Kinetic boundary layers for the Boltzmann equation on discrete velocity lattices

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WE CONSIDER families of discrete velocity models with physical collision invariants, and develop algebraic criteria for well-posedness of the linearized kinetic boundary layer problem. Using the obtained criteria we discuss various hierarchies of symmetric discrete velocity models, and calculate analytical and numerical slip coefficients for the representants of the hierarchies.

Key words: kinetic boundary layers, discrete velocity models, linearized Boltzmann equation, slip coefficients

1. Introduction

FOR MANY FLUID dynamic applications, a correct description of the real phenomena occurring in fluid flows in the vicinity of obstacles (e.g. supersonic, hypersonic airplanes, space shuttles, reentry problems) in rarefied flows is essential to calculate proper values of the temperature and pressure fields on the surface of the body.

In particular, numerical calculations based on the compressible Navier–Stokes equations with the non-slip boundary conditions do not provide the proper description of the shocks for such flows. It amounts to the fact that fluid dynamic equations are not valid in the thin region in vicinity of the obstacles, usually of the order of the mean free path. In this *boundary layer* region the Boltzmann equation describes properly the flow and provides correct boundary conditions for the flow outside the boundary layer, cf. [1].

Let M be a macroscopic physical quantity (mass, bulk velocity, energy), with known macroscopic gradients at infinity (outside the boundary layer). These gradients are known, for example, from numerical calculations based on fluid dynamic equations. Thus (with the x-axis being the direction perpendicular to the wall), the relevant quantity can be written as:

$$M = xr + \Delta(x),$$

where $\Delta(x)$ has vanishing gradients for $x \to \infty$. For a correct fluid dynamic description it is important to know the limit values of M at x = 0, which means the value $\Delta(0)$. As an illustration, let M = T be a fluid temperature. For fluid dynamic calculations we need T(x = 0) as a boundary condition. It would be reasonable to use the wall temperature as T(0). However, it turns out that it has to be corrected due to kinetic effects in the boundary layer. In fluid dynamic calculations we do not want to use the detailed description of the kinetic model. The influence of the kinetic layer enters into the fluid dynamic correction as a jump coefficient, defined as a difference between the wall temperature and the effective fluid temperature at x = 0.

The Boltzmann equation [2] is a complicated integro-differential equation, and its solution is a formidable numerical task. Deterministic numerical schemes of solving the Boltzmann equation require discretization of the velocity space. The reader is referred to e.g. [3–10] and the references therein for various computational and theoretical aspects of the discretization of the original Boltzmann equation.

In computations, the discretized velocity space has to be finite. The relevant Discrete Velocity Models should possess specific properties, necessary for the consistence of the models and the correct description of physics, cf. [11]. In general, for arbitrary discretization of the velocity space, velocities of the particles after the collision do not need to belong to the velocity lattice, from which the velocities of the pre-colliding particles have been chosen. Thus, the first essential property of the admissible collisions (binary as well as higher-order collisions) is that the underlying discrete lattice is invariant under all such collisions. The second essential requirement for the discrete lattice is that mass, momentum and energy are conserved in the admissible collisions. In addition, one requires that there are no other conserved quantities, i.e. there are no spurious conservation laws in the considered model., cf. [12]. In other words, the number of collision invariants is the same as for the original Boltzmann equation with continuum velocity space.

Additional requirements for a model construction follow from the physics of the considered problem. In particular, in order to obtain the proper numerical scheme for the boundary layer, first the problem of well-posedness of the kinetic boundary layer problem should be solved, cf. [13, 14].

In the case of a linearized Boltzmann equation with continuum velocity space, this problem has been solved in [18]. The authors proved existence and uniqueness (in a weighted L_2 space) of the boundary value problem for the linearized Boltzmann equation in one spatial dimension, with given mass flux through an arbitrary wall x = const., integrable inflow distribution at x = 0, and prescribed gradients of velocity and temperature at $x \to \infty$. The solution can be decomposed into three parts: the hydrodynamic part (linear in x, i.e. with constant gradients), the constant part which is orthogonal to the null space of the linearized Boltzmann operator and does not contribute to macroscopic quantities (the so-called fluctuation part), and the exponentially decaying boundary layer part, which is a solution of an adequate Milne problem. Any discrete velocity counterpart of the considered boundary value problem should conserve this structure of the solution, cf. [14]. It is precisely this structure which is analyzed in the present paper and which can be applied, e.g. for the derivation of diffusion limits within thin gaps [15]. The assumptions introduced are physically reasonable and turn out to be valid for discrete velocity models used for the numerical simulation of rarefied gas flows, like that described in [16, 17].

In this paper we discuss general algebraic criteria for the discretized Boltzmann collision operator, and several families of general discrete velocity lattices, which satisfy the above requirements and provide sufficient conditions for the well-posedness of the linearized kinetic boundary layer problem. We study sufficient conditions for discretization schemes, which provide the same qualitative behavior of the distribution function as that found in the original linearized Boltzmann equation. We consider various hierarchies of discrete models and calculate the relevant slip coefficients of adequate macroscopic quantities for representatives of two such hierarchies: 12-velocity model and 13-velocity model. The latter hierarchy admits, beyond usual binary collisions, also the collisions of higher order, in particular the so-called ternary (triple) collisions, in which three particles take part in the collision. This means that both the pre-collisional and post-collisional velocities of the three particles belong to the lattice. We assume that the usual conservation laws are satisfied for such collisions.

We investigate the influence of higher order collisions on the properties of the considered boundary layers, in particular on their thickness and the numerical values of slip coefficients. In addition, we also present exact analytical and numerical results for the simplest, nontrivial in the context of the kinetic boundary layer model – a plane 8 – velocity model, in which triple collisions are necessary to preserve proper structure of the kinetic boundary layer.

The paper is organized as follows. In the first section we consider various algebraic aspects of the linearized problem and prove the relevant mathematical results. In the second section we introduce two general hierarchies of the discrete velocity lattices, which have the required theoretical properties. The next sections deal with analytical and numerical calculations for the representative examples of the hierarchies considered. We also shortly discuss some other, well-known discrete models, such as 8-velocity or 6-velocity planar models. In the last section we discuss the results and their possible generalizations.

2. Linearized kinetic boundary layers

2.1. Discrete Velocity Models

We consider Discrete Velocity Models consisting of 2N+K discrete velocities $\mathbf{v}_1, \ldots, \mathbf{v}_{2N+K}$ in \mathbb{R}^d (d = 2, 3). We denote by v_i the *x*-component of \mathbf{v}_i , with the *x*-axis being the direction normal to the wall.

Introducing a binary collision model, we arrive at a set of (nonlinear) kinetic equations. Here, we are interested only in the stationary, spatially onedimensional version given by

(2.1)
$$v_i \partial_x f_i = \sum_{jkl=1}^{2N+K} A_{ij}^{kl} (f_k f_l - f_i f_j).$$

Linearization around a constant equilibrium state $m = (m_i)_{i=1}^{2N+K}$ readily yields the following system (we denote the linearized part of f_i also by f_i):

(2.2)
$$v_i \partial_x f_i = \sum_{jkl=1}^{2N+K} A_{ij}^{kl} (m_k f_l + m_l f_k - m_i f_j - m_j f_i).$$

Physically relevant collision models follow certain (symmetry) principles (like rotational invariance of the collision rates, invariance with respect to reflection at a plane etc.), and the principle of micro-reversibility (stating that the rate for a collision $(v, w) \rightarrow (v', w')$ is the same as that for the reverse collision $(v', w') \rightarrow (v, w)$). Properties like these are reflected in the Assumptions 1 and 2 to follow.

ASSUMPTION 1. (a) Symmetries of collision coefficients:

(2.3)
$$A_{ij}^{kl} = A_{ji}^{kl} = A_{kl}^{ij};$$

if $i \in \{j, k, l\}$, then $A_{ij}^{kl} = 0$.

(b) Symmetries of velocities: The velocities are arranged in such a way that for i = 1, ..., N, $v_{i+N} = -v_i$; (other components of \mathbf{v}_i and of \mathbf{v}_{i+N} are assumed to be equal, i.e. \mathbf{v}_{i+N} is obtained from \mathbf{v}_i by reflection at the plane x = 0); furthermore, $v_i > 0$. For i = 2N + 1, ..., 2N + K, $v_i = 0$.

We write the linearized equations in the form

$$(2.4) V \cdot \partial f = Mf$$

with $V = \text{diag}(v_i, i = 1, ..., 2N + K)$ and decompose M in the form

(2.5)
$$M = \begin{pmatrix} A_1 & B_1 & C_1 \\ B_2 & A_2 & C_2 \\ D_1 & D_2 & E \end{pmatrix}$$

with the $N \times N$ -matrices A_1, B_1, B_2, A_2 .

