Journal of Statistical Physics, Vol. 98, Nos. 1/2, 2000

New Discrete Model Boltzmann Equations for Arbitrary Partitions of the Velocity Space

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Received January 13, 1999; final June 24, 1999

Modified discrete Boltzmann equations for arbitrary partitions of the velocity space are established. The new equations can be derived from the continuous Boltzmann equation and are a generalization of previous discrete-velocity models. They preserve mass, momentum, and energy, and an H-theorem holds. The new model equations are tested by comparing their solutions with the analytical ones of the continuous Boltzmann equation for the Krook–Wu and the very hard particle models.

KEY WORDS: Kinetic theory; Boltzmann equation; discrete-velocity models.

1. INTRODUCTION

The famous Boltzmann equation,[(1)] describing rarefied gases in equilibrium and in non-equilibrium states, can be solved exactly only for idealized special cases (see ref. 2 and references herein). Realistic problems, however, require modified transport equations with a simpler mathematical structure to overcome the computational complexity. All of these model-equations have to fulfill at least the basic properties of the full Boltzmann equation, namely the conservation laws and an H-theorem.

Such simple models are, for example, the so-called discrete velocity models. In these models the particle velocities can attain only a finite number of lattice points. A summary of the theory of discrete velocity models and their applications is given by Monaco and Preziosi[(3)] and Bellomo and Gustafson.[(4)] Although the idea of discretizing the velocity space is rather old,[(5)] it was not before the 60's that Broadwell[(6, 7)] succeeded in using a discrete velocity model of the Boltzmann equation. A decade later,

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0022-4715/00/0100-0419$18.00/0

Gatignol[8] and Cabannes[9] developed a systematic and rigorous foundation of the discrete kinetic theory. They analyzed in detail the relevant aspects of this theory such as modeling, analysis of thermodynamic equilibrium, and application to fluiddynamic problems. In their pioneering work only a few particle speeds were used, but a sufficient modeling of arbitrary velocity distributions was left open. To treat physically relevant problems, multi-speed models[10] are needed in order to describe adequately macroscopic quantities such as pressure, temperature, etc.

By creating a discrete velocity model, one has to pay attention to the conservation laws, which restrict the freedom of modeling dramatically. Furthermore, if we want to describe real gases with the help of discrete velocities, we have to introduce a partition of the continuous velocity space. Each discrete velocity vector represents the velocities within its corresponding domain. The partition permits the discretization of a given continuous initial distribution density. In previous works,[3, 11] the discrete Boltzmann equation has governed number densities without taking into account a partition of the velocity space. Our intention is now to link the continuous Boltzmann equation to an adequate discrete model Boltzmann equation. We aim to evaluate the temporal evolution of continuous particle distributions by means of discrete equations. Therefore, our approach can be seen as a generalization of the original discrete Boltzmann equations.

It has been proved by Bobylev, Palczewski, and Schneider in a series of papers[12–14] that the usual discrete Boltzmann equation[3, 8, 11] converges, but only very slowly, to the continuous Boltzmann equation on a regular grid in three dimensions. However, for the two-dimensional case they have shown that the discrete Boltzmann equation does not converge to the continuous one. It should be noted that we do not intend to prove that our model equation approaches the full Boltzmann equation asymptotically, because we consider our model to be an approximation and still refer to the continuous state function which is represented by a discrete velocity distribution. Numerical solutions to the discrete Boltzmann equation on a regular grid can be found for the two-and three-dimensional case in the papers of Innamuro and Sturtevant,[15] Rogier and Schneider,[16] and Buet.[17]

In this paper, we show in detail the connection between the continuous and the discrete theory and set up the corresponding discrete Boltzmann equations. For a given velocity model, we introduce appropriate velocity domains (cells) to cover the whole physically relevant velocity space.

In Section 2 we obtain a new "weighted" discrete Boltzmann equation derived from the continuous one. Establishing an H-theorem requires certain symmetry relations concerning the transition rates. This in turn must be consistent with the fact that the size of the cells is not uniform.

Section 3 is devoted to the two-dimensional "Union Jack" model. This simple hierarchical model allows mixing speed collisions and makes relaxation towards a Maxwellian possible.

We then apply the new discrete Boltzmann equation to the Union Jack model for the spatial homogenous case. By assuming the Krook–Wu scattering model, we compare in Section 4 the discrete temporal evolution obtained from the numerical integration with an exact solution of the Boltzmann equation, namely, the famous BKW mode. In Section 5 a comparison with discrete results is made for the Very Hard Particle (VHP) model, which can be solved analytically for arbitrary initial distributions.

2. CONNECTING THE CONTINUOUS AND THE DISCRETE THEORY

2.1. The Continuous Boltzmann Equation

For rarefied gases the temporal and spatial evolution of the distribution function $f(\mathbf{x}, \mathbf{v}, t)$ is governed by the nonlinear Boltzmann equation[18, 19]

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla}\right) f(\mathbf{x}, \mathbf{v}, t) = G[f] - L[f] \tag{2.1}$$

where the loss term $L[f]$ is given by

$$L[f] = \int d\mathbf{w}\, |\mathbf{v} - \mathbf{w}| \int d\boldsymbol{\Omega}'\, \sigma_c(|\mathbf{v} - \mathbf{w}|, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')\, f(\mathbf{x}, \mathbf{v}, t)\, f(\mathbf{x}, \mathbf{w}, t) \tag{2.2}$$

and the gain term $G[f]$ reads

$$G[f] = \int d\mathbf{w}\, |\mathbf{v}' - \mathbf{w}'| \int d\boldsymbol{\Omega}'\, \sigma_c'(|\mathbf{v}' - \mathbf{w}'|, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})\, f(\mathbf{x}, \mathbf{v}', t)\, f(\mathbf{x}, \mathbf{w}', t) \tag{2.3}$$

Here $\sigma_c(|\mathbf{v} - \mathbf{w}|, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')$ and $\sigma_c'(|\mathbf{v}' - \mathbf{w}'|, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})$ denote the differential cross sections for the direct collision and its corresponding inverse collision. The total cross section given by

$$S(|\mathbf{v} - \mathbf{w}|) = \int d\boldsymbol{\Omega}'\, \sigma_c(|\mathbf{v} - \mathbf{w}|, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') = \int d\boldsymbol{\Omega}'\, \sigma_c'(|\mathbf{v}' - \mathbf{w}'|, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}) \tag{2.4}$$

depends only on the relative speed of the particles. The unit vectors $\boldsymbol{\Omega}$ and $\boldsymbol{\Omega}'$ indicate the direction of the relative velocities of the particles before and after collision.

2.2. The Modified Discrete Boltzmann Equation

In order to establish a discrete velocity model for the continuous Boltzmann equation, we choose a set of velocities $\mathbf{v}_i$ $(i=1, 2,..., M)$ and subdivide the physically relevant velocity space $\mathscr{V} \subset \mathbb{R}^d$ into a disjoint set of M arbitrary domains $\Delta\mathscr{V}_i$ with the properties $\mathbf{v}_i \in \Delta\mathscr{V}_i$ and $\mathscr{V} = \bigcup_{i=1}^{M} \Delta\mathscr{V}_i$. Physically relevant means that we consider only velocities up to a maximal speed $v_{\max}$. We neglect the number of particles with speeds greater than $v_{\max}$ and apply the approximation $f(\mathbf{x}, \mathbf{v}_i, t)\, \Delta v_i \equiv f_i\, \Delta v_i = N_i \approx \int_{\Delta\mathscr{V}_i} d\mathbf{v}\, f(\mathbf{x}, \mathbf{v}, t)$ within each domain $\Delta\mathscr{V}_i$, where f_i denotes the discrete distribution function $f(\mathbf{x}, \mathbf{v}_i, t)$, N_i the number of particles in $\Delta\mathscr{V}_i$, and $\Delta v_i = \int_{\Delta\mathscr{V}_i} d\mathbf{v}$ represents the size of the cell $\Delta\mathscr{V}_i$.

