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Discrete Kinetic Models in the Fluid Dynamic Limit

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Abstract

We investigate discrete kinetic models in the Fluid dynamic limit described by the Euler system and the Navier-Stokes correction obtained by the Chapman Enskog procedure. We show why reliable "small" systems can be expected only for small Mach numbers and derive a calculus for designing models for given Prandtl numbers.

Key words: Boltzmann equation, numerical simulation, discrete kinetic model, fluid dynamic limit.

MSC classification: 82C40, 82C80, 76P05

1 Introduction

The Boltzmann equation provides a mathematical description of gas flows on a mesoscopic level and is useful in a number of applications like the modelling of microflows. Due to the complexity of the equation (the Boltzmann collision operator requires the calculation of a five-dimensional integral to be evaluated pointwise in phase space) it is hard to construct efficient numerical schemes based on the classical numerical discretization concepts. One way out is the use of Monte Carlo methods. This approach is not discussed here. Another way is the derivation of highly *reduced discrete kinetic models*.

Concepts for discrete kinetic models on regular lattices have been proposed and investigated by a number or authors. The paper [16] provides an attempt to discretize the collision operator on a Cartesian grid. However, the order of consistency is extremely low (see the investigations in [15, 13]). Another possibility is the construction of classes of models which as a minimal requirement satisfy the correct physical conservation laws [9, 10]. However, we do not know of any results confirming their use as a numerical tool. An attempt to construct discrete collision dynamics which in a sense are optimally adapted to a given lattice have been introduced in [2] as the socalled *Lattice Group Models*. They turn out to be applicable to produce reliable numerical results in a number of test cases [3, 4].

Discrete kinetic models are also used as a tool for *macroscopic* simulation. A commonly applied technique represent the *Lattice Boltzmann Systems* [18, 14] which have been proven to be consistent with the Navier-Stokes equations. At present there seem to be two separate scientific communities with not much overlap applying kinetic schemes either from the view point of rarefied gas dynamics or of fluid dynamics. The present paper is intended to overcome this gap. We derive a framework for discrete kinetic models on the basis of two-particle collisions and then apply it in the fluid dynamic limit. The scope of the paper is this. In section 2 we define two-particle collisions on general discrete grids and introduce an appropriate representation for the nonlinear ant the linearized collision operators. Furthermore we establish the concept of the pseudo inverse. In section 3 we investigate the moment system and give arguments why discrete models on (small) grids can only be expected to yield useful results in the small Mach number limit. Applying the classical Chapman Enskog procedure we derive the Navier Stokes system. Section 4 is devoted to 2D velocity models with rotational symmetry. We derive systems comparable to the *single relaxation time* (SRT) and to the *multiple relaxation time* (MRT) models used in Lattice Boltzmann schemes. A few numerical examples are presented in section 5 demonstrating the need for further investigations

concerning instabilities when passing to the fluid dynamics regime.

2 Discrete kinetic models: Mathematical framework

2.1 The nonlinear collision operator

Let $\mathcal{I}$ be a finite index set, $|\mathcal{I}| = N$ and define $\mathcal{V} = \{\mathbf{v}_i, i \in \mathcal{I}\} \subset \mathbb{R}^d$ ($d \in \{2,3\}$) as a set of N pairwise different points ("velocities") in $\mathbb{R}^d$. Suppose given a quadruple $\alpha = (i,j,k,l) \in \mathcal{I}$. We call a transition

$$(\mathbf{v}_i, \mathbf{v}_j) \leftrightarrow (\mathbf{v}_k, \mathbf{v}_l) \tag{2.1}$$

between velocity pairs a *two-particle collision*. The collision is called *momentum and energy conserving* (short: an *elastic collision*), if

$$\mathbf{v}_i + \mathbf{v}_j = \mathbf{v}_k + \mathbf{v}_l, \tag{2.2}$$

$$|\mathbf{v}_i|^2 + |\mathbf{v}_j|^2 = |\mathbf{v}_k|^2 + |\mathbf{v}_l|^2. \tag{2.3}$$

The following result is well-known and elementary.

2.1 Lemma: The collision is elastic iff the polygone connecting $\mathbf{v}_i$, $\mathbf{v}_k$, $\mathbf{v}_j$, $\mathbf{v}_l$ is a rectangle in $\mathbb{R}^d$.

Related to the collision is the nonlinear *elementary collision operator* $J_\alpha : \mathbb{R}^{\mathcal{V}} \to \mathbb{R}^{\mathcal{V}}$,

$$(J_\alpha f)_m = \left\{ \begin{array}{ccc} f_k f_l - f_i f_j & \text{for} & m \in \{i,j\} \\ f_i f_j - f_k f_l & \text{for} & m \in \{k,l\} \\ 0 & \text{for} & m \in \mathcal{I} \setminus \{i,j,k,l\} \end{array} \right\} = (f_k f_l - f_i f_j) \cdot \mathbf{s}_\alpha, \tag{2.4}$$

where $\mathbf{s}_\alpha$ is the α-index vector defined by

$$\mathbf{s}_\alpha = \mathbf{e}_i + \mathbf{e}_j - \mathbf{e}_k - \mathbf{e}_l, \tag{2.5}$$

with $\mathbf{e}_m$ being the m-th canonical unit vector in $\mathbb{R}^{\mathcal{V}}$. In the following, $\mathcal{A} \subset \mathcal{I}^4$ denotes the set of all quadruples $\alpha = (i,j,k,l)$ corresponding to elastic collisions. Writing elements $\mathbf{v}$ of $\mathcal{V}$ componentwise in the form $\mathbf{v} = (v_x, v_y)$ for $d = 2$ resp. $\mathbf{v} = (v_x, v_y, v_z)$ for $d = 3$, we define the moment vectors $m_i \in \mathbb{R}^N$, $i = 0, \ldots, d+1$ by

$$m_0 = \mathbb{1} = (1, \ldots, 1)^T, \tag{2.6}$$

$$m_1 = \mathbf{v}_x = (v_x, \mathbf{v} \in \mathcal{V})^T, \tag{2.7}$$

$$m_2 = \mathbf{v}_y = (v_y, \mathbf{v} \in \mathcal{V})^T, \tag{2.8}$$

$$m_3 = \mathbf{v}_z = (v_z, \mathbf{v} \in \mathcal{V})^T \quad (\text{if } d = 3), \tag{2.9}$$

$$m_{d+1} = 0.5\mathbf{v}^2 = (0.5|\mathbf{v}|^2, \mathbf{v} \in \mathcal{V})^T, \tag{2.10}$$

the matrix

$$M := (m_i, i = 0, \ldots, d+1) \in \mathbb{R}^{N \times (d+2)}, \tag{2.11}$$

and the subspace

$$\mathcal{M} = \text{span}(m_i, i = 0, \ldots, d+1) \subseteq \mathbb{R}^{\mathcal{V}}. \tag{2.12}$$

An immediate consequence of the conservation laws (2.2) and (2.3) is

2.2 Lemma: $\alpha \in \mathcal{A} \Leftrightarrow M^T \mathbf{s}_\alpha = 0 \Leftrightarrow \mathbf{s}_\alpha \in \mathcal{M}^\perp$.

2.3 Definition: (a) A subset $\mathcal{A}_0 \subseteq \mathcal{A}$ is called *regular*, if

$$\text{span}(\mathbf{s}_\alpha, \alpha \in \mathcal{A}_0) = \mathcal{M}^\perp. \tag{2.13}$$

(b) A *collision operator* $J : \mathbb{R}^{\mathcal{V}} \to \mathbb{R}^{\mathcal{V}}$

$$J := \sum_{\alpha \in \mathcal{A}} \pi_\alpha J_\alpha \tag{2.14}$$

with *collision frequencies* $\pi_\alpha \geq 0$ is called *regular* if the set $\mathcal{A}_J := \{\alpha \in \mathcal{A} : \pi_\alpha > 0\}$ is regular.

The evolution equation on $\mathbb{R}^{\mathcal{V}}$

$$\partial_t f = Jf \tag{2.15}$$

with regular collision operator J is called a *(homogeneous) Boltzmann equation*. Consider the initial value problem (IVP)

$$\partial_t f = Jf, \quad f(0) = f^{(0)} \in \mathbb{R}_+^{\mathcal{V}} \tag{2.16}$$

for a Boltzmann equation with strictly positive initial condition $f^{(0)}$ ($\mathbb{R}_+$ denotes the open interval $(0, \infty)$). Applying the classical arguments from kinetic theory (e.g. [12], with adaptation to discrete models like in [2]) one can prove the following standard results.

