Discrete model collision operators of Boltzmann type

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Received 29 May 1998; received in revised form 30 November 1998

Abstract

In the present paper we develop a new kind of discrete velocity models to discretize the Boltzmann collision operator. The chosen approach is situated between the macroscopic ansatz of the BGK-Model and the microscopic ansatz of usual discrete velocity models. Beside questions of the solvability and the form of the solutions of the arising optimization problems, the weak convergence of the discrete collision operators to the original operator is proved. © 1999 Published by Elsevier Science B.V. All rights reserved.

MSC: 76P05; 41A99; 65D99

Keywords: Collision operator; Discrete velocity model

1. Introduction

Direct simulation Monte Carlo (or DSMC) methods are used for solving evolution problems of the Boltzmann equation. They are both mathematically well-understood and used with great success in many cases of application (see [3]). Discrete velocity models are the methods of choice, if results of high accuracy have to be obtained. Such high accuracy is needed for coupling kinetic and fluid dynamic solutions. This is hardly possible by DSMC methods because of their stochastic character. Furthermore, DSMC methods are still not very well-understood for calculation of stationary flows. Systematic errors occur here as well as artificial details of solutions (see [1]). Also in this case, it is necessary to prefer deterministic methods, based on a classical discretization of the collision operator.

So our aim is the discretization of the Boltzmann operator fulfilling the property of mass, impulse and energy conservation to construct a powerful deterministic scheme for solving the Boltzmann equation, especially in the case of stationary solutions. Besides this, we want to ensure the convergence of this method to the continuous equation for fine grids $\Omega_h$.

The paper is structured as follows: In Section 2 we introduce the mesoscopic view of moment conservation which is the main concept of our approach. This concept leads us in Section 3 to a
weak transformation of the gain term of the collision operator and to its discretization on a given
grid \( \Omega_h \). After this we set our focus on the solvability and some properties of the solutions of the
arising optimization systems in Section 4. Questions of special types of these solutions and the weak
convergence of the constructed discrete operators to the continuous one are considered in Section 5.

2. Principles of moment conservation

The starting point of our considerations is the Boltzmann collision operator

\[
J(f) = \int_{\mathbb{R}^3} \int_{S^2} K(\xi - \xi_*, \eta) [f(\xi') f(\xi'_*) - f(\xi) f(\xi_*)] \, d\mu(\eta) \, d\xi_*. \tag{1}
\]

In this definition \( \mu \) is the unit measure on \( S^2 \) and \( K(\xi - \xi_*, \eta) \) the collision kernel. The post-collision velocities \( \xi' \) and \( \xi'_* \) result from the pre-collision velocities \( \xi \) und \( \xi_* \) due to the transformation \( T_\eta \):

\[
\begin{align*}
\xi' &= \xi - (\xi - \xi_*, \eta) \eta, \\
\xi'_* &= \xi_* + (\xi - \xi_*, \eta) \eta,
\end{align*}
\]

with \( \eta \in S^2 \) and \((\cdot, \cdot)\) as the scalar product in \( \mathbb{R}^3 \). \( T_\eta \) is linear, and obviously \( T_{\eta^{-1}} = T_\eta \) holds. The following properties of (1) represent conservation of mass, moments and energy in the collisions of the particles. For the purpose of abbreviation we define

\[
F(f) := K(\xi - \xi_*, \eta) [f(\xi') f(\xi'_*) - f(\xi) f(\xi_*)]
\]

Now let

\[
I(\phi) := \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{S^2} \phi(\xi) F(f) \, d\eta \, d\xi_* \, d\xi
\]

be a linear functional on \( C(\mathbb{R}^3, \mathbb{R}) \). Then for \( I(\phi) \) the equations

\[
I(\phi) = - \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{S^2} \phi(\xi') F(f) \, d\eta \, d\xi_* \, d\xi
\]

\[
= \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{S^2} \phi(\xi_*) F(f) \, d\eta \, d\xi_* \, d\xi
\]

\[
= - \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{S^2} \phi(\xi'_*) F(f) \, d\eta \, d\xi_* \, d\xi
\]

hold. Hence we have

\[
I(\phi) = \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{S^2} (\phi(\xi) + \phi(\xi_*) - \phi(\xi') - \phi(\xi'_*)) F(f) \, d\eta \, d\xi_* \, d\xi.
\]

A function \( \phi \in C(\mathbb{R}^3, \mathbb{R}) \) is called summation or collision invariant (see [5]), if

\[
I(\phi) = 0.
\]

This means from the

- macroscopic point of view,

\[
\int_{\mathbb{R}^3} \phi(\xi) J(f) \, d\xi = 0; \tag{3}
\]
mesoscopic point of view,
\[
\int_{S^2} \phi(\xi) + \phi(\xi_*) - \phi(\xi') - \phi(\xi_*) \, d\mu(\eta) = 0 \quad \forall \xi, \xi_* \tag{4}
\]

microscopic point of view,
\[
\phi(\xi) + \phi(\xi_*) - \phi(\xi') - \phi(\xi_*) = 0 \quad \forall \xi, \xi_*, \quad (\xi', \xi_*)^T = T_0(\xi, \xi_*). \tag{5}
\]

The linear subspace of all collision invariants has the basis
\[
\begin{align*}
\phi_0(\xi) &= 1, \\
\phi_1(\xi) &= \xi_1, \\
\phi_2(\xi) &= \xi_2, \\
\phi_3(\xi) &= \xi_3, \\
\phi_4(\xi) &= |\xi|^2.
\end{align*}
\]

We will try to conserve these collision invariants for our model collision operators (see [2]). In contrast to the strategy in [6], conservation of mass, moments and energy from the mesoscopic point of view (4) will be used. This is an advantage, because in general the post-collision velocities do not lie on the discretization grid. However, having post-collision velocities on the grid is necessary for microscopic conservation of mass, moments and energy (5). We also will preserve the frame of two-particle collisions to be contrary to the BGK model, which is based on a macroscopic point of view of conservation (3). In the following, we will state the scheme of discretization and its weak convergence to the Boltzmann collision operator. Therefore, we restrict ourselves to the two-dimensional case
\[
J(f) = \int_{\mathbb{R}^2} \int_{S^1} K(\xi - \xi_*, \eta)[f(\xi')f(\xi_*) - f(\xi)f(\xi_*)] \, d\mu(\eta) \, d\xi_* \tag{6}
\]
and assume \(K(\xi - \xi_*, \eta) \equiv 1\) for simplicity. Referring to this a generalization is straightforward and the proof of convergence is transferable although some detail questions are to be clarified.