ASSUMPTION 2. ("left-right-symmetry") (a) The collision coefficients satisfy for $1 \le i, j, k, l \le N$ the conditions

(2.6)
$$A_{ij}^{kl} = A_{i+N,j+N}^{k+N,l+N}, \quad A_{i,j+N}^{kl} = A_{i+N,j}^{k+N,l+N}, \quad A_{i+N,j+N}^{kl} = A_{i,j}^{k+N,l+N}.$$

(b) For i > 2N and $1 \le j, k, l \le N$,

$$(2.7) A_{ij}^{kl} = A_{i,j+N}^{k+N,l+N}, A_{i,j+N}^{kl} = A_{i,j}^{k+N,l+N}, A_{i,j}^{k,l+N} = A_{i,j+N}^{k+N,l}.$$

(c) The linearized system is obtained by linearization around an equilibrium solution satisfying the condition

(2.8)
$$m_i = m_{i+N}, \quad i = 1, \dots, N.$$

A simple consequence of these assumptions is the following:

LEMMA 1. (a) M takes the form

$$M = \begin{pmatrix} \bar{A} & \bar{B} & C \\ \bar{B} & \bar{A} & C \\ C^T & C^T & E \end{pmatrix}$$

with $A_1 = A_2 =: \overline{A}, B_1 = B_2 =: \overline{B}, and C_1 = C_2 = D_1^T = D_2^T =: C$. The coefficients of $\overline{A}, \overline{B}, C$ and E are given by

(2.9)
$$\bar{a}_{ii} = -\sum_{j,k,l)=1}^{2N+K} A_{ij}^{kl} m_j,$$

(2.10)
$$\bar{a}_{ij} = 2 \sum_{k,l=1}^{2N+K} A_{ik}^{jl} m_l - \sum_{k,l=1}^{2N+K} A_{ij}^{kl} m_i,$$

(2.11)
$$\bar{b}_{ii} = 0,$$

(2.12)
$$\bar{b}_{ij} = 2 \sum_{k,l=1}^{2N+K} A_{ik}^{j+N,l} m_l - \sum_{k,l=1}^{2N+K} A_{i,j+N}^{kl} m_i,$$

(2.13)
$$c_{ij} = 2 \sum_{k,l=1}^{2N+K} A_{ik}^{j+2N,l} m_l - \sum_{k,l=1}^{2N+K} A_{i,j+2N}^{kl} m_i \quad ,$$

(2.14)
$$e_{ij} = 2 \sum_{k,l=1}^{2N+K} A_{i+2N,k}^{j+2N,l} m_l - \sum_{k,l=1}^{2N+K} A_{i+2N,j+2N}^{kl} m_{i+2N} .$$

(b) If $m_i = m_j$ for all i, j = 1, ..., 2N + K, then \overline{A} , \overline{B} and E are symmetric.

A special treatment is necessary for the algebraic equations

$$(2.15) \qquad \left(\begin{array}{cc} C^T & C^T & E\end{array}\right)f = 0.$$

If the $K \times K$ -matrix E is regular, then the components $f^{(alg)} := (f_{2N+1}, \ldots, f_{2N+K})^T$ can be obtained from $f^{(1)} := (f_1, \ldots, f_N)^T$ and $f^{(2)} := (f_{N+1}, \ldots, f_{2N})^T$ by

(2.16)
$$f^{(alg)} = -E^{-1}(C^T f^{(1)} + C^T f^{(2)}).$$

This means that the algebraic components can be removed in order to obtain a regular differential system.

COROLLARY 1. If E is invertible, then the linearized equations for $f^{(1)}$ and $f^{(2)}$ read

(2.17)
$$V_1 \partial_x f^{(1)} = (\bar{A} - CE^{-1}C^T)f^{(1)} + (\bar{B} - CE^{-1}C^T)f^{(2)},$$

(2.18)
$$-V_1 \partial_x f^{(2)} = (\bar{B} - C E^{-1} C^T) f^{(1)} + (\bar{B} - C E^{-1} C^T) f^{(2)},$$

where $V_1 = \text{diag}(v_1, \dots, v_N)$. If $m_i = m_j$ for $1 \le i, j \le 2N + K$, then

(2.19)
$$A := \bar{A} - CE^{-1}C^T$$
 and $B := \bar{B} - CE^{-1}C^T$

are symmetric.

2.2. A system of ordinary differential equations

According to the results of previous section, we consider the system

$$(2.20) V \cdot \partial_x f = Mf$$

where now f is the distribution function related to 2N velocities,

(2.21)
$$V = \begin{pmatrix} \operatorname{diag}(\nu_1, \dots, \nu_N) & 0\\ 0 & \operatorname{diag}(-\nu_1, \dots, -\nu_N) \end{pmatrix} =: \begin{pmatrix} V_1 & 0\\ 0 & -V_1 \end{pmatrix},$$
$$\nu_i > 0,$$

and

$$(2.22) M = \begin{pmatrix} A & B \\ B & A \end{pmatrix}$$

Our main concern here is the eigenspace structure and with this, the Jordan normal form of $V^{-1}M$. Denote

(2.23)
$$|V| := \begin{pmatrix} V_1 \\ V_1 \end{pmatrix}, \quad |V|^{\pm \frac{1}{2}} := \begin{pmatrix} V_1^{\pm \frac{1}{2}} \\ V_1^{\pm \frac{1}{2}} \end{pmatrix}.$$

Then $V^{-1}M$ is similar to the matrix

(2.24)
$$\tilde{M} := |V|^{1/2} (V^{-1}M) |V|^{-1/2} = \begin{pmatrix} \tilde{A} & \tilde{B} \\ -\tilde{B} & -\tilde{A} \end{pmatrix}$$

with

(2.25)
$$\tilde{A} = V_1^{-1/2} A V_1^{-1/2}$$
, and $\tilde{B} = V_1^{-1/2} B V_1^{-1/2}$.

For us it is more convenient to work with \tilde{M} rather than $V^{-1}M$. We notice that

(2.26)
$$\tilde{M}^2 = \begin{pmatrix} \tilde{A}^2 - \tilde{B}^2 & \tilde{A}\tilde{B} - \tilde{B}\tilde{A} \\ \tilde{A}\tilde{B} - \tilde{B}\tilde{A} & \tilde{A}^2 - \tilde{B}^2 \end{pmatrix}.$$

Let us begin with some clarifying remarks. In the following, we will call a vector \mathbf{z} with block structure of the form $\mathbf{z} = (z_1, z_2)$ even, if $z_1 = z_2$, and odd, if $z_1 = -z_2$, where z_1, z_2 are N-dimensional vectors.

REMARKS (a) Suppose $\mathbf{z} = (z_1, z_2)^T \in \ker(\tilde{M})$. Then \mathbf{z} can be written uniquely as the sum of an even vector \mathbf{z}^+ and an odd vector \mathbf{z}^- . These vectors are given as

$$\mathbf{z}^{+} = \frac{1}{2} \begin{pmatrix} z_1 + z_2 \\ z_1 + z_2 \end{pmatrix}$$
 and $\mathbf{z}^{-} = \frac{1}{2} \begin{pmatrix} z_1 - z_2 \\ -(z_1 - z_2) \end{pmatrix}$

A simple calculation shows that $\mathbf{z} \in \ker(\tilde{M})$ if and only if $(z_1 + z_2) \in \ker(\tilde{A} + \tilde{B})$ and $(z_1 - z_2) \in \ker(\tilde{A} - \tilde{B})$.

(b) For realistic models linearized around a symmetric equilibrium state, the even eigenvectors are the mass, y-impulse and energy vector; the only odd eigenvector is the x-impulse vector.

The eigenspaces of \tilde{M} corresponding to nonzero real eigenvalues are related to the eigenspaces of $(\tilde{A} + \tilde{B})(\tilde{A} - \tilde{B})$ and $(\tilde{A} - \tilde{B})(\tilde{A} + \tilde{B})$ as follows.

LEMMA 2. For a given real number $\lambda \neq 0$, the following statements are equivalent:

(i) λ^2 is an eigenvalue of $(\tilde{A} + \tilde{B})(\tilde{A} - \tilde{B})$,

- (ii) λ^2 is an eigenvalue of $(\tilde{A} \tilde{B})(\tilde{A} + \tilde{B})$,
- (iii) λ is an eigenvalue of M,
- (iv) $-\lambda$ is an eigenvalue of M.

P r o o f. We note that necessary and sufficient condition for a vector $(y + z, y - z)^T \neq 0$ to be an eigenvector of \tilde{M}^2 with eigenvalue λ^2 is that y and z should be eigenvectors of $(\tilde{A} - \tilde{B})(\tilde{A} + \tilde{B})$ resp. of $(\tilde{A} + \tilde{B})(\tilde{A} - \tilde{B})$ with the same eigenvalue.

It follows that both (iii) and (iv) imply that at least one of the conditions (i) or (ii) holds. On the other hand, suppose that (i) is satisfied with an eigenvector z. Then

(2.27)
$$y := \frac{1}{\lambda} (\tilde{A} - \tilde{B}) z$$

is an eigenvector of $(\tilde{A} - \tilde{B})(\tilde{A} + \tilde{B})$ with the same eigenvalue λ^2 , and

(2.28)
$$z = \frac{1}{\lambda} (\tilde{A} + \tilde{B})y.$$

Similarly, if (ii) is satisfied with an eigenvector y, then

(2.29)
$$z := \frac{1}{\lambda} (\tilde{A} + \tilde{B}) y$$

is an eigenvector of $(\tilde{A} + \tilde{B})(\tilde{A} - \tilde{B})$ satisfying

(2.30)
$$y = \frac{1}{\lambda} (\tilde{A} - \tilde{B}) z.$$

If $(y, z)^T$ is a pair of eigenvectors satisfying (2.28) resp. (2.30), then $(y+z, y-z)^T$ is an eigenvector of \tilde{M} with eigenvalue λ , and $(y-z, y+z)^T$ is one with eigenvalue $-\lambda$.

