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Discrete Velocity Models for Mixtures

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Models of discrete velocity gases have been used for a long time, but only in the last few years have they become a tool to construct sequences converging to solutions of the Boltzmann equation. It appears that the case of mixtures has been rarely considered and only a couple of models, which are trivial in a sense to be explained in this paper, have been introduced. Here we thoroughly investigate the matter, and supply examples of models with both finitely and infinitely many velocities.

KEY WORDS: Discrete velocity models; Boltzmann equation; kinetic theory.

1. INTRODUCTION

In the last twenty years research on discrete models of the Boltzmann equation has flourished. On the one hand the lattice gas (with discrete positions, velocities and time) has been introduced as a computational tool for problems of ordinary hydrodynamics;[1,2] on the other hand the research on merely discrete velocity gases (with continuous space-time), started in the mid-seventies,[3,4] has continued to be investigated. In the last eight years it started to become clear that the discrete velocity models (DVM) were also becoming a tool to approximate the solutions of the Boltzmann equation, at a theoretical if not at a practical level.[5-8]

A breakthrough came two years ago when Palczewski, Schneider and one of the authors proved a consistency result for the DVM as an approximation of the Boltzmann equation.[9] The other author of the present paper must apologize for not realizing that this result was available

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and thus for writing the following sentence in a paper prepared a few months after ref. 9 had appeared: "there is not a known procedure to approximate in arbitrary fashion the continuous case by a sequence of discrete models."[10] Another sentence of that paper ("their extension to mixtures seems hard if not impossible, especially when the ratio of masses is irrational (in fact I do not know of any discrete velocity model of the traditional kind for mixtures, with the exception of the case when all the momenta have the same magnitude and hence conservation of energy follows from the conservation of the number of particles)") was however correct, as far as we know, and is the motivation for the present work.

The extension of DVM to mixtures seems impossible when the ratio of masses is irrational, but poses no special problems for the case of a rational ratio (this limitation is, of course, irrelevant in practice). Yet, the fact that only trivial models (in a sense to be specified below) have appeared so far, stimulated us to write the present paper.

2. DISCRETE VELOCITY MODELS FOR MIXTURES

According to standard definitions, a discrete velocity model of a gas is a system of partial differential equations of hyperbolic type (discrete Boltzmann equation), having the following form:

$$\partial f_{\mathbf{n}}/\partial t + \mathbf{v}_{\mathbf{n}} \cdot \partial f_{\mathbf{n}}/\partial \mathbf{x} = Q_{\mathbf{n}}(f, f) \tag{2.1a}$$

$$Q_{\mathbf{n}}(f, f) = \sum_{\mathbf{lk}} c_{\mathbf{nlk}} f_{\mathbf{l}} f_{\mathbf{k}} - \sum_{\mathbf{m}} k_{\mathbf{nm}} f_{\mathbf{n}} f_{\mathbf{m}} \tag{2.1b}$$

where $\mathbf{v}_{\mathbf{n}}$ are the discrete velocities (vectors of R^d) belonging to a prearranged discrete set, $c_{\mathbf{nlk}}$ and $k_{\mathbf{nl}}$ are positive constants and the vector indices run over a discrete set of vectors with integer components, symmetrical with respect to the origin, whereas $f_{\mathbf{n}}$ are the probabilities (per unit volume) of finding a molecule at time t at position $\mathbf{x}$ with velocity $\mathbf{v}_{\mathbf{n}}$. We shall occasionally write f, as done in (2.1b), for the collection $\{f_{\mathbf{n}}\}$.

We certainly must assume that the collision term $Q_{\mathbf{n}}(f, f)$ satisfies the restrictions needed to guarantee the conservation of mass, momentum and energy and the entropy inequality. We remark that this would be a generalization with respect to the traditional concept of a discrete velocity gas,[3,4] where it is assumed that each single collision satisfies momentum and energy conservation.

However if we only assume that

$$\sum_{\mathbf{n}} Q_{\mathbf{n}}(f, f)\, \psi_{\alpha\mathbf{n}} = 0 \qquad (\alpha = 0, 1, 2, 3, 4, 5) \tag{22}$$

where ψ_α ($\alpha = 0, 1, 2, 3, 4$) are the five collision invariants ($1, v_1, v_2, v_3, |v|^2$) and v_j ($j = 1, 2, 3$) are the Cartesian components of $\mathbf{v}$, we lose several important properties of the Boltzmann equation.

