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A numerical model for the Boltzmann equation with applications to micro flows

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Abstract

Given an integer lattice $\mathcal{L} \subset \mathbb{R}^d$, we define G as the orthogonal group leaving $\mathcal{L}$ invariant. Starting from a basic kinetic model on G we construct a collision operator on $\mathcal{L}$ which keeps all the essential features of the classical Boltzmann collision operator. For a particular 3D lattice we demonstrate the suitability of this discrete model for the numerical simulation of rarefied flows. For several examples, e.g. in the context of micro flows, we find a good qualitative and quantitative agreement of our simulation results with test data.

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

MSC classification: 82C40, 82C80, 76P05

1 Introduction

The classical Boltzmann equation describes on a mesoscopic level the evolution of a large system of small identical particles interacting via elastic short-range two-particle collisions. An elastic collision is the momentum exchange of two particles in such a way that total momentum and (kinetic) energy remain conserved. Formally this can be described by a transition of a pair of velocities $v, w \in \mathcal{V} = \mathbb{R}^d$ (where $d \in \{2, 3\}$ describes the dimension of the velocity space),

$$(v, w) \longrightarrow (v', w') \tag{1.1}$$

such that

$$v + w = v' + w' \qquad \text{(momentum conservation)} \tag{1.2}$$

$$\|v\|^2 + \|w\|^2 = \|v'\|^2 + \|w'\|^2 \qquad \text{(energy conservation)} \tag{1.3}$$

(with $\|.\|$ Euclidean norm). Define S^{d-1} as the unit sphere in $\mathbb{R}^d$. Then a simple calculation shows the following: Given $(v, w) \in \mathbb{R}^d$, define the center

$$c := (v + w)/2 \tag{1.4}$$

and $r := \|v - c\|$. Then due to the conservation laws the relation between the velocities v, w, v', w' is given by

$$v = c + r\eta \quad , \quad w = c - r\eta \tag{1.5}$$

$$v' = c + r\xi \quad , \quad w' = c - r\xi \tag{1.6}$$

with $\eta, \xi \in S^{d-1}$. The domain where all these collisions act is the sphere

$$S_{(c,v)} := c + rS^{d-1} = \{c + r\xi, \xi \in S^{d-1}\} \tag{1.7}$$

Thus the Boltzmann collision operator may be written in the form

$$J[f](c + r\eta) = \int_{c \in \mathbb{R}^d} \int_{\xi \in S^{d-1}} k(r, \theta)(f(c + r\xi)f(c - r\xi) - f(c + r\eta)f(c - r\eta))d\omega(\theta)dc \tag{1.8}$$

where θ is the angle between η and ξ. (For details concerning the classical Boltzmann equation, see e.g. [8, 16].)

The fact that collision events are defined on spheres causes troubles when designing numerical schemes for the Boltzmann collision operator on the basis of a regular grid on $\mathcal{V}$. This is because regular grids are not efficient in resolving the spheres $S_{(c,v)}$. Problems arising in this context are in the focus of a paper by Rogier and Schneider [15] in an attempt to establish a numerical algorithm. Later this was investigated in more detail in [7] with the result that the poor match of the spheres on the grid cause an extremely poor order of consistency. A more recent paper [11] (for $d = 2$) concerns the number $n(r)$ of sphere points on a Cartesian grid as a quite irregular function of the radius r. It is obviously this problem which prevents models on regular grids to be established as efficient numerical schemes. There have been alternative approaches like that of Görsch [12], which smears out the collision results onto some neighborhood of the circle by introducing weights. This provides the correct conservation laws, but the H-theorem is violated, and a numerical scheme needs to work with many megabytes of weight data – even for $d = 2$. We are not aware of any interesting space dependent application which could be solved efficiently with one of the above algorithms. Thus other attempts aim at alternative approaches like spectral methods; an overview of recent advances may be extracted from [13].

The present paper proposes a different idea which is based on adjusting the dynamics to a given grid rather than adjusting the grid to a given collision dynamics. The key observation is the following. All we need to formulate the collision dynamics (1.5), (1.6) is a reflection operator τ,

$$v = c + r\eta \rightarrow \tau(v) = c - \tau\eta \tag{1.9}$$

determining the collision partner of v on $S_{(c,v)}$, and a rotation operator $\rho[.]$,

$$v = c + r\eta \rightarrow \rho[\theta](v) = c - \tau\xi \tag{1.10}$$

where $\theta \in S^{d-1}$ is the angle between η and ξ. Using these, the inner integral of the collision operator may be reformulated as

$$\int_{S^{d-1}} k(r,\theta)(f(\rho[\theta](v))f(\rho[\theta](\tau v)) - f(v)f(\tau v))d\omega(\theta) \tag{1.11}$$

Rotations and reflections generate a group in $S_{(c,v)}$ – the automorphism group. Thus it should be possible to describe collisional details in terms of a Boltzmann equation on the automorphism group. Being prepared to accept this point, there is only a small step to a discretized collision operator. Given a regular lattice $\mathcal{V}$ on $\mathbb{R}^d$, determine the automorphism group G (i.e. the set of orthogonal matrices leaving $\mathcal{V}$ invariant), and formulate a collision dynamics on G which in turn induces a collision dynamics on $\mathcal{V}$. An algorithm based on this has been for $d = 2$ proposed using a hexagonal grid [1]. It has been demonstrated that a corresponding numerical code is efficient and yields at least *qualitatively* good results [3, 4, 5]. It is the aim of the present paper to derive a general framework and to provide a numerical scheme for $d = 2$ which is efficient and provides also *quantitatively* good results.

We should emphasize that we have to pay a price for this approach. If we decrease the grid size h of a given lattice and turn to the limit $h \searrow 0$, then the result is not the classical Boltzmann collision operator but one in which the inner integral is not described by the usual surface measure $d\omega(\xi)$ but by a discrete approximation $d\omega_{discrete}$ (see [3]). However, it is widely accepted in the scientific community, that for reasons of numerical efficiency the inner integral is modified; e.g. the commonly used VHS (*variable diameter hard sphere*) model is accepted as one of the main models for applications, although it does not provide the correct picture for any of the established interaction potentials. Whether a model will be accepted for numerical purposes should be decided through numerical experiments and benchmarks.

The paper is organized as follows. In section 2 we describe the framework for the definition of a collision operator. This is general enough to include besides binary collisions (which are the main topic in rarefied gas dynamics) also linear, ternary etc. interactions. Inherent to these models is an H-Theorem; the set of collision invariants is easily derived. In section 3, this model is applied to regular lattices $\mathcal{V}$; we derive its main properties. For $d = 3$ we investigate in detail a special model which is useful for numerical purposes. It satisfied the H-Theorem, has the correct collision invariants and has Maxwellians as its equilibrium solutions. This model is used in section 4 to establish numerical results for a 1D heat layer problem and for 2D microchannel flows. These examples show that the numerical scheme is capable to provide qualitatively as well as quantitatively good results.

2 Kinetic models on groups

2.1 Collision operators

Let G be a finite multiplicative group with neutral element η, and H a subgroup. Define the equivalence relation on G,

$$g \sim g' \Leftrightarrow g{g'}^{-1} \in H \tag{2.1}$$

The equivalence classes are the right coset classes of H, and $G/\sim := \{[g], g \in G\}$ denotes the set of equivalence classes. The order of $G/\sim$ (resp. the *index* of H) is

$$|G/\sim| = \mathrm{idx}_G H = \frac{|G|}{|H|} \tag{2.2}$$

Given a function $f \in \mathbb{R}^G$, we define

$$\Pi_g f = \Pi_{[g]} f := \Pi_{g' \in [g]} f(g') \tag{2.3}$$

For $z \in G$, we define $f \circ z \in \mathbb{R}^G$ by $f \circ z(g) = f(gz)$.

A kinetic model on G is defined as a *collision operator* on $\mathbb{R}^G$, which is constant on equivalence classes and given by

$$J[f](g) = J[f]([g]) = (J_+[f] - J_-[f])(g) = \sum_{[g'] \in G/\sim} \alpha_{[g'],[g]} \cdot \Pi_{g'} f - \alpha \cdot \Pi_g f. \tag{2.4}$$

with appropriate positive coefficients $\alpha_{[g'],[g]}$ and α.

