Theory of Non-uniform Gases.* Cambridge University Press, Cambridge, 1952.

[9] E.M. Shakhov. *Fluid Dynam.*, 3:95–96, 1968.

[10] Y. Sone. *Molecular Gas Dynamics.* Birkhäuser, Boston, 2007.

[11] V. A. Titarev. Application of model kinetic equations to hypersonic rarefied gas flows. *Computers & Fluids*, 169:62–70, 2018.