By integrating Eq. (2.1) with respect to $\mathbf{v}$ over $\Delta\mathscr{V}_i$, we obtain for the left hand side

$$\int_{\Delta\mathscr{V}_i} d\mathbf{v} \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f(\mathbf{x}, \mathbf{v}, t) \approx \left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \nabla \right) f_i\, \Delta v_i \tag{2.5}$$

Performing the same integration for the loss term, Eq. (2.2), yields

$$\int_{\Delta\mathscr{V}_i} d\mathbf{v}\, L[f] \approx \Delta v_i \sum_{j=1}^{M} \Delta v_j\, |\mathbf{v}_i - \mathbf{v}_j| \int d\mathbf{\Omega}'\, \sigma_c(|\mathbf{v}_i - \mathbf{v}_j|, \mathbf{\Omega}_{(i,j)} \cdot \mathbf{\Omega}')\, f_i f_j \tag{2.6}$$

where $\sigma_c(|\mathbf{v}_i - \mathbf{v}_j|, \mathbf{\Omega}_{(i,j)} \cdot \mathbf{\Omega}')$ indicates that the velocities $\mathbf{v}$ and $\mathbf{w}$ of the incident particles have already been discretized. To express the discretization of the post-collisional velocities $\mathbf{v}'$ and $\mathbf{w}'$, it is necessary to represent the differential cross section by means of Dirac's δ-function as

$$\sigma_c(|\mathbf{v}_i - \mathbf{v}_j|, \mathbf{\Omega}_{(i,j)} \cdot \mathbf{\Omega}') = \sum_{(k,l)} S(|\mathbf{v}_i - \mathbf{v}_j|)\, a_{(i,j)}^{(k,l)}\, \delta(\mathbf{\Omega}' - \mathbf{\Omega}'^{(k,l)}_{(i,j)}) \tag{2.7}$$

The symbol $\sum_{(k,l)}$ denotes the summation over all possible pairs of particles (k, l) with discrete velocities $\mathbf{v}_k$ and $\mathbf{v}_l$ after collision. Inserting Eq. (2.7) into Eq. (2.4) yields that the probabilities $a_{(i,j)}^{(k,l)}$ are normalized to one

$$\sum_{(k,l)} a_{(i,j)}^{(k,l)} = 1 \tag{2.8}$$

In this way, we finally obtain for the loss term

$$\int_{\Delta\mathscr{V}_i} d\mathbf{v}\, L[f] \approx \sum_{j=1}^{M} \Delta v_i\, \Delta v_j\, |\mathbf{v}_i - \mathbf{v}_j|\, S(|\mathbf{v}_i - \mathbf{v}_j|) \sum_{(k,l)} a_{(i,j)}^{(k,l)} f_i f_j \tag{2.9}$$

The integration of the gain term, Eq. (2.3), results in

$$\int_{\Delta\mathscr{V}_i} d\mathbf{v}\, G[f] \approx \Delta v_i \sum_{j=1}^{M} \Delta v_j\, |\mathbf{v}_i - \mathbf{v}_j| \int d\boldsymbol{\Omega}'\, \sigma_c'(|\mathbf{v}_i - \mathbf{v}_j|, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}^{(i,j)})$$
$$\times f(\mathbf{x}, \tfrac{1}{2}(\mathbf{v}_i + \mathbf{v}_j) + \tfrac{1}{2}\,|\mathbf{v}_i - \mathbf{v}_j|\, \boldsymbol{\Omega}', t)$$
$$\times f(\mathbf{x}, \tfrac{1}{2}(\mathbf{v}_i + \mathbf{v}_j) - \tfrac{1}{2}\,|\mathbf{v}_i - \mathbf{v}_j|\, \boldsymbol{\Omega}', t) \qquad (2.10)$$

where $\sigma_c'(|\mathbf{v}_i - \mathbf{v}_j|, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}^{(i,j)})$ indicates that the velocities $\mathbf{v}$ and $\mathbf{w}$ of the scattered out particles have already been discretized. To express the discretization of the pre-collisional velocities $\mathbf{v}'$ and $\mathbf{w}'$, it is again necessary to represent the differential cross section with the help of Dirac's δ-function as

$$\sigma_c'(|\mathbf{v}_i - \mathbf{v}_j|, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}^{(i,j)}) = \sum_{(k,l)} S(|\mathbf{v}_i - \mathbf{v}_j|)\, a'^{(i,j)}_{(k,l)}\, \delta(\boldsymbol{\Omega}' - \boldsymbol{\Omega}'^{(i,j)}_{(k,l)})$$

where $\sum_{(k,l)} a'^{(i,j)}_{(k,l)} = 1$ which is consistent with Eq. (2.4). We obtain for the gain term

$$\int_{\Delta\mathscr{V}_i} d\mathbf{v}\, G[f] \approx \sum_{j=1}^{M} \Delta v_i\, \Delta v_j\, |\mathbf{v}_i - \mathbf{v}_j|\, S(|\mathbf{v}_i - \mathbf{v}_j|) \sum_{(k,l)} a'^{(i,j)}_{(k,l)} f_k f_l \qquad (2.11)$$

and can finally write the discrete Boltzmann equation using Eqs. (2.5), (2.9), and (2.11) in the form

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \boldsymbol{\nabla}\right) f_i\, \Delta v_i$$
$$= \sum_{j=1}^{M} \Delta v_i\, \Delta v_j\, |\mathbf{v}_i - \mathbf{v}_j|\, S(|\mathbf{v}_i - \mathbf{v}_j|) \sum_{(k,l)} (a'^{(i,j)}_{(k,l)} f_k f_l - a^{(k,l)}_{(i,j)} f_i f_j) \qquad (2.12)$$

The probabilities $a^{(k,l)}_{(i,j)}$ and $a'^{(i,j)}_{(k,l)}$ are yet to be determined. Being aware that $\sum_{(k,l)}$ is equivalent to $\frac{1}{2}\sum_{k=1}^{M}\sum_{l=1}^{M}$ and introducing the transition coefficients

$$A^{(k,l)}_{(i,j)} := \Delta v_i\, \Delta v_j\, |\mathbf{v}_i - \mathbf{v}_j|\, S(|\mathbf{v}_i - \mathbf{v}_j|)\, a^{(k,l)}_{(i,j)} \qquad (2.13a)$$
$$A'^{(i,j)}_{(k,l)} := \Delta v_i\, \Delta v_j\, |\mathbf{v}_i - \mathbf{v}_j|\, S(|\mathbf{v}_i - \mathbf{v}_j|)\, a'^{(i,j)}_{(k,l)} \qquad (2.13b)$$

we can express Eq. (2.12) in the compact form

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \boldsymbol{\nabla}\right) f_i\, \Delta v_i = \frac{1}{2} \sum_{j,k,l=1}^{M} (A'^{(i,j)}_{(k,l)} f_k f_l - A^{(k,l)}_{(i,j)} f_i f_j) \qquad (2.14)$$

The coefficients $A_{(i,j)}^{(k,l)}$ and the probabilities $a_{(i,j)}^{(k,l)}$ have the property that $A_{(i,j)}^{(k,l)} \neq 0$ and $a_{(i,j)}^{(k,l)} \neq 0$ if and only if $\mathbf{v}_i + \mathbf{v}_j = \mathbf{v}_k + \mathbf{v}_l$ and $\mathbf{v}_i^2 + \mathbf{v}_j^2 = \mathbf{v}_k^2 + \mathbf{v}_l^2$. Furthermore, the relations $A_{(i,j)}^{(k,l)} = A_{(j,i)}^{(k,l)} = A_{(i,j)}^{(l,k)} = A_{(j,i)}^{(l,k)}$ imply that $a_{(i,j)}^{(k,l)} = a_{(j,i)}^{(k,l)} = a_{(i,j)}^{(l,k)} = a_{(j,i)}^{(l,k)}$. For the term $A'^{(i,j)}_{(k,l)}$ analog relations hold. It should be noted that we have not yet established a relation between $A_{(i,j)}^{(k,l)}$ and $A_{(k,l)}^{(i,j)}$. Such a symmetry is necessary to obtain an H-theorem.