These remarks should justify the following assumptions.

ASSUMPTION 3. (i) The zero-eigenspace of M is spanned by n_0 odd eigenvectors $b_i^- = (e_i^-, -e_i^-)^T$, $i = 1, \ldots, n_0$, and $n_0 + r_0$ even eigenvectors $b_i^+ = (e_i^+, e_i^+)^T$, $i = 1, \ldots, n_0 + r_0$.

(ii) $(\tilde{A} + \tilde{B})(\tilde{A} - \tilde{B})$ is diagonizable, and all eigenvalues are real and nonnegative. It is not clear whether this is a consequence of some intrinsic properties of all "reasonable" collision models. In all the particular regular models which we have investigated, \tilde{M}^2 turns out to be diagonizable.

Under this assumption, we are able to determine, as a first main result, the Jordan normal form of \tilde{M} . At first we have to analyze the zero eigenspace.

LEMMA 3. Under the Assumptions 3, the following holds. (a) $\text{Defect}(\tilde{A} - \tilde{B}) = n_0$ and $\text{defect}(\tilde{A} + \tilde{B}) = n_0 + r_0$. (b) Define the integer $q_0 \ge 0$ by

(2.31)
$$\dim[R(\tilde{A} - \tilde{B}) + \ker(\tilde{A} + \tilde{B})] = N - q_0.$$

Then

(2.32)
$$\dim[R(A - B) \cap \ker(A + B)] = r_0 + q_0$$

and

(2.33)
$$\operatorname{defect}[(A + B)(A - B)] = n_0 + r_0 + q_0.$$

(c) If \tilde{A} and \tilde{B} are symmetric, then also

(2.34)
$$\operatorname{defect}[(\tilde{A} - \tilde{B})(\tilde{A} + \tilde{B})] = n_0 + r_0 + q_0,$$

and

(2.35)
$$\dim[R(\tilde{A} + \tilde{B}) \cap \ker(\tilde{A} - \tilde{B})] = q_0.$$

P r o o f. (a) An odd vector $(v, -v)^T$ is in the kernel of M iff $v \in \ker(A-B)$. Thus a basis of $\ker(A-B)$ is given by e_i^- , $i = 1, ..., n_0$, and $V^{1/2}e_i^-$, $i = 1, ..., n_0$ is a basis of $\ker(\tilde{A} - \tilde{B})$. Similarly, $V^{1/2}e_i^+$, $i = 1, ..., n_0 + r_0$, is a basis of $\ker(\tilde{A} + \tilde{B})$.

(b) Suppose $v \in \ker[(\tilde{A} + \tilde{B})(\tilde{A} - \tilde{B}]$. Then either $v \in \ker(\tilde{A} - \tilde{B})$ or $(\tilde{A} - \tilde{B})v \in \ker(\tilde{A} + \tilde{B}) \setminus \{0\}$. Thus

(2.36)
$$\operatorname{defect}[(A+B)(A-B)] = \operatorname{defect}(\tilde{A}-\tilde{B}) + \operatorname{dim}[R(\tilde{A}-\tilde{B}) \cap \operatorname{ker}(\tilde{A}+\tilde{B})].$$

From the formula for general subspaces U, U',

$$\dim(U) + \dim(U') = \dim(U + U') + \dim(U \cap U')$$

follows

(2.37)
$$\dim[R(\tilde{A} - \tilde{B}) \cap \ker(\tilde{A} + \tilde{B})]$$
$$= \dim[R(\tilde{A} - \tilde{B})] + \operatorname{defect}(\tilde{A} + \tilde{B}) - \dim[R(\tilde{A} - \tilde{B}) + \ker(\tilde{A} + \tilde{B})]$$
$$= (N - n_0) + (n_0 + r_0) - (N - q_0) = r_0 + q_0.$$

With (2.36) follows (2.33).

(c) If \tilde{A} and \tilde{B} are symmetric, then

(2.38)
$$[(\tilde{A} + \tilde{B})(\tilde{A} - \tilde{B})]^T = [(\tilde{A} - \tilde{B})(\tilde{A} + \tilde{B})],$$

and (2.34) follows from (2.33). (2.35) is an immediate consequence of (2.34) and defect $(\tilde{A} + \tilde{B}) = n_0 + r_0$.

The general normal form is now given as follows.

THEOREM 1. If $q_0 = 0$ or if \tilde{A} and \tilde{B} are symmetric, then \tilde{M} has a Jordan normal form $\tilde{M} = TJT^{-1}$, where T is a nonsingular transformation matrix, and

(2.39)
$$J = \begin{pmatrix} \Lambda & & & & \\ & -\Lambda & & & & \\ & & J_1 & & & \\ & & \ddots & & & \\ & & & \ddots & & \\ & & & J_{r_0+q_0} & & \\ & & & & 0 & \\ & & & & & 0 \end{pmatrix},$$

where

(2.40)
$$\Lambda = \operatorname{diag}(\tilde{\lambda}_i, i = 1, \dots, N - (n_0 + r_0 + q_0)), \quad \tilde{\lambda}_i > 0,$$

and the Jordan blocks

(2.41)
$$J_1 = \dots = J_{r_0+q_0} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

P r o o f. We have to construct a basis of $\mathbb{R}^{2N},$ under which \tilde{M} acts as given by J.

(i) First, we construct the eigenvectors of \tilde{M} with nonzero eigenvalues. For this, denote by z_i , $i = 1, \ldots, N - (n_0 + r_0 + q_0)$, linearly independent eigenvectors of $(\tilde{A} + \tilde{B})(\tilde{A} - \tilde{B})$ with eigenvalues $\lambda_i^2 > 0$. (Compare Assumption 3 (ii) and Eq. (2.33).) With $\lambda_i \cdot y_i := (\tilde{A} - \tilde{B})z_i$, the vectors $(y_i + z_i, y_i - z_i)^T$ resp. $(y_i - z_i, y_i + z_i)^T$ are linearly independent eigenvectors of \tilde{M} with eigenvalues $\pm \lambda_i$.

(ii) We need a collection of pairs (v_i, w_i) of independent vectors, $i = 1, \ldots, r_0 + 2q_0$, which correspond to the Jordan blocks J_i . From (2.32) it follows that there are $r_0 + q_0$ vectors x_i such that $y_i := (\tilde{A} - \tilde{B})x_i$ are linearly independent elements of ker $(\tilde{A} + \tilde{B})$. Denote

(2.42)
$$v_i := \begin{pmatrix} x_i \\ -x_i \end{pmatrix}$$
 and $w_i := \begin{pmatrix} y_i \\ y_i \end{pmatrix}$.

Then $w_i = \tilde{M}v_i$ and $\tilde{M}w_i = 0$. Similarly, the existence of q_0 additional pairs follows from formula (2.35).

(iii) In (ii), $r_0 + q_0$ resp. q_0 elements of ker $(\tilde{A} + \tilde{B})$ resp. of ker $(\tilde{A} - \tilde{B})$ have been used to construct the basis elements related to J. We supplement these with

 $n_0 - q_0$ linearly independent vectors $b_i \in \ker(\tilde{A} + \tilde{B})$ and $n_0 - q_0$ independent elements $c_i \in \ker(\tilde{A} - \tilde{B})$, and complete the basis in \mathbb{R}^{2N} by $(b_i, b_i)^T$ and $(c_i, -c_i)^T$.

REMARK. We consider a Discrete Velocity Model to reveal the correct physical behavior, if the Jordan normal form reflects the structure of the full (i.e. continuous) system. Corresponding to [18], this means that there are two (in 2D) resp. 3 (in 3D) 2×2 -Jordan blocks, and two further zero-eigenvectors; the latter ones are the mass vector (even) and normal momentum ρv_x (odd). The Jordan blocks are related to the tangential moment components and to the energy vector.

2.3. Boundary layers and jump conditions

As worked out in the previous section, solutions of the system (2.4) on the half-space $[0, \infty)$ can be presented in the form

(2.43)
$$\Phi(x) = T \cdot \exp(xJ) \cdot T^{-1} \Phi_0,$$

where $\exp(xJ)$ is a block diagonal matrix

$$\exp(xJ) = \operatorname{diag}(\exp(x\Lambda), \exp(-x\Lambda), \exp(xJ_1), \dots, \exp(xJ_{r_0+q_0}), I)$$

consisting of an exponentially increasing part $\exp(x\Lambda)$, an exponentially decreasing part $\exp(-x\Lambda)$, the blocks

$$\exp(xJ_1) = \dots = \exp(xJ_{r_0+q_0}) = \begin{pmatrix} 1 & x \\ 0 & 1 \end{pmatrix}$$

and a lower-dimensional unit matrix I. Φ_0 represents the solution at x = 0. We call a solution of the form (2.43) a *boundary layer*, if Φ_0 is such that the exponentially increasing part is vanishing.