We pause a moment to discuss what the physical interpretation of these extended discrete velocity models could be. If we accept Eq. (2.2) as the only restriction on $Q_{\mathbf{n}}(f, f)$, a collision is a more complicated process than in the continuous velocity model. When two particles meet they undergo a not completely deterministic process, in the sense that we cannot guarantee that another pair will emerge from the collision with certain velocities but only that the pre-collision momentum and energy will be distributed with a certain probability to a number of pairs; this is true even in the continuous Boltzmann equation because the collision parameters also determine the post-collisional velocities. Here we would go a step further because Eq. (2.2) does not require that we exhibit possible pairs of these velocities; thus there are no elementary processes where mass momentum and energy are conserved, but we only ensure that momentum and energy are conserved globally.

We need, however, also assume the validity of an H-theorem and this can be shown to require the conservation of momentum and energy in each single collision, thus ruling out the possibility that we have just discussed. As a consequence, however, we can also show the existence of a Maxwellian distribution $\mathcal{M}_{\mathbf{n}}$, such that $Q(\mathcal{M}, \mathcal{M}) = 0$ and $\log \mathcal{M}$ is a linear combination of the collision invariants.

We shall henceforth assume that[3]

$$c_{\mathbf{nlk}} = \sum_{\mathbf{m}} A_{\mathbf{n},\mathbf{m}}^{\mathbf{k},\mathbf{l}} \tag{2.3}$$

$$k_{\mathbf{nm}} = \sum_{\mathbf{k},\mathbf{l}} A_{\mathbf{n},\mathbf{m}}^{\mathbf{k},\mathbf{l}} \tag{2.4}$$

with

$$A_{\mathbf{n},\mathbf{m}}^{\mathbf{k},\mathbf{l}} = A_{\mathbf{k},\mathbf{l}}^{\mathbf{n},\mathbf{m}} = A_{\mathbf{l},\mathbf{k}}^{\mathbf{m},\mathbf{n}} \geqslant 0 \tag{2.5}$$

These assumptions make it easy to satisfy the conservation equations and the H-theorem and might be slightly relaxed.

We now introduce a regular lattice as a grid in velocity space with step h such that the grid points will have position vectors

$$\mathbf{v}_{\mathbf{n}} = \mathbf{n}h \tag{2.6}$$

Henceforth we shall consider this set of velocity vectors or some subset of the said set. When we consider the entire set, Galilei invariance is lost but can be replaced by a discrete symmetry (invariance with respect to translation rectilinear motions having velocity $\mathbf{n}_0 h$ where $\mathbf{n}_0$ is any chosen vector with integer components).

The coefficients $A_{\mathbf{l},\mathbf{k}}^{\mathbf{m},\mathbf{n}}$ must vanish if the following conservation equations are not satisfied:

$$\mathbf{l}+\mathbf{k}=\mathbf{m}+\mathbf{n} \tag{2.7}$$

$$|\mathbf{l}|^2+|\mathbf{k}|^2=|\mathbf{m}|^2+|\mathbf{n}|^2 \tag{2.8}$$

We remark that there are three different kinds of such models for the general Boltzmann equation, plus a simple model for a very special case in two dimensions with a "perpendicular law of scattering" (see ref. 11 for a review).

The most natural and popular model was first proposed by Goldstein. Sturtevant and Broadwell in 1989.[5] The proof of consistency for this model was provided in ref. 9 (see also refs. 12 and 13).

Let us now show that we can generalize this kind of model (and the proof of consistency) to the case of mixtures.

To this end, we consider a mixture with rational masses $m_1, m_2,..., m_s$ where s is the number of species. If we exclude irrational ratios for the masses, without loss of generality we can assume the masses to be given by integers, by a suitable choice of the mass unit.