Considered carefully, there are some relations between the approach in [4] of regularization of the Boltzmann collision operator and our method. But our theory is well adapted to numerical schemes because of its discrete character. There already exists a numerical realization, which is used with great success in several test problems. Furthermore, all quantities in our scheme are independent of the distribution function \(f\). So the feasibility of the method in [4] has to be proved.

3. Measure replacement and discretization

The collision operator \(J(f)\) in (6) contains two terms, which have to be handled differently in view of a discretization. This motivates the subdivision of \(J(f)\) in the gain operator \(g(f)\):
\[
g(f(\xi)) = \int_{\mathbb{R}^2} \int_{S^1} f(\xi')f(\xi_*) \, d\mu(\eta) \, d\xi_*. \tag{7}
\]
and the loss operator \(l(f)\)
\[
l(f(\xi)) = \int_{\mathbb{R}^2} f(\xi)f(\xi_*) \, d\xi_. \tag{8}
\]
Thus it follows that
\[ J(f) = g(f) - l(f). \]  
(9)

We will drop the \( f \)-dependence of \( g \) and \( l \), instead we use the notation \( g(f(\zeta)) = g(\zeta) \). Let \( \phi \in C^1(\mathbb{R}^2, \mathbb{R}) \) be a test function. Then the gain operator (7) can be transformed in weak equivalence yielding (see [2])
\[
\int_{\mathbb{R}^2} \phi(\zeta)g(\zeta) \, d\zeta = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \int_{S^1} \phi(\zeta) f(\zeta') f(\xi') \, d\mu(\eta) \, d\xi' \, d\zeta
= \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \int_{S^1} \phi(\zeta') f(\zeta') f(\xi) \, d\mu(\eta) \, d\xi \, d\zeta'.
\]  
(10)

To prepare a discretization in the velocity space one has to replace \( S^1 \) by \( \mathbb{R}^2 \). Furthermore, we substitute the unit measure \( \mu(\eta) \) on \( S^1 \) by the singular measure \( \mu(z, \xi, \xi_*) \). So we end up with
\[
\int_{\mathbb{R}^2} \phi(\zeta)g(\zeta) \, d\zeta = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \phi(z) f(\xi) f(\xi_*) \, d\mu(z, \xi, \xi_*) \, d\xi \, d\xi_*, \quad \forall \zeta, \xi_*, \, \in \mathbb{R}^2, \quad i = 0, \ldots, 3
\]  
(11)

to preserve the summation invariants \( \phi_0 = 1, \phi_1(\zeta) = \zeta_1, \phi_2(\zeta) = \zeta_2, \phi_3(\zeta) = |\zeta|^2 \). This results in the following expression for \( g(z) \):
\[
g(z) = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} f(\xi) f(\xi_*) \, d\mu(z, \xi, \xi_*) \, d\xi_*. \]

For numerical purposes it is necessary to restrict the method to bounded domains as well as to use a grid instead of the continuum in the velocity space. So the bounded domain \( \Omega \subset \mathbb{R}^2 \) replaces \( \mathbb{R}^2 \) and is discretized by the grid \( \Omega_{h_1, h_2} \subset \Omega \), e.g.
\[
\Omega_{h_1, h_2} = \{ \bar{\zeta}^i = \zeta^i | \bar{\zeta}^j = (\zeta^1 + h_1(i - 1), \zeta^2 + h_2(j - 1)), \quad k = (i - 1)n_2 + j, \quad 1 \leq i, j \leq n_1, n_2 \},
\]  
(12)

where
\[
h_1 = \frac{\bar{\zeta}_1 - \bar{\zeta}_1}{n_1 - 1}, \quad h_2 = \frac{\bar{\zeta}_2 - \bar{\zeta}_2}{n_2 - 1}.
\]

If \( h_1 = h_2 = h \) we will write \( \Omega_h \). The number of points in the grid is denoted by \( n = n_1n_2 \). The discretization \( g^h \) of \( g \) on this grid has the form
\[
g_k^h = \sum_{i,j} f_i f_j M^h_{ij} L,
\]
where the tensor \( M^h_{ij} \) represents the measure \( \mu(z, \xi, \xi_*) \). The discretized form \( l^h \) of the loss operator \( l \) results in
\[
l_k^h = f_k \sum_{i} f_i L.
\]
Here and in the following let \( 1 \leq k \leq n \) and \( L = |\Omega|/n \).
4. Determination of the tensor \( M^k_{ij} \)

The next step is to determine the quantities \( M^k_{ij} \). This is the aim of this section. By limitation to the grid \( \Omega_h \) the conditions (11) to \( \mu(z, \xi, \zeta) \) transform into

\[
\sum_k M^k_{ij} = 1, \\
\sum_k \xi^k M^k_{ij} = \frac{1}{2}(\xi^i + \xi^j), \\
\sum_k \zeta^k M^k_{ij} = \frac{1}{2}(\zeta^i + \zeta^j), \\
\sum_k |\xi^k|^2 M^k_{ij} = \frac{1}{2}(|\xi^i|^2 + |\xi^j|^2)
\]

or

\[
A(n)M_{ij} = b_{ij}
\]

as the determination system of the quantities \( M^k_{ij} \) with

\[
A(n) = \begin{pmatrix}
\frac{1}{|\xi|^2} & \frac{1}{|\xi|^2} & \cdots & \frac{1}{|\xi|^2} \\
\frac{1}{|\xi|^2} & \frac{1}{|\xi|^2} & \cdots & \frac{1}{|\xi|^2} \\
\cdots & \cdots & \cdots & \cdots \\
\frac{1}{|\xi|^2} & \frac{1}{|\xi|^2} & \cdots & \frac{1}{|\xi|^2}
\end{pmatrix}, \quad b_{ij} = \frac{1}{2} \begin{pmatrix}
\xi^i + \xi^j \\
\xi^i + \xi^j \\
\cdots \\
\xi^i + \xi^j
\end{pmatrix}.
\]

Now we collect some useful properties of the solutions of the system (13). The following lemma gives the shift invariance of those solutions.