As a first simple illustration consider a four-velocity model with two velocities pointing to the right (i.e. $v_x > 0$) and two – to the left. In this case, N = 2, K = 0. We assume the existence of one Jordan block, i.e. $r_0 = 1$ and thus $n_0 = q_0 = 0$. The Jordan normal form reads

$$J = \begin{pmatrix} \lambda & & \\ & -\lambda & \\ & & 0 & 1 \\ & & & 0 \end{pmatrix},$$

and

(2.44)
$$\Phi(x) = T \cdot \begin{pmatrix} \exp(\lambda x) & & \\ & \exp(-\lambda x) & \\ & & \begin{pmatrix} 1 & x \\ & 1 \end{pmatrix} \end{pmatrix} \cdot T^{-1} \Phi_0.$$

Denoting by \mathbf{t}_i the *i*-th column of the transformation matrix T, and the initial vector as

(2.45)
$$\Phi_0 = \sum_{i=1}^4 r_i \mathbf{t}_i,$$

the Eq. (2.44) is given as

(2.46)
$$\Phi(x) = r_1 \exp(\lambda x) \mathbf{t}_1 + r_2 \exp(-\lambda x) \mathbf{t}_2 + (r_3 + r_4 x) \mathbf{t}_3 + r_4 \mathbf{t}_4.$$

Notice that \mathbf{t}_3 is the component related to one of the ("even") conservation laws (e.g. energy, *y*-velocity). Using the terminology of [14, 18], the component \mathbf{t}_4 is called a *fluctuation part*.

Usually, a kinetic boundary layer is prescribed by some boundary condition at x = 0, concerning the inflow part Φ_0^+ (i.e. the restriction of Φ_0 to the velocities with $v_x > 0$). In our case, these are given by two conditions. The third condition comes from the definition of a boundary layer and reads $r_1 = 0$. The fourth condition is left and is used to prescribe the gradient of \mathbf{t}_3 at infinity, which fixes the component r_4 of the fluctuation part. With these requirements, the solution is in general uniquely described. In particular, r_3 is fixed what determines the value of the physically relevant component \mathbf{t}_3 at x = 0. This quantity is called the *jump condition* for \mathbf{t}_3 and is usually not to be read off directly from the boundary condition for Φ_0^+ . (In particular, it can not be determined in the full system from the wall temperature in the case of kinetic energy, or in the form of a zero-velocity condition for a wall at rest.)

3. Hierarchies of discrete lattices

3.1. Hierarchy 1

Hierarchy 1 is defined as a geometrical superposition of two sub-lattices E (with even coordinates of the velocities), and O (with odd velocity coordinates) in \mathbb{R}^d , with d = 2 or 3. For d = 2, the sub-lattices are defined as follows:

(3.1)
$$E = \{ (v_1, v_2) \in \mathbb{R}^2 : v_1 = \mp 2k, v_2 = \mp 2l, k, l \in \{0, 1...L\} \},\$$

(3.2)
$$O = \{ (v_1, v_2) \in R^2 : v_1 = \mp (2k+1), \\ v_2 = \mp (2l+1), k, l \in \{0, 1...L-1\} \}$$

with obvious generalization to three dimensions, and for the lattices with unequal number of nodes along different coordinate axes. The integer $L \in \{1, 2, ...\}$ determines the size of the lattice.

For given L and d, the number of nodes is $(2L + 1)^d + (2L)^d$. Thus, with L = 1 the simplest two-dimensional model is the (9 + 4) velocity model. In the notation of Subsection 2.1, the model is the (2*5+3)-velocity model, with three algebraic equations (K = 3). The subsequent two-dimensional model is the (2*18+5)-velocity model with K = 5 algebraic equations. In three dimensions (d = 3), the simplest model is the (2*13+9)-velocity model with 9 algebraic equations.

For future discussion we define "strong mixing" collisions as such, for which the pre-collisional and post-collisional velocity vectors of the collision partners are different. One can verify by inspection the existence of the binary strong mixing collisions in the models of Hierarchy 1, as well as the existence of higher-order (triple, quadruple) strong-mixing collisions. Explicit examples will be considered in Sec. 4.

3.2. Hierarchy 2

Hierarchy 2 is defined as a superposition of "strips", parallel to the coordinate axes. For d = 2, Hierarchy 2 consists of two strips:

The "horizontal" strip, the set of velocity vectors:

(3.3)
$$H = \{ [\mp (2k+1), -1], [\mp (2k+1), +1], k = 0, ...L \}$$

and the "vertical" strip, the set of velocity vectors:

$$(3.4) \quad V = \{ [-1, \mp(2k+1),], [1, \mp(2k+1)], k = 0, \dots L \}, \ L = 0, 1, \dots$$

Note that all the velocity vectors of Hierarchy 2 have all the components different from zero. For a given N, the number of different velocity vectors (lattice nodes) is 8(L+1) + 4. The simplest model corresponds to L = 0, which gives a symmetric 12-velocity model.

Analogous formulas can be derived in 3 dimensions. In that case the general model for Hierarchy 2 has 8 + 24L velocities. The simplest example is the 32-velocity model. Generalization for lattices with different number of velocity nodes along the coordinate axes is straightforward.

We define a "weak mixing collision" as the one, when pre-collisional and post-collisional velocities are from different strips. Weak mixing exists in both hierarchies, whereas strong mixing only in Hierarchy 1. Moreover, one can prove that increase of the number of nodes in Hierarchy 2 is always accompanied by the appearance of a new type of weak mixing collisions.

LEMMA 4. Let us consider the general 8L + 4 model of Hierarchy 2. Then, for any $L \in \{2, 3, ...\}$ there exists a weak mixing collision, not present in the relevant lattice with smaller L. P r o o f. For a given L value, which determines the size of the lattice, the velocities forming the horizontal (i.e. parallel to the x-axis) strip, belong to the set:

(3.5)
$$\{ [-(2k+1), -1], [(2k+1), -1], [-(2k+1), 1], [(2k+1), 1], \\ k = 0, \dots L \}.$$

The velocities forming the vertical strip, belong to the set:

(3.6)
$$\left\{ \left[-1, -(2k+1), \right], \left[-1, (2k+1) \right], \left[1, -(2k+1) \right], \left[1, (2k+1) \right], k = 0, \dots L \right\} \right\}$$

Let us choose [-(2(L-1)+1), 1] and [(2L+1), 1] as the pre-collisional pair, and [-1, -(2(L-1)+1)] and [1, (2L+1)] as the post-collisional one. One verifies by inspection that the conservation laws are satisfied, therefore this choice gives a weak mixing collision in which two particles from the "L" lattice, and two from the "L - 1" lattice participate.

4. Examples

In this section we report the results of analytical and numerical calculations of the kinetic boundary layers, obtained on the basis of theoretical considerations of the first section. We discuss three examples: one for each of the introduced hierarchies, and the kinetic boundary layer from an 8-velocity model on a plane. We calculate the relevant algebraic properties of the matrices defining the corresponding linearized operators, obtain expressions for the boundary layer thickness, and calculate the slip coefficients for the considered models.

As the first example we discuss the algebraic differential model with 13 velocities, with three algebraic equations resulting from the zero velocity projections of three velocity nodes of the lattice, which corresponds to K = 3 in notation of Sec. 2. The second example provides the differential model with all the velocity components different from zero, i.e. the model without the algebraic part, which corresponds to K = 0. Finally we consider a 8-velocity planar model, which does not belong to any of the considered hierarchies, however it gives the proper structure of the kinetic boundary layer, and exact analytic expressions for the slip coefficients.

4.1. Example of Hierarchy 1: (9 + 4)-velocity model with binary and triple collisions

This 2-dimensional discrete velocity lattice is obtained from the general Hierarchy 1 for L = 1, with 9 velocity vectors of the "even" sub-lattice E, and 4 velocity vectors of the "odd" hierarchy *O*. The relevant one-dimensional steady discrete velocity model equations read, after suitable rearrangement of the numbering of the velocity vectors:

(4.1)
$$v_x^i \partial_x f_i = Q_i, \quad i = 1, \dots 13$$

with

(4.2) $v_x^i = +2, i = 1, 2, 3, \quad v_x^i = +1, i = 4, 5, \quad v_x^i = -2, i = 6, 7, 8,$

(4.3)
$$v_x^i = -1, i = 9, 10, \quad v_x^i = 0, i = 11, 12, 13,$$

Note that the last three equations are algebraic, what corresponds to the algebraic part of Sec. 2 with K = 3.

The collision terms take into account all admissible binary and nontrivial (cf. Appendix A) triple collisions which conserve mass, momentum and energy for the considered lattice. For example,

(4.4)
$$Q_1 = c(f_3f_6 - f_1f_8) + e(f_2f_6 - f_1f_7) + e(f_3f_{11} - f_1f_{12}) + g(f_2f_{11} - f_1f_{13}) + t_2(f_2f_8f_{11} - f_1f_7f_{12})$$

The collision rates c, e, g are assumed to be proportional to the moduli of differences of the velocities of colliding particles in the case of binary collisions, cf. [10]. The coefficient t_2 describes the influence of triple collisions. Complete definitions and explanation of all the collision terms are given in Appendix A.