2.1 Assumptions: We assume the coefficients to satisfy

(a) *group invariance*: There is a mapping $\tilde{\alpha} : G/R \to \mathbb{R}_+ = (0,\infty)$ such that

$$\alpha_{[g'],[g]} = \tilde{\alpha}_{[g'g^{-1}]} \tag{2.5}$$

(b) *mass conservation*:

$$\sum_{[g]\in G/\sim} \tilde{\alpha}_{[g]} = \alpha \tag{2.6}$$

(c) *microreversibility (symmetry)*: For all $g \in G$,

$$\tilde{\alpha}_{[g]} = \tilde{\alpha}_{[g^{-1}]} \tag{2.7}$$

2.2 Lemma: J is invariant under actions in G in the sense that

$$J[f \circ z] = J[f] \circ z \quad \text{for all} \quad z \in G. \tag{2.8}$$

Proof: Since $\tilde{g} \in [g'] \Leftrightarrow \tilde{g}z^{-1} \in [g'z^{-1}]$, we conclude with $g'' = g'z^{-1}$

$$J_+[f] \circ z(g) = J_+[f](gz) = \sum_{[g']} \tilde{\alpha}_{[g'z^{-1}g^{-1}]}\Pi_{g'} f = \sum_{[g'']} \tilde{\alpha}_{[g''g^{-1}]}\Pi_{g''} f \circ z = J_+[f \circ z](g)$$

and

$$J_-[f] \circ z(g) = J_-[f](gz) = \alpha\Pi_{gz} f = \alpha\Pi_g f \circ z = J_-[f \circ z](g) \qquad \square$$

2.3 Remark: In the case $H = G$ (i.e. $\mathrm{idx}_G H = 1$) the collision operator takes the trivial form $J[f] \equiv 0$. On the other hand, if $H = \{\eta\}$, then $J[f]$ is a *linear collision operator* given by

$$J[f](g) = \sum_{g'\in G} \alpha_{g',g} f(g') - \alpha f(g), \quad \alpha = \sum_{g\in G} \alpha_{g',g} \tag{2.9}$$

The case of *binary collisions* is obtained if G has even order. Then we define H as a subgroup with order 2, $H = \{\eta, g_0\}$ with $g_0 \neq \eta$, $g_0^2 = \eta$. For $g \in G$ we write g^* for the unique element $g^* \neq g$ in G satisfying gRg^*. Then collecting in $\tilde{G} \subset G$ a unique representative for each equivalence class we find

$$J[f](g) = \sum_{g' \in \tilde{G}} \alpha_{[g'],[g]} f(g') f(g'^*) - \alpha f(g) f(g^*) \tag{2.10}$$

A vector $m \in \mathbb{R}^G$ is called *collision invariant*, if

$$\langle m, J[f] \rangle = 0 \quad \text{for all} \quad f \in \mathbb{R}^G_+. \tag{2.11}$$

2.4 Lemma: (a) $\mathbb{1}_G = (1)_{g \in G}$ is a collision invariant.
(b) Choose an equivalence class $[z]$ and a vector $\lambda = (\lambda_h)_{h \in H} \in \mathbb{1}_H^\perp = \{\lambda \in \mathbb{R}^H : \sum_{h \in H} \lambda_h = 0\}$. Then

$$m[\lambda, z]_g := \begin{cases} \lambda_h & \text{if} \quad g = hz \in [z] \\ 0 & \text{if} \quad g \notin [z] \end{cases} \tag{2.12}$$

is a collision invariant.
(c) The space C_H of collision invariants is spanned by $\mathbb{1}_G$ and the vectors $m[\lambda, z]$, $[z] \in G/R$, $\lambda \in \mathbb{1}_H^\perp$. Its dimension is

$$\dim(C_H) = \mathrm{idx}_G H \cdot (|H| - 1) + 1. \tag{2.13}$$

(d) For $g, g' \in G$ and $m \in C_H$,

$$\sum_{\tilde{g} \in [g]} m(\tilde{g}) = \sum_{\tilde{g} \in [g']} m(\tilde{g}) \tag{2.14}$$

(e) For all $z \in G$, $C_H = C_H \circ z$.

Proof: (a) Because of the mass conservation property (2.6),

$$\begin{aligned} \langle \mathbb{1}_G, J[f] \rangle &= \sum_{g \in G} \left(\sum_{[g'] \in G/\sim} \alpha_{[g'],[g]} \cdot \Pi_{[g']} f - \alpha \cdot \Pi_g f \right) \\ &= \mathrm{idx}_G H \cdot \left(\sum_{[g] \in G/\sim} \sum_{[g'] \in G/\sim} \alpha_{[g'],[g]} \cdot \Pi_{[g']} f - \sum_{[g] \in G/\sim} \alpha \cdot \Pi_{[g]} f \right) \end{aligned} \tag{2.15}$$

$$= \quad \mathrm{idx}_G H \cdot \left(\sum_{[g]\in G/\sim} \sum_{[g']\in G/\sim} \alpha_{[g'],[g]} \cdot \Pi_{[g']} f - \sum_{[g]\in G/\sim} \sum_{[g']\in G/\sim} \alpha_{[g],[g']} \cdot \Pi_{[g]} f \right) = 0$$

(b) Since $J[f]$ is constant on $[z]$,

$$J[f](g) = J[f]([z]) \tag{2.16}$$

for all $g \in [z]$ we find

$$\langle m[\lambda, z], J[f] \rangle = \left(\sum_{g\in[z]} m[\lambda, z]_g \right) \cdot J[f]([z]) = \left(\sum_{h\in H} \lambda_h \right) \cdot J[f]([z]) = 0 \tag{2.17}$$

(c) Let $m \in C_H$. We have to show that m is a linear combination of the above invariants. Without restriction we may assume that

$$\langle m, \mathbb{1}_G \rangle = 0 \tag{2.18}$$

For any $[g] \in G/\sim$ define $m_{[g]} := \sum_{g'\in[g]} m(g')$. The proof is complete after showing that $m_{[g]} = 0$ for all $[g] \in G/\sim$. Because of microreversibility,

$$\begin{aligned}
\langle m, J[f] \rangle &= \sum_{g\in G} m(g) J[f](g) = \sum_{[g]\in G/\sim} m_{[g]} J[f]([g]) \\
&= \sum_{[g]\in G/\sim} m_{[g]} \left(\sum_{[g']\in G/\sim} \alpha_{[g'],[g]} \cdot \Pi_{[g']} f - \sum_{[g']\in G/\sim} \alpha_{[g],[g']} \cdot \Pi_{[g]} f \right) \\
&= \sum_{[g]\in G/\sim} \sum_{[g']\in G/\sim} \alpha_{[g'],[g]} \cdot (m_{[g]} - m_{[g']})(\Pi_{[g']} f - \Pi_{[g]} f)
\end{aligned} \tag{2.19}$$

Choosing $\Pi_{[g]} f = m_{[g]} + C$ with any constant $C \in \mathbb{R}$ we see that m is collision invariant only if $m_{[g]} = m_{[g']}$ and because of (2.18), $m_{[g]} = 0$. The formula for the dimension of C_H follows from $\dim(\mathbb{1}_H^\perp) = |H| - 1$.

(d) was shown in the proof of (c).