**Lemma 4.1.** The set of solutions of this system is invariant under the transformation

\[
S(\xi) = \alpha \xi + \beta, \quad \alpha \in \mathbb{R}_+, \quad \beta \in \mathbb{R}^2.
\]

**Proof.** Let \( S(\xi) \) be the transformation

\[
S(\xi) = \alpha \xi + \beta
\]

as stated above. Let \( x \) be a solution of (13), i.e.

\[
A(n)x = b_{ij}, \quad x \geq 0.
\]

Then the second and third equations in (13) give

\[
\sum S(\xi^k)x^k = \alpha \sum \xi^k x^k + \beta
\]

and

\[
\frac{1}{2}(S(\xi^i) + S(\xi^j)) = \frac{1}{2}(\xi^i + \xi^j) + \beta.
\]

The fourth condition leads to

\[
\sum |S(\xi^k)|^2 x^k = \sum (\alpha^2 |\xi^k|^2 + |\beta|^2 + 2x^T \beta^T \xi^k)x^k
\]
= x^2 \sum_k |\xi_k|^2 x^k + \alpha \beta^T (\xi^i + \xi^j) + |\beta|^2

and
\frac{1}{2}(S(\xi^i)^2 + |S(\xi^j)|^2) = x^2 \frac{1}{2}(|\xi^i|^2 + |\xi^j|^2) + \alpha \beta^T (\xi^i + \xi^j) + |\beta|^2.

Thus \( x \) is a solution of the transformed system, too. \( \Box \)

For an unbounded grid we already know a solution as Lemma 4.2 shows.

**Lemma 4.2.** Let \( \Omega_h := h \mathbb{Z}^2 \) and \( \tilde{\xi} = \frac{1}{2}(\xi^i + \xi^j) \). Then it follows that
\[
M_{ij}^k = h^2 \frac{c_i^2}{c_2} e^{-|\xi^i - \tilde{\xi}|^2/2c_2^2}
\]
is a solution of (13).

**Proof.** In the proof we will need the two kinds of numbering of the grid points \( \xi_k \) and \( \xi^{mn} \), following the definition in (12). In a first step a constant \( c_1 > 0 \) has to be determined, such that the condition
\[
\sum_k M_{ij}^k = 1
\]
is fulfilled. This is possible for all \( c_2 > 0 \):
\[
\sum_k h^2 \frac{c_i^2}{c_2} e^{-|\xi^i - \tilde{\xi}|^2/2c_2^2} = \sum_m h \frac{c_i}{c_2} e^{-(\xi^i_1 - \tilde{\xi}_1)^2/2c_2^2} \sum_n h \frac{c_i}{c_2} e^{-(\xi^i_2 - \tilde{\xi}_2)^2/2c_2^2} = \left( \sum_m h \frac{c_i}{c_2} e^{-(\xi^i - \tilde{\xi})^2/2c_2^2} \right)^2.
\]
With \( c_2 \hat{u}^m_1 = \tilde{\xi}_1^m \) and \( c_2 \tilde{h} = h \) we get
\[
\sum_k h^2 \frac{c_i^2}{c_2} e^{-|\xi^i - \tilde{\xi}|^2/2c_2^2} = \left( \sum_m h c_1 e^{-\hat{u}^m_1^2/2} \right)^2.
\]
From the second condition \( \sum_k \xi_k^i M_{ij}^k = \xi_1^i \) we calculate
\[
h^2 \frac{c_i^2}{c_2} \sum_k \xi_k^i e^{-|\xi^i - \tilde{\xi}|^2/2c_2^2} = h \frac{c_i}{c_2} \sum_m \xi_1^m e^{-(\xi^i_1 - \tilde{\xi}_1)^2/2c_2^2} h \frac{c_i}{c_2} \sum_n e^{-(\xi^i_2 - \tilde{\xi}_2)^2/2c_2^2} = h \frac{c_i}{c_2} \sum_m e^{-(\xi^i_1 - \tilde{\xi}_1)^2/2c_2^2} = h \frac{c_i}{c_2} \sum_m e^{-(\hat{u}^m_1)^2/2c_2^2}.
\]
By setting \( \hat{u}^m_1 = \xi^m_1 - \tilde{\xi}_1 \) we end up with
\[
h^2 \frac{c_i^2}{c_2} \sum_k \xi_k^i e^{-|\xi^i - \tilde{\xi}|^2/2c_2^2} = h \frac{c_i}{c_2} \sum_m (\hat{u}^m_1 + \xi^i_1) e^{-(\hat{u}^m_1)^2/2c_2^2} = \tilde{\xi}_1^i.
\]
The proof of \( \sum_k \xi_k^2 M_{ij}^k = \tilde{z} \) is analogous. The equation
\[
|\xi|^2 M_{ij} = 2
\]
gives the constant \( c_2 \) by the calculation
\[
\sum_k |\xi|^2 h^2 \frac{c_1}{c_2} e^{-|\xi|^2/2c_2} = \frac{1}{4} |\xi|^2 + 2 \sum_m (u^m_i + \tilde{z}_i)^2 h \frac{c_1}{c_2} e^{-|u^m|^2/2c_2} = \frac{1}{4} |\xi|^2 + 2 \sum_m (u^m_i + \tilde{z}_i)^2 h \frac{c_1}{c_2} e^{-|u^m|^2/2c_2}
\]
c_2 has to be determined, such that
\[
\frac{1}{4} |\xi|^2 - |\xi|^2 = 2 \sum_m (u^m_i + \tilde{z}_i)^2 h \frac{c_1}{c_2} e^{-|u^m|^2/2c_2}
\]
holds. \( \Box \)

**Remark 4.1.** The Maxwell distributions in Lemma 4.2 do not solve the bounded problem because one has to take boundary effects into considerations.

**Lemma 4.3.** System (13) has a positive solution.

**Proof.** By the Lemma of Farkas (see [7]) we only have to prove that for all \( y \in \mathbb{R}^4 \) with \( y^T A^{(a)} > 0 \), \( y^T b_{ij} > 0 \) holds. But this is a trivial fact because \( b_{ij} \) is a positive linear combination of the columns of \( A^{(a)} \). \( \Box \)

At the end of this section we are able to construct a discretization of the Boltzmann operator both on bounded and unbounded grids. But by now we can not say anything about the approximation properties of these discrete operators with respect to the original operator.