2.4 Remark: (a) *Existence and uniqueness:* For all $t \geq 0$ there exists a unique solution of the IVP in $\mathbb{R}_+^{\mathcal{V}}$.
(b) *Conservation laws:* The only invariants are mass, moments and energy, i.e. the quantities $\langle m_i f(t) \rangle$, $i = 0, \ldots, d+1$. (For vectors $f, g \in \mathbb{R}^q$ we denote by $\langle fg \rangle$ the usual

scalar product $f^T g$ in $\mathbb{R}^q$.)
(c) *H-Theorem:* The *H-functional*

$$Hf(t) = \langle f(t)\ \ln(f(t))\rangle \tag{2.17}$$

is monotonously decreasing and strictly decreasing as long $f(t)$ is not a *Maxwellian*, i.e. a function of the form

$$f(\mathbf{v}) = a \cdot \exp(-s|\mathbf{v} - \mathbf{b}|^2). \tag{2.18}$$

(d) *Equilibria:* The only functions $f \in \mathbb{R}_+^{\mathcal{V}}$ satisfying $Jf = 0$ are Maxwellians. (This latter statement is not generally true for initial values $f^{(0)} \in \overline{\mathbb{R}_+}^{\mathcal{V}}$.)

2.2 The linearized collision operator

Consider an elementary collision operator

$$J_\alpha f = -(f_i f_j - f_k f_l) \cdot \mathbf{s}_\alpha \tag{2.19}$$

and choose an arbitrary Maxwellian $a \cdot e(\mathbf{v})$ with $a > 0$ and

$$e(\mathbf{v}) = \exp(-s|\mathbf{v} - \mathbf{b}|^2) = (e_i, i \in \mathcal{I}) \in \mathbb{R}_+^{\mathcal{V}} \tag{2.20}$$

which we keep fixed in the following. Then $J_\alpha e = 0$, and for $f = e + \epsilon\phi$ the linearization of J_α for ϵ small is given by $a \cdot L_\alpha \phi$ with

$$L_\alpha \phi = -(e_i\phi_j + e_j\phi_i - e_k\phi_l - e_l\phi_k) \cdot \mathbf{s}_\alpha. \tag{2.21}$$

Taking into account the conservation laws (2.2), (2.3) we find that

$$e_i e_j = e_k e_l = \exp(-s\left[(|\mathbf{v}_i|^2 + |\mathbf{v}_j|^2 - 2\langle \mathbf{b}(\mathbf{v}_i + \mathbf{v}_j)\rangle + 2|\mathbf{b}|^2\right]) =: q_\alpha > 0. \tag{2.22}$$

Thus defining the matrix $E := \mathrm{diag}(e(\mathbf{v}), \mathbf{v} \in \mathcal{V}) \in \mathbb{R}^{N\times N}$, we can write the linearization in matrix vector form as

$$L_\alpha \phi = -q_\alpha \mathbf{s}_\alpha \cdot (e_i^{-1}\phi_i + e_j^{-1}\phi_j - e_k^{-1}\phi_k - e_l^{-1}\phi_l) = -q_\alpha \mathbf{s}_\alpha \mathbf{s}_\alpha^T E^{-1}\phi. \tag{2.23}$$

Now let J be a regular collision operator with A_J given as in definition 2.3(b). Define a fixed subset $\mathcal{A}_0 \subseteq \mathcal{A}_J$ (which we keep fixed in the following) such that

$$\{\mathbf{s}_\alpha, \alpha \in \mathcal{A}_0\}$$

is a basis of $\mathcal{M}^\perp$, and define the matrix

$$S = (\mathbf{s}_\alpha, \alpha \in \mathcal{A}_0) \in \mathbb{R}^{N\times(N-d-2)}.$$

By definition of $\mathcal{A}_0$ we find for arbitrary $\alpha \in \mathcal{A}_J$ a unique vector $\mathbf{c}_\alpha \in \mathbb{R}^{N-d-2}$ such that $\mathbf{s}_\alpha = S\mathbf{c}_\alpha$. Thus the corresponding linearized elementary collision operator takes the form

$$L_\alpha = -q_\alpha S\mathbf{c}_\alpha \mathbf{c}_\alpha^T S^T E^{-1}.$$

This proves the following representation result for the linearized regular collision operator

$$L = \sum_{\alpha\in\mathcal{A}} \pi_\alpha L_\alpha.$$

2.5 Lemma: With the symmetric positive definite matrix

$$C = \sum_{\alpha\in\mathcal{A}_J} \pi_\alpha q_\alpha \mathbf{c}_\alpha \mathbf{c}_\alpha^T \in \mathbb{R}^{(N-d-2)\times(N-d-2)}$$

L takes the form

$$L = -SCS^T E^{-1}.$$

Important for the characterization of L is the following decomposition of vectors $f \in \mathbb{R}^{\mathcal{V}}$.

2.6 Lemma: For $f \in \mathbb{R}^{\mathcal{V}}$ there exist unique vectors $f_\parallel \in \mathbb{R}^{d+2}$ and $f_\perp \in \mathbb{R}^{N-d-2}$ such that

$$f = Sf_\perp + EMf_\parallel. \tag{2.24}$$

These are given as

$$f_\parallel = (M^T EM)^{-1} M^T f, \tag{2.25}$$
$$f_\perp = (S^T E^{-1} S)^{-1} S^T E^{-1} f. \tag{2.26}$$

Proof: Since the columns of M (resp. S) are a basis of $\mathcal{M}$ (resp. $\mathcal{M}^\perp$, existence and uniqueness of a decomposition are evident. The inverses of $S^T E^{-1} S$ and $M^T EM$ exist, since S and M have maximal dimension. Now suppose that f has the representation

(2.24). Multiplication with M^T and the fact that $M^T S = 0$ yield $f_\parallel$. Similarly, multiplication with $S^T E^{-1}$ gives the expression for $f_\perp$. $\square$

This leads to the following description of L.

2.7 Theorem: (a) The range of L is $R(L) = \mathcal{M}^\perp$. The nullspace is $\ker(L) = E\mathcal{M}$.
(b) $g = Lf$ has the decomposition $g = Sg_\perp + EMg_\parallel$ with

$$g_\perp = -CS^T E^{-1} S f_\perp, \tag{2.27}$$
$$g_\parallel = 0. \tag{2.28}$$

Proof: (a) From $R(L) \subseteq \mathcal{M}^\perp$, the regularity of C, and from the fact that the columns of S span $\mathcal{M}^\perp$ follows $R(L) = \mathcal{M}^\perp$. Furthermore, $\ker(L) \subseteq E\mathcal{M}$, and the dimension of $\ker(L)$ is $d+2$ from which we conclude that $\ker(L) = E\mathcal{M}$.
(b) follows from (a) and Lemma 2.6. $\square$

2.8 Definition: The *pseudo-inverse* $L^\dagger$ is defined as the operator on $\mathbb{R}^{\mathcal{V}}$ with $\ker(L^\dagger) = E\mathcal{M}$ such that $L^\dagger L f = L L^\dagger f = S f_\perp$.

From (2.27) we conclude

2.9 Corollary: The pseudo-inverse of L is given as

$$L^\dagger = -S(S^T E^{-1} S)^{-1} C^{-1} (S^T E^{-1} S)^{-1} S^T E^{-1} \tag{2.29}$$

Proof: Define

$$\tilde{L} := -S(S^T E^{-1} S)^{-1} C^{-1} (S^T E^{-1} S)^{-1} S^T E^{-1} \tag{2.30}$$

Then $EM \subseteq \ker(\tilde{L})$, and

$$\tilde{L} L f = L \tilde{L} f \tag{2.31}$$
$$= S(S^T E^{-1} S)^{-1} S^T E^{-1} f = S(S^T E^{-1} S)^{-1} S^T E^{-1} (S f_\perp + EM f_\parallel) = S f_\perp \quad \square$$

3 Fluid dynamic limits

3.1 The Euler system

Consider the space inhomogeneous rescaled Boltzmann equation for a density function $f(t, \mathbf{x}, \mathbf{v})$,

$$(\partial_t + \mathbf{v}\nabla_{\mathbf{x}})f = \frac{1}{\epsilon}Jf. \tag{3.32}$$

Multiplication with the transpose M^T of the moment matrix yields the non-closed system of moment equations

$$\begin{aligned}
\partial_t\rho + \nabla_{\mathbf{x}} \cdot (\rho\overline{\mathbf{v}}) &= 0, && (3.33)\\
\partial_t(\rho\overline{\mathbf{v}}) + \nabla_{\mathbf{x}}(\rho\overline{\mathbf{v}} \otimes \overline{\mathbf{v}} + P) &= 0, && (3.34)\\
\partial_t\left(\rho(e_{int} + \frac{1}{2}|\overline{\mathbf{v}}|^2)\right) + \nabla_{\mathbf{x}}\left(\rho\mathbf{v}(e_{int} + \frac{1}{2}|\overline{\mathbf{v}}|^2) + P\overline{\mathbf{v}} + \mathbf{q}\right) &= 0, && (3.35)
\end{aligned}$$

with the moments

$$\begin{aligned}
\text{density} \quad \rho &= \langle f\rangle,\\
\text{momentum vector} \quad \rho\overline{\mathbf{v}} &= \langle \mathbf{v}f\rangle,\\
\text{and specific internal energy} \quad e_{int} &= \langle|\mathbf{v} - \overline{\mathbf{v}}|^2 f\rangle/\rho.
\end{aligned}$$