(e) From $\mathbb{R}_+^G = (\mathbb{R}_+^G) \circ z$ and Lemma (2.2) follows

$$\langle m, J[f] \rangle = \langle m \circ z, J[f] \circ z \rangle = \langle m \circ z, J[f \circ z] \rangle \tag{2.20}$$

from which we conclude

$$m \in C_H \Leftrightarrow m \circ z \in C_H \qquad \square \tag{2.21}$$

2.2 The Boltzmann equation

The system of differential equation on $\mathbb{R}^G$,

$$\partial_t f = J[f] \tag{2.22}$$

is called *Boltzmann equation* on G. Given a density $f \in \mathbb{R}_+^G$ we define the H-functional as

$$Hf := \langle f, \ln(f) \rangle \tag{2.23}$$

$e \in \mathbb{R}_+^G$ is called *equilibrium solution* if

$$J[e] \equiv 0 \tag{2.24}$$

2.5 Proposition: (a) For any $f_0 \in \mathbb{R}_+^G$, there exists a global unique solution of the initial value problem (IVP)

$$\partial_t f = J[f], \quad f(0) = f_0 \tag{2.25}$$

It is strictly positive and satisfies

$$\langle m, f(t) \rangle = const \quad \text{for all} \quad m \in C_H \tag{2.26}$$

(b) For the solution $f(t)$ of (a), $Hf(t)$ is monotonously decreasing.
(c) For $e \in \mathbb{R}_+^G$ holds

$$e \text{ equilibrium solution } \Leftrightarrow \forall g, g' \in G : \Pi_g e = \Pi_{g'} e \Leftrightarrow \ln e \text{ is collision invariant} \tag{2.27}$$

Proof: (a) The Boltzmann collision operator is locally Lipschitz continuous in $\mathbb{R}_+^G$; thus there exists a local solution of IVP. As long as $f(t)$ remains positive, because of the definition of collision invariants, $\langle m, f(t) \rangle$ is constant for all $m \in C_H$. In particular, since $\mathbb{1}_G \in C_H$, we conclude

$$\|f(t)\|_\infty \leq \langle \mathbb{1}_G, f_0 \rangle \tag{2.28}$$

As a consequence, with $C := \alpha \cdot \langle \mathbb{1}_G, f_0 \rangle^{|H|}$

$$J[f] + Cf > 0 \tag{2.29}$$

which proves that

$$f(t) \geq f_0 \cdot \exp(-Ct) > 0 \tag{2.30}$$

Therefore the local solution $f(t)$ can be extended to a global solution.

(b) Obviously, because $\mathbb{1}_G \in C_H$,

$$\begin{aligned}
\partial_t H f(t) &= \langle J[f(t)], \ln(f(t)) + 1\rangle = \langle J[f(t)], \ln(f(t))\rangle && (2.31)\\
&= \sum_{[g]\in G/\sim} \sum_{\tilde{g}\in[g]} \ln(f(t,\tilde{g})) \cdot J[f(t)]([g]) = \sum_{[g]\in G/\sim} \ln\left(\Pi_{[g]} f(t)\right) \cdot J[f(t)]([g])\\
&= \sum_{[g]\in G/\sim} \sum_{[g']\in G/\sim} \alpha_{[g'],[g']} \ln\left(\Pi_{[g]} f(t)\right) \cdot \left(\Pi_{[g']} f - \Pi_{[g]} f\right)\\
&= \frac{1}{2} \sum_{[g]\in G/\sim} \sum_{[g']\in G/\sim} \alpha_{[g'],[g']} \left(\ln\left(\Pi_{[g]} f(t)\right) - \ln\left(\Pi_{[g']} f(t)\right)\right) \cdot \left(\Pi_{[g']} f - \Pi_{[g]} f\right)\\
&\leq 0 && (2.32)
\end{aligned}$$

Inequality (2.32) holds since for any real numbers $x, y > 0$,

$$(\ln(x) - \ln(y)) \cdot (y - x) \leq 0 \tag{2.33}$$

Equality holds if and only if $x = y$.

(c) If e is equilibrium solution, then $f(t) = e$ is a steady solution of the Boltzmann equation. Thus

$$\begin{aligned}
0 &= \partial_t H f(t) && (2.34)\\
&= \frac{1}{2} \sum_{[g]\in G/\sim} \sum_{[g']\in G/\sim} \alpha_{[g'],[g']} \left(\ln\left(\Pi_{[g]} e\right) - \ln\left(\Pi_{[g']} e\right)\right) \cdot \left(\Pi_{[g']} e - \Pi_{[g]} e\right)
\end{aligned}$$

Following inequality (2.32) and the subsequent remark, this is true if and only if

$$\forall g, g' \in G : \Pi_g e = \Pi_{g'} e \tag{2.35}$$

Now choose $e \in \mathbb{R}_+^G$ and define $m := \ln e + c\mathbb{1}_G$ with $c \in \mathbb{R}$ such that

$$\langle m, \mathbb{1}_G\rangle = 0 \tag{2.36}$$

Then

$$\begin{aligned}
&\forall g, g' : \Pi_{[g']} e = \Pi_{[g]} e \Leftrightarrow \forall g, g' : \sum_{\tilde{g}\in[g']} m(\tilde{g}) = \sum_{\tilde{g}\in[g]} m(\tilde{g}) && (2.37)\\
&\Leftrightarrow \forall g : \sum_{\tilde{g}\in[g]} m(\tilde{g}) = 0 \Leftrightarrow m \in C_H \setminus \{\mathbb{1}_G\} \qquad \square
\end{aligned}$$

2.3 Induced collision operators

Suppose G induces a group operation on some set X, i.e. a mapping from $G \times X$ to X satisfying $\eta x = x$ and $(gg')x = g(g'x)$ for all $x \in X$ and $g, g' \in G$. Assume further that for some fixed $\hat{x} \in X$ (and thus for all), $G\hat{x} = X$. However, the mapping $\hat{\psi} : G \to X$, $g \to g\hat{x}$ need not be injective. Given a density vector f on X, i.e. $f \in \mathbb{R}_+^X$, $\hat{\psi}$ induces a density vector $f \circ \hat{x}$ on G by

$$f \circ \hat{x}(g) := f(g\hat{x}) \tag{2.38}$$

We now define a collision operator $\hat{J}$ on $\mathbb{R}_+^X$ by

$$\begin{aligned} \hat{J}[f](x) &:= \sum_{g \in \hat{\psi}^{-1}(x)} J[f \circ \hat{x}](g) \\ &= \sum_{g \in \hat{\psi}^{-1}(x)} \left(\sum_{[g'] \in G/\sim} \alpha_{[g'],[g]} \cdot \Pi_{[g']} f \circ \hat{x} - \alpha \cdot \Pi_{[g]} f \circ \hat{x} \right) \end{aligned} \tag{2.39}$$

2.6 Lemma: The definition of $\hat{J}$ is independent of the choice of $\hat{x}$.

Proof: Choose $\tilde{x} = \tilde{g}\hat{x} \in X$ and define $\tilde{\psi}(g) := g\tilde{x}$ and

$$\tilde{J}[f](x) := \sum_{g \in \tilde{\psi}^{-1}(x)} J[f \circ \tilde{x}](g) \tag{2.40}$$

Because of $f \circ \tilde{x} = (f \circ \hat{x}) \circ \tilde{g}$ and from Lemma 2.2 follows

$$\begin{aligned} \tilde{J}[f](x) &= \sum_{g \in \tilde{\psi}^{-1}(x)} J[f \circ \hat{x}] \circ \tilde{g}(g) = \sum_{g \in \tilde{\psi}^{-1}(x)} J[f \circ \hat{x}](g\tilde{g}) \\ &= \sum_{g \in \hat{\psi}^{-1}(x)} J[f \circ \hat{x}](g) = \hat{J}[f](x) \end{aligned} \tag{2.41}$$

Here we have used

$$g \in \tilde{\psi}^{-1}(x) \Leftrightarrow g\tilde{x} = x \Leftrightarrow g\tilde{g}\hat{x} = x \Leftrightarrow g\tilde{g} \in \hat{\psi}^{-1}(x) \qquad \square \tag{2.42}$$

Since the definition of the collision operator does not depend on $\hat{x}$, we write again $J[.]$ instead of $\hat{J}[.]$. In analogy to (2.23) we define the H-functional on $\mathbb{R}_+^X$ as

$$Hf := \langle f, \ln f \rangle = \sum_{x \in X} f(x) \ln f(x) \tag{2.43}$$

Denote by C_X the set of collision invariants. For $m \in \mathbb{R}^X$,

$$\begin{aligned} \langle m, J[f] \rangle &= \sum_{x \in X} m(x) \sum_{g \in \hat{\psi}^{-1}(x)} J[f \circ \hat{x}](g) = \sum_{g \in G} m(g\hat{x}) m(g\hat{x}) J[f \circ \hat{x}](g) & (2.44) \\ &= \sum_{g \in G} m \circ \hat{x}(g) \cdot J[f \circ \hat{x}](g) & (2.45) \end{aligned}$$

Thus we find as a sufficient (but not necessary) condition for C_X

$$m \circ \hat{x} \in C_H \Rightarrow m \in C_X \tag{2.46}$$

In particular, $\mathbb{1}_X \in C_X$.