We linearize the equations around the symmetric Maxwellian $m_i = 1$, i = 1, ...13:

(4.5)
$$f_i = m_i + \tilde{f}_i, \quad i = 1, ... 13.$$

The last three algebraic equations i = 11, 12, 13 are used to reduce the system to the one with ten linear differential equations:

(4.6)
$$V \cdot \partial F = MF, \quad F = (f_1, \dots f_{10})^T,$$

with $V = \text{diag}(v_i, i = 1, ... 10)$ and

$$(4.7) M = \begin{pmatrix} A & B \\ B & A \end{pmatrix}$$

with the 5×5 -matrices A, B, cf. Subs. 2.2.

The coefficients of the matrices A and B are rather complicated algebraic expressions, nonlinearly depending on the collision rates. Their explicit values are given in Appendix B.

Using symbolic calculations we calculate:

(4.8)
$$\operatorname{Ker}(A+B) = \operatorname{span}\left\{ \left[-2, 0, 0, 0, 1 \right], \left[0, 0, 1, \frac{-1}{2}, 0 \right], \left[3, 1, 0, \frac{3}{2}, 0 \right] \right\}$$

(4.9)
$$\operatorname{Ker}(A-B) = \operatorname{span}\{[2, 2, 2, 1, 1]\},\$$

what confirms the correct structure of matrices obtained from the collision operators for the considered model, as discussed in Sec. 2.

We note that the correct structure of the matrices does not depend in this model on the existence of the triple collisions, cf. the 8-velocity planar model discussed in the next section, where the correct structure of the relevant matrices can be obtained only in the presence of triple collisions.

Eigenvalues of (A + B)(A - B):

$$\begin{split} \lambda_1^2 &:= \frac{7}{6} \, 18 \, t + 33, \\ \lambda_2^2 &:= \frac{9}{2} \frac{15 + 16 \, t + 4 \, t^2}{13 + 6 \, t} \end{split}$$

where $t = t_1 + t_2$ determines the contribution of both types of triple collisions to the boundary layer thickness, cf. discussion below and in Appendix A.

With explicit values of the collision rates: a = 1, b = 1, c = 2, d = 1, $e = 2, f = 1, g = 1, t_1 = t_2 = 1$ we obtain, using symbolic calculus, the following approximate values for the velocity and energy jumps across the boundary layer:

 V_y (perpendicular) velocity jump = 0.14 β ,

energy jump = $-0.14 \,\delta - 2.02 \,\alpha$,

where the constants α , β , δ are obtained from numerical calculations based on fluid dynamical equations, as discussed in the Introduction.

REMARK 1. Analysis of the eigenvalues shows that the thickness of the boundary layer, being proportional to the smaller of both eigenvalues is, for any positive t, greater than for t = 0; thus the triple collisions diminish the thickness of the boundary layer. Therefore, with the triple collisions taken into account, the region of validity of the description based on the fluid dynamical equations, enlarges. We point out however that in the considered model, triple collisions are not necessary to preserve the correct structure of the kinetic boundary layer.

4.2. Example 2: Hierarchy 2: (4 + 8)-velocity model

This 2 – dimensional discrete velocity model is obtained from the general Hierarchy 2 for L = 0. The velocity vectors are denoted $v^i = (v_x^i, v_y^i), i = 1, ...6, 9, ...14$, with

(4.10)
$$v_x^i = +3, i = 1, 3, v_x^i = +1, i = 2, 4, 5, 6, v_x^i = -3, i = 9, 11,$$

 $v_x^i = -1, i = 10, 12, 13, 14,$

(4.11)
$$v_y^i = +3, i = 5, 13, v_y^i = +1, i = 1, 2, 9, 10, v_y^i = -3, i = 6, 14,$$

 $v_y^i = -1, i = 3, 4, 11, 12.$

The relevant one-dimensional steady discrete velocity model equations read:

(4.12)
$$v_x^i \partial_x f_i = Q_i, \quad i = 1, \dots, 6, 9, \dots, 14.$$

Note that in this model the algebraic part vanishes.

The collision terms take into account all the admissible binary and nontrivial quadruple collisions (contrary to the previously considered model, this one does not admit nontrivial triple collisions), which conserve mass, momentum and energy for the considered lattice. Thus, e.g.

$$(4.13) Q_1 = -A_1 - B_1 - C_1 + F_1 + G_1 - G_4,$$

(4.14)
$$A_1 = a(f_1f_4 - f_2f_3), \quad B_1 = b(f_1f_{12} - f_3f_{10}),$$

(4.15)
$$C_1 = c(f_1f_{13} - f_3f_9), \quad F_1 = f(f_4f_5 - f_1f_{10}),$$

(4.16)

$$G_1 = g(f_2 f_4 f_6 f_9 - f_1 f_{10} f_{12} f_{14}),$$

$$G_4 = g(f_1 f_2 f_{10} f_{14} - f_3 f_4 f_{12} f_{13}).$$

The collision frequencies a, b, c, f are assumed to be proportional to the moduli of differences of the velocities of colliding particles in the case of binary collisions, cf. [10]. The operators G_i describe the influence of the quadruple collisions, cf. Appendix C for details.

We linearize the equations around the symmetric Maxwellian $m_i = 1$, i = 1, ...6, 9, ...14:

$$(4.17) f_i = m_i + \tilde{f}_i,$$

and obtain the linear differential system of 12 equations

$$(4.18) V \cdot \partial F = MF,$$

with $V = \text{diag}(v_i, i = 1, ...6, 9, ...14), \quad F = (f_1, ...f_6, f_9, ...f_{14})^T$, and

(4.19)
$$M = \begin{pmatrix} A & B \\ B & A \end{pmatrix}.$$

Using symbolic calculations we obtain:

$$A := \begin{bmatrix} -\frac{1}{3}a - \frac{1}{3}b - c - \frac{1}{3}f, \frac{1}{3}a, \frac{1}{3}a + \frac{1}{3}b + \frac{1}{3}c, -\frac{1}{3}a + \frac{1}{3}f, \frac{1}{3}c + \frac{1}{3}f, \frac{1}{3}c \\ a, -2a - 2b - d - 2f, -a + f, a + b + d, a, b - f \\\\ \frac{1}{3}a + \frac{1}{3}b + \frac{1}{3}c, -\frac{1}{3}a + \frac{1}{3}f, -\frac{1}{3}a - \frac{1}{3}b - c - \frac{1}{3}f, \frac{1}{3}a, \frac{1}{3}c, \frac{1}{3}c + \frac{1}{3}f \\\\ -a + f, a + b + d, a, -2a - 2b - d - 2f, b - f, a \\\\ c + f, a, c, b - f, -a - b - 3c - f, c \\\\ c, b - f, c + f, a, c, -a - b - 3c - f \end{bmatrix}$$

$$\begin{bmatrix} 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ -b & -d+2f & b-f & a+b+d & -b & -a+f \\ c & -a+f & c & -b & a+b+c & -3c \\ c & -b & c & -a+f & -3c & a+b+c \end{bmatrix}$$

$$\begin{split} &\operatorname{Ker}(A+B) = \operatorname{span}\{[-1,-1,0,0,-2,1],[2,1,1,0,3,0],[0,1,0,1,0,0]\},\\ &\operatorname{Ker}(A-B) = \operatorname{span}\{[3,1,3,1,1,1]\}. \end{split}$$

For the choice of the collision rates: a = 3 : b = 4 : c = 2 : d = 3 : f = 4, g = 0, corresponding to the closest integral number approximation of the values of collision rates for hard spheres, we obtain the following approximate values for perpendicular bulk velocity and energy:

 $V_y \text{ jump} = 0.04 \beta,$

energy jump = $-2.14 \alpha - .04 \delta$.

For a = b = c = d = f = 1 we obtain:

 V_y jump = 0.10 β ,

energy jump = $-2.16 \alpha - 0.13 \delta$.

Note the qualitative agreement of the results with those obtained from the previously considered model of Hierarchy 1.

4.3. Example 3: Plane 8v-model

This model seems to be the simplest one which gives the proper structure of the kinetic boundary layer. For this model, which does not belong to any of the above-defined hierarchies of regular models, one can obtain exact analytical expressions for the relevant jump coefficients. Six velocity vectors of the model $v^i = (v_x^i, v_y^i)$ are distributed regularly on a circle of radius 2, and have the following coordinates:

(4.20)
$$v^0 = (2,0), \quad v^1 = (1,\sqrt{3}), \quad v^5 = (-1,\sqrt{3}),$$

(4.21)
$$v^4 = (-2, 0), \quad v^7 = (-1, -\sqrt{3}), \quad v^3 = (1, -\sqrt{3}),$$

and the remaining two velocity vectors are

(4.22)
$$v^2 = (1.0), v^6 = (-1,0).$$

We denote the distribution functions of the particles with the above velocity vectors by: $f_0, f_2, \dots f_7$.