(3.2) to (3.4) does not represent a closed system, since the *stress tensor* $P = (p_{\nu\nu'})$, the pressure p and the *heat-flow vector* $\mathbf{q} = (q_\nu)$ defined by

$$\begin{aligned}
p_{\nu\nu'} &= \langle(v_\nu - \overline{v}_\nu)(v_{\nu'} - \overline{v}_{\nu\nu'})f\rangle, && (3.36)\\
p &= \frac{1}{d}\sum_{\nu=1}^{d} p_{\nu\nu}, && (3.37)\\
q_\nu &= \frac{1}{2}\sum_{\nu'=1}^{d}\langle(v_\nu - \overline{v}_\nu)(v_{\nu'} - \overline{v}_{\nu\nu'})^2 f\rangle && (3.38)
\end{aligned}$$

cannot be expressed by ρ, $\rho\overline{\mathbf{v}}$ and e_{int}. Formally, the system can be closed by passing to the limit $\epsilon \searrow 0$ and replacing the density function f in the definitions (3.5), ..., (3.7) by the equilibrium $a \cdot \exp(-s|\mathbf{v} - \mathbf{b}|^2)$ with the same density, momentum and internal energy as f. For small values of $\mathbf{b}$ (and thus small flow velocities $\overline{\mathbf{v}}$) we can use the Taylor expansion around the *centered Maxwellian*

$$e_0(\mathbf{v}) = \exp(-s|\mathbf{v}|^2) \tag{3.39}$$

to obtain

$$e(\mathbf{v}) = \exp(-s|\mathbf{v}-\mathbf{b}|^2) \;\; = \;\; e_0(\mathbf{v}) \cdot \big(1 + 2s\langle \mathbf{vb}\rangle - s|\mathbf{b}|^2 + 2s^2\langle \mathbf{vb}\rangle^2\big) + \mathcal{O}(|\mathbf{b}|^3) \quad (3.40)$$

In the following we need some symmetry conditions for the velocity set $\mathbf{V}$. For a multiindex $\mathbf{n} = (n_\nu, \nu = 1, \ldots, d)$ of nonnegative integers define the $\mathbf{n}$-moment of f by

$$\langle \mathbf{v}^{\mathbf{n}} f\rangle := \big\langle \Pi_{\nu=1}^d v_\nu^{n_\nu} f\big\rangle$$

If π is a permutation of $\{1, \ldots, d\}$, then write for short $\mathbf{n}_\pi := (n_{\pi(\nu)}, \nu = 1, \ldots, d)$. From now on we assume the follwing assumptions to be satisfied.

3.1 Symmetry assumptions: (a) Moments of centered Maxwellians e_0 are invariant under permutations π, i.e. $\langle \mathbf{v}^{\mathbf{n}_\pi} e_0\rangle = \langle \mathbf{v}^{\mathbf{n}} e_0\rangle$.
(b) $\langle \mathbf{v}^{\mathbf{n}} e_0\rangle = 0$ whenever one of the numbers n_ν is odd.

Obviously these conditions are satisfied it $\mathcal{V}$ is invariant under reflection along and under rotation of 45° around the coordinate axes of $\mathbb{R}^d$.

3.2 Lemma: For Maxwellians $e(\mathbf{v}) = \exp(-s|\mathbf{v}-\mathbf{b}|^2)$ and for $\nu, \nu' \in \{1, \ldots, d\}$, $\nu \neq \nu'$, the coefficients of the stress tensor satisfy

$$p_{\nu\nu} - p_{\nu'\nu'} \;\; = \;\; 2s^2(b_\nu^2 - b_{\nu'}^2)\left(\langle v_\nu^4 e_0\rangle - \langle v_\nu^2 v_{\nu'}^2 e_0\rangle - 2\frac{\langle v_\nu^2 e_0\rangle^2}{\langle e_0\rangle}\right) + \mathcal{O}(|\mathbf{b}|^3) \quad (3.41)$$

$$p_{\nu\nu'} \;\; = \;\; 4s^2 b_\nu b_{\nu'}\left(\langle v_\nu^2 v_{\nu'}^2 e_0\rangle - \frac{\langle v_\nu^2 e_0\rangle^2}{\langle e_0\rangle}\right) + \mathcal{O}(|\mathbf{b}|^3) \quad (3.42)$$

Proof: A straightforward calculation yields

$$\begin{aligned} p_{\nu\nu} &= \langle v_\nu^2 e\rangle - \overline{v}_\nu^2\langle e\rangle \\ &= (1 - s|\mathbf{b}|^2)\langle v_\nu^2 e_0\rangle + 2s^2 b_\nu^2\left(\langle v_\nu^4 e_0\rangle - \langle v_\nu^2 v_{\nu'}^2 e_0\rangle - 2\frac{\langle v_\nu^2 e_0\rangle^2}{\langle e_0\rangle}\right) \\ &\quad + 2s^2|\mathbf{b}|^2\langle v_\nu^2 v_{\nu'}^2 e_0\rangle + \mathcal{O}(|\mathbf{b}|^3) \end{aligned}$$

From this and the symmetry assumptions follows the first formula. The calculations for $p_{\nu\nu'}$ are similar. $\square$

In classical fluid dynamics, the stress tensor takes the form

$$P = p \cdot I \quad (3.43)$$

with the pressure p depending on the density and the *temperature* T defined by

$$T = \frac{2}{d} e_{int}, \tag{3.44}$$

but not on bulk velocity $\overline{\mathbf{v}}$ which in first order is proportional to $\mathbf{b}$ (3.16). Thus in discrete models, which do not satisfy the two conditions

$$\langle v_\nu^2 v_{\nu'}^2 e_0 \rangle = \frac{1}{3} \langle v_\nu^4 e_0 \rangle = \frac{\langle v_\nu^2 e_0 \rangle^2}{\langle e_0 \rangle} \tag{3.45}$$

there is a structural error of the order $\mathcal{O}(|\mathbf{b}|^2)$ related to the stress tensor. This means that such models can yield useful results only in the limit $|\mathbf{b}| \searrow 0$. In the following calculations we take into account only terms up to the order $\mathcal{O}(|\mathbf{b}|)$. We verify easily the following formulas relating ρ, $\overline{\mathbf{v}}$ and T to the parameters a, $\mathbf{b} = (b_\nu)$ and s,

$$\begin{aligned}
\rho &= a\langle e_0 \rangle + \mathcal{O}(|\mathbf{b}|^2), && (3.46)\\
\rho \overline{\mathbf{v}} &= 2as\langle v_\nu^2 e_0 \rangle \mathbf{b} + \mathcal{O}(|\mathbf{b}|^3), && (3.47)\\
s\mathbf{b} &= \frac{\langle e_0 \rangle}{2\langle v_\nu^2 e_0 \rangle} \cdot \overline{\mathbf{v}} + \mathcal{O}(|\mathbf{b}|^3), && (3.48)\\
\partial_s T &= \frac{\langle |\mathbf{v}|^2 e_0 \rangle^2 - \langle |\mathbf{v}|^4 e_0 \rangle \langle e_0 \rangle}{2\langle e_0 \rangle^2} + \mathcal{O}(|\mathbf{b}|^2). && (3.49)
\end{aligned}$$

3.2 The Navier-Stokes correction

The Navier-Stokes correction presents a modification of the right hand side of the Euler system described above. In classical fluid dynamics, it is given by

$$\begin{pmatrix} 0 \\ \mu \left[\sum_{\nu'} \partial_{x_{\nu'}} \left(\frac{\partial \overline{v}_\nu}{\partial_{x_{\nu'}}} + \frac{\partial \overline{v}_{\nu'}}{\partial_{x_\nu}} \right) - \frac{2}{d} \partial_{x_\nu} \left(\nabla_{\mathbf{x}} \cdot \overline{\mathbf{v}} \right) \right], \quad \nu = 1, \ldots, d \\ \lambda \Delta_{\mathbf{x}} T \end{pmatrix} \tag{3.50}$$

[17] with viscosity μ and thermal conductivity λ. For our discrete models we derive it here applying the classical formal Chapman-Enskog procedure. To this end we decompose the solution f of the rescaled Boltzmann equation (3.1) like in section 2 in the form

$$f = ae + \epsilon S f_\perp \tag{3.51}$$

with $e(\mathbf{v}) = \exp(-s|\mathbf{v} - \mathbf{b}|^2)$, and with a, $\mathbf{b}$ and s depending on t, $\mathbf{x}$ and ϵ. Inserting this ansatz in the Boltzmann equation and neglecting terms of the order $\mathcal{O}(\epsilon)$ yields

$$(\partial_t + \mathbf{v} \nabla_{\mathbf{x}})(ae) = aLSf_\perp. \tag{3.52}$$

Here, L is the linearized operator related to the local Maxwellian $e(t, \mathbf{x})$. Thus

$$Sf_\perp = \frac{1}{a} L^\dagger (\partial_t + \mathbf{v}\nabla_\mathbf{x})(ae). \tag{3.53}$$

Plugging this into the Boltzmann equation and multiplying with M^T yields as the Navier-Stokes correction the vector

$$-\epsilon M^T (\partial_t + \mathbf{v}\nabla_\mathbf{x}) \left(\frac{1}{a} L^\dagger (\partial_t + \mathbf{v}\nabla_\mathbf{x})(ae) \right). \tag{3.54}$$

In several steps we are going to simplify this expression.