Solutions of the Boltzmann equation on X are characterized as follows.

2.7 Proposition: The IVP for the Boltzmann equation on B for given initial condition $f_0 \in \mathbb{R}_+^X$ possesses a unique global solution $f(t)$. $f(t)$ is strictly positive; moreover, mass is conserved, i.e.

$$\langle \mathbb{1}_X, f(t) \rangle = \langle \mathbb{1}_X, f_0 \rangle \tag{2.47}$$

The H-functional $Hf(t)$ is monotonously decreasing. A density $e \in \mathbb{R}_+^X$ is equilibrium solution if and only if

$$\Pi_g e \circ \hat{x} = \Pi_{g'} e \circ \hat{x} \quad \text{for all} \quad g, g' \in G \tag{2.48}$$

Proof: The evolution of the H-functional is given by

$$\partial_t Hf \;=\; \langle \ln(f), J[f] \rangle = \sum_{g \in G} \ln(f \circ \hat{x}(g)) \cdot J[f \circ \hat{x}](g) \leq 0 \tag{2.49}$$

All further arguments may be taken from the proof of Proposition 2.5 . □

3 Kinetic models on integer lattices

3.1 Integer lattices and discrete spheres

Let $\mathcal{C} \subset \mathbb{R}^d$ ($d \geq 2$) be an integer lattice spanned by normed vectors $b_i, i = 1, \ldots, d$, i.e.

$$\mathcal{C} = \left\{ \sum_{i=1}^{d} k_i b_i : k_i \in \mathbf{Z} \right\} \tag{3.1}$$

and $G \subset \mathbb{R}^{d \times d}$ the group of orthogonal transformations leaving $\mathcal{C}$ invariant (resp. a subgroup containing point reflection $-\mathrm{id} : x \in \mathcal{C} \to -x$). The orthogonal groups of the most common integer lattices may be found in [10]. Furthermore, define a subset $\emptyset \neq \mathcal{V} \subseteq \mathcal{C}$ satisfying the invariance laws

$$\mathcal{V} = -\mathcal{V} \tag{3.2}$$

$$\mathcal{V} = (v_1 - v_2) + \mathcal{V} \quad \text{for all} \quad v_1, v_2 \in \mathcal{V}, \tag{3.3}$$

$$c + G(v - c) \subset \mathcal{V} \quad \text{for all} \quad v \in \mathcal{V}, \quad c \in \mathcal{C} \tag{3.4}$$

It is (a finite subset of) the grid $(\mathcal{V}, \mathcal{C})$ on which we establish a kinetic model in the next section.

3.1 Remarks: (a) In the case $\mathcal{C} = \mathcal{V}$, the conditions (3.2) to (3.4) are satisfied.
(b) Given $\mathcal{C}$, define the even part of the lattice by

$$\mathcal{C}_{\text{even}} := \left\{ \sum_{i=1}^{d} k_i b_i : k_i \in \mathbf{Z}, \sum_{i=1}^{d} k_i \text{ even} \right\} \tag{3.5}$$

If G leaves $\mathcal{C}_{\text{even}}$ invariant, then for the choice $\mathcal{V} = \mathcal{C}_{\text{even}}$ the above conditions are satisfied.
(c) An example for $d \geq 2$ is the Cartesian grid with b_i being the i-th canonical unit vector. Another example for $d = 2$ is the hexagonal lattice $\mathcal{C}$ described in [1] with $b_1 = \exp(i\pi/6)$ and $b_2 = \exp(i\pi/3)$, and $\mathcal{V} = \mathcal{C}_{\text{even}}$. (Here we have identified $\mathbb{R}^2$ with $\mathbb{C}$.) Our main example concerns the case $d = 3$ and is treated in detail in the next section.

Given $(c, v) \in \mathcal{C} \times \mathcal{V}$, $c \neq v$, define the *discrete ball around c through v* as the set

$$S_{(c,v)} := c + G \times (v - c) \subset \mathcal{V} \tag{3.6}$$

Obviously, for all $v' \in S_{(c,v)}$, $|v' - c| = |v - c|$. It is easy to prove

3.2 Lemma: The mapping from $G \times S_{(c,v)}$ to $S_{(c,v)}$,

$$(g, v') = (g, c + g'(v - c)) \to c + gg'(v - c) \tag{3.7}$$

describes a group operation on $S_{(c,v)}$.

3.2 A Boltzmann equation

Define the subgroup $H := \{\mathrm{id}, -\mathrm{id}\}$ of G and consider the collision operator J_G on G related to H as defined in section 2.2. Due to Lemma 3.2, J_G induces on each discrete sphere $S_{(c,v)}$ via the mapping

$$\psi(g) := (g, v) = c + g(v - c) \tag{3.8}$$

a collision operator $J_{(c,v)}$ as described in section 2.3. In the following we denote with an asterisk the collision partner of a velocity under the operator $J_{(c,v)}$; e.g. if $v' = \psi(g', v)$, then $v'^* = \psi(-g', v')$. The explicit form of $J_{(c,v)}$ is then given by

$$\begin{aligned} J_{(c,v)}[f](\tilde{v}) &= \sum_{g \in \psi^{-1}(\tilde{v})} \left(\sum_{[g'] \in G/\sim} \alpha_{[g'],[g]} \cdot f(\psi(g'))f(\psi(-g')) - \alpha \cdot f(\tilde{v})f(\tilde{v}^*) \right) \\ &= \sum_{g \in \psi^{-1}(\tilde{v})} \left(\frac{1}{2} \sum_{g' \in G} \alpha_{[g'],[g]} \cdot f(\psi(g'))f(\psi(-g')) - \alpha \cdot f(\tilde{v})f(\tilde{v}^*) \right) \\ &= \sum_{v' \in S_{(c,v)}} \alpha_{v',\tilde{v}} \left(f(v')f(v'^*) - f(\tilde{v})f(\tilde{v}^*) \right) \end{aligned} \tag{3.9}$$

where we have defined

$$\alpha_{v',\tilde{v}} := \frac{1}{2} \sum_{\tilde{g} \in \psi^{-1}(\tilde{v})} \sum_{g' \in \psi^{-1}(v')} \alpha_{[g'],[\tilde{g}]} \tag{3.10}$$

We extend this operator in a convenient way to an operator on $\mathbb{R}_+^{\mathcal{V}}$ by setting

$$J_{(c,v)}[f](v) := \begin{cases} J_{(c,v)}\left[f|_{S_{c,v}}\right](v) & \text{if} \quad v \in S_{(c,v)} \\ 0 & \text{else} \end{cases} \tag{3.11}$$

Like for the continuous Boltzmann collision operator we find the classical results

3.3 Lemma: (a) A function $m \in \mathbb{R}^{\mathcal{V}}$ is a collision invariant of $J_{(c,v)}$ if and only if for all $v', \tilde{v} \in S_{(c,v)}$

$$m(v') + m(v'^*) = m(\tilde{v}) + m(\tilde{v}^*) \tag{3.12}$$

In particular, $\mathbb{1}_{\mathcal{V}}$, v and $|v|^2$ are invariants.
(b) A density $e \in \mathbb{R}_+^{\mathcal{V}}$ is equilibrium function of $J_{(c,v)}$ if and only if $\ln e$ is a collision invariant.