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The relevant one-dimensional steady discrete velocity model equations read:

(4.23)
$$v_x^i \partial_x f_i = Q_i, \quad i = 0, ...7,$$

with

(4.24)
$$Q_0 = -B_2 + B_3 - T, Q_1 = A_1 + B_1 + B_2 + T$$

(4.25)
$$Q_2 = -A_1 + A_2,$$
$$Q_3 = -A_2 - B_1 - B_3 + T,$$
$$Q_4 = B_2 - B_2 - T$$

(4.26)

$$Q_5 = A_1 + B + 1 + B_3 + T,$$

$$Q_6 = -A_1 + A_2,$$

$$Q_7 = -A_2 + B_1 - B_2 + T,$$

and with the binary collisional operators:

(4.27)
$$A_1 = a(f_2f_5 - f_1f_6), \quad A_2 = a(f_3f_6 - f_2f_7),$$

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$$(4.28) \quad B_1 = b(f_3f_5 - f_1f_7), \quad B_2 = b(f_0f_4 - f_1f_7) \quad B_3 = b(f_3f_5 - f_0f_4)$$

a, b being the collision rates for the relevant types of binary collisions. $T = t(f_0f_5f_7 - f_1f_3f_4)$ is the operator of triple collisions, with t – the collision rate for triple collisions. In this model triple collisions are necessary for the correct number of collision invariants, cf. Subs. 4.3.2. For this model we obtain exact expressions for the jumps in parametric form.

4.3.1. Plane 8-velocity model with triple collisions. We linearize the equations around the symmetric maxwellian $m_i = m$, i = 0, ...7:

(4.29)
$$f_i = m + \tilde{f}_i,$$

and obtain the system of 8 linear differential equations

$$(4.30) V \cdot \partial F = MF,$$

with $V = \text{diag}(v_i, i = 0, ...7), \quad F = (f_0 ... f_7)^T$, and

(4.31)
$$M = \begin{pmatrix} A & B \\ B & A \end{pmatrix}.$$

Using symbolic calculations we obtain:

$$A := \begin{bmatrix} -b - \frac{1}{2}t & \frac{1}{2}b + \frac{1}{2}t & 0 & \frac{1}{2}b + \frac{1}{2}t \\ b + t & -m - 2b - t & 1 & b - t \\ 0 & m & -2 & m \\ b + t & b - t & 1 & -m - 2b - t \end{bmatrix}$$
$$B := \begin{bmatrix} -b + \frac{1}{2}t & \frac{1}{2}b - \frac{1}{2}t & 0 & \frac{1}{2}b - \frac{1}{2}t \\ b - t & m + b + t & -1 & -2b + t \\ 0 & -m & 2 & -m \\ b - t & -2b + t & -1 & m + b + t \end{bmatrix}$$

Basis of Ker(A + B):

$$[1, 2, 0, 0], [0, 0, 1, 0], [0, -1, 0, 1]$$

Basis of Ker(A - B):

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 V_y and energy collisional invariants for 8v model:

$$\left[0, \frac{1}{2}\sqrt{3}, 0, -\frac{1}{2}\sqrt{3}, 0, \frac{1}{2}\sqrt{3}, 0, -\frac{1}{2}\sqrt{3}\right], [4, 4, 1, 4, 4, 4, 1, 4].$$

Eigenvalue of (A + B)(A - B):

$$\lambda^2 = 18\,b\,t + 4\,m\,b.$$

Note that the presence of ternary collisions decreases the boundary layer thickness, as it already has been discussed in Example 1. V_y jump is

$$\frac{1}{2}\frac{\beta}{3b+m}$$

and energy jump: $-\frac{1}{6} \left(-32 \,\delta \,m - 16 \,\delta \,m^2 - 189 \,\delta \,t^2 + 1080 \,t^2 \,\alpha + 216 \,\sqrt{2} \,c1 \,t \,\alpha - 72 \,\delta \,t + 54 \,t^2 \,\alpha \,m - 8 \,\sqrt{2} \,c1 \,\delta \,m - 102 \,\delta \,t \,m + 264 \,t \,\alpha \,m + 12 \,t \,\alpha \,m^2 + 12 \,\sqrt{2} \,c1 \,t \,\alpha \,m - 36 \,\sqrt{2} \,c1 \,\delta \,t \right) / \left(t \,(2 \,m^2 + 9 \,m \,t + 2 \,\sqrt{2} \,c1 \,m + 54 \,t + 12 \,\sqrt{2} \,c1 + 12 \,m) \right), \text{ where } c1 = \sqrt{b(9t + 2m)}.$

Note, as in the previously considered examples of Hierarchies 1 and 2, the correct, linear dependence of the velocity and energy jumps on the fluid dynamics coefficients α , β , δ .

4.3.2. Plane 8-velocity model without triple collisions. In this case the algebraic structure of the linearized problem is different. In particular, the E = A - B matrix has a two-dimensional zero eigenspace, which reflects existence of a spurious collision invariant. Nevertheless the general structure is conserved, with the energy jump zero as a necessary condition for the existence of the kinetic layer solution.

Eigenvectors of A + B:

$$[1, 2, 0, 0], [0, 0, 1, 0], [0, -1, 0, 1].$$

Eigenvectors of A - B:

Eigenvalue of (A + B)(A - B):

$$\lambda^2 = 2 \, m \, b.$$

In this case the energy jump vanishes, and V_y jump is

$$\frac{1}{2}\frac{\beta}{m+3b}.$$

5. Conclusions

We have derived algebraic criteria under which discrete velocity models lead to qualitatively correct boundary layers. These criteria include not only correct number of the conserved quantities, but also allow to model gradients of fluid quantities at infinity, and to calculate the jump conditions. We have tested the theory in a number of cases. As it turns out, the relevant algebraic details are readily calculated through application of computer algebra tools. They allow to determine the physical relevance of a given model and in particular, to answer the questions, which type of collisions can be dropped, thus simplifying the model, and which are essential to preserve the correct structure of the kinetic boundary layer. The explicit formulas derived in the theory allow to determine all the quantities relevant for the coupling with fluid dynamics, like layer thickness, flow gradients and jump conditions.

Included in the framework are also the models described by differential algebraic rather than only differential equations. The theory is flexible enough to include several of more general classes, like three-particle interaction models. It can be also applied for discrete velocity models of mixtures [19].

Acknowledgments

T.P. acknowledges the financial support granted by the KBN Grant No. 2 P03 A 007 17, and by the Alexander von Humboldt Stiftung during his stay at the Technical University Ilmenau, where the main part of the paper has been completed.

Appendix A.

We present expressions for the collision operators Q_i for the (9+4)-velocity model of Hierarchy 1.

(A.1)
$$Q_{2} = e(f_{1}f_{7} - f_{2}f_{6}) + b(f_{11}f_{12} - f_{2}f_{6}) + d(f_{4}f_{12} - f_{2}f_{10}) + d(f_{5}f_{11} - f_{2}f_{9}) + e(f_{3}f_{7} - f_{2}f_{8}) + f(f_{4}f_{5} - f_{2}f_{13}) + g(f_{1}f_{13} - f_{2}f_{11}) + g(f_{3}f_{13} - f_{2}f_{12}) + t_{1}(f_{7}f_{4}f_{5} - f_{2}f_{9}f_{11}) + t_{2}(f_{1}f_{7}f_{12} - f_{8}f_{2}f_{11}) + t_{2}(f_{3}f_{7}f_{11} - f_{6}f_{2}f_{12})$$

(A.2)
$$Q_3 = c(f_1 f_8 - f_6 f_3) + e(f_1 f_{12} - f_3 f_{11}) + e(f_2 f_8 - f_3 f_7) + g(f_2 f_{12} - f_3 f_{11}) + t_2(f_6 f_2 f_{12} - f_3 f_7 f_{11}) + t_2(f_1 f_7 f_{12} - f_8 f_2 f_{11}).$$

(A.3)
$$Q_4 = d(f_2 f_{10} - f_4 f_{12}) + a(f_9 f_5 - f_4 f_{10}) + d(f_{10} f_{11} - f_4 f_7) + f(f_{11} f_{13} - f_4 f_9) + f(f_2 f_{13} - f_4 f_5) + t_1(f_2 f_9 f_{10} - f_7 f_4 f_5) + t_1(f_{11} f_{10} f_5 - f_{12} f_4 f_9).$$

(A.4)
$$Q_5 = d(f_2 f_9 - f_5 f_{11}) + a(f_4 f_{10} - f_5 f_9) + d(f_9 f_{12} - f_5 f_7) + f(f_2 f_{13} - f_4 f_5) + f(f_{12} f_{13} - f_5 f_{10}) + t_1(f_2 f_9 f_{10} - f_7 f_4 f_5) + t_1(f_{12} f_{14} f_9 - f_{11} f_{10} f_5).$$

(A.5)
$$Q_6 = c(f_1 f_8 - f_6 f_3) + e(f_1 f_7 - f_2 f_6) + e(f_8 f_{11} - f_6 f_{12}) + g(f_7 f_{11} - f_6 f_{13}) + t_2(f_3 f_7 f_{11} - f_6 f_2 f_{12})$$

$$(A.6) Q_7 = e(f_2f_6 - f_1f_7) + b(f_{11}f_{12} - f_2f_7) + d(f_2f_9 - f_4f_7) + d(f_2f_{10} - f_5f_7) + e(f_2f_8 - f_3f_7) + f(f_7f_{10} - f_3f_{13}) + g(f_6f_{13} - f_7f_{11}) + g(f_8f_{13} - f_7f_{12}) + t_2(f_8f_2f_{11} - f_1f_7f_{12}) + t_2(f_6f_2f_{12} - f_3f_7f_{11}) + t_1(f_2f_9f_{10} - f_7f_4f_5)$$