2.3. *H*-Theorem

Before proving an H-theorem for Eq. (2.14), we introduce a diagonal matrix B with entries $B_{ii} := \mathbf{v}_i \cdot \nabla$ as well as a vector $\mathbf{F}$ with components

$$F_i(\mathbf{U}, \mathbf{U}) := \frac{1}{2} \sum_{j,k,l=1}^{M} \left(A'^{(i,j)}_{(k,l)} U_k U_l - A_{(i,j)}^{(k,l)} U_i U_j \right) \tag{2.15}$$

Let $\mathbf{N}$ be the vector with components N_i and $\mathbf{f}$ the vector with components f_i. Then, one can express the discrete Boltzmann equation (2.14) in convenient vector notation as

$$\frac{\partial \mathbf{N}}{\partial t} + \mathsf{B}\mathbf{N} \equiv \frac{d\mathbf{N}}{dt} = \mathbf{F}(\mathbf{f}, \mathbf{f}) \tag{2.16}$$

For an arbitrary vector $\boldsymbol{\phi}$ with components ϕ_i, we define its scalar product

$$\langle \boldsymbol{\phi}, \mathbf{F}(\mathbf{U}, \mathbf{U}) \rangle := \sum_{i=1}^{M} \phi_i F_i(\mathbf{U}, \mathbf{U})) = \frac{1}{2} \sum_{i,j,k,l=1}^{M} \phi_i \left(A'^{(i,j)}_{(k,l)} U_k U_l - A_{(i,j)}^{(k,l)} U_i U_j \right) \tag{2.17}$$

which can also be written as

$$\begin{aligned} \langle \boldsymbol{\phi}, \mathbf{F}(\mathbf{U}, \mathbf{U}) \rangle = {} & \frac{1}{8} \sum_{i,j,k,l=1}^{M} (\phi_i + \phi_j) \left(A'^{(i,j)}_{(k,l)} U_k U_l - A_{(i,j)}^{(k,l)} U_i U_j \right) \\ & - \frac{1}{8} \sum_{i,j,k,l=1}^{M} (\phi_k + \phi_l) \left(A_{(k,l)}^{(i,j)} U_k U_l - A'^{(k,l)}_{(i,j)} U_i U_j \right) \end{aligned} \tag{2.18}$$

If we now require that

$$A'^{(i,j)}_{(k,l)} = A_{(k,l)}^{(i,j)} \qquad \text{and} \qquad A'^{(k,l)}_{(i,j)} = A_{(i,j)}^{(k,l)} \tag{2.19}$$

then Eq. (2.18) reduces to

$$\langle \boldsymbol{\phi}, \mathbf{F}(\mathbf{U}, \mathbf{U}) \rangle = \tfrac{1}{8} \sum_{i,\, j,\, k,\, l=1}^{M} (\phi_i + \phi_j - \phi_k - \phi_l)(A_{(k,\, l)}^{(i,\, j)} U_k U_l - A_{(i,\, j)}^{(k,\, l)} U_i U_j) \tag{2.20}$$

We introduce the H-function

$$H = \sum_{i=1}^{M} N_i \ln f_i \tag{2.21}$$

With the help of Eqs. (2.16) and (2.20) and by setting $\phi_i = 1 + \ln f_i$, its time derivative reads as

$$\frac{dH}{dt} = \frac{1}{8} \sum_{i,\, j,\, k,\, l=1}^{M} \left(\ln \frac{f_i f_j}{f_k f_l} \right) (A_{(k,\, l)}^{(i,\, j)} f_k f_l - A_{(i,\, j)}^{(k,\, l)} f_i f_j) \tag{2.22}$$

If we now require that

$$A_{(k,\, l)}^{(i,\, j)} = A_{(i,\, j)}^{(k,\, l)} \tag{2.23}$$

then it follows from Eq. (2.13) that

$$\Delta v_i \, \Delta v_j \, a_{(i,\, j)}^{(k,\, l)} = \Delta v_k \, \Delta v_l \, a_{(k,\, l)}^{(i,\, j)} \tag{2.24}$$

and Eq. (2.22) can be written in the form

$$\frac{dH}{dt} = \frac{1}{8} \sum_{i,\, j,\, k,\, l=1}^{M} \left(\ln \frac{f_i f_j}{f_k f_l} \right) \left(1 - \frac{f_i f_j}{f_k f_l} \right) A_{(k,\, l)}^{(i,\, j)} f_k f_l \tag{2.25}$$

Equation (2.23) is a consequence of microreversibility and the fact that we are dealing with central interactions typical of a monoatomic gas. Hence, we can dispose of reverse collisions. By introducing the quantities

$$b_{(i,\, j)}^{(k,\, l)} = \frac{a_{(i,\, j)}^{(k,\, l)}}{\Delta v_k \, \Delta v_l}, \qquad b_{(k,\, l)}^{(i,\, j)} = \frac{a_{(k,\, l)}^{(i,\, j)}}{\Delta v_i \, \Delta v_j} \tag{2.26}$$

and applying Eqs. (2.13), (2.19), and (2.23), the discrete Boltzmann equation (2.14) now becomes

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \boldsymbol{\nabla} \right) f_i \, \Delta v_i = \frac{1}{2} \sum_{j,\, k,\, l=1}^{M} \Delta v_i \, \Delta v_j \, \Delta v_k \, \Delta v_l \, |\mathbf{v}_i - \mathbf{v}_j| \; S(|\mathbf{v}_i - \mathbf{v}_j|) \, b_{(i,\, j)}^{(k,\, l)} (f_k f_l - f_i f_j) \tag{2.27}$$

an Eq. (2.24) simply reads

$$b_{(i,j)}^{(k,l)} = b_{(k,l)}^{(i,j)} \tag{2.28}$$

As the probabilities $a_{(i,j)}^{(k,l)}$ have to fulfill the condition given by Eq. (2.8), the coefficients $b_{(i,j)}^{(k,l)}$ must obey the relation

$$\sum_{(k,l)} b_{(i,j)}^{(k,l)} \Delta v_k \, \Delta v_l = 1 \tag{2.29}$$

Since the product $(\ln(f_i f_j / f_k f_l))(1 - (f_i f_j / f_k f_l)) \leqslant 0$, the equilibrium is given by $\hat{f}_i \hat{f}_j = \hat{f}_k \hat{f}_l$, which implies the discrete Maxwell Boltzmann distribution

$$\hat{f}_i = C \exp(-E(\mathbf{v}_i - \mathbf{D})^2) \tag{2.30}$$

where $C = C(\mathbf{x})$, $\mathbf{D} = \mathbf{D}(\mathbf{x})$, and $E = E(\mathbf{x})$ are constants to be determined from the macroscopic quantities defined by

$$n(\mathbf{x}, t) = \sum_{i=1}^{M} f(\mathbf{x}, \mathbf{v}_i, t) \, \Delta v_i \tag{2.31a}$$

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{n} \sum_{i=1}^{M} \mathbf{v}_i f(\mathbf{x}, \mathbf{v}_i, t) \, \Delta v_i \tag{2.31b}$$

$$e_{\text{th}} = \frac{1}{n} \sum_{i=1}^{M} \frac{m_{\text{p}}(\mathbf{v}_i - \mathbf{u})^2}{2} f(\mathbf{x}, \mathbf{v}_i, t) \, \Delta v_i \tag{2.31c}$$

Here, $n(\mathbf{x}, t)$ is the total number density of the particles, $\mathbf{u}(\mathbf{x}, t)$ the bulk velocity, e_{th} the average thermal energy, and m_{p} the particles mass. It should be noted that the concept of temperature in kinetic theory has not a clear status due to the lack of Galilei invariance of discrete velocity models as discussed in detail in ref. 20. For this reason, we use the term average thermal energy e_{th} instead.