Let us consider any pair of molecules with masses m_i, m_j and let us put $m_i=m$, $m_j=M$ $(m<M)$. The usual Boltzmann equation for mixtures (with continuous velocities) has the following form

$$\partial f_i/\partial t+\mathbf{v}\cdot\partial f_i/\partial\mathbf{x}=\sum_j Q_{ij} \tag{2.9}$$

where

$$Q_{ij}=\int_{R_d\times S_{d-1}} d\mathbf{v}\,d\boldsymbol{\omega}\,|\mathbf{u}|\,\sigma(\mu\,|\mathbf{u}|^2/2,\,\mathbf{u}\cdot\boldsymbol{\omega}/|\mathbf{u}|)[f(\mathbf{v}')\,F(\mathbf{w}')-f(\mathbf{v})\,F(\mathbf{w})] \tag{2.10}$$

where $d=2, 3,...,$ $f(\mathbf{v})=f_i(\mathbf{v})$, $F(\mathbf{v})=f_j(\mathbf{w})$, and

$$\mathbf{u}=\mathbf{v}-\mathbf{w}, \qquad \mu=\frac{mM}{m+M} \tag{2.11}$$

$$\begin{aligned}\mathbf{v}'&=\frac{m\mathbf{v}+M\mathbf{w}}{m+M}+\frac{\mu}{m}\,|\mathbf{u}|\,\boldsymbol{\omega}\\ \mathbf{w}'&=\frac{m\mathbf{v}+M\mathbf{w}}{m+M}-\frac{\mu}{M}\,|\mathbf{u}|\,\boldsymbol{\omega}\end{aligned} \tag{2.12}$$

The first step toward obtaining a form of the collision term suitable for arriving at a discrete velocity model is to adopt $\mathbf{u} = \mathbf{v} - \mathbf{w}$ as an integration variable. We obtain:

$$Q_{ij} = \int d\mathbf{u}\, d\boldsymbol{\omega}\, |\mathbf{u}|\, \sigma(\mu\, |\mathbf{u}|^2/2, \mathbf{u} \cdot \boldsymbol{\omega}/|\mathbf{u}|)[f(\mathbf{v}')\, F(\mathbf{w}') - f(\mathbf{v})\, F(\mathbf{v} - \mathbf{u})] \tag{2.13}$$

where the primed variables must be expressed according to

$$\begin{aligned} \mathbf{v}' &= \mathbf{v} + \frac{M}{m + M}(|\mathbf{u}|\, \boldsymbol{\omega} - \mathbf{u}) \\ \mathbf{w}' &= \mathbf{v} - \mathbf{u} - \frac{m}{m + M}(|\mathbf{u}|\, \boldsymbol{\omega} - \mathbf{u}) \end{aligned} \tag{2.14}$$

We change again the variables by letting $\mathbf{u} = (m + M)\, \tilde{\mathbf{u}}$ and then omitting the tilda. The result reads as follows:

$$\begin{aligned} Q_{ij} = (m + M)^{d+1/2} \int & d\mathbf{u}\, d\boldsymbol{\omega}\, |\mathbf{u}|\, \sigma(mM(m + M)\, |\mathbf{u}|^2/2, \mathbf{u} \cdot \boldsymbol{\omega}/|\mathbf{u}|) \\ & \times [f(\mathbf{v} - M\mathbf{u} + M\, |\mathbf{u}|\, \boldsymbol{\omega})\, F(\mathbf{v} - M\mathbf{u} - m\, |\mathbf{u}|\, \boldsymbol{\omega}) \\ & - f(\mathbf{v})\, F(\mathbf{v} - (M + m)\, \mathbf{u})] \end{aligned} \tag{2.15}$$

In the following it will be useful, for any vector $\mathbf{u}'$, to use the following notation:

$$\begin{aligned} \Psi(\mathbf{u}, \mathbf{u}') = {} & |\mathbf{u}|\, \sigma(mM(m + M)\, |\mathbf{u}|^2/2, \mathbf{u} \cdot \mathbf{u}'/|\mathbf{u}|^2) \\ & \times [f(\mathbf{v} - M\mathbf{u} + M\mathbf{u}')\, F(\mathbf{v} - M\mathbf{u} - m\mathbf{u}') - f(\mathbf{v})\, F(\mathbf{v} - (M + m)\, \mathbf{u})] \end{aligned} \tag{2.16}$$