5. Weak convergence statements

This section deals with the approximation qualities of the constructed discrete Boltzmann operators. In this field the main question is if we can approximate the integral over \( S^1 \) by an integration formula on the grid \( \Omega_h \), i.e.
\[
\forall \varepsilon > 0 \ \exists n_0(\varepsilon) \ \forall n > n_0(\varepsilon): \left| \int_{S^1} \phi(\xi) \mathrm{d}\mu(\eta) - \sum_{k=1}^n \phi(\xi_k) M_{ij}^k \right| \leq \varepsilon \quad (14)
\]
for all pairs \( (\xi, \xi_*) \in \Omega \times \Omega \), with \( [\xi] = \xi^j, [\xi_*] = \xi^j \). The way we will go now can be described as follows. After some definitions concerning the approximation of a circle by linear splines we state
some lemmata to solve the problem (14). Lemma 5.1 gives the general method on the convergence rate of such an approximation formula. Lemma 5.2 recognizes the conservation of mass, momentum and energy in this context and Theorem 5.1 put these two approaches together by giving a positive solution of the approximation problem which fulfills the system (13), too. To prove the uniform convergence of the integral approximation for all pairs \((\xi, \xi_*)\) \(\in \Omega \times \Omega\) is the last step towards a convergence theorem for the gain term of the Boltzmann operator after all these preparations. So let us start with some definitions, which are necessary for our further investigations.

As we will see, we can not prove the statement above for all pairs \((\xi, \xi_*)\) \(\in \Omega \times \Omega\). So to avoid these boundary effects we restrict ourselves to pairs \((\xi, \xi_*)\) \(\in \Omega \times \Omega\), where the domain \(\Omega \times \Omega\) is defined by

\[
\Omega \times \Omega \subset \{(\xi, \xi_*) \in \mathbb{R}^2 \times \mathbb{R}^2 : Z^1(\xi, \xi_*) \subset \Omega\}.
\]

Eqs. (2) give a procedure to calculate the post-collision velocities \(\xi'\) and \(\xi_*'\) from the pre-collision velocities \(\xi, \xi_*\) \(\in \mathbb{R}^2\) and the unit vector \(\eta \in S^1\). This results in

**Definition 5.1.** Let \(S^1\) be the unit sphere in \(\mathbb{R}^2\). We say \(Z^1(\xi, \xi_*)\) is the set of post-collision velocities with respect to the pair \((\xi, \xi_*)\) if

\[
Z^1(\xi, \xi_*) = \{\xi' : \xi' = \xi - (\xi - \xi_*) \eta, \eta \in S^1\}.
\]

Because of this definition we often identify the set \(Z^1(\xi, \xi_*)\) with \(S^1\) keeping in mind that there always exist two \(\eta \in S^1\) producing the same \(\xi' \in Z^1(\xi, \xi_*)\) (see Definition 5.2). Furthermore, we write \(Z^1\) instead of \(Z^1(\xi, \xi_*)\) if \(\xi\) and \(\xi_*\) are fixed. The first step to approximate the integral over \(S^1\) is its discretization and the generation of the resulting set of post-collision velocities. So we add

**Definition 5.2.** We define the set \(Z^1_m = Z^1_m(\xi, \xi_*), m \in \mathbb{N}, (\xi, \xi_*) \in \Omega \times \Omega\) by

\[
Z^1_m(\xi, \xi_*) = \left\{\xi_m^i : \xi_m^i = \xi'(\eta^i) = \xi'\left(\frac{2\pi}{2m}i\right), \eta^i = \frac{2\pi}{2m}i, 1 \leq i \leq 2m\right\}.
\]

Because of the fact that many points of \(Z^1_m\) do not lie on the grid \(\Omega_h\), we introduce another family of point sets.

**Definition 5.3.** We call the set \(Z^1_{m,n} = Z^1_{m,n}(\xi, \xi_*), (\xi, \xi_*) \in \Omega \times \Omega\) defined by

\[
Z^1_{m,n}(\xi, \xi_*) = \left\{\xi_m^i_n : \xi_m^i_n = [\xi_m^i], \xi_m^i_n \in Z^1_m(\xi, \xi_*)\right\}
\]

with

\[
[\xi] = \xi', \quad |\xi - \xi_*'|_2 = \min_{\xi^k \in \Omega_h} |\xi - \xi^k|_2
\]

a grid approximation of \(Z^1(\xi, \xi_*)\).

If we want to guarantee that \(Z^1_m\) contains \(m\) pairwise distinct points, we have to take \(n\) large enough, which means the grid \(\Omega_h\) should be fine enough. An inner and an outer grid approximation of \(Z^1\) are the last constructions we will need.
Fig. 1. A special set $Z^1_{m,n}(\xi, \xi_*)$.

Fig. 2. Special sets $Z^1_{m,n}(\xi, \xi_*)$ and $Z^1_{m,n}(\xi, \xi_*)$.

**Definition 5.4.** The point set

$$Z^1_{m,n} = \{ \zeta^k: \xi_i = [\xi^k_m, \xi^k_m] \in Z^1_m \}$$

is called inner grid approximation of $Z^1$ and the set

$$Z^1_{m,n} = \{ \zeta^k: \xi_i = [\xi^k_m, \xi^k_m] \in Z^1_m \}$$

outer grid approximation of $Z^1$ with Fig. 1

$$\xi = [\xi], \quad |\xi - \xi|_2 = \min_{\xi^k \in \tilde{A}} |\xi - \xi^k|_2$$

$$\xi = [\xi], \quad |\xi - \xi|_2 = \min_{\xi^k \in \tilde{A}} |\xi - \xi^k|_2$$

and $A = \Omega_b \cap B(\frac{1}{2}(\xi + \xi_*), \frac{1}{2}|\xi - \xi_*|)$.