3. A HIERARCHICAL DISCRETE VELOCITY MODEL

We now apply the new modified discrete Boltzmann equation (2.27) to the two-dimensional "Union Jack" model shown in Fig. 1. The model was first introduced by Grieshnig[21, 22] and is the simplest hierarchical model that allows mixing speed collisions, where at least one of the post-collisional speeds differs from both pre-collisional ones. This means that energy can be transferred among different hierarchies.

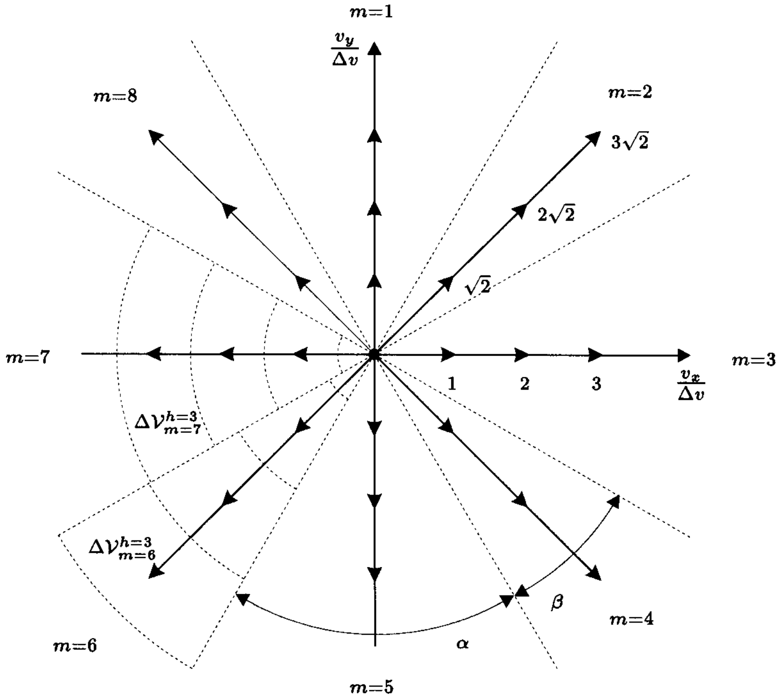

Fig. 1. The two-dimensional Union Jack model.

The eight possible directions are indicated with the subscript m. Along the v_x- and v_y-axes, the speeds are given by $v^h_{m=1,3,5,7} = h\,\Delta v$ with $\Delta v = v_{\max}/h_{\max}$ and $h = 1, 2,..., h_{\max}$. Along the diagonals, the speeds are $v^h_{m=2,4,6,8} = \sqrt{2}\,h\,\Delta v$. The hierarchy $h = 0$ consists only of the velocity $\mathbf{v}^0_0 = 0$. The maximum hierarchy $h_{\max}$ is associated with the maximum discrete speed $v_{\max}$ (along the axes $m = 1, 3, 5, 7$). We choose $v_{\max}$ corresponding to a maximum energy of 50 e_{th}. Thus the maximum speed is 10 if v is measured in units of $\sqrt{e_{\text{th}}/m_p}$. It should be noted that from one mole of gas in the equilibrium state, only approximately 2500 particles have energies larger than 50 e_{th}.

The Union Jack model permits the following bimolecular collisions:

$$(\mathbf{v}^h_1, \mathbf{v}^h_5) \leftrightarrow (\mathbf{v}^h_3, \mathbf{v}^h_7) \tag{3.1a}$$

$$(\mathbf{v}^h_2, \mathbf{v}^h_6) \leftrightarrow (\mathbf{v}^h_4, \mathbf{v}^h_8) \tag{3.1b}$$

$$(\mathbf{v}^h_1, \mathbf{v}^h_4) \leftrightarrow (\mathbf{v}^h_2, \mathbf{v}^h_5) \tag{3.1c}$$

$$(\mathbf{v}^{2h}_1, \mathbf{v}^h_4) \leftrightarrow (\mathbf{v}^{2h}_3, \mathbf{v}^h_8) \tag{3.1d}$$

$$(\mathbf{v}_1^h, \mathbf{v}_3^h) \leftrightarrow (\mathbf{v}_2^h, \mathbf{v}_0^0) \tag{3.1e}$$

$$(\mathbf{v}_2^h, \mathbf{v}_4^h) \leftrightarrow (\mathbf{v}_3^{2h}, \mathbf{v}_0^0) \tag{3.1f}$$

$$(\mathbf{v}_1^h, \mathbf{v}_3^g) \leftrightarrow (\mathbf{v}_2^{(h+g)/2}, \mathbf{v}_8^{(h-g)/2}) \qquad \text{with} \quad 1 \leqslant g < h \tag{3.1g}$$

For Eqs. (3.1c)–(3.1g) the corresponding symmetric collisions must also be considered. The collision scheme, Eqs. (3.1), is very simple. Only two possible outputs exist for each collision. One of them is the trivial collision $(\mathbf{v}_i, \mathbf{v}_j) \rightarrow (\mathbf{v}_i, \mathbf{v}_j)$, which does not contribute to the right hand side of Eq. (2.27) and must be considered only in the determination of the probabilities $a_{(i,j)}^{(k,l)}$. The number of possible collisions grows moderately with $\mathcal{O}(h_{\max}^2)$.

With the above collision scheme the model is regular for $h_{\max} \geqslant 1$. It possesses 4 collisional invariants, which correspond to preservation of mass, momentum in x- and y-direction, and energy. Consequently, the model does not decompose into independent subsystems.