Proof: (a) A straightforward calculation yields

$$\begin{aligned} \langle m, J_{(c,v)}[f]\rangle &= \frac{1}{2}\sum_{\tilde{v}\in S_{(c,v)}} (m(\tilde{v}) + m(\tilde{v}^*))J_{(c,v)}[f] \qquad (3.13)\\ &= \frac{1}{2}\sum_{\tilde{v}\in S_{(c,v)}} f(\tilde{v})f(\tilde{v}^*)\cdot \sum_{v'\in S_{(c,v)}} \alpha_{v',\tilde{v}}[m(v') + m(v'^*) - m(\tilde{v}) - m(\tilde{v}^*)] \end{aligned}$$

Now suppose that (3.12) is not satisfied. Then there exists $v_0 \in S_{(c,v)}$ such that

$$C := \sum_{v'\in S_{(c,v)}} \alpha_{v',v_0}[m(v') + m(v'^*) - m(v_0) - m(v_0^*)] \neq 0 \tag{3.14}$$

Now choose $f \in S_{(c,v)}$ by

$$f(v') := \begin{cases} 1 & \text{if} \quad v' \in \{v_0, v_0^*\} \\ \epsilon & \text{else} \end{cases} \tag{3.15}$$

Then for ϵ small,

$$\langle m, J_{(c,v)}[f]\rangle = C + \mathcal{O}(\epsilon) \neq 0 \tag{3.16}$$

and thus m is no collision invariant.
(b) If $\ln e$ is collision invariant then $e(v')e(v'^*) = e(\tilde{v})e(\tilde{v}^*)$ for all $v', \tilde{v} \in S_{(c,v)}$. Thus e is equilibrium. On the other hand, if e is equilibrium, then

$$\begin{aligned} \langle \ln e, J[e]\rangle &= \frac{1}{4}\sum_{v',\tilde{v}\in S_{(c,v)}} \alpha_{v',\tilde{v}}\,(\ln(e(\tilde{v})e(\tilde{v}^*) - \ln(e(v')e(v'^*))\cdot(e(v')e(v'^*) - e(\tilde{v})e(\tilde{v}^*)) \\ &= 0 \qquad (3.17) \end{aligned}$$

and thus $e(v')e(v'^*) = e(\tilde{v})e(\tilde{v}^*)$ for all $v', \tilde{v} \in S_{(c,v)}$. According to (a), $\ln e$ is a collision invariant. $\square$

Finally, summing up over all discrete balls, we may define a collision operator on $\mathbb{R}_+^{\mathcal{V}}$ by

$$Jf(v) := \sum_{c\in\mathcal{C}} \gamma(c, |v-c|)C_{(c,v)}f(v) \tag{3.18}$$

with properly chosen nonnegative coefficients $\gamma(c, |v-c|)$. However, since we are interested in discrete models for purposes of numerics we restrict to finite sums as follows. Suppose $\mathcal{S}$ is a finite subset of $(\mathcal{C}, \mathcal{V})$ containing only pairs (c, v) with $c \neq v$. We interpret $\mathcal{S}$ as indicating a finite number of discrete spheres and define

$$\mathcal{V}_{\mathcal{S}} := \bigcup_{(c,v)\in S} S_{(c,v)} \tag{3.19}$$

as the finite subset of $\mathcal{V}$ containing all these discrete spheres. We now define the collision operator $J_{\mathcal{S}}$ on $\mathcal{V}_{\mathcal{S}}$ by

$$J_{\mathcal{S}}f(v) := \sum_{c\in\mathcal{C}_{\mathcal{S}}(v)} \gamma(c, |v-c|)J_{(c,v)}f(v) \tag{3.20}$$

with positive parameters $\gamma(c, |v-c|)$, where

$$\mathcal{C}_{\mathcal{S}}(v) := \{c \in \mathcal{C} : \exists g \in G : (c, gx) \in \mathcal{S}\} \tag{3.21}$$

describes the set of centers of all discrete spheres through v indicated by $\mathcal{S}$. We conclude

3.4 Theorem: (a) The IVP given by the collision operator $J_{\mathcal{S}}$ and any initial condition $f_0 \in \mathbb{R}_+^{\mathcal{S}}$ has a unique global solution $f(t)$. $f(t)$ is strictly positive; mass $\langle \mathbb{1}_{\mathcal{S}}, f\rangle$, momentum $\langle v, f\rangle$ and energy $\langle 0.5|v|^2, f\rangle$ are conserved. The H-functional $Hf(t)$ is monotonously decreasing.
(b) A function $m \in \mathbb{R}^{\mathcal{S}}$ is a collision invariant if and only if the restriction $m|_{S_{(c,v)}}$ is collision invariant of $J_{(c,v)}$ for all $(c, v) \in \mathcal{S}$.
(c) A density $e \in \mathbb{R}^{\mathcal{S}}$ is an equilibrium solution if and only if the restriction $e|_{S_{(c,v)}}$ is equilibrium solution of $J_{(c,v)}$ for all $(c, v) \in \mathcal{S}$.

Proof: (a) and (c) follow with Lemma 3.3 by applying the same arguments as in Propositions 2.5 and 2.8.

(b) Suppose $(c, v) \in \mathcal{S}$ arbitrary but fixed, and $m \in \mathbb{R}^{\mathcal{S}}$ such that $m|_{S_{(c,v)}}$ is no collision invariant of $J_{(c,v)}$. Define the mapping (g, v') as in Lemma 3.2, and $m_{[g]} := m((g, v)) + m((-g, v))$. From

$$\begin{aligned} \langle m|_{S_{(c,v)}}, J_{(c,v)} f \rangle &= \sum_{[g] \in G/\sim} m_{[g]} J_{(c,v)}[f \circ v]([g]) \\ &= \sum_{[g] \in G/\sim} \sum_{[g'] \in G/\sim} \alpha_{[g'],[g]} \Pi_{[g]} f \circ v \cdot (m_{[g']} - m_{[g]}) \not\equiv 0 \quad \text{on} \quad \mathbb{R}_{+}^{S_{(c,v)}} \end{aligned} \tag{3.22}$$

follows that

$$\min\{m_{[g]} | [g] \in G/\sim\} \neq \max\{m_{[g]} | [g] \in G/\sim\} \tag{3.23}$$

Choose g_0 and g_1 such that $m_{[g_0]} = \max\{m_{[g]} | [g] \in G/\sim\}$ and $m_{[g_1]} = \min\{m_{[g]} | [g] \in G/\sim\}$ and define f on $S_{(c,v)}$ by

$$f(v') := \begin{cases} 1 & \text{if} \quad v' \in \{-g_0 v, g_0 v\} \\ \epsilon & \text{else} \end{cases} \tag{3.24}$$

Then

$$\langle m|_{S_{(c,v)}}, J_{(c,v)} f \rangle = \alpha_{[g_1],[g_0]} \cdot (m_{[g_1]} - m_{[g_0]}) + \mathcal{O}(\epsilon) < 0 \tag{3.25}$$

for ϵ sufficiently small. If we now extend f to $\mathbb{R}_{+}^{\mathcal{S}}$ by $f(v') := \epsilon$ for $v' \notin S_{(c,v)}$, then again

$$\langle m, J_{\mathcal{S}} f \rangle = \alpha_{[g_1],[g_0]} \cdot (m_{[g_1]} - m_{[g_0]}) + \mathcal{O}(\epsilon) < 0 \tag{3.26}$$

for ϵ small proving that m is no collision invariant. □

3.3 A 3D example

Denote by $\mathcal{C} \subset \mathbb{R}^3$ the Cartesian lattice spanned by the three canonical unit vectors b_i. Define $\mathcal{V}$ as the even part of $\mathcal{C}$ (see Remark 2.1 (b)). $\mathcal{V}$ is the well-known *face-centered cubic* (fcc) lattice, see [10]. Both $\mathcal{C}$ and $\mathcal{V}$ have the same orthogonal group consisting of 48 elements (see [10]) which means that all discrete spheres consist of at most 48 elements. We show that $\mathcal{V}$ satisfies (3.2) to (3.4) by proving

3.5 Lemma: $G\mathcal{V} = \mathcal{V}$.

Proof: Suppose $(k,l,m) \in \mathcal{V}$ and $(k',l',m') = g(k,l,m)$, $g \in G$. Since g is orthogonal,

$$k^2 + l^2 + m^2 = k'^2 + l'^2 + m'^2 \tag{3.27}$$

Write $k + l + m =: 2q$, $q \in \mathbb{N}$; then

$$k^2 + l^2 + m^2 = 2k^2 + 2l^2 + 4q^2 - 4q(k+l) \quad \text{is even} \tag{3.28}$$

For $(a,b,c) \notin \mathcal{V}$, $a + b + c = 2p + 1$,

$$a^2 + b^2 + c^2 = 2a^2 + 2b^2 + (2p+1)^2 - 2(2p+1)(a+b) \quad \text{is odd} \tag{3.29}$$

Thus $(k',l',m') \in \mathcal{V}$. $\square$

We are going to construct finite restrictions $\overline{\mathcal{S}}$ and $\overline{\mathcal{V}}$ of $\mathcal{C} \times \mathcal{V}$ resp. $\mathcal{V}$ for which the set of collision invariants is the physically correct one, i.e. is spanned by $\mathbb{1}_{\overline{\mathcal{V}}}$, v and $|v|^2$. In the following we write $|z| := |z_1| + |z_2| + |z_3|$ for $z = (z_1, z_2, z_3) \in \mathbf{Z}^3$.