In this definition $B(x_0, r)$ denotes the open ball around $x_0$ with radius $r$ with respect to the norm $|\cdot|_2$. After these definitions we first ask the question, how can we approximate an integral over $S^1$ by a summation over a grid $\Omega_b$? Therefore we prove Fig. 2
Lemma 5.1. Let \( \phi \in C^1(\mathbb{R}^2, \mathbb{R}) \) be a test function and the distribution \( \delta_{Z^1}(\phi) \) be defined by

\[
\delta_{Z^1}(\phi) := \int_{Z^1} \phi(\xi') \, d\mu(\eta),
\]

where the pair \((\xi, \xi') \in \omega \times \omega\) is fixed. Let \( Z_{m,n}^1 \) form an approximation of \( Z^1 \) of \( m \) points of the grid \( \Omega_k \) in the sense of Definition 5.3. To get this let \( h \leq h_0(m) \) and \( |\Omega_k| = n \geq n_0(m) \). Further the distributions \( \delta_{Z_{m,n}^1} \)

\[
\delta_{Z_{m,n}^1}(\phi) := \sum_{k} \phi(\xi) \chi_{Z_{m,n}^1}(\xi) \frac{1}{m}
\]

are defined on \( Z_{m,n}^1 \), where \( \chi_{Z_{m,n}^1}(\xi) \) denotes the characteristic function of \( Z_{m,n}^1 \). Then

\[
\lim_{m,n \to \infty} \delta_{Z_{m,n}^1}(\phi) = \delta_{Z^1}(\phi), \quad \forall \phi \in C^1(\mathbb{R}^2, \mathbb{R})
\]

holds and

\[
|\delta_{Z_{m,n}^1}(\phi) - \delta_{Z^1}(\phi)| = o(h).
\]

Proof. The sequence of the distributions \( \delta_{Z_{m,n}^1} \) is given by

\[
\delta_{Z^1}(\phi) := \sum_{i=1}^{m} \phi(\xi_m) \frac{1}{m}.
\]

So the relation \( \lim_{m,n \to \infty} \delta_{Z_{m,n}^1} = \delta_{Z^1} \) holds. (That is a simple consequence of Definition 5.2.) To prove the lemma the following fact is applied: For every \( \delta_{Z^1} \) Definition 5.3 provides a sequence \( \{Z_{m,n}^1\}_{n=n_0(m)}^{+\infty} \), which fulfills the condition

\[
\lim_{n \to \infty} \delta_{Z_{m,n}^1}(\phi) = \delta_{Z^1}(\phi), \quad \forall \phi \in C^1(\mathbb{R}^2, \mathbb{R}),
\]

since for all \( \xi \in Z_{m,n}^1 \) there exists a sequence of grid points \( \{\xi_{m,n}\}_{n=n_0(m)}^{+\infty} \) with the property

\[
\lim_{n \to \infty} \xi_{m,n} = \xi.
\]

Then the set of the \( \{\xi_{m,n}\}_{i=1}^{m} \) forms the set \( Z_{m,n}^1 \) for a fixed \( n \). Therefore for a test function \( \phi \in C^1(\mathbb{R}^2, \mathbb{R}) \) it follows that

\[
0 \leq |\delta_{Z_{m,n}^1}(\phi) - \delta_{Z^1}(\phi)| \leq |\delta_{Z_{m,n}^1}(\phi) - \delta_{Z_{m,n}^1}(\phi)| + |\delta_{Z_{m,n}^1}(\phi) - \delta_{Z^1}(\phi)|.
\]

The second addend has the explicit representation

\[
0 \leq |\delta_{Z_{m,n}^1}(\phi) - \delta_{Z_{m,n}^1}(\phi)|
\]

\[
\leq \sum_{k=1}^{m} \frac{1}{m} |\phi(\xi_{m,n}) - \phi(\xi_{m})|
\]

\[
\leq ||\phi||_{C^1(\mathbb{R}^2, \mathbb{R})} \sum_{k=1}^{m} \frac{1}{m} |\xi_{m,n} - \xi_{m}|.
\]

(15)

First we choose \( m \geq m_1 \) in a way that \( |\delta_{Z^1}(\phi) - \delta_{Z^1}(\phi)| \leq \varepsilon/2 \) holds. Subsequently, \( n \geq n_1(\varepsilon, m) \) has to be fixed to guarantee \( ||\phi||_{C^1(\mathbb{R}^2, \mathbb{R})} \sum_{i=1}^{m} \frac{1}{m} |\xi_{m,n} - \xi_{m}| \leq \varepsilon/2 \). So we get

\[
0 \leq |\delta_{Z_{m,n}^1}(\phi) - \delta_{Z^1}(\phi)| < \varepsilon \quad \text{if} \quad m > m_1, \ n > n_1.
\]
and

\[ |\delta_{x_{1}^{*}}(\phi) - \delta_{z_{1}}(\phi)| = O(h). \]

Remark 5.1. Eq. (15) shows that Lemma 5.1 can not be applied if \( Z_{1}^{2} \) and \( z_{1}^{2} \) are not situated within the domain \( \Omega \) and if they are not captured therefore by the grid \( \Omega_{\eta} \), so the restrictions we made are necessary. All of the following convergence statements only refer to balls \( Z_{1}^{2}(\xi_{1}^{2}, \xi_{2}^{2}) \) completely lying in \( \Omega \).

Lemma 5.1 does not take the conditions (13) into consideration. Hence, we will try now to get its statement for integration formulae fulfilling these conditions. A first step in this direction is

Lemma 5.2. Let \( Z_{m_{n}, n}^{2} \) and \( z_{m_{n}, n}^{2} \) be defined as in Lemma 5.1. Additionally, \( \delta_{z_{m_{n}, n}^{2}}^{*} \) represents the nearest solution to \( \delta_{z_{m_{n}, n}^{2}}^{2} \) regarding \( || \cdot || := || \cdot ||_{2} \) of the system (13). Then the statements

\[ \lim_{m_{n} \to \infty} |\delta_{z_{m_{n}, n}^{2}}^{*}(\phi) - \delta_{z_{m_{n}, n}^{2}}(\phi)| = 0, \forall \phi \in C^{1}(\mathbb{R}^{2}, \mathbb{R}) \]

hold.