We suggest a partition of the velocity space as indicated by the dotted lines in Fig. 1. The domains $\Delta\mathcal{V}_m^h$ are radially centered to each discrete velocity vector $\mathbf{v}_m^h$. For the domain sizes Δv_m^h the conditions $\Delta v_1^h = \Delta v_3^h = \Delta v_5^h = \Delta v_7^h$ and $\Delta v_2^h = \Delta v_4^h = \Delta v_6^h = \Delta v_8^h$ hold because of the symmetry of the model. The chosen partition yields the following relations between the domain angles

$$\alpha = \frac{\pi}{r+2}, \qquad \beta = \frac{\pi}{2}\frac{r}{r+2}, \qquad \alpha + \beta = \frac{\pi}{2}$$

and the ratio of the domain sizes

$$r = \frac{\Delta v_{m=2,4,6,8}^h}{\Delta v_{m=1,3,5,7}^h} \tag{3.2}$$

In detail, the domain sizes are given by

$$\Delta v_0^0 = \pi \frac{(\Delta v)^2}{2}\frac{r+1}{r+2}, \qquad \Delta v_{1,3,5,7}^h = (\Delta v)^2 \frac{\pi h}{r+2}, \qquad \Delta v_{2,4,6,8}^h = r\,\Delta v_{1,3,5,7}^h$$

The study of the temporal evolution of a non-equilibrium distribution towards equilibrium obtained by applying the discrete Boltzmann equation (2.27) as well as the continuous one shows that the relaxation time τ_{relax} for the discrete model is slower (cf. "BKW Mode" and "DVM ($K=1$)" in Fig. 4). In Fig. 2 the relaxation time (in our case defined by the time that has elapsed until deviation from equilibrium is smaller than 2 percent)

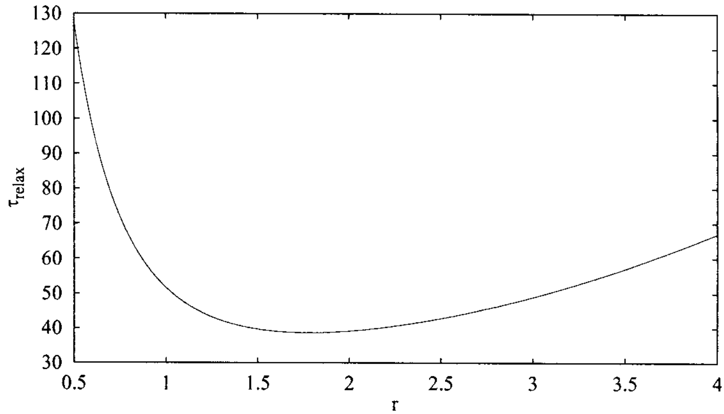

Fig. 2. Relaxation time τ_{relax} obtained from the discrete Boltzmann equation (2.27) for the BKW mode Eq. (4.5) depending on the cell size ratio r.

obtained from the discrete Boltzmann equation (2.27) is shown for the two-dimensional BKW mode Eq. (4.5) depending on different cell size ratios r. We select the value of $r = 1.7$, where τ_{relax} becomes a minimum. This choice of r corresponds to the domain angles $\alpha = 48.65°$ and $\beta = 41.35°$. It should be noted that this minimum of τ_{relax} at $r = 1.7$ can also be observed for other initial conditions.

The reason why we apply the partition shown in Fig. 1 is that for a normalized continuous two-dimensional Maxwell Boltzmann distribution with $\mathbf{u} = 0$,

$$\hat{f}(\mathbf{v})\, d\mathbf{v} = \frac{1}{2\pi} \exp\left(-\frac{v^2}{2}\right) d\mathbf{v} \tag{3.4}$$

the corresponding discrete equilibrium distribution reads for the Union Jack model

$$\hat{f}_i = C_1 \frac{1}{2\pi} \exp\left(-C_2 \frac{v_i^2}{2}\right) \tag{3.5}$$

with coefficients

$$C_1 = 1 - \frac{r+1}{6(r+2)} (\Delta v)^2 + \mathcal{O}((\Delta v)^4) \tag{3.6a}$$

$$C_2 = 1 - \frac{r+1}{12(r+2)} (\Delta v)^2 + \mathcal{O}((\Delta v)^4) \tag{3.6b}$$

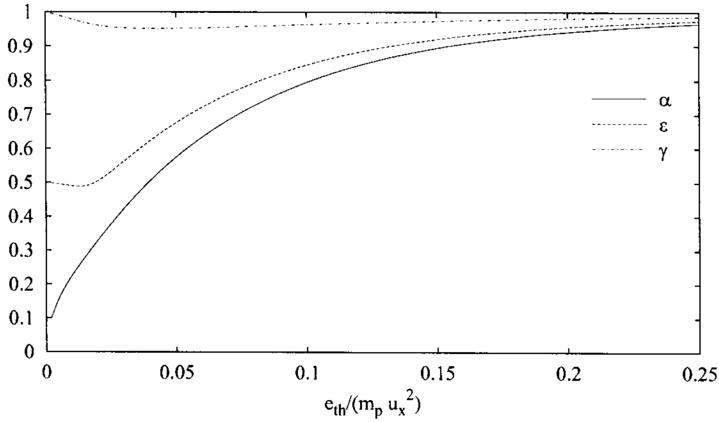

Fig. 3. Factors α, ε, γ in Eq. (3.7) dependent on average thermal energy e_{th}.

obtained from Eqs. (2.31) after some tedious calculation. If the interval Δv approaches zero, then both C_1 and C_2 tend towards 1 and consequently Eq. (3.5) approaches Eq. (3.4) asymptotically.

In the case $\mathbf{u} \neq 0$, the discrete equilibrium distribution can be written as

$$\hat{f}_i = \alpha \frac{n m_{\mathrm{p}}}{2\pi e_{\mathrm{th}}} \exp\left(-\varepsilon \frac{m_{\mathrm{p}}}{2 e_{\mathrm{th}}} \left((v_{i,x} - \gamma u_x)^2 + v_{i,y}^2 \right) \right) \tag{3.7}$$

where we assume that $\mathbf{u}$ has only a component u_x along the x-axis. The terms α, ε, and γ are a measure for the deviation from the continuous Maxwellian. These three factors are calculated from the macroscopic quantities Eqs. (2.31) with a multidimensional, globally convergent Newton method[23] for 200, 2000, and 20000 hierarchies. This study shows that α, ε, and γ barely depend on the number $h_{\max}$ of hierarchies if $h_{\max}$ is large. Their dependence on average thermal energy e_{th} is shown in Fig. 3. As expected, all three values tend to 1 if e_{th} becomes large compared to the energy $m_{\mathrm{p}} u_x^2/2$. However, for relatively small values of e_{th}, the deviation from the continuous equilibrium distribution is significant. It should be noted that the value of γ is not far from 1 which means that the value of $\mathbf{D}$ in Eq. (2.30) is almost the bulk velocity $\mathbf{u}$.

4. COMPARISON WITH THE BKW MODE

In this section we test the Union Jack model as well as the new modified discrete Boltzmann equation by applying them to the Krook–Wu scattering model.[24, 25]

It is now useful to introduce the abbreviation $f_m^h := f(\mathbf{x}, \mathbf{v}_m^h, t)$. In this and the following section, we will only deal with a spatial homogenous gas with bulk velocity $\mathbf{u} = 0$. Hence, we set $f_1^h = f_3^h = f_5^h = f_7^h$ and $f_2^h = f_4^h = f_6^h = f_8^h$. In this case only the three collision types Eqs. (3.1e), (3.1f), and (3.1g) contribute in a nontrivial manner to the discrete Boltzmann equation (2.27). The total number of nontrivial collisions is given by $h_{\max}^2/4 + h_{\max}$.