We start with a smallest setting (*basic configuration*) given as follows. Define the indicator set

$$\mathcal{S}^{(0)} := \{((0,0,0),(1,1,0))\} \cup \{(c, 2c) : c \in \mathcal{C}, |c| = 1\} \tag{3.30}$$

representing seven discrete spheres with centers $(0,0,0)$ resp. $(\pm1,0,0)$, $(0,\pm1,0)$ and $(0,0,\pm1)$ consisting of 6 (for $|c| = 1$) resp. 12 elements (for $c = 0$), and the corresponding velocity set

$$\mathcal{V}^{(0)} := \bigcup_{(c,v)\in\mathcal{S}^{(0)}} S_{(c,v)} = \{v \in \mathcal{V}, |v| \le 2\} \tag{3.31}$$

Following the lines of [1], we call a pair $(\mathcal{S}^{(j+1)}, \mathcal{V}^{(j+1)})$ a *basic extension* of $(\mathcal{S}^{(j)}, \mathcal{V}^{(j)})$ if $\mathcal{S}^{(j+1)} = \mathcal{S}^{(j)} \cup \{(c^{(j)}, v^{(j)})\}$ for some $(c^{(j)}, v^{(j)}) \in \mathcal{C} \times \mathcal{V}$ and

$$\mathcal{V}^{(j+1)} = \bigcup_{(c,v)\in\mathcal{S}^{(j+1)}} S_{(c,v)} \tag{3.32}$$

such that

(a) for all $g \in G$, one of the vectors $v = c^{(j)} + g(v^{(j)} - c^{(j)})$ and $v^* = c^{(j)} - g(v^{(j)} - c^{(j)})$ is in $\mathcal{V}^{(j)}$,

(b) there exists $g \in G$ such that both $v, v^* \in \mathcal{V}^{(j)}$.

A pair $(\overline{\mathcal{S}}, \overline{\mathcal{V}})$ is called an *extension* of $(\mathcal{S}^{(0)}, \mathcal{V}^{(0)})$ if $(\overline{\mathcal{S}}, \overline{\mathcal{V}}) = (\mathcal{S}^{(0)}, \mathcal{V}^{(0)})$ or if there is a finite chain

$$(\mathcal{S}^{(0)}, \mathcal{V}^{(0)}), \dots (\mathcal{S}^{(j)}, \mathcal{V}^{(j)}), \dots, (\mathcal{S}^{(n)}, \mathcal{V}^{(n)}) = (\overline{\mathcal{S}}, \overline{\mathcal{V}}) \tag{3.33}$$

such that $(\mathcal{S}^{(j+1)}, \mathcal{V}^{(j+1)})$ is a basic extension of $(\mathcal{S}^{(j)}, \mathcal{V}^{(j)})$.

3.6 Theorem: Let $(\overline{\mathcal{S}}, \overline{\mathcal{V}})$ be an extension of $(\mathcal{S}^{(0)}, \mathcal{V}^{(0)})$, $\overline{J} := J_{\mathcal{S}}$ the corresponding collision operator and $C_{\overline{J}}$ the set of collision invariants.

(a) $C_{\overline{J}}$ is spanned by $\mathbb{1}_{\overline{\mathcal{V}}}$, v and $|v|^2$.

(b) $e \in \mathbb{R}_+^{\overline{\mathcal{V}}}$ is equilibrium solution of $\overline{J}$ if and only if $\ln e \in C_{\overline{J}}$, i.e. if there exist $\lambda_{\mathbb{1}}, \lambda_{|v|^2} \in \mathbb{R}$, $\lambda_v \in \mathbb{R}^3$ such that

$$e(v) = \exp\left(\lambda_{\mathbb{1}} \cdot \mathbb{1}_{\overline{\mathcal{V}}} + \langle \lambda_v, v \rangle + \lambda_{|v|^2} |v|^2\right) \tag{3.34}$$

Proof: We start with the case $(\overline{\mathcal{S}}, \overline{\mathcal{V}}) = (\mathcal{S}^{(0)}, \mathcal{V}^{(0)})$. Suppose $m \in C_{\overline{J}}$. We write for short $m_{klm} := m((k,l,m))$ for $(k,l,m) \in \overline{\mathcal{V}}$. According to Theorem 2.4 and Lemma 2.3, m has to satisfy the following equations related to each of the seven discrete spheres:

$$c = (0,0,0): \ m^{(0)} := m_{110} + m_{-1-10} = m_{1-10} + m_{-110} = m_{101} + m_{-10-1} \tag{3.35}$$

$$= m_{10-1} + m_{-101} = m_{011} + m_{0-1-1} = m_{01-1} + m_{0-11}$$

$$c = (1,0,0): \ m^{(1)} := m_{000} + m_{200} = m_{110} + m_{1-10} = m_{101} + m_{10-1} \tag{3.36}$$

$$c = (-1,0,0): \ m^{(2)} := m_{000} + m_{-200} = m_{-110} + m_{-1-10} = m_{-101} + m_{-10-1} \tag{3.37}$$

$$c = (0,1,0): \ m^{(3)} := m_{110} + m_{-110} = m_{000} + m_{020} = m_{011} + m_{01-1} \tag{3.38}$$

$$c = (0,-1,0): \ m^{(4)} := m_{1-10} + m_{-1-10} = m_{000} + m_{0-20} = m_{0-11} + m_{0-1-1} \tag{3.39}$$

$$c = (0,0,1): \ m^{(5)} := m_{101} + m_{-101} = m_{011} + m_{0-11} = m_{000} + m_{002} \tag{3.40}$$

$$c = (0,0,-1): \ m^{(6)} := m_{10-1} + m_{-10-1} = m_{01-1} + m_{0-1-1} = m_{000} + m_{00-2} \tag{3.41}$$

Now suppose e.g. the five quantities $\alpha_0 := m_{000}$, $\alpha_1 := m_{002}$, $\alpha_2 := m_{011}$, $\alpha_3 := m_{-1-10}$ and $\alpha_4 := m_{101}$ are given. Then

$$(3.35) \;\Rightarrow\; m_{0-1-1} = m^{(0)} - \alpha_2 \tag{3.42}$$

$$(3.35) \;\Rightarrow\; m_{110} = m^{(0)} - \alpha_3 \tag{3.43}$$

$$(3.35) \;\Rightarrow\; m_{-10-1} = m^{(0)} - \alpha_4 \tag{3.44}$$

$$(3.36) \;\Rightarrow\; m_{200} = m^{(1)} - \alpha_0 \tag{3.45}$$

$$(3.36) \;\Rightarrow\; m_{10-1} = m^{(1)} - \alpha_4 \tag{3.46}$$

$$(3.35) \;\Rightarrow\; m_{-101} = m^{(0)} - m_{10-1} = m^{(0)} - m^{(1)} + \alpha_4 \tag{3.47}$$

$$(3.37) \;\Rightarrow\; m^{(2)} = m_{-101} + m_{-10-1} = 2m^{(0)} - m^{(1)} \tag{3.48}$$

$$(3.37) \;\Rightarrow\; m_{-110} = m^{(2)} - \alpha_3 = 2m^{(0)} - m^{(1)} - \alpha_3 \tag{3.49}$$