3.3 Lemma: The Navier-Stokes correction is

$$-\epsilon M^T \mathbf{v}\nabla_\mathbf{x} \left(L^\dagger (\mathbf{v}\nabla_\mathbf{x}) e \right). \tag{3.55}$$

Proof: (a) One verifies quickly that $\partial_t(ae) \in E\mathcal{M}$. Thus $S^T E^{-1} \partial_t(ae) = 0$ and $L^\dagger \partial_t(ae) = 0$.
(b)Furthermore, from the definition of $L^\dagger$ follows that $L^\dagger$ maps into $\mathcal{M}^\perp$. Thus $M^T L^\dagger \psi = 0$ for arbitrary ψ.
(c) Since $(\mathbf{v}\nabla_\mathbf{x} a) \cdot e = \sum_\nu (\partial_{x_\nu} a) v_\nu e \in E\mathcal{M}$, we find finally $L^\dagger (\mathbf{v}\nabla_\mathbf{x})(ae) = a L^\dagger (\mathbf{v}\nabla_\mathbf{x}) e$.
□

Notice that

$$\mathbf{v}\nabla_\mathbf{x} e = \sum_{\nu'} v_{\nu'} \left(-|\mathbf{v}|^2 \partial_{x_{\nu'}} s + \sum_{\tilde{\nu}} v_{\tilde{\nu}} \partial_{x_{\nu'}} (s b_{\tilde{\nu}}) + \partial_{x_{\nu'}} |\mathbf{b}|^2 \right) e. \tag{3.56}$$

Defining the diagonal matrices $V_\nu := \mathrm{diag}(v_\nu, \mathbf{v} \in \mathcal{V}$ and $|V| := \mathrm{diag}(|\mathbf{v}|, \mathbf{v} \in \mathcal{V}$, and writing $e = E\mathbb{1}$, we can write (3.24) in matrix vector form as

$$-\epsilon \sum_{\nu,\nu'} M^T V_\nu \partial_{x_\nu} \left(L^\dagger E V_{\nu'} [-|V|^2 \partial_{x_{\nu'}} s + \sum_{\tilde{\nu}} V_{\tilde{\nu}} \partial_{x_{\nu'}} (s b_{\tilde{\nu}})] \right) \mathbb{1}. \tag{3.57}$$

For reasons discussed above, we consider grid models useful only for small bulk velocities. Suppose the local Maxwellians are given in the form ae where $e = e(t, \mathbf{x}, \mathbf{v}) = \exp(-s|\mathbf{v} - \mathbf{b}|^2)$ deviates only slightly from a global central Maxwellian $e_0(\mathbf{v}) = \exp(-s_0|\mathbf{v}|^2)$ (with s_0 being a fixed constant). We are going to derive the linear approximation (in terms of $\Delta s = s - s_0$ and $\mathbf{b}$) of the Navier-Stokes correction.

3.4 Lemma: Denote $E_0 := \mathrm{diag}(e_0(\mathbf{v}), \mathbf{v} \in \mathcal{V})$. Then $(S^T E^{-1} S)^{-1}$ is a perturbation of $(S^T E_0^{-1} S)^{-1}$ which up to linear order is given as

$$(S^T E^{-1} S)^{-1} \;=\; (S^T E_0^{-1} S)^{-1} - (S^T E_0^{-1} S)^{-1} \Xi (S^T E_0^{-1} S)^{-1} \tag{3.58}$$

with the first order correction term

$$\Xi = S^T E_0^{-1} \left(\Delta s \cdot |V|^2 - 2s_0 \sum_{\nu=1}^{d} b_\nu V_\nu \right) S \tag{3.59}$$

Proof: Taylor expansion up to first order yields

$$E^{-1} = E_0^{-1} \cdot \left(I + \Delta s \cdot |V|^2 - 2s_0 \sum_{\nu=1}^{d} b_\nu V_\nu \right)$$

and

$$\begin{aligned} S^T E^{-1} S &= S^T E_0^{-1} S + \Xi \\ &= (S^T E_0^{-1} S)^{1/2} \left(I + (S^T E_0^{-1} S)^{-1/2} \Xi (S^T E_0^{-1} S)^{-1/2} \right) (S^T E_0^{-1} S)^{1/2} \end{aligned}$$

(Notice that $(S^T E_0^{-1} S)^{-1}$ is symmetric and positive definite; thus $(S^T E_0^{-1} S)^{-1/2}$ exists.) The required result follows from inverting while inserting

$$I - (S^T E_0^{-1} S)^{-1/2} \Xi (S^T E_0^{-1} S)^{-1/2}$$

as a first order approximation of

$$(I + (S^T E_0^{-1} S)^{-1/2} \Xi (S^T E_0^{-1} S)^{-1/2})^{-1} \qquad \square$$

This result allows us to replace in the representation of Corollary 2.7 the matrix E by E_0 and to shift the derivative ∂_{x_ν} in (3.26) to the right. Applying the formulas (3.17) and (3.18) we find the general form of the correction term.

3.5 Theorem: Up to linear order in $\overline{\mathbf{v}}$ and $T - T_0$, the Navier-Stokes correction reads

$$\begin{aligned} &\epsilon \sum_{\nu,\nu'} M^T V_\nu S (S^T E_0^{-1} S)^{-1} C^{-1} (S^T E_0^{-1} S)^{-1} S^T V_{\nu'} \\ &\cdot \left(\frac{\langle e_0 \rangle}{2 \langle v_\nu^2 e_0 \rangle} \sum_{\tilde{\nu}} V_{\tilde{\nu}} \partial_{x_\nu x_{\nu'}} \overline{v}_{\tilde{\nu}} + \frac{2 \langle e_0 \rangle^2}{\langle |\mathbf{v}|^4 e_0 \rangle \langle e_0 \rangle - \langle |\mathbf{v}|^2 e_0 \rangle^2} |V|^2 \partial_{x_\nu x_{\nu'}} T \right) \end{aligned} \tag{3.60}$$

4 2D Cartesian lattices

In the following we derive kinetic models on sublattices $\mathcal{V}^N$ of the 2D-integer grid $\mathcal{V} = \mathbf{Z} \times \mathbf{Z}$, exploiting rotational symmetry. Rotation around 45° (counterclockwise) is given

by the operator

$$R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{4.1}$$

4.1 Rotational symmetry

Let $(\mathbf{v}_n, n \in \mathbb{N}_0)$ be a bijection from $\mathbb{N}_0 = \{0, 1, \ldots\}$ to $\mathcal{V}$ with properties stated below. Given this mapping we define $(N+1)$-velocity sets by

$$\mathcal{V}^N = \{\mathbf{v}_n, n = 0, \ldots, N\}. \tag{4.2}$$

To define a kinetic model on $\mathcal{V}^N$ we have to define a set $\mathcal{A}_0^N$ of rectangles $\alpha = (i, j, k, l)$ given by the diagonals $\overline{\mathbf{v}_i\mathbf{v}_j}$ and $\overline{\mathbf{v}_k\mathbf{v}_l}$, resp. a basis of the $(N-3)$-dimensional subspace $\mathcal{M}^\perp$ of $\mathbb{R}^{|\mathcal{V}^N|}$ of vectors of the form $\mathbf{s}_\alpha = \mathbf{e}_i + \mathbf{e}_j - \mathbf{e}_k - \mathbf{e}_l$. To exploit symmetries, the bijection $(\mathbf{v}_n, n \in \mathbb{N}_0)$ and the set $\mathcal{A}_0$ have to follow the rules given below. We say that a quadrupel (i, j, k, l) of velocities is *in cyclic order*, if

$$\mathbf{v}_j = R\mathbf{v}_i, \quad \mathbf{v}_k = R\mathbf{v}_j, \quad \mathbf{v}_l = R\mathbf{v}_k. \tag{4.3}$$

We say that a quadrupel $(\alpha_p, \alpha_q, \alpha_r, \alpha_s)$ of rectangles with $\alpha_m = (i_m, j_m, k_m, l_m)$, $m = p, q, r, s$, is *in cyclic order*, if each of the quadrupels (i_p, i_q, i_r, i_s), (j_p, j_q, j_r, j_s), (k_p, k_q, k_r, k_s) and (l_p, l_q, l_r, l_s) is in cyclic order, i.e. if each of the rectangles arises from its predecessor by application of R.