We consider Maxwell molecules with isotropic scattering. Hence, in the two-dimensional case $d = 2$ the differential cross section reads

$$\sigma_c(|\mathbf{v} - \mathbf{w}|, \mathbf{\Omega} \cdot \mathbf{\Omega}') = \frac{K}{2\pi\, |\mathbf{v} - \mathbf{w}|}$$

leading to the total cross section

$$S(|\mathbf{v} - \mathbf{w}|) = \frac{K}{|\mathbf{v} - \mathbf{w}|} \tag{4.1}$$

by applying Eq. (2.4). Setting $K = 1$, the Boltzmann equation (2.1) then simplifies in the spatial homogenous case to

$$\frac{\partial}{\partial t} f(v, t) = \int d\mathbf{w} \int d\mathbf{\Omega}' \, \frac{1}{2\pi} \, [f(v', t)\, f(w', t) - f(v, t)\, f(w, t)] \tag{4.2}$$

In accordance with Ernst,[2] an exact solution of Eq. (4.2), namely the two-dimensional BKW mode, can be written as

$$f_{\mathrm{BKW}}^{d=2}(v)\, d\mathbf{v} = \frac{1}{2\pi} \exp\left(-\frac{v^2}{2s}\right) \left[\frac{2s-1}{s^2} + \frac{1-s}{2s^3}\, v^2\right] d\mathbf{v} \tag{4.3}$$

with

$$s(t) = 1 + \eta \exp\left(-\frac{t}{8}\right); \qquad -\frac{1}{2} \leqslant \eta \leqslant 0; \qquad \frac{1}{2} \leqslant s \leqslant 1 \tag{4.4}$$

It is assumed in Eq. (4.3) that the microscopic and macroscopic quantities are measured in units such that $m_{\mathrm{p}} = 1$, $n = 1$, and $e_{\mathrm{th}} = 1$.

The discrete analogue of the continuous BKW mode is given by

$$f_{\mathrm{BKW}}^{d=2}(v_i) = \frac{C_1}{2\pi} \exp\left(-C_2 \frac{v_i^2}{2s}\right) \left[\frac{2s-1}{s^2} + \frac{1-s}{2s^3}\, C_2 v_i^2\right] \tag{4.5}$$

where C_1 and C_2 are normalization constants. By applying Eqs. (2.31), we find after some algebra

$$C_1 = 1 - \frac{2s-1}{6s^2} \frac{r+1}{r+2} (\Delta v)^2 + \mathcal{O}((\Delta v)^4) \tag{4.6a}$$

$$C_2 = 1 - \frac{2s-1}{12s^2} \frac{r+1}{r+2} (\Delta v)^2 + \mathcal{O}((\Delta v)^4) \tag{4.6b}$$

It should be noted that Eqs. (3.6) are special cases of Eqs. (4.6) for $s=1$. For $t \to \infty$ and consequently $s \to 1$ the BKW mode approaches the Maxwell Boltzmann distribution. Since in the limiting case, $\Delta v \to 0$, both C_1 and C_2 tend towards 1, the discrete distribution function, Eq. (4.5), approaches the continuous solution, Eq. (4.3), asymptotically.

The discrete version of Eq. (4.2) can be simply obtained by inserting the total cross section, Eq. (4.1), into Eq. (2.27):

$$\frac{\partial}{\partial t} f_i \, \Delta v_i = \frac{1}{2} \sum_{j,k,l=1}^{M} \Delta v_i \, \Delta v_j \, \Delta v_k \, \Delta v_l \, K b_{(i,j)}^{(k,l)} (f_k f_l - f_i f_j) \tag{4.7}$$

The next step consists in determining the probabilities $a_{(i,j)}^{(k,l)}$ needed for evaluating the coefficients $b_{(i,j)}^{(k,l)}$ by means of Eq. (2.26). The collision scheme, Eqs. (3.1), shows that two possible outputs always exist for a collision

$$(\mathbf{v}_i, \mathbf{v}_j) \to \begin{cases} (\mathbf{v}_i, \mathbf{v}_j) \\ (\mathbf{v}_k, \mathbf{v}_l) \end{cases} \qquad \text{and the inverse collision} \qquad (\mathbf{v}_k, \mathbf{v}_l) \to \begin{cases} (\mathbf{v}_k, \mathbf{v}_l) \\ (\mathbf{v}_i, \mathbf{v}_j) \end{cases}$$

The probabilities a have to fulfill the relations given by Eqs. (2.8) and Eqs. (2.24)

$$a_{(i,j)}^{(i,j)} + a_{(i,j)}^{(k,l)} = 1, \qquad a_{(k,l)}^{(i,j)} + a_{(k,l)}^{(k,l)} = 1, \qquad \Delta v_i \, \Delta v_j \, a_{(i,j)}^{(k,l)} = \Delta v_k \, \Delta v_l \, a_{(k,l)}^{(i,j)} \tag{4.8}$$

These are three equations for four unknowns. Since the scattering is isotropic, the probabilities a do not depend on the domain sizes of the pre-collisional velocities but only on the domain sizes of the velocities after collision. Hence, setting

$$a_{(i,j)}^{(i,j)} = \text{const}_1 \, \Delta v_i \, \Delta v_j, \qquad a_{(i,j)}^{(k,l)} = \text{const}_1 \, \Delta v_k \, \Delta v_l$$

$$a_{(k,l)}^{(i,j)} = \text{const}_2 \, \Delta v_i \, \Delta v_j, \qquad a_{(k,l)}^{(k,l)} = \text{const}_2 \, \Delta v_k \, \Delta v_l$$

results in $\text{const}_1 = \text{const}_2 = 1/(\Delta v_i\,\Delta v_j + \Delta v_k\,\Delta v_l)$, and from Eq. (2.26) it follows that

$$b^{(k,\,l)}_{(i,\,j)} = b^{(i,\,j)}_{(k,\,l)} = b^{(i,\,j)}_{(i,\,j)} = b^{(k,\,l)}_{(k,\,l)} = \frac{1}{\Delta v_i\,\Delta v_j + \Delta v_k\,\Delta v_l}$$

By integrating Eq. (4.7) numerically, we obtain the temporal evolution of the discrete distribution function shown in Fig. 4. We choose $\eta = -\frac{1}{2}$ in Eq. (4.4). This corresponds to an initial condition with $f(\mathbf{v}=0, t=0)=0$, showing a maximum deviation from the Maxwell Boltzmann distribution. The discrete velocity distribution splits into two branches corresponding to particles with velocities along the axis and diagonals, respectively. This means that the relaxation differs for those two directions. Moreover, the average relaxation for $K=1$ is too slow compared with the BKW-mode. This is a general problem of two-dimensional models as has been proved by Bobylev *et al.*[12–14] To overcome this shortcoming, we adjust the total

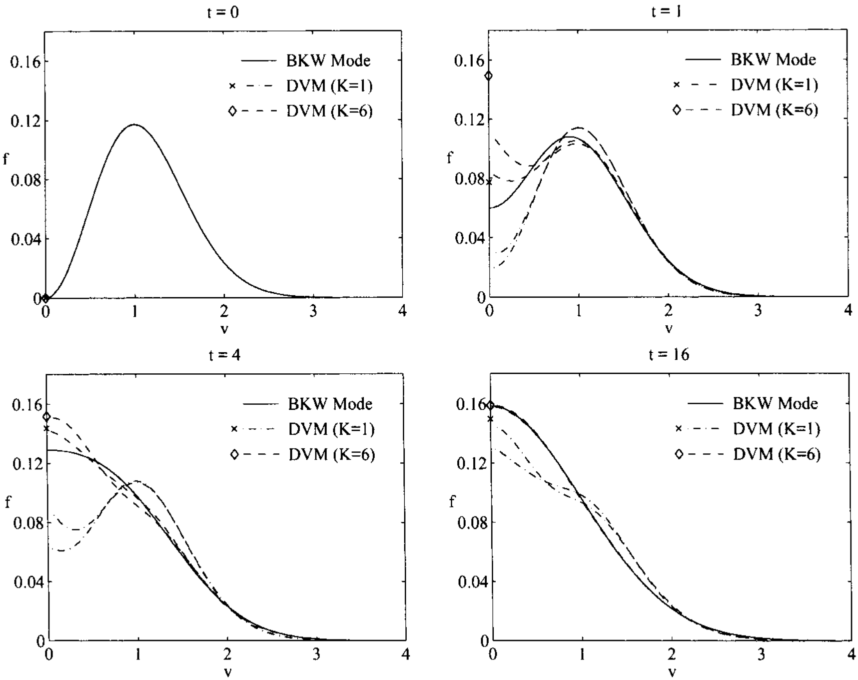

Fig. 4. Temporal evolution of the two-dimensional BKW mode given by Eq. (4.3) and of the numerical solution of the corresponding discrete Boltzmann equations (4.7) applied to the Union Jack velocity model (DVM).