$$(3.35) \;\Rightarrow\; m_{1-10} = m^{(0)} - m_{-110} = -m^{(0)} + m^{(1)} + \alpha_3 \tag{3.50}$$

$$(3.37) \;\Rightarrow\; m_{-200} = m^{(2)} - \alpha_0 = 2m^{(0)} - m^{(1)} - \alpha_0 \tag{3.51}$$

$$(3.38) \;\Rightarrow\; m^{(3)} = m_{110} + m_{-110} = 3m^{(0)} - m^{(1)} - 2\alpha_3 \tag{3.52}$$

$$(3.38) \;\Rightarrow\; m_{020} = m^{(3)} - \alpha_0 = 3m^{(0)} - m^{(1)} - 2\alpha_3 - \alpha_0 \tag{3.53}$$

$$(3.38) \;\Rightarrow\; m_{01-1} = m^{(3)} - \alpha_2 = 3m^{(0)} - m^{(1)} - \alpha_2 - 2\alpha_3 \tag{3.54}$$

$$(3.35) \;\Rightarrow\; m_{0-11} = m^{(0)} - m_{01-1} = -2m^{(0)} + m^{(1)} + \alpha_2 + 2\alpha_3 \tag{3.55}$$

$$(3.39) \;\Rightarrow\; m^{(4)} = m_{1-10} + m_{-1-10} = -m^{(0)} + m^{(1)} + 2\alpha_3 \tag{3.56}$$

$$(3.39) \;\Rightarrow\; m_{0-20} = m^{(4)} - \alpha_0 = -m^{(0)} + m^{(1)} - \alpha_0 + 2\alpha_3 \tag{3.57}$$

$$(3.40) \;\Rightarrow\; m_{101} + m_{-101} = m_{011} + m_{0-11} \Rightarrow m^{(1)} = 1.5m^{(0)} - \alpha_2 - \alpha_3 + \alpha_4 \tag{3.58}$$

$$(3.40) \;\Rightarrow\; m^{(5)} = \alpha_0 + \alpha_1 \Rightarrow m^{(0)} = -2\alpha_0 - 2\alpha_1 + 2\alpha_2 + 2\alpha_3 + 2\alpha_4 \tag{3.59}$$

$$(3.41) \;\Rightarrow\; m^{(6)} = m_{10-1} + m_{-10-1} = -5\alpha_0 - 5\alpha_1 + 4\alpha_2 + 4\alpha_3 + 4\alpha_4 \tag{3.60}$$

$$(3.41) \;\Rightarrow\; m_{00-2} = -6\alpha_0 - 5\alpha_1 + 4\alpha_2 + 4\alpha_3 + 4\alpha_4 \tag{3.61}$$

In this way we find that all quantities m_{klm} can be expressed by α_i, $i = 0, \dots, 4$. Thus the dimension of $C_{\overline{J}}$ is at most five. From Theorem 3.4 and Lemma 3.3 we conclude

$$C_{\overline{J}} = \mathrm{span}(\mathbb{1}, v, |v|^2) \tag{3.62}$$

Now consider $(\overline{\mathcal{S}}, \overline{\mathcal{V}})$ arbitrary and choose a chain of basic extensions $(\mathcal{S}^{(j)}, \mathcal{V}^{(j)})$ as in (3.32). Suppose given $m \in C_{\overline{\mathcal{J}}}$ and suppose $m|_{\mathcal{V}^{(j)}}$ is known. Choose $g_0, g \in G$ such that

$$c^{(j)} \pm g_0(v^{(j)} - c^{(j)}), \quad c^{(j)} + g(v^{(j)} - c^{(j)}) \in \mathcal{V}^{(j)} \tag{3.63}$$

Then $m(c^{(j)} - g(v^{(j)} - c^{(j)}))$ can be calculated from

$$\begin{aligned} & m(c^{(j)} + g(v^{(j)} - c^{(j+1)})) + m(c^{(j)} - g(v^{(j)} - c^{(j)})) \\ = \; & m(c^{(j)} + g_0(v^{(j)} - c^{(j)})) + m(c^{(j)} - g_0(v^{(j)} - c^{(j)})) \end{aligned} \tag{3.64}$$

Thus by the definition of a basic extension, $m|_{\mathcal{V}^{(j+1)}}$ is completely determined by $m|_{\mathcal{V}^{(j)}}$. This proves (a).

(b) follows from the fact that $\ln e$ is a collision invariant. □

3.7 Remark: It is a straightforward calculation to prove that for $R \geq 2$ and the velocity sets

$$\overline{\mathcal{V}} = \mathcal{V} \cap \{v : |v| \leq R\} \tag{3.65}$$

and

$$\overline{\mathcal{V}} = \mathcal{V} \cap \{v = (v_1, v_2, v_3) : v_1^2 + v_2^2 + v_3^2 \leq R^2\} \tag{3.66}$$

$(\overline{\mathcal{S}}, \overline{\mathcal{V}})$ is an extension of $(\mathcal{S}^{(0)}, \mathcal{V}^{(0)})$ if $\overline{\mathcal{S}}$ contains all discrete spheres in $\overline{\mathcal{V}}$ with $|c-v| = 1$ and $|c-v| = 2$. Including further spheres does not change the set of collision invariants.

At this point we want to mention that a different approach concerning kinetic models on the *fcc*-lattice is taken in [2] which does not make use of the group structure of the lattice.

4 Numerical examples

In [3, 4, 5] we have demonstrated that the 2D hexagonal model is useful for the purpose of at least *qualitative* studies of rarefied flows. *Quantitative* comparisons hard to obtain due to the lack of data of two-dimensional velocity spaces. In this section we present some first qualitative and quantitative results for the 3D model based on the *fcc* lattice $\mathcal{V}_{fcc}$ as described in section 3.3. For numerical purposes we truncate it by

$$\overline{\mathcal{V}} = \mathcal{V}_{fcc} \cap \{v_1^2 + v_2^2 + v_3^2 \leq R^2\} \quad , \quad R = 4 \tag{4.1}$$

ending up with a 141-velocity model.

One difficulty in the comparison of results lies in the fact that the mean free path of a continuous model with uniform angle distribution is not realized in the discrete model which favors small angles. So we can calculate the exact mean free path mfp_{ex} of the discrete model e.g. by calculating the L^1-norm of the loss term during run time, but for comparison with e.g. experimental or DSMC data we have to use an effective mean free path

$$mfp_{eff} = \lambda_{eff} \cdot mfp_{ex} \tag{4.2}$$

In all what follows we choose $\lambda_{eff} = 2$. More detailed investigations into this point will follow in future papers.

All of the following calculations have been carried out on a conventional DELL Inspiron 8600 portable computer with Intel Mobile Pentium M processor.

4.1 A heat layer problem

As a first benchmark we consider a spatially 1D heat layer problem as it has been treated in [14] with the DSMC (*Direct Simulation Monte Carlo*) method by Bird [6]. It concerns an Argon gas in a gap of width 1mm between walls with temperatures 223.15 K and 323.15 K. Initially, the gas is in global equilibrium with a mean free path of Kn=0.024 (which corresponds to a pressure of 266.644 Pa). We choose an equidistant grid of 100 intervals. The temperature profile of our calculation is given in Fig. 1. It is almost undistinguishable from that of [14]. One of the test quantities is the heat flux. [14] reports 1512 W/m^2 as the correct value. Our calculations yield 1501 W/m^2.

The temperature jumps at the walls are +6.7 K at the cold and -7.06 K at the warm wall (compared to approximately 4 K reported in [14]). The computations required a calculation time of 7 min.