Proof. First we get

\[ |\delta_{z_{m_{n}, n}^{2}}^{*}(\phi) - \delta_{z_{m_{n}, n}^{2}}(\phi)| = \left| \sum_{k} (M_{ij}^{k} - M_{ij}^{k}) \phi(\xi_{1}^{k}) \right| \leq ||\phi||_{C^{1}(\mathbb{R}^{2}, \mathbb{R})} \sum_{k} |M_{ij}^{k} - M_{ij}^{k}|. \]

For the difference \( \delta_{z_{m_{n}, n}^{2}}^{*} - \delta_{z_{m_{n}, n}^{2}} \) it follows that

\[ \delta_{z_{m_{n}, n}^{2}}^{*} - \delta_{z_{m_{n}, n}^{2}} = \sum_{i=0}^{3} \alpha_{i} \frac{\phi_{i}}{||\phi_{i}||}, \]

where \( N(A^{(n)})^{\perp} = \text{Span}\{\phi_{0}, \ldots, \phi_{3}\} \). If \( A^{(n)} \delta_{z_{m_{n}, n}^{2}}^{*} - b = e = e(n) \) holds, we calculate

\[ -e = \sum_{i=0}^{3} \frac{\alpha_{i}}{||\phi_{i}||} A^{(n)} \phi_{i}, \]

or in detail

\[ -e_{0} = \alpha_{0} ||\phi_{0}|| + \alpha_{3} \frac{\phi_{0} \phi_{3}}{||\phi_{3}||}, \]

\[ -e_{1} = \alpha_{1} ||\phi_{1}||, \]

\[ -e_{2} = \alpha_{2} ||\phi_{2}||, \]

\[ -e_{3} = \alpha_{3} ||\phi_{3}|| + \alpha_{0} \frac{\phi_{0} \phi_{3}}{||\phi_{0}||}. \]
One can choose $\delta_{Z_{1,m,n}^\ast}$ in a way that $\xi = (0, 0, 0, \delta_3)^T$. So we get $x_1 = 0$, $x_2 = 0$ and

$$x_0 = -\delta_3 \frac{||\phi_0|| (\phi_0, \phi_3)}{||\phi_0||^2 ||\phi_3||^2 - (\phi_0, \phi_3)^2}.$$  

$$x_3 = \delta_3 \frac{||\phi_0||^2 ||\phi_3||}{||\phi_0||^2 ||\phi_3||^2 - (\phi_0, \phi_3)^2}.$$  

Hence it follows that

$$x_0 = -\frac{(\phi_0, \phi_3)}{||\phi_0|| ||\phi_3||} x_3.$$  

Thus we have $|x_3| > |x_0|$ and $x_0 x_3 < 0$. To determine the rate of convergence we consider

$$\delta_3 = x_3 \frac{||\phi_3||^2 ||\phi_0||^2 - (\phi_0, \phi_3)^2}{||\phi_0||^2 ||\phi_3||}.$$  

A short calculation for a grid $\xi = (i/m, j/m)$, $i, j = -m, \ldots, m$, $(2m + 1)^2 = n$ results in

$$||\phi_3||^2 = \frac{2(2m + 1)(-3 + 5m + 50m^2 + 70m^3 + 28m^4)}{45m^3},$$  

$$(\phi_0, \phi_3) = \frac{2m(m + 1)(2m + 1)^2}{3m},$$  

$$||\phi_0||^2 = (2m + 1)^2.$$  

Now we obtain the order of the coefficients of the correction

$$x_0 = x_3 = O\left(\frac{\delta_3}{m}\right)$$  

and consequently

$$||\delta_{Z_{1,m,n}^\ast}^\ast - \delta_{Z_{1,m,n}^\ast}||_1 \leq \sqrt{n} ||\delta_{Z_{1,m,n}^\ast}^\ast - \delta_{Z_{1,m,n}^\ast}||_2$$  

$$\leq \sqrt{n} (|x_0|^2 + |x_3|^2)^{1/2}$$  

$$= O(\epsilon_3)$$  

$$= O\left(\frac{1}{\sqrt{n}}\right).$$  

Of course, there is no guarantee that $\delta_{Z_{1,m,n}^\ast}^\ast$ is a positive solution of the system (13). But in order to avoid numerical instabilities we have to determine positive integration weights. Theorem 5.1 solves this problem.

**Theorem 5.1.** Let $\xi$ and $\tilde{\xi}$ be points of the grid $\Omega$, such that $Z^1(\tilde{\xi}, \xi) \subset \Omega$, e.g. $(\xi, \tilde{\xi}) \in \omega \times \omega$ (Fig. 3). Further we choose an inner grid approximation $Z_{m,n}^{1,1}$ and an outer grid approximation $Z_{m,n}^{1,0}$ of $Z^1(\xi, \tilde{\xi})$. They have to be symmetric with respect to the center $\frac{1}{2}(\xi + \tilde{\xi})$ of $Z^1(\xi, \tilde{\xi})$. This means that if $\xi \in Z_{m,n}^{1,1}$ then $\xi^* = \xi + \tilde{\xi} - \xi^0 \in Z_{m,n}^{1,1}$, too. We claim the same property for $Z_{m,n}^{1,0}$. Then
for all those $\tilde{z}_i$ and $\tilde{z}_j$ there exists a positive solution $\delta^+_{Z_{2m,n}}$ of the system (13) yielding

$$\lim_{m,n \to \infty} \delta^+_{Z_{2m,n}}(\phi) = \delta_{Z_1}(\phi), \quad \forall \phi \in C^1(\mathbb{R}^2, \mathbb{R})$$

and

$$|\delta^+_{Z_{2m,n}}(\phi) - \delta_{Z_1}(\phi)| = C(h)$$

with $Z_{2m,n}^1 = Z_{m,n}^{1,1} \cup Z_{m,n}^{1,0}$.

**Proof.** Without loss of generality we assume that $\frac{1}{2}(\tilde{z}_i^1 + \tilde{z}_j^1) = 0$. To achieve this we are allowed to shift the grid $\Omega_h$. With Lemma 4.1 we get that the set of solutions of the system (13) is not influenced by this procedure.