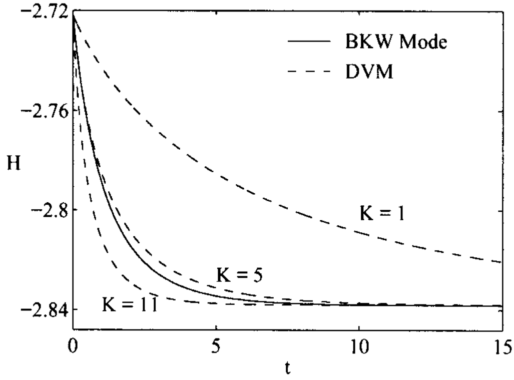

Fig. 5. The H-functions of the two-dimensional BKW mode given by Eq. (4.3) and of the numerical solution of the corresponding discrete Boltzmann equations (4.7) for different total cross sections (DVM).

cross section in such a way that the discrete macroscopic quantities, e.g., the H-function, show the same relaxation behavior as the continuous macroscopic quantities. This is demonstrated for various total cross sections in Fig. 5. For a value of $K=6$, the H-function obtained from the analytical solution, Eq. (4.3), and the discrete one obtained from integration of Eq. (4.7) show the same temporal behavior. The correction factor $K=6$ is also the best match for other values of η in Eq. (4.4), which correspond to different initial distributions.

The numerical calculations have been performed with a maximum hierarchy $h_{\max}=200$ using a Cash–Karp Runge Kutta routine as well as a Bulirsch–Stoer integration routine taken from ref. 23.

5. COMPARISON WITH THE VHP-MODEL

The two-dimensional and exactly solvable VHP model is discussed in details in ref. 2. By introducing an energy like scalar $x=v^2/2$, $x\in[0,\infty)$, the energy distribution function reads for an isotropic velocity distribution

$$F(x,t)\,dx=f(v,t)\,d\mathbf{v}$$

For a differential cross section given by

$$\sigma_c(|\mathbf{v}-\mathbf{w}|,\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')=|\mathbf{v}-\mathbf{w}|\,\frac{|\sin(\chi)|}{8}\tag{5.1}$$

we obtain by applying Eq. (2.4) the total cross section

$$S(|\mathbf{v}-\mathbf{w}|)=\tfrac{1}{2}\,|\mathbf{v}-\mathbf{w}| \tag{5.2}$$

The spatial homogenous Boltzmann equation can be written as

$$\frac{\partial}{\partial t} f(v,t)=\int d\mathbf{w}\,|\mathbf{v}-\mathbf{w}|^2 \int d\mathbf{\Omega}' \,\frac{|\sin(\chi)|}{8}\,[f(v',t)\,f(w',t)-f(v,t)\,f(w,t)] \tag{5.3}$$

where $\chi=\arccos(\mathbf{\Omega}\cdot\mathbf{\Omega}')$ denotes the scattering angle in the center of mass system. By performing the Laplace transform $G(z,t)=\int_0^\infty dx\,\mathrm{e}^{-zx}F(x,t)$, Eq. (5.3) reduces to the simple equation

$$(\partial_t-\partial_z+1)\,G(z,t)=\frac{1}{z}\,(1-G^2)$$

The general solution

$$G(z,t)=\frac{\psi(z+t)+(z-1)\,\mathrm{e}^{-t}}{(z+1)\,\psi(z+t)-\mathrm{e}^{-t}} \tag{5.4}$$

can be expressed with the help of the function

$$\psi(z)=\frac{G(z,0)+z-1}{(z+1)\,G(z,0)-1}$$

which is determined from the initial distribution $F(x,0)$ or its Laplace transform $G(z,0)$, respectively. The distribution function $F(x,t)$ is then gained by applying the Laplace inversion of Eq. (5.4).

The discrete version of Eq. (5.3) is obtained by inserting the total cross section, Eq. (5.2), into Eq. (2.27),

$$\frac{\partial}{\partial t} f_i\,\Delta v_i=\frac{1}{2}\sum_{j,k,l=1}^{M} \Delta v_i\,\Delta v_j\,\Delta v_k\,\Delta v_l\,\frac{K}{2}\,|\mathbf{v}_i-\mathbf{v}_j|^2\,b_{(i,j)}^{(k,l)}(f_k f_l-f_i f_j) \tag{5.5}$$

where we have introduced a correction factor K as done in the previous section.

Again there is the problem of how the coefficients $b_{(i,j)}^{(k,l)}$ should be determined. Contrary to the Krook–Wu model, the scattering in the VHP model is not isotropic. The differential cross section, Eq. (5.1), exhibits no forward scattering and approaches a maximum for a scattering angle $\chi=\pi/2$.

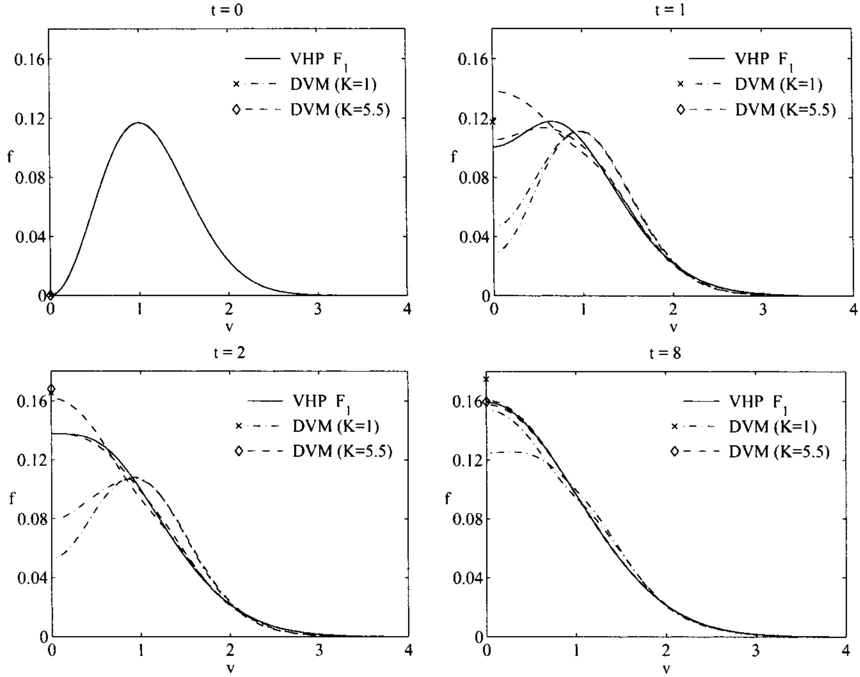

Fig. 6. Temporal evolution of the initial condition given by Eq. (5.7a) for the Very Hard Particle model (VHP F_1) and of the numerical solution of the corresponding discrete Boltzmann equations (5.5) applied to the Union Jack velocity model (DVM).