4.1 Assumptions: The bijection $(\mathbf{v}_n, n \in \mathbb{N}_0)$ from $\mathbb{N}_0$ to $\mathcal{V}$ satisfies

(R1) $\mathbf{v}_0 = (0, 0), \quad \mathbf{v}_1 = (1, 0), \quad \mathbf{v}_5 = (1, 1) \quad \mathbf{v}_9 = (2, 0)$.

(R2) For $m \in \mathbb{N}_0$, the quadrupel $(\mathbf{v}_{4m+n}, n = 1, \ldots, 4)$ is in cyclic order.

The set $\mathcal{A}_0 = \{\alpha_n, n \in \mathbb{N}_0\}$ satisfies

(R3) $\alpha_0 = (1, 3, 2, 4), \quad \alpha_1 = (0, 5, 1, 2), \quad \alpha_5 = (0, 9, 5, 8)$.

(R4) For $m \geq 0$, the quadrupels $(\alpha_{4m+n}, n = 1, \ldots, 4)$ are in cyclic order.

(R5) If $m \geq 2$ and $\alpha_{4m+1} = (i, j, k, l)$, then $j = 4m{+}5$ and $i, k, l \in \{1, \ldots, 4m{+}4\}$.

We denote

$$\mathcal{A}_0^N := \{\alpha_n, n = 0, \ldots, N\}. \tag{4.4}$$

Notice that the rule (R5) guarantees that the vectors $\mathbf{s}_\alpha$ are pairwise linearly independent.

4.2 Example: Figure 1 illustrates one choice of $\mathbf{v}_0, \ldots, \mathbf{v}_{40}$ such that $(R1)$ and $(R2)$ are satisfied. For $N = 8, 12, 20, 24, 36, 40$, $\mathcal{V}^N$ is R-invariant and thus the symmetry assumptions 3.1 are satisfied. In addition, the velocities are semi-ordered by $|\mathbf{v}_{n+1}| \geq |\mathbf{v}_n|$. The corresponding set $\mathcal{A}_0^8$ is given by (R3), (R4) as $\{(1,3,2,4), (0,5,1,2), (0,6,2,3), (0,7,3,4), (0,8,4,1)\}$. For $\mathcal{A}_0^{12}$ we have to add $(0,9,5,8), (0,10,6,5), (0,11,7,6), (0,12,8,7)$. Higher indices may be chosen according to (R5) as $\alpha_9 = (1,13,5,9)$, $\alpha_{13} = (2,17,5,10)$, $\alpha_{17} = (5,21,13,17)$, $\alpha_{21} = (1,25,13,20)$, etc.

				38				
			30	26	33			
		22	14	10	17	21		
	34	18	6	2	5	13	29	
39	27	11	3	0	1	9	25	37
	31	15	7	4	8	20	36	
		23	19	12	16	24		
			35	28	32			
				40				

FIGURE 1. Numbering of $\mathbf{Z} \times \mathbf{Z}$

The cyclic ordering of α_n leads to a special structure of the matrices S_N given by the index vectors $\mathbf{s}_n$ of α_n $(n = 0, \ldots, N)$. E.g., in the above example, the transpose is for $N = 12$ given as

$$S^T = \left(\begin{array}{c|cccc|cccc|cccc} 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 1 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ \hline 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 1 \end{array}\right) \tag{4.5}$$

Define the 4×4-matrices

$$G = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad I_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{4.6}$$

and the vector

$$\mathbb{1}_- = (1, -1, 1, -1)^T. \tag{4.7}$$

Then G generates a multiplicative group of order 4 (i.e. $G^4 = I_4$), and S has the 4×4-block structure

$$S^T = \left(\begin{array}{c|ccc} 0 & \mathbb{1}_-^T & 0 & 0 \\ \hline \mathbb{1} & -I_4 - G & I_4 & 0 \\ \mathbb{1} & 0 & -I_4 - G^3 & I_4 \end{array}\right)$$

These observations can be generalized. For $N = 4m \geq 8$ and $S_N = (s_{ij}, 0 \leq i \leq N-4, 0 \leq j \leq N)$ define the submatrices

$$\begin{aligned} S_{0,n} &= (s_{0,4n-3}, \ldots, s_{0,4n}) \quad \text{for} \quad n \geq 1 \\ S_{m,0} &= (s_{4m-3,0}, \ldots, s_{4m,0})^T \quad \text{for} \quad m \geq 1 \\ S_{ij} &= (s_{ij}, 4m-3 \leq i \leq 4m, 4n-3 \leq j \leq 4n) \quad \text{for} \quad m, n \geq 1 \end{aligned}$$

which give the block structure of S_N,

$$S_N = \left(\begin{array}{c|ccc} s_{00} & \cdots & S_{0n} & \cdots \\ \hline \vdots & & \vdots & \\ S_{m0} & \cdots & S_{mn} & \cdots \\ \vdots & & \vdots & \end{array}\right) \tag{4.8}$$

Then from (R3), (R4) and (R5) immediately follows

4.3 Lemma: Let $N \geq 8$ be a multiple of 4.
(a) $s_{00} = 0$, and

$$S_{0n} = \begin{cases} \mathbb{1}_-^T & \text{for} \quad n = 1 \\ 0 & \text{for} \quad n > 1 \end{cases} \tag{4.9}$$

(b) The left column is given by

$$S_{m0} = \begin{cases} \mathbb{1} & \text{for} \quad m = 1, 2 \\ 0 & \text{for} \quad m > 2 \end{cases} \tag{4.10}$$

(c) The 4×4-submatrices are polynomials in G with coefficients in $\{-1, 0, 1\}$ and satisfy

$$S_{mn} = \begin{cases} I_4 & \text{for} \quad n = m+1 \\ 0 & \text{for} \quad m > n+1 \text{ or } (m,n) = (1,2) \end{cases} \tag{4.11}$$

Denote by $\mathcal{P}(G)$ the set of all polynomials in G. Since $G^4 = I_4$, the most general form of a polynome is

$$P(G) = p_0 I_4 + p_1 G + p_2 G^2 + p_3 G^3 \tag{4.12}$$

Furthermore, $G^3 = G^T$ and thus $(P(G))^T = P(G^T)$. $\mathcal{P}(G)$ is a commutative ring with unit element I_4. We call an element $P(G)$ *invertible*, if there exists $Q \in \mathcal{P}(G)$ with $PQ = I_4$. An invertible element P is denoted as *positive* if there exists $Q \in \mathcal{P}(G)$ such that $P(G) = Q(G)Q(G^T)$. Useful are the following formulas.

4.4 Calculus in $\mathcal{P}(G)$: Let $P, Q, R \in \mathcal{P}(G)$ with coefficients p_i, q_i and r_i, $i = 0, 1, 2, 3$. (a) Multiplication: If $PQ = R$ then

$$\begin{aligned} r_0 &= p_0 q_0 + p_1 q_3 + p_2 q_2 + p_3 q_1 && (4.13)\\ r_1 &= p_0 q_1 + p_1 q_0 + p_2 q_3 + p_3 q_2 && (4.14)\\ r_2 &= p_0 q_2 + p_1 q_1 + p_2 q_0 + p_3 q_3 && (4.15)\\ r_3 &= p_0 q_3 + p_1 q_2 + p_2 q_1 + p_3 q_0 && (4.16) \end{aligned}$$

(b) $P \in \mathcal{P}(G)$ is invertible iff $|p_0 + p_2| \neq |p_1 + p_3|$ and $|p_0 - p_2|^2 + |p_1 - p_3|^2 \neq 0$. The coefficients of $R(G) = P^{-1}(G)$ are given by

$$\begin{aligned} r_0 + r_2 &= = \frac{p_0 + p_2}{(p_0 + p_2)^2 - (p_1 + p_3)^2} && (4.17)\\ r_0 - r_2 &= \frac{p_0 - p_2}{(p_0 - p_2)^2 + (p_1 - p_3)^2} && (4.18)\\ r_1 + r_3 &= = \frac{-(p_1 + p_3)}{(p_0 + p_2)^2 - (p_1 + p_3)^2} && (4.19)\\ r_1 - r_3 &= \frac{-(p_1 - p_3)}{(p_0 - p_2)^2 + (p_1 - p_3)^2} && (4.20) \end{aligned}$$