(A.7)
$$Q_8 = c(f_6f_3 - f_1f_8) + e(f_3f_7 - f_2f_8) + e(f_6f_{12} - f_8f_{11}) + g(f_7f_{12} - f_8f_{13}) - t_2(f_8f_2f_{11} - f_1f_7f_{12}).$$

(A.8)
$$Q_9 = d(f_4 f_7 - f_2 f_9) + a(f_4 f_{10} - f_5 f_9) + d(f_{11} f_{10} - f_9 f_{12}) + f(f_{11} f_{13} - f_4 f_9) + f(f_7 f_{13} - f_9 f_{10}) + t_1(f_7 f_4 f_5 - f_2 f_9 f_{10}) + t_1(f_{10} f_{11} f_5 - f_{12} f_4 f_9).$$

(A.9)
$$Q_{10} = d(f_5f_7 - f_2f_{10}) + a(f_9f_5 - f_4f_{11}) + d(f_9f_{12} - f_{11}f_{10}) + f(f_7f_{13} - f_9f_{10}) + f(f_{12}f_{13} - f_5f_{10}) + t_1(f_7f_4f_5 - f_2f_9f_{10}) + t_1(f_{12}f_4f_9 - f_{11}f_{10}f_5).$$

(A.10)
$$Q_{11} = e(f_1f_{12} - f_3f_{11}) + b(f_2f_7 - f_{11}f_{12}) + e(f_6f_{12} - f_8f_{11}) + d(f_2f_9 - f_5f_{11}) + d(f_4f_7 - f_{10}f_{11}) + f(f_4f_7 - f_{11}f_{13}) + g(f_1f_{13} - f_2f_{11}) + g(f_6f_{13} - f_7f_{11}) + t_1(f_{12}f_{14}f_9 - f_{11}f_{10}f_5) + t_2(f_1f_7f_{12} - f_8f_2f_{11}) + t_2(f_6f_2f_{12} - f_3f_7f_{11}).$$

(A.11)
$$Q_{12} = e(f_3f_{11} - f_1f_{12}) + b(f_2f_7 - f_{11}f_{12}) + e(f_8f_{11} - f_6f_{12}) + d(f_2f_{10} - f_4f_{12}) + d(f_5f_7 - f_9f_{12}) + f(f_5f_{10} - f_{12}f_{13}) + g(f_8f_{13} - f_7f_{12}) + g(f_3f_{13} - f_2f_{12}) + t_1(f_{10}f_{11}f_5 - f_{12}f_4f_9) + t_2(f_8f_2f_{11} - f_1f_7f_{12}) + t_2(f_3f_7f_{11} - f_6f_2f_{12}).$$

(A.12)
$$Q_{13} = f(f_4 f_5 + f_4 f_9) + f_9 f_{10} + f_5 f_{10} - f_2 f_{13} - f_{11} f_{13} - f_7 f_{11} - f_6 f_{13}) + g(f_2 f_{11} - f_1 f_{13}) + g(f_7 f_{11} - f_6 f_{13}) + g(f_7 f_{12} - f_8 f_{13}) + g(f_2 f_{12} - f_3 f_{13})$$

In all the terms corresponding to the triple collisions we have assumed that the post-collisional velocities of the colliding particles are different from the precollisional ones, in order to eliminate the so-called triple collisions with a "spectator", in which one of the velocities remains unchanged (note that we assume that particles are indistinguishable).

Appendix B.

We give expressions for the matrices A and B of the linearized system of equations obtained from the 13-velocity model of Hierarchy 1.

$$A := \begin{bmatrix} -\frac{1}{2}c - e - \frac{1}{2}g + \frac{1}{2}z11 - \frac{1}{2}t2, & \frac{1}{2}e + \frac{1}{2}g + \frac{1}{2}z12 + \frac{1}{2}t2, \\ & \frac{1}{2}c + \frac{1}{2}e + \frac{1}{2}z13, & \frac{1}{2}z14, \frac{1}{2}z15 \\ & a21, & a22, & a23, & a24, & a25 \\ \\ & \frac{1}{2}c + \frac{1}{2}e + \frac{1}{2}z31, & \frac{1}{2}e + \frac{1}{2}g + \frac{1}{2}z32 + \frac{1}{2}t2, \\ & -\frac{1}{2}c - e - \frac{1}{2}g + \frac{1}{2}z33 - \frac{1}{2}t2, & \frac{1}{2}z34, \frac{1}{2}z35 \\ & z41, d + f + z42 + t1, z43, -2d - a - 2f + z44 - 2t1, \\ & a - f + z45 \\ & z51, & d + f + z52 + t1, & z53, a - f + z54, \\ & -2d - a - 2f + z55 - 2t1 \end{bmatrix}$$

$$B := \begin{bmatrix} \frac{1}{2}c + \frac{1}{2}e + \frac{1}{2}z16, -\frac{1}{2}e + \frac{1}{2}z17 - \frac{1}{2}t2, -\frac{1}{2}c + \frac{1}{2}z18 + \frac{1}{2}t2, \\ & \frac{1}{2}z19, \frac{1}{2}z10 \\ b21, b22, b23, b24, b25 \\ -\frac{1}{2}c + \frac{1}{2}z36 + \frac{1}{2}t2, -\frac{1}{2}e + \frac{1}{2}z37 - \frac{1}{2}t2, \frac{1}{2}c + \frac{1}{2}e + \frac{1}{2}z38, \\ & \frac{1}{2}z39, \frac{1}{2}z30 \\ z46, -d + z47 - t1, z48, a - f + z49, 2d - a + z40 + 2t1 \\ z56, -d + z57 - t1, z58, 2d - a + z59 + 2t1, a - f + z50 \end{bmatrix}$$

The remaining unknown parameters in these expressions are defined as follows:

$$\begin{split} a21 &:= \frac{1}{2}e + \frac{1}{2}g + \frac{1}{2}z21 + \frac{1}{2}t2, \\ a22 &:= -\frac{1}{2}b - d - \frac{1}{2}f - g - e + \frac{1}{2}z22 - \frac{1}{2}t1 - t2, \\ a23 &:= \frac{1}{2}e + \frac{1}{2}g + \frac{1}{2}z23 + \frac{1}{2}t2, \\ a24 &:= \frac{1}{2}d + \frac{1}{2}f + \frac{1}{2}z24 + \frac{1}{2}t1, \\ a25 &:= \frac{1}{2}d + \frac{1}{2}f + \frac{1}{2}z25 + \frac{1}{2}t1, \\ b21 &:= -\frac{1}{2}e + \frac{1}{2}z26 - \frac{1}{2}t2, \\ b22 &:= e - \frac{1}{2}b + \frac{1}{2}z27 + \frac{1}{2}t1 + t2, \\ b23 &:= -\frac{1}{2}e + \frac{1}{2}z28 - \frac{1}{2}t2, \\ b24 &:= -\frac{1}{2}d + \frac{1}{2}z29 - \frac{1}{2}t1, \\ b25 &:= -\frac{1}{2}d + \frac{1}{2}z20 - \frac{1}{2}t1, \end{split}$$

where

z21 := (p1 + r1) (b - g + d) + s1 (2g - f);
z22 := (p2 + r2) (b - g + d) + s2 (2g - f);
z23 := (p3 + r3) (b - g + d) + s3 (2g - f);
z24 := (p4 + r4) (b - g + d) + s4 (2g - f);
z25 := (p5 + r5) (b - g + d) + s5 (2g - f);
z26 := (p6 + r6) (b - g + d) + s6 (2g - f)
$z2\mathcal{I} := (p\mathcal{I} + r\mathcal{I}) (b - g + d) + s\mathcal{I} (2g - f);$
z28 := (p8 + r8) (b - g + d) + s8 (2g - f);
z29 := (p9 + r9) (b - g + d) + s9 (2g - f);
z20 := (p10 + r10) (b - g + d) + s10 (2g - f);
z31 := -p1 e + r1 (e + g) - s1 g + t2 (r1 - p1);
z32 := -p2 e + r2 (e + g) - s2 g + t2 (r2 - p2);
z33 := -p3 e + r3 (e + g) - s3 g + t2 (r3 - p3);
z34 := -p4 e + r4 (e + g) - s4 g + t2 (r4 - p4);
z35 := -p5 e + r5 (e + g) - s5 g + t2 (r5 - p5);
z36 := -p6 e + r6 (e + g) - s6 g + t2 (r6 - p6);
z37 := -p7 e + r7 (e + g) - s7 g + t2 (r7 - p7);
z38 := -p8 e + r8 (e + g) - s8 g + t2 (r8 - p8);
z39 := -p9 e + r9 (e+g) - s9 g + t2 (r9 - p9);
z30 := -p10 e + r10 (e + g) - s10 g + t2 (r10 - p10);
z41 := p1 (d+f) - r1 d + 2 s1 f + t1 (p1 - r1);
z42 := p2 (d+f) - r2 d + 2 s2 f + t1 (p2 - r2);
z43 := p3 (d+f) - r3 d + 2 s3 f + t1 (p3 - r3);
z44 := p4 (d+f) - r4 d + 2 s4 f + t1 (p4 - r4);
z45 := p5 (d+f) - r5 d + 2 s5 f + t1 (p5 - r5);
z46 := p6 (d+f) - r6 d + 2 s6 f + t1 (p6 - r6);
z 47 := p7 (d+f) - r7 d + 2 s7 f + t1 (p7 - r7)
z48 := p8 (d+f) - r8 d + 2 s8 f + t1 (p8 - r8;
z49 := p9 (d+f) - r9 d + 2 s9 f + t1 (p9 - r9);