The probabilities a have to fulfill the relations given by Eqs. (4.8). In the spatial homogenous case, only Eqs. (3.1e)–(3.1g) contribute to the discrete Boltzmann equation (5.5). For these collisions the scattering angle χ is either 0 or $\pi/2$. If we express the fact that no forward scattering appears simply by setting $a_{(i,j)}^{(i,j)} = 0$ and $a_{(i,j)}^{(k,l)} = 1$, then we obtain for the two remaining probabilities with regard to Eq. (4.8)

$$a_{(k,l)}^{(i,j)} = \frac{\Delta v_i \, \Delta v_j}{\Delta v_k \, \Delta v_l} \qquad \text{and} \qquad a_{(k,l)}^{(k,l)} = 1 - a_{(k,l)}^{(i,j)}$$

This is possible only if $\Delta v_i \, \Delta v_j \leqslant \Delta v_k \, \Delta v_l$ in order to ensure that $a_{(k,l)}^{(i,j)} \leqslant 1$. In the case that $\Delta v_i \, \Delta v_j \geqslant \Delta v_k \, \Delta v_l$, we set $a_{(k,l)}^{(k,l)} = 0$ and $a_{(k,l)}^{(i,j)} = 1$, which results in

$$a_{(i,j)}^{(k,l)} = \frac{\Delta v_k \, \Delta v_l}{\Delta v_i \, \Delta v_j} \qquad \text{and} \qquad a_{(i,j)}^{(i,j)} = 1 - a_{(i,j)}^{(k,l)}$$

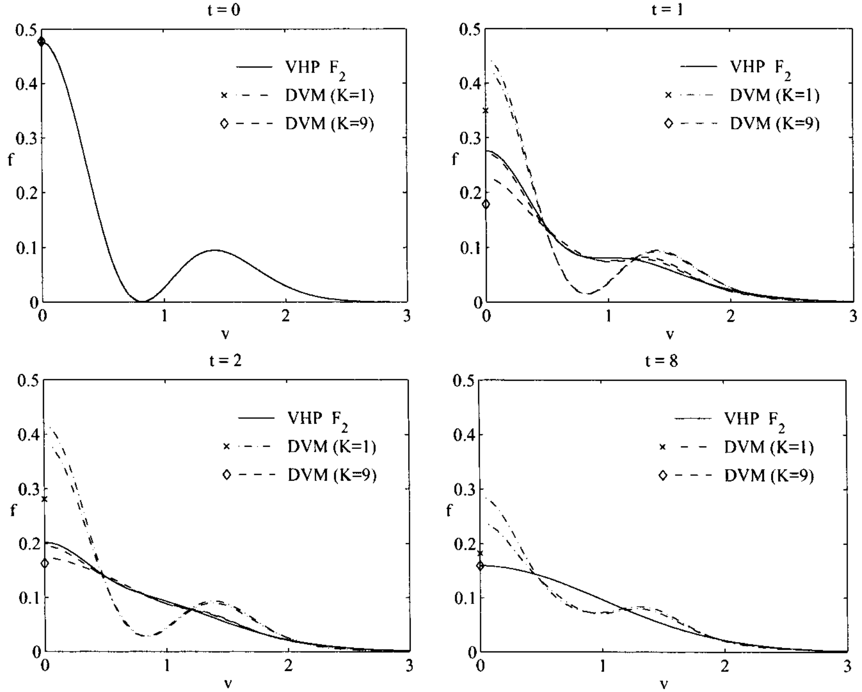

Fig. 7. Temporal evolution of the initial condition given by Eq. (5.7b) for the Very Hard Particle model (VHP F_2) and of the numerical solution of the corresponding discrete Boltzmann equations (5.5) applied to the Union Jack velocity model (DVM).

By inserting these equations into Eq. (2.26), we finally obtain

$$b_{(i,\,j)}^{(k,\,l)} = b_{(k,\,l)}^{(i,\,j)} = \frac{1}{\max(\Delta v_i\, \Delta v_j,\, \Delta v_k\, \Delta v_l)} \tag{5.6}$$

We solved Eq. (5.5) numerically with a maximum hierarchy $h_{\max} = 200$ for two totally different initial distributions, namely

$$F_1(x, 0) = 4x\, e^{-2x} \tag{5.7a}$$

corresponding to $\psi_1(z) = -z - 3$, and

$$F_2(x, 0) = (27x^2 - 18x + 3)\, e^{-3x} \tag{5.7b}$$

corresponding to $\psi_2(z) = (z^2 + 8z + 21)/(2z - 6)$. The microscopic and macroscopic quantities are again measured in units such that $m_p = 1$, $n = 1$, and $e_{th} = 1$. The distribution functions $F(x, t)$ can be obtained analytically

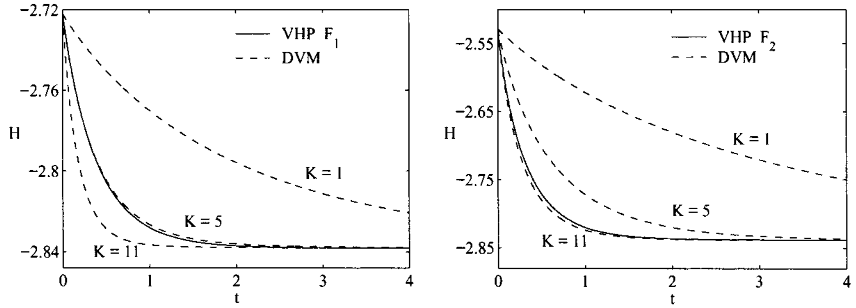

Fig. 8. The H-functions of two different solutions for the Very Hard Particle Model (VHP F_1 and VHP F_2 for the initial conditions Eqs. (5.7a) and (5.7b), respectively) and of the numerical solution of the corresponding discrete Boltzmann equations (4.7) for different total cross sections (DVM).

but their lengthy expressions are not cited here. It should be noted that $F_1(x, 0)$ is the same initial condition which has been chosen for the BKW-mode in the previous section. As shown in Figs. 6 and 7, the distribution function splits again into two branches and the relaxation for $K = 1$ is again too slow compared with the analytical solution. The H-functions obtained from the analytical solutions and from the integration of Eq. (5.5) exhibit the same temporal behavior for values of $K = 5.5$ (initial condition $F_1(x, 0)$) and $K = 9.0$ (initial condition $F_2(x, 0)$), respectively, as displayed in Fig. 8. Since the scattering mechanism is very efficient at high energies, the relaxation to equilibrium is faster than for the BKW mode.

6. CONCLUSION

This paper establishes discrete Boltzmann equations for arbitrary partitions of the velocity space. The new approach permits relating results of the discrete Boltzmann equations to continuous velocity distributions of real gases. The discrete transport equations are derived from the continuous Boltzmann equation and conserve mass, momentum, and energy. The subdivision of the velocity space requires a representation of the differential cross section by means of generalized functions, where the occurring discrete scattering probabilities must obey symmetry relations in order to obtain an H-theorem in the form $H = \sum_{i=1}^{M} N_i \ln f_i$. This new H-theorem corresponds to a Maxwellian for the discrete distribution function f_i.

We apply the new discrete Boltzmann equation to the two-dimensional hierarchical Union Jack model, which is the simplest regular discrete velocity model with mixing speed collisions. The partition of the velocity space allows us to minimize the relaxation time by choosing the domain angles properly. The discrepancy of the solutions to the discrete Boltzmann equations from the solutions to the continuous one requires us to adjust the total cross section for the discrete model, which leads to the same temporal behavior in both cases.

Using two properly scaled "Union Jacks," the new model can be extended to binary mixtures as well. A detailed investigation will be carried out in future work.

ACKNOWLEDGMENT

This work has been supported by the Fonds zur Förderung der wissenschaftlichen Forschung, Vienna, under contract No. P10879-TEC.

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