**Step 1.** First we will construct the solution $\delta^+_{Z_{2m,n}}$. To do so, we assign each point $z_k^{q_i} \in Z_{m,n}^{1,0}$ to a point $z_k^{q_i} \in Z_{m,n}^{1,1}$. This assignment has to be done in a way that the following fact is guaranteed. If $z_k^{q_i} \in Z_{m,n}^{1,1}$ is assigned to the point $z_k^{q_i} \in Z_{m,n}^{1,1}$ so the point $z_k^{q_i} \in Z_{m,n}^{1,0}$ has to be assigned to $z_k^{q_i} \in Z_{m,n}^{1,1}$ where $q_i$ is the index of the point $\tilde{z}_i^1 + \tilde{z}_j^1 - \tilde{z}_o^1$. Then we claim

$$\gamma_o z_o^k |z_o^k|^2 + \gamma_i z_i^k |z_i^k|^2 = |\tilde{z}_o^i|^2 + |\tilde{z}_i^j|^2,$$

$$\gamma_o + \gamma_i = 2$$

(16)

for $k = 1, \ldots, m$. Because of the symmetry we have $|\tilde{z}_o^i|^2 = |\tilde{z}_i^j|^2 = r^2$, where $r$ is the radius of $Z^1(\tilde{z}_i^j, \tilde{z}_o^i)$. Now we set the $m$ weights on $Z_{2m,n}^{1,0}$ to $\frac{1}{2m} \gamma_o$ and on $Z_{2m,n}^{1,1}$ to $\frac{1}{2m} \gamma_i$. This leads to

$$\sum_{p=1}^{2m} \frac{1}{2m} \gamma_p = \sum_{k=1}^{m} \frac{1}{2m} (\gamma_o^k + \gamma_i^k) = \sum_{k=1}^{m} \frac{1}{m} = 1.$$
The conservation of moments is also fulfilled:

\[
\sum_{p=1}^{2m} \frac{1}{2m} \eta^p \xi^p = \frac{1}{2m} \sum_{q=1}^{m} \eta^q (\xi^q + \xi^q^*)
\]

where \(q^*\) is the index of the point \(-\xi^q + \xi^q + \xi^q.i\). This equation holds because of the symmetric assignment of \(\xi^w_o\) and \(\xi^w_i\). Therefore the solutions of the system (16) are equal, e.g. \(\eta^q_o = \eta^q_o^*\) and \(\eta^q_i = \eta^q_i^*\). The last condition reads

\[
\sum_{p=1}^{2m} \frac{1}{2m} \eta^p |\xi^p|^2 = \sum_{k=1}^{m} \frac{1}{2m} (\eta^o |\xi^o|^2 + \eta^i |\xi^i|^2)
\]

\[
= m \frac{1}{m} r^2
\]

\[
= r^2 = \frac{1}{2} (|\xi^o|^2 + |\xi^i|^2).
\]

So \(\delta^2_{\eta_{o,m}}\) is a positive solution of system (13).

**Step 2.** To complete the first step we have to prove that the conditions (16) are admissible. If \(|\xi^o| = |\xi^i| = r\) then we set \(\eta^k = \eta^k.o = 1\), otherwise we determine \(\eta^k_o\) to

\[
\eta^k_o = 2 - \eta^k.
\]

A short calculation gives

\[
\eta^k = \frac{2(r^2 - |\xi^o|^2)}{|\xi^o|^2 - |\xi^i|^2}.
\]

Because of \(|\xi^o|^2 < r^2 > |\xi^i|^2\) the inequalities

\[
0 < \eta^k_o < 2,
\]

\[
0 < \eta^k_i < 2
\]

hold for all \(k = 1, \ldots, m\). Under the assumptions for \(Z_{m,n.o}^1\) and \(Z_{m,n.i}^1\) the system (16) has always a positive solution.

**Step 3.** The proof of convergence is analogous to the proof of Lemma 5.1. So we only repeat the estimation of

\[
|\delta^2_{\eta_{o,m}}(\phi) - \delta^2_{\eta^*}(\phi)|.
\]
It holds that

\[\delta_{Z_{2m,n}}^+(\phi) - \delta_{Z_m}^+(\phi) = \sum_{p=1}^{2m} \frac{1}{2m} \gamma^p \phi(\xi^p) - \sum_{k=1}^{m} \frac{1}{m} \phi(\xi_m^k)\]

\[= \sum_{k=1}^{m} \frac{1}{2m} \left[ \gamma^k \phi(\xi_0^k) - \gamma^k \phi(\xi_1^k) \right] - \sum_{k=1}^{m} \frac{1}{m} \phi(\xi_m^k)\]

\[= \sum_{k=1}^{m} \frac{1}{2m} \left[ \gamma^k \phi(\xi_0^k) - \gamma^k \phi(\xi_1^k) \right] - \sum_{k=1}^{m} \frac{1}{2m} \left( \gamma^k + \gamma^k \right) \phi(\xi_m^k)\]

and therefore

\[|\delta_{Z_{2m,n}}^+(\phi) - \delta_{Z_m}^+(\phi)| \leq \sum_{k=1}^{m} \frac{1}{2m} \gamma^k |\phi(\xi_0^k) - \phi(\xi_m^k)| + \sum_{k=1}^{m} \frac{1}{2m} \gamma^k |\phi(\xi_1^k) - \phi(\xi_m^k)|\]

\[\leq ||\phi|| \left[ \sum_{k=1}^{m} \frac{1}{2m} \gamma^k |\xi_0^k - \xi_m^k| + \sum_{k=1}^{m} \frac{1}{2m} \gamma^k |\xi_1^k - \xi_m^k| \right]\]

\[= \mathcal{O}(h).\]

This completes the proof. Now the tensor $M_{ij}^k$ can easily be assembled. For fixed $i$ and $j$ the components $M_{ij}^k$ are set to zero, if $\xi_m^k \notin Z_{m,n}^{i,1} \cup Z_{m,n}^{i,0}$ and otherwise set to the weights determined above. \(\square\)

With this result we finish the main discussion of the problem (14). The following lemma is the last step of answering the question of approximation of the integral over $S^1$ by an integration formula on the grid $\Omega_h$ and the first step to prove the weak convergence of the discrete Boltzmann operators to the original one. It shows that it is possible to make this approximation uniformly for all pairs $(\xi, \xi_*)$ of a bounded domain $\omega \subset \Omega.$