(c) Necessary for positiveness is $p_1 = p_3$. Sufficient for positiveness of an invertible element is that $p_1 = p_3$ and in addition $p_0 > p_2$ and $|p_1| < \frac{1}{2}(p_0 + p_2)$. In this case a root $Q(G) = q_0 I_4 + q_1 G + q_2 G^2 + q_3 G^3$ is given by

$$\begin{aligned} q_0 &= \frac{1}{2}\left(\frac{1}{2}(\sqrt{p_0 + 2p_1 + p_2} + \sqrt{p_0 - 2p_1 + p_2}) + \sqrt{p_0 - p_2}\right) && (4.21)\\ q_1 = q_3 &= \frac{1}{4}\left(\sqrt{p_0 + 2p_1 + p_2} - \sqrt{p_0 - 2p_1 + p_2}\right) && (4.22)\\ q_2 &= \frac{1}{2}\left(\frac{1}{2}(\sqrt{p_0 + 2p_1 + p_2} + \sqrt{p_0 - 2p_1 + p_2}) - \sqrt{p_0 - p_2}\right) && (4.23) \end{aligned}$$

Proof: (a) follows from elementary calculations. For the other results, the following transformation is useful. Define the orthogonal matrix

$$Q = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \end{pmatrix} \tag{4.24}$$

satisfying $Q = Q^{-1}$, and the transformed matrix $\hat{G} = QGQ$. Then

$$\hat{G} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad \hat{G}^2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \hat{G}^3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Thus $P(G)$ transforms into

$$P(\hat{G}) = \mathrm{diag}\left(p_0 + p_1 + p_2 + p_3, \begin{pmatrix} p_0 - p_2 & -p_1 + p_3 \\ p_1 - p_3 & p_0 - p_2 \end{pmatrix}, p_0 - p_1 - p_2 + p_3\right) \tag{4.25}$$

The inverse $P^{-1}(G)$ follows now easily from inverting $P(\hat{G})$ which leads to

$$\begin{aligned} r_0 + r_2 &= \frac{1}{2}\left(\frac{1}{p_0 + p_1 + p_2 + p_3} + \frac{1}{p_0 - p_1 + p_2 - p_3}\right) \\ r_0 - r_2 &= \frac{p_0 - p_2}{(p_0 - p_2)^2 + (p_1 - p_3)^2} \\ r_1 + r_3 &= \frac{1}{2}\left(\frac{1}{p_0 + p_1 + p_2 + p_3} - \frac{1}{p_0 - p_1 + p_2 - p_3}\right) \\ r_1 - r_3 &= \frac{-(p_1 - p_3)}{(p_0 - p_2)^2 + (p_1 - p_3)^2} \end{aligned}$$

and thus to (4.16) to (4.19). Similarly the results (4.20) to (4.22) are obtained. □

Given N as a multiple of 4, we denote by $\mathcal{B}_N(P)$ the set of all matrices $A = (a_{ij}, 1 \le i, j \le N)$ for which the block-submatrices

$$A_{mn} = (a_{ij}, 4m - 3 \le i \le 4m, 4n - 3 \le j \le n), \quad 1 \le m, n \le N/4$$

are elements of $\mathcal{P}(G)$. We call $A \in \mathcal{B}_N(P)$ *invertible in* $\mathcal{B}_N(P)$, if A is regular as an element of $\mathbb{R}^{N \times N}$ and if $A^{-1} \in \mathcal{B}_N(P)$. $A \in \mathcal{B}_N(P)$ is called *Cholesky-decomposable* if

there exists $C \in \mathcal{B}_N(P)$ with C_{nn} positive and $C_{mn} = 0$ for $m < n$ such that $A = CC^T$. In this case A is *invertible in* $\mathcal{B}_N(P)$, since we can use the decomposition to construct A^{-1}. A special role for our collision models plays the matrix $S^T E_0^{-1} S$. Since

$$E_0 = \mathrm{diag}(1, e_0(\mathbf{v}_{4m}) \cdot I_4, 1 \le m \le k)$$

it has the structure

$$S^T E_0^{-1} S = \left(\begin{array}{c|c} \sigma & 0 \\ \hline 0 & \Sigma \end{array} \right)$$

with $\sigma \in \mathbb{R}_+$ and $\Sigma \in \mathcal{B}_{N-4}(P)$. The above calculus simplifies significantly the construction of specific models. An example is given in the following subsection.

4.2 The collision matrix for the nine-velocity model

We are going to establish the collision matrix C for the nine-velocity lattice $\mathcal{V}^8$. The five elements of $\mathcal{A}_0$ (and with these the column vectors $\mathbf{s}_0, \ldots, \mathbf{s}_4$) are chosen as given in (R3) and represent collisions with (positive) collision probabilities π_0 (for α_0) and π_1 (for $\alpha_1, \ldots, \alpha_4$). However, there are more rectangles which have to be taken into account. Four of these are given by $(1, 6, 3, 5)$ (represented by $\mathbf{s}_2 - \mathbf{s}_1$) and three more obtained by rotation. We attach to these the collision frequency $\tilde{\pi}_1 \ge 0$. A final collision $(5, 7, 6, 8)$ (with frequency $\tilde{\pi}_2 \ge 0$) is given by $\mathbf{s}_1 - \mathbf{s}_2 + \mathbf{s}_3 - \mathbf{s}_4$. Define the centered Maxwellian $e_0(\mathbf{v}) = \exp(-s|\mathbf{v}|^2)$ and the corresponding diagonal matrix E_0. With $\xi := \exp(-s)$, C takes the form

$$\begin{aligned} C &= \xi^2 \cdot \left(\begin{array}{cc} \pi_0 & \\ & (\pi_1 + 2\tilde{\pi}_1\xi + \tilde{\pi}_2\xi^2) \cdot I_4 - (\tilde{\pi}_1\xi + \tilde{\pi}_2\xi^2) \cdot (G + G^3) + \tilde{\pi}_2\xi^2 \cdot G^2 \end{array} \right) \\ &=: \xi^2 \cdot \left(\begin{array}{cc} c_{00} & \\ & P_C(G) \end{array} \right) \end{aligned} \tag{4.26}$$

The matrix $S^T E_0^{-1} S$ is given as

$$S^T E_0^{-1} S = \left(\begin{array}{cc} 4\xi^{-1} & \\ & P_S(G) \end{array} \right) \tag{4.27}$$

with

$$P_S(G) = \eta^2 I_4 + \eta(G + G^3) + G^2, \quad \eta = 1 + \xi^{-1}. \tag{4.28}$$

Its inverse is

$$(S^T E_0^{-1} S)^{-1} = \left(\begin{array}{cc} \xi/4 & \\ & P_S^{-1}(G) \end{array} \right) \tag{4.29}$$

with

$$P_S^{-1}(G) = (\eta^2 - 1)^{-2}(\eta^2 I_4 - \eta(G + G^3) + G^2). \tag{4.30}$$

Crucial for the adequate modelling are the following results.

4.5 Theorem: (a) If

$$\pi_1 \neq \tilde{\pi}_2 \xi^2 \tag{4.31}$$

then the matrix $(S^T E_0^{-1} S)^{-1} C^{-1} (S^T E_0^{-1} S)^{-1}$ takes the form

$$(S^T E_0^{-1} S)^{-1} C^{-1} (S^T E_0^{-1} S)^{-1} = \begin{pmatrix} \ell_{00} & \\ & \ell_0 I_4 + \ell_1 (G + G^3) + \ell_2 G^2 \end{pmatrix} \tag{4.32}$$

The Navier-Stokes correction part of Theorem 3.5 is

$$\begin{pmatrix} 0 \\ \frac{1+2\xi}{\xi} \left[\ell_{00} (\partial_{xx}(\overline{v}_x) - \partial_{xy}(\overline{v}_y)) + (\ell_0 - 2\ell_1 + \ell_2)(\partial_{xy}(\overline{v}_y) + \partial_{yy}(\overline{v}_x)) \right] \\ \frac{1+2\xi}{\xi} \left[\ell_{00} (\partial_{yy}(\overline{v}_y) - \partial_{xy}(\overline{v}_x)) + (\ell_0 - 2\ell_1 + \ell_2)(\partial_{xx}(\overline{v}_y) + \partial_{xy}(\overline{v}_x)) \right] \\ \frac{2(1+2\mu)^2}{\mu} (\ell_0 - \ell_2)(\partial_{xx} + \partial_{yy}) T \end{pmatrix} \tag{4.33}$$