z40 := p10 (d + f) - r10 d + 2 s10 f + t1 (p10 - r10); z51 := -p1 d + r1 (f + d) + 2 s1 f + t1 (r1 - p1);z52 := -p2 d + r2 (f + d) + 2 s2 f + t1 (r2 - p2);

$$\begin{split} z53 &:= -p3 \ d + r3 \ (f + d) + 2 \ s3 \ f + t1 \ (r3 - p3) \ ; \\ z54 &:= -p4 \ d + r4 \ (f + d) + 2 \ s4 \ f + t1 \ (r4 - p4) \\ z55 &:= -p5 \ d + r5 \ (f + d) + 2 \ s5 \ f + t1 \ (r5 - p5) \ ; \\ z56 &:= -p6 \ d + r6 \ (f + d) + 2 \ s6 \ f + t1 \ (r6 - p6) \\ z57 &:= -p7 \ d + r7 \ (f + d) + 2 \ s7 \ f + t1 \ (r7 - p7) \ ; \\ z58 &:= -p8 \ d + r8 \ (f + d) + 2 \ s8 \ f + t1 \ (r8 - p8) \\ z59 &:= -p9 \ d + r9 \ (f + d) + 2 \ s9 \ f + t1 \ (r9 - p9) \ ; \\ z50 &:= -p10 \ d + r10 \ (f + d) + 2 \ s10 \ f + t1 \ (r10 - p10) \end{split}$$

with

$$\begin{split} w1 &:= \frac{f}{4(f+g)}; \quad w2 := \frac{g}{4(f+g)}; \\ h &:= \frac{1}{4e+2d+f+2g+2(t1+2t2)}; \\ k &:= 2b+2g+2d+f - \frac{(2g-f)^2}{2(f+g)}; \quad l := \frac{2g-f}{k}; \\ m &:= \frac{1+h\left(b-2e\right) - \frac{h\left(2g-f\right)^2}{4(f+g)} - h\left(t1+2t2\right)}{k}; \quad n := \frac{1-mk}{k}; \\ lf &:= 1 + \frac{l\left(2g-f\right)}{2(f+g)}; \quad mf := \frac{(2g-f)\left(2m-h\right)}{4(f+g)}; \\ nf &:= \frac{(2g-f)\left(2n+h\right)}{4(f+g)}; \\ nf &:= \frac{(2g-f)\left(2n+h\right)}{4(f+g)}; \\ p1 &:= -lw2 + m\left(e+g+t2\right) + n\left(-e-t2\right); \\ p2 &:= l\left(-w1 + 2w2\right) + (m+n)\left(b-g+d\right); \\ p3 &:= -lw2 + m\left(-e-t2\right) + n\left(e+g+t2\right); \\ p4 &:= l2w1 + m\left(d+f+t1\right) + n\left(-d-t1\right); \end{split}$$

$$\begin{split} p5 &:= l\,2\,w1 + m\,(-d-t1) + n\,(d+t1+f)\,; \\ p6 &:= p1\,; \quad p7 := p2\,; \end{split}$$

$$p8 := p3; p9 := p4; p10 := p5;$$

$$\begin{split} r1 &:= -l \ w2 + (m-h) \ (e+g+t2) + (n+h) \ (-e-t2) \ ; \\ r2 &:= l \ (-w1 + 2 \ w2) + (m+n) \ (b-g+d) \ ; \\ r3 &:= -l \ w2 + (m-h) \ (-e-t2) + (n+h) \ (e+g+t2) \ ; \\ r4 &:= l \ 2 \ w1 + (m-h) \ (d+f+t1) + (n+h) \ (-d-t1) \ ; \\ r5 &:= l \ 2 \ w1 + (m-h) \ (-d-t1) + (n+h) \ (d+t1+f) \ ; \\ r6 &:= r1 \ ; \ r7 &:= r2 \ ; \ r8 &:= r3 \ ; \ r9 &:= r4 \ ; \ r10 &:= r5 \ ; \\ s1 &:= -lf \ w2 + mf \ (e+g+t2) + nf \ (-e-t2) \ ; \\ s2 &:= lf \ (-w1 + 2 \ w2) + (mf+nf) \ (b-g+d) \ ; \\ s3 &:= -lf \ w2 + mf \ (-e-t2) + nf \ (e+g+t2) \ ; \\ s4 &:= lf \ 2 \ w1 + mf \ (-e-t2) + nf \ (e+g+t2) \ ; \\ s4 &:= lf \ 2 \ w1 + mf \ (-e-t2) + nf \ (e+g+t2) \ ; \\ s4 &:= lf \ 2 \ w1 + mf \ (-d-t1) + nf \ (d+t1+f) \ ; \\ s5 &:= s1 \ ; \ s7 &:= s2 \ ; \ s8 &:= s3 \ ; \ s9 &:= s4 \ ; \ s10 \ := s5 \ ; \\ z11 &:= p1 \ (e+g) - r1 \ e-s1 \ g+t2 \ (p1-r1) \ ; \\ z12 &:= p2 \ (e+g) - r2 \ e-s2 \ g+t2 \ (p2-r2) \ ; \\ z13 &:= p3 \ (e+g) - r3 \ e-s3 \ g+t2 \ (p3-r3) \ ; \\ z14 &:= p4 \ (e+g) - r4 \ e-s4 \ g+t2 \ (p4-r4) \ ; \\ z15 &:= p5 \ (e+g) - r5 \ e-s5 \ g+t2 \ (p5-r5) \ ; \\ z16 &:= p6 \ (e+g) - r6 \ e-s6 \ g+t2 \ (p6-r6) \ ; \\ z17 &:= p7 \ (e+g) - r7 \ e-s7 \ g+t2 \ (p7-r7) \ ; \\ z18 &:= p8 \ (e+g) - r8 \ e-s8 \ g+t2 \ (p8-r8) \ ; \\ z19 &:= p9 \ (e+g) - r9 \ e-s9 \ g+t2 \ (p9-r9) \ ; \\ z10 &:= p10 \ (e+g) - r10 \ e-s10 \ g+t2 \ (p10-r10). \end{split}$$

Appendix C

The remaining collision terms $Q_2, ..., Q_{14}$ of the (4 + 8)-velocity model are defined as follows:

$$\begin{aligned} Q_2 &= A_1 - D - B_2 + A_3 + B_4 + F_2 + F_4 - G_1 + G_2 - G_3 - G_4, \\ Q_3 &= A_1 + B_1 + C_1 - F_4 + G_3 + G_4, \\ Q_4 &= -A_1 + D + B_2 - B_3 - A_4 - F_1 + F_3 - G_1 - G_2 - G_3 + G_4, \\ Q_5 &= -A_3 + B_3 - C_2 - F_1 - G_2 - G_3, \end{aligned}$$

$$\begin{split} Q_6 &= C_2 + A_4 + F_4 - G_1 + G_2, \\ Q_9 &= C_1 + B_2 + A_2 + F_2 - G_1 + G_2, \\ Q_{10} &= B_1 + D - A_2 - A_3 + B_4 + F_1 - F_3 + G_1 + G_2 + G_3 - G_4, \\ Q_{11} &= C_1 - B_2 - A_2 + F_3 - G_2 - G_3, \\ Q_{12} &= -B_1 - D + A_2 + B_3 + A_4 - F_2 - F_4 + G_1 - G_2 + G_3 + G_4, \\ Q_{13} &= A_3 + C_2 - F_2 + G_3 + G_4, \\ Q_{14} &= -C_2 + B_4 - A_4 - F_3 + G_1 - G_4, \end{split}$$

where

$$\begin{split} D &= d(f_2 f_{12} - f_4 f_{10}), \quad B_2 = b(f_2 f_{11} - f_4 f_9), \\ A_2 &= a(f_{10} f_{11} - f_9 f_{12}), \quad A_3 = a(f_5 f_{10} - f_2 f_{13}), \\ A_4 &= a(f_4 f_{14} - f_6 f_{12}), \\ B_3 &= b(f_4 f_{13} - f_5 f_{12}), \quad B_4 = b(f_6 f_{10} - f_2 f_{14}), \\ C_2 &= b(f_5 f_{14} - f_6 f_{13}), \\ F_2 &= f(f_{12} f_{13} - f_2 f_9), \quad F_3 = c(f_{10} f_{14} - f_{11} f_4), \\ F_4 &= f(f_3 f_{12} - f_2 f_6), \\ G_2 &= g(f_4 f_5 f_{11} f_{12} - f_2 f_6 f_9 f_{10}), \quad G_3 = g(f_2 f_4 f_5 f_{11} - f_3 f_{10} f_{12} f_{13}) \end{split}$$

The collision frequencies a, b, c, d, f are assumed to be proportional to the moduli of differences of the velocities of colliding particles in the case of binary collisions, cf. [10]. The operators G_i describe the influence of quadruple collisions, g being the parameter describing the collision rate for the quadruple collisions.

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Received July 2, 2007; revised version January 16, 2008.