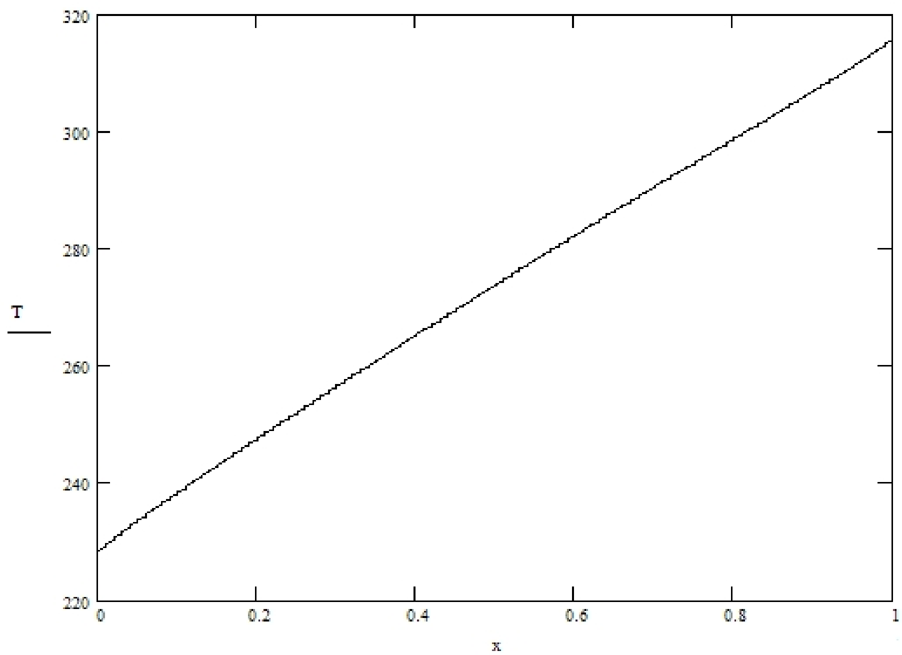

Fig. 1: Temperature profile.

4.2 The Knudsen minimum problem

Consider a long thin channel connected to two vessels at different pressures. The pressure difference causes a flux through the channel. Now keep the pressure ratio (or the pressure difference) constant while decreasing the average pressure. Then a decreasing (rescaled) flow rate should be expected. However, it turns out, that the rate exhibits a minimum at a certain Knudsen number and increases again when further reducing the pressure. This phenomenon (called in literature the *Knudsen minimum problem* or the *Knudsen paradox*) is a rarefied gas effect caused by particles reflected at the walls into velocities close to parallel to the wall. At low pressures, only few of these particles suffer collisions and so contribute much to the channel flow. In [9], model calculations based on the linearized Boltzmann equation for a flow between parallel planes are performed predicting a minimum flow around Kn=1 and a diverging flow in the limit Kn$\searrow$ 0.

We performed calculations on a 160 × 20 grid. The flow rates are shown in Fig. 2. We recognize a distinct minimum at Kn=1.1 which is in agreement with Cercignani's result. In contrast to [9], we do not find a rapid increase for larger Knudsen numbers. Instead, the curve becomes even slightly concave for Kn∼ 10 and presumably takes a maximum for larger values (which in fact is the case for the 2D hexagonal model). The reason for this is that velocities close to tangential are resolved only roughly in our 141-velocity grid.

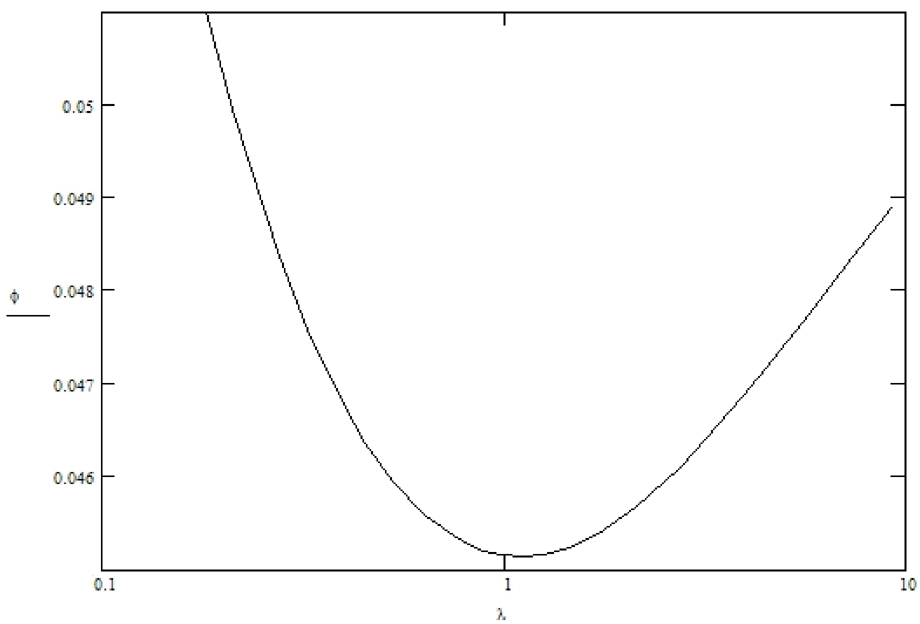

Fig. 2: Flow as function of Knudsen number.

4.3 Thermal creep flow

A well-known rarefied gas effect is *thermal creep flow*, a flow induced by a gradient of the wall temperature. As a particular example, we consider an infinite periodic channel with a periodic temperature profile at the upper wall with alternatingly (linearly) increasing and decreasing temperatures and specular reflection at the lower wall. To demonstrate this effect we performed a calculation on a 150 × 30 spatial grid. The resulting flow field is shown in Fig. 3 which covers a little bit more than a whole period, with the maximum wall temperature in the middle of the upper wall. We clearly recognize convection rolls induced by the temperature gradient.

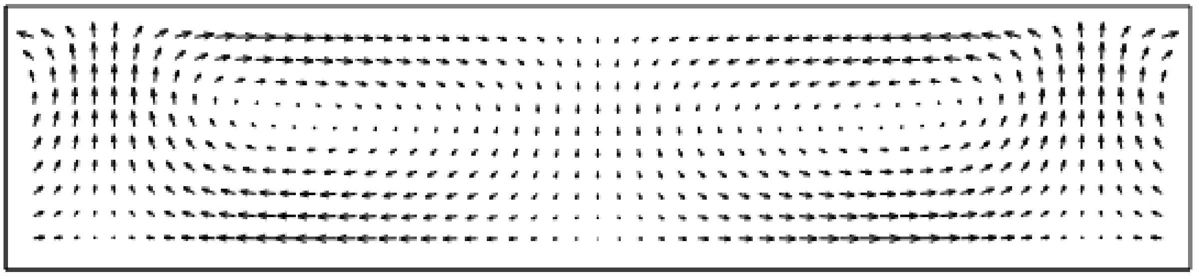

Fig. 3: Flow induced by temperature gradient.

This effect may be used for so called Knudsen pumps for micro flows. These are compressors without moving parts inducing a net flow in an arrangement with zero average gradient. For demonstration, we introduce a step in one half period of Fig. 3, as shown in Fig. 4. In the unperturbed region, we find a convection roll close to that of Fig. 3. In the step region however, the shape of the roll is more affected. As a result, an average flow is induced from the left to the right. In [16] one may find a more detailed description and model calculations for Knudsen compressors. An analogous 2D result based on a hexagonal grid may be found in [5].

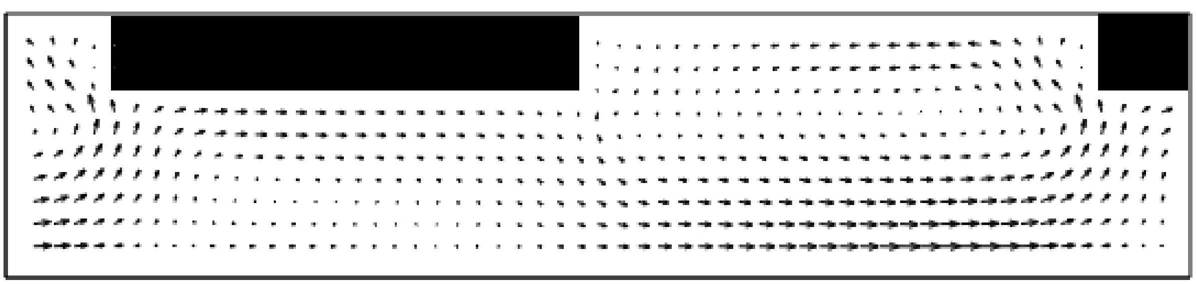

Fig. 4: Net flow induced by temperature gradient and step.

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