(b) The correction term (4.32) is of the form (3.19) iff

$$\ell_{00} = (\ell_0 - 2\ell_1 + \ell_2). \tag{4.34}$$

In this case the nine-velocity model describes a system with viscosity

$$\mu = \frac{1 + 2\xi}{\xi} \ell_{00} \tag{4.35}$$

and thermal conductivity

$$\lambda = \frac{2(1 + 2\mu)^2}{\mu} (\ell_0 - \ell_2). \tag{4.36}$$

Proof: (a) Because of 4.4, $P_C(G)$ is invertible if $\pi_1 \neq \tilde{\pi}_2 \xi^2$. Since $\mathcal{P}(G)$ is closed with respect to multiplication, (4.31) is satisfied. (4.32) follows from straight evaluation of (3.29), taking into account the moments

$$\langle e_0 \rangle = (1 + 2\xi)^2, \tag{4.37}$$

$$\langle |\mathbf{v}|^2 e_0 \rangle = 4\xi(1 + 2\xi), \tag{4.38}$$

$$\langle |\mathbf{v}|^4 e_0 \rangle = 4\xi(1 + 4\xi). \tag{4.39}$$

(b) For $d = 2$, (3.19) can be reformulated as

$$\begin{pmatrix} 0 \\ \mu\left[(\partial_{xx}(\overline{v}_x) - \partial_{xy}(\overline{v}_y)) + (\partial_{xy}(\overline{v}_y) + \partial_{yy}(\overline{v}_x))\right] \\ \mu\left[(\partial_{yy}(\overline{v}_y) - \partial_{xy}(\overline{v}_x)) + (\partial_{xx}(\overline{v}_y) + \partial_{xy}(\overline{v}_x))\right] \\ \lambda(\partial_{xx} + \partial_{yy})T \end{pmatrix}. \qquad \square \tag{4.40}$$

We are now able to construct models which asymptotically describe the classical Navier-Stokes system (for this, (4.33) has to be satisfied), and which has a specified Prandtl number

$$Pr = \frac{\mu}{\lambda}. \tag{4.41}$$

4.6 Example (Single relaxation time, SRT): If we choose $C = (S^T E_0 S)^{-1}$, then the linearized equation

$$\partial_t f = Lf \tag{4.42}$$

describes a system relaxing exponentially to the equilibrium (*single relaxation time, SRT system*). It corresponds to the BGK system of classical fluid dynamics. In this case the matrix (4.31) is given by $(S^T E_0^{-1} S)^{-1}$, i.e.

$$\ell_{00} = \xi/4, \quad (\ell_0, \ell_1, \ell_2, \ell_3) = (\eta^2 - 1)^{-2} \cdot (\eta^2, -\eta, 1, -\eta). \tag{4.43}$$

Thus $\ell_0 - (\ell_1 + \ell_3) + \ell_2 = \xi^2$, and (4.33) is satisfied iff

$$\xi = 1/4. \tag{4.44}$$

The collision frequencies turn out as

$$\pi_0 = 1, \quad \pi_1 = \tilde{\pi}_1 = \tilde{\pi}_2 = 4/9. \tag{4.45}$$

Viscosity and thermal conductivity are

$$\mu = \lambda = 3/4$$

thus yielding Prandtl number $Pr = 1$. This is the same as the Prandtl number for classical BGK systems [17] as well as for the SRT Lattice Boltzmann system citeSucci.

Since λ depends on $\ell_0 - \ell_2$ but not on $\ell_0 + \ell_2$ while the opposite is true for μ, it is easy

to construct systems with variable Prandtl numbers.

4.7 Example (Variable Prandtl number): The ansatz

$$C^{-1} = (S^T E_0^{-1} S) \cdot \begin{pmatrix} 1 & \\ & (1+\epsilon) \cdot I_4 - \epsilon \cdot G^2 \end{pmatrix} \tag{4.46}$$

leads to the representation (4.31) with ℓ_{00}, $\ell_0 + \ell_2$ and $\ell_1 + \ell_3$ as in Example 4.6. Thus viscosity is the same as before. $\ell_0 - \ell_2$ and thermal conductivity change by a factor $(1+\epsilon)$ giving rise to the new Prandtl number

$$Pr = (1+\epsilon)^{-1}. \tag{4.47}$$

The new collision frequencies can be easily calculated as

$$\pi_0 = 1, \quad (\pi_1, \tilde{\pi}_1, \tilde{\pi}_2) = \frac{4}{9 \cdot (1+2\epsilon)} \cdot (1-\epsilon, 1+2\epsilon, 1+26\epsilon). \tag{4.48}$$

E.g. for a hard sphere gas with $Pr = 2/3$ we find the frequencies

$$\pi_0 = 1, \quad \pi_1 = 1/9, \quad \tilde{\pi}_1 = 4/9, \quad \tilde{\pi}_2 = 28/9. \tag{4.49}$$

5 Numerical examples

After having studied the algebraic structure of (linearized) discrete kinetic models we are going to discuss some of their numerical properties. We restrict to the nine-velocity model ($N = 8$) since this is comparable to the standard D2Q9 relaxation models for Boltzmann Lattice systems.

5.1 Heat layer and Couette flow

The simplest nontrivial flows to investigate for the $N+1$-velocity systems are the heat layer and the Couette flow between two parallel plates, considered here to be placed at $x = -1$ and $x = 1$. Both are given by the $(N+1)$-dimensional steady Boltzmann system

$$v_x \partial_x f = \gamma J(f) \tag{5.1}$$

with inflow boundary conditions at $x = \pm 1$. This describes an index-1 differential-algebraic system of equation which can be transformed into an $(N+1-n)$-dimensional differential two-point boundary value system, where n is the dimension of the algebraic

part. In the case of the nine-velocity model, the algebraic part has dimension 3 (number of velocities with vanishing v_x-components), and the differential system has dimension 6. Denote by

$$e_0(\mathbf{v}) = a_0 \cdot \exp(-s|\mathbf{v}|^2) \tag{5.2}$$

a central Maxwellian and by L the corresponding linearized collision operator. Eliminating the algebraic part, the linearized problem is governed by a differential system of the form

$$\partial_x \phi = \gamma \hat{L} \phi \tag{5.3}$$

In [7] (for the continuous case) and in [1, 6] (for discrete models with certain symmetry conditions which are satisfied in our case) flows satisfying this equation have been analyzed and shown to consist of exponentially decaying boundary layers, of a linear macroscopic profile and an orthogonal macroscopically non-observable part. This is due to the Jordan normal form of $\hat{L}$ which is given by

$$N = \mathrm{diag}(\Lambda, -\Lambda, N_0, N_0, 0, 0) \tag{5.4}$$

Here, Λ is a diagonal matrix with positive diagonal entries, and

$$N_0 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{5.5}$$

is an elementary Jordan block with eigenvalue 0. Solutions of the linearized system are given by the exponential

$$\exp(xN) = \mathrm{diag}\left(\exp(x\Lambda), \exp(-x\Lambda), \begin{pmatrix} 1 & x \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & x \\ 0 & 1 \end{pmatrix}, 1, 1\right) \tag{5.6}$$

The blocks corresponding to $\exp(\pm x\Lambda)$ establish the boundary layers, and the other blocks the 6-dimensional linear macroscopic part. Obviously the nine-velocity system has a dimension too low to produce boundary layers. Thus only linear profiles are to be expected. Figure 2 shows the temperature profile of a heat layer problem with the inflow boundary conditions

$$f_{in}(\pm 1) = a_\pm \cdot \exp(-(s \pm \Delta s)|\mathbf{v}|^2) \tag{5.7}$$

$\mathbf{b} = (0, b_y)^T$, and the velocity profile of a Couette problem with boundary conditions

$$f_{in}(\pm 1) = a \cdot \exp(-s|\mathbf{v} \pm \mathbf{b}|^2), \tag{5.8}$$

For these calculations we have chosen a spatial discretization $\Delta x = 0.01$, a collision frequency $\gamma = 0.002$, and a ratio between space and time discetization parameter $\Delta t/\Delta x = 0.5$. We denote the corresponding Knudsen number as Kn_0.