**Lemma 5.3.** Let $\phi \in C^1(\mathbb{R}^2, \mathbb{R})$ be a fixed test function. The functions $u(\xi, \xi_*)$ and $u^h([\xi], [\xi_*])$ are defined by

\[u(\xi, \xi_*) := \int_{S^1} \phi(\xi) \, d\mu(\eta)\]

and

\[u^h([\xi], [\xi_*]) := \sum_k \phi(\xi_m^k) M_{ij}^k.\]

Then it follows that

\[\lim_{h \to 0} ||u([\xi], [\xi_*]) - u^h([\xi], [\xi_*])||_{C(\omega \times \omega)} = 0\]
and
\[ \|u([\zeta], [\zeta]) - u^h([\zeta], [\zeta])\|_{C_0 \times C_0} = \mathcal{O}(h). \]

**Proof.** We prove only the convergence. The rate of convergence follows directly from formula (15).

Given an \( \varepsilon > 0 \) we determine a radius \( r_0 = r_0(\varepsilon) \) such that for all pairs \( (\xi, \xi') \in \omega \times \omega \) which generate a set \( Z^1(\xi, \xi') \) with radius \( r < r_0 \)
\[ \left| \frac{1}{2}(\phi(\xi) + \phi(\xi')) - \int_{\xi}^{\xi'} \phi(\eta) \, d\mu(\eta) \right| < \varepsilon \]
holds. This is possible because of \( \phi \in C^1(\mathbb{R}^2, \mathbb{R}) \). For all pairs \( (\xi, \xi') \in \omega \times \omega \) with radius \( r \) of \( Z^1(\xi, \xi') \) greater than \( r_0 \), we guarantee with \( \xi' = [\xi] \) and \( \xi'' = [\xi'] \)
\[ \left| \sum_\xi \phi(\xi) M_{ij}^k - \int_{\xi}^{\xi''} \phi(\eta) \, d\mu(\eta) \right| < \varepsilon \]
by choosing \( m > m_0 \) and \( n > n_0(m, \varepsilon) \) as we did in Lemma 5.1. The tensor \( M_{ij}^k \) results from Theorem 5.1.

After this we are able to prove the weak convergence theorem.

**Theorem 5.2.** Let the functions \( u(\xi, \xi') \) and \( u^h([\xi], [\xi']) \) be defined as in Lemma 5.3. Furthermore, we assume
\[ \int_{\omega} \int_{\omega} |f(\xi)f(\xi') - f([\xi])f([\xi'])| \, d\xi \, d\xi' = \mathcal{O}(h) \]
for the distribution function \( f \). Then the following error estimation for the gain operator \( g(\xi) \) with \( f = f_{\omega} \):
\[ \left| \int_{\Omega} g(\xi)\phi(\xi) \, d\xi - \sum_k \sum_{i,j} f_i f_j M_{ij}^k \phi_k L^2 \right| = \mathcal{O}(h). \]
holds.

**Proof.** We keep the relations (10) and \( f = f_{\omega} \) in mind and consider the term
\[ \left| \int_{\Omega} g(\xi)\phi(\xi) \, d\xi - \sum_k \sum_{i,j} f_i f_j M_{ij}^k \phi_k L^2 \right| \]
\[ \leq \left| \int_{\omega} \int_{\omega} f(\xi)f(\xi')u(\xi, \xi') \, d\xi \, d\xi' - \int_{\omega} \int_{\omega} f(\xi)f(\xi')u^h([\xi], [\xi']) \, d\xi \, d\xi' \right| \]
\[ + \left| \int_{\omega} \int_{\omega} f(\xi)f(\xi')u^h([\xi], [\xi']) \, d\xi \, d\xi' - \sum_{i,j} f_i f_j u^h(\xi, \xi') L^2 \right| \]
\[ = E_1 + E_2. \]
Both error parts $E_1$ and $E_2$ will be estimated separately. We get

$$E_1 \leq \int_0^1 \int_0^1 f(\xi)f(\xi_*)u(\xi, \xi_*) - u^h([\xi],[\xi_*]) \, d\xi \, d\xi_* \leq ||f||^2_{L_2(\omega \times \omega)} ||u(\xi, \xi_*) - u^h([\xi],[\xi_*])||_{C(\omega \times \omega)}.$$ 

Since

$$||u(\xi, \xi_*) - u^h([\xi],[\xi_*])||_{C(\omega \times \omega)} \leq ||u(\xi, \xi_*) - u([\xi],[\xi_*])||_{C(\omega \times \omega)} + ||u([\xi],[\xi_*]) - u^h([\xi],[\xi_*])||_{C(\omega \times \omega)}$$

holds, the result is

$$||u(\xi, \xi_*) - u^h([\xi],[\xi_*])||_{C(\omega \times \omega)} = O(h).$$

The following calculation gives for $E_2$,

$$E_2 = \int_0^1 \int_0^1 f(\xi)f(\xi_*)u^h([\xi],[\xi_*]) \, d\xi \, d\xi_* - \sum_{i,j} f_i f_j u^h(\xi^i, \xi^j) L^2_i \leq ||u^h([\xi],[\xi_*])||_{C(\omega \times \omega)} ||f(\xi)f(\xi_*) - f([\xi])f([\xi_*])||_{L_2(\omega \times \omega)}$$

$$\leq c ||f(\xi)f(\xi_*) - f([\xi])f([\xi_*])||_{L_2(\omega \times \omega)} = O(h).$$

**Remark 5.2.** The error $E_1$ is obviously determined by the approximation quality of the integral of the test function $\phi$ on the ball $Z^1(\xi^i, \xi^j)$ as well as by the approximation quality of $Z^1(\xi^i, \xi^j)$ by the grid $\Omega_h$.

**Remark 5.3.** The error $E_2$ is determined by the quality of approximation of the function $f$ by step functions on the grid $\Omega_h$.

6. Conclusion

As we have seen it is possible to construct a discrete velocity model which is close to the original Boltzmann operator in the sense of distributions as well as easy to realize in a numerical scheme. The main advantage of our method is that we do not need to have the post-collision velocities on the grid in the velocity space. So we can reach a required accuracy for the approximation with less grid points than other discrete velocity models. This is very important with respect to the complexity of the collision operator. But the main disadvantage is that for our scheme the H-Theorem is not yet proven.

At the present time we develop a scheme for the 3D velocity space and general collision kernels to generalize our approach for a wider range of application. A paper concerning this topic is being prepared.
References