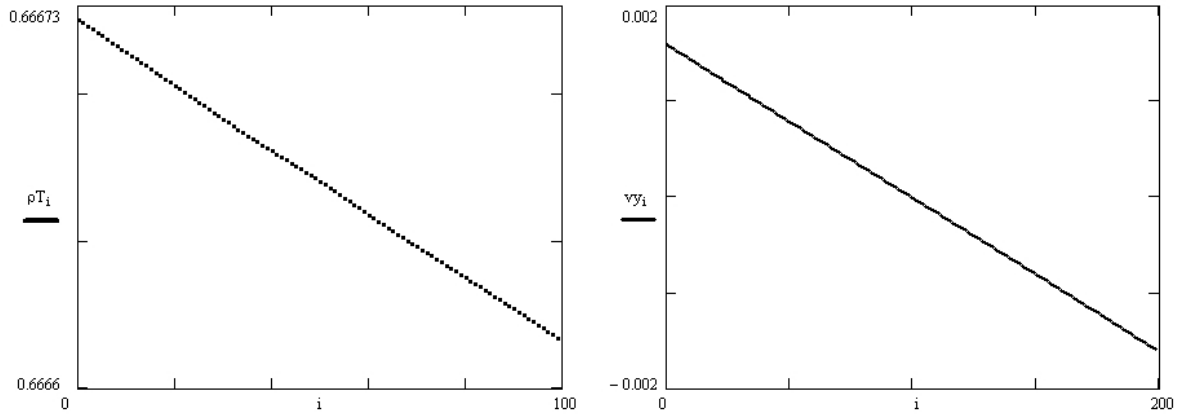

FIGURE 2. Linear profiles for (a) heat layer and (b) Couette flow problem.

In order to show that the situation is more complex than shown above, we modify parameters. (We restrict to the Couette problem.) In the Lattice Boltzmann case one is interested in the Navier-Stokes equations, i.e. in small Knudsen numbers. To this end we choose $\Delta t/\Delta x = 0.1$ and $\gamma = 0.02$ which results in a Knudsen number $0.02Kn_0$. While the Navier-Stokes correction to the Euler equation predicts a linear profile similar to that above, we find vanishing flow velocity in the main part, supplemented with boundary layers (Figure 3(a)). This shows that the Chapman-Enskog procedure does not produce the correct results. Passing to large Knudsen numbers the situation again changes completely. The flow pattern now exhibits a shock profile. In Figure 3(b) we have chosen $\gamma = 0.00002$ ($Kn_0 = 20$). Increasing the mean free path even more with $\Delta x = 0.0025$, $\gamma = 10^{-7}$ and $\Delta t/\Delta x = 0.1$ produces a double shock. This situation needs further theoretical investigation which will follow in some future work.

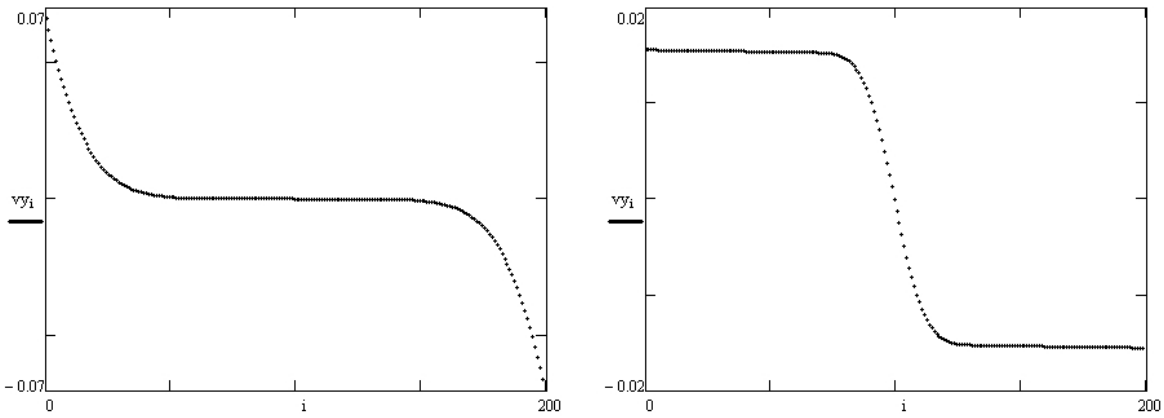

FIGURE 3. Degenerate profiles for (a) small (b) large Knudsen numbers.

5.2 Lid-driven flow

In [5] a 2D simulation of a thermal creep flow with the nine-velocity model was demonstrated, showing a tendency to instability in a certain parameter range. Here, we shortly illustrate an example of a lid-driven flow, i.e. a flow in a square cavity with one moving wall (upper wall) generating a circular flow. This is a favorite test case for lattice Boltzmann simulations, e.g. [11]. In 2D simulations it turns out that large Knudsen numbers as those taken above lead to artificial flow profiles due to the low number of velocities. Thus we have to restrist to reasonably small mean free paths. Lid driven cavities lead to typical flow patterns like that in Figure 4(a) which was obtained on a 40×40 spatial grid with a ration $\Delta t/\Delta x = 5$ and a relaxation time of $\tau = 1.15$. The flow pattern in the upper right corner on a 150×150 grid with $\Delta t/\Delta x = 1$ and $\tau = 0.015$ is given in Figure 4(b). Figure 5 shows the pressure profile for this situation. It turns out that the circular pattern is superimposed by a plane perturbation. Phenomena like these will be studied in future work. In particular it will have to be investigated how far the results are affected by the choice of the collision models.

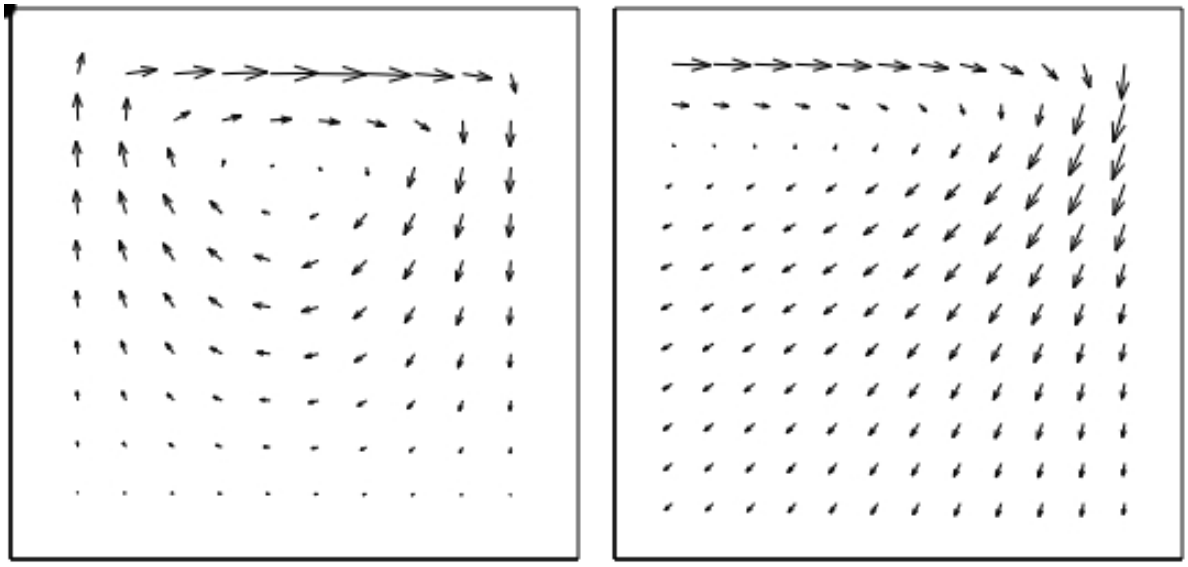

FIGURE 4. Lid-driven flow at (a) large (b) small Knudsen numbers.

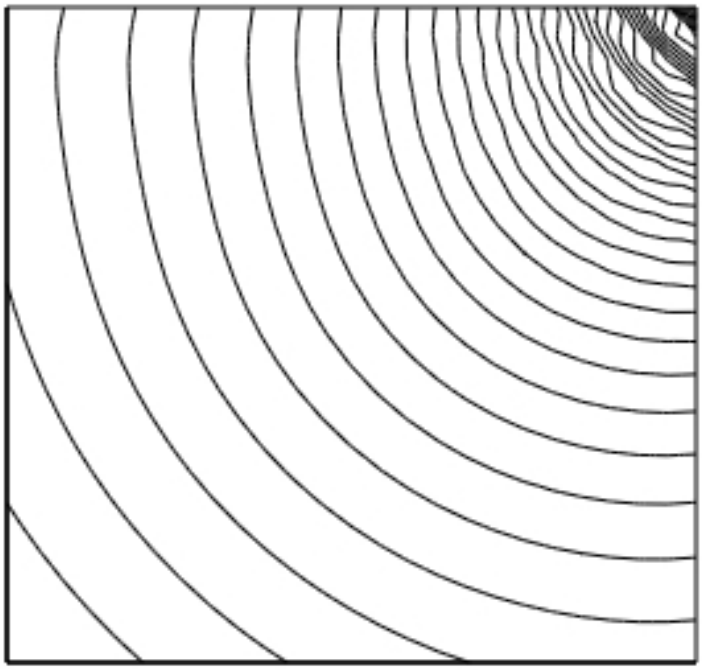

FIGURE 5. Pressure field of lid-driven flow.

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