We have the following lemma of discrete approximation:

Lemma. Let $\Psi(\mathbf{u}, \mathbf{u}')$: $\Re^d \times \Re^d \Rightarrow \Re$ be continuous and have a compact support. Let, for any $d \geqslant 3$:

$$S_h(\Psi) = \sum_{\mathbf{n} \in \mathbf{Z}^d} h^d \frac{|\Omega_{d-1}|}{r_d(|\mathbf{n}|^2)} \sum_{|\mathbf{m}|^2 = |\mathbf{n}|^2} \Psi(\mathbf{n}h, \mathbf{m}h) \tag{2.17}$$

where $|\Omega_{d-1}|$ is the area of the unit sphere in d dimensions and $r_d(|\mathbf{n}|^2)$ denotes the number of the roots of the equation $|\mathbf{m}|^2 = |\mathbf{n}|^2$ where the vectors with integer components **m** and **n** denote, respectively an unknown and a given vector. Then

$$S_h(\Psi) \to \int d\mathbf{u}\, d\boldsymbol{\omega}\, \Psi(\mathbf{u}, |\mathbf{u}|\, \boldsymbol{\omega}) \qquad \text{as} \quad h \to 0 \tag{2.18}$$

This lemma provides the desired approximation and hence a rule to construct discrete velocity models for mixtures with arbitrarily many velocities.

We remark that the previous lemma is a slight generalization of a statement first made in ref. 13 and is related to classical problems of number theory.[14, 15] The problem is full of subtleties and one can also provide an estimate of the error in the quadrature formula given above.[9] The starting point is that any number which is not congruent to 7 (mod. 8) can be represented as a sum of three squares and the number of possible representations grows sufficiently fast with the size of the number. The main problems do not arise from numbers congruent to 7 (mod. 8) (in fact they never arise since we equate the sum of three squares to a number which is known already to be the sum of three squares) but from special sequences of the form $\{4^n m_0\}$, where m_0 is a fixed number prime with 4 and n grows; in fact for these sequences the number of roots $r_d(4^n m_0)$ grows rather slowly with n. The difficulty can be easily overcome. A key point of the proof is the strong number-theoretical result (uniform distribution of integer points on the surface of a 3D sphere) obtained by Iwaniec in 1987 (see refs. 12–15 for details).

For $d = 2$ matters are more complicated (there are much less integers which are sums of two, rather than three, squares) and the proof of the above lemma does not hold.

In the next section we shall investigate how to construct models with a small number of velocities.

3. COLLISION MODELS WITH A SMALL NUMBER OF VELOCITIES

Although we have a rule, it is not so easy to apply it to obtain models with a small number of velocities. In fact, if the number of velocities is too small we obtain models with some undesirable properties. In order to keep matters at a simple level we shall exhibit only models for binary mixtures in two dimensions.

The simplest models are given by Monaco and Preziosi in their book.[16] They are not satisfactory (as indicated by the authors [16, p. 74]), because no exchange of energy between the species occurs. It is just what we mean when we say that they are trivial.

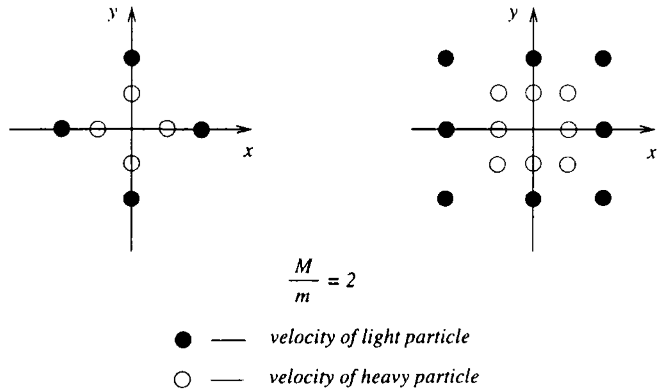

Fig. 1. The discrete velocities for the two trivial models.

The simplest model has $4+4$ velocities defined as follows:

$$\begin{aligned} &\mathbf{v}_{1,3} = \{\pm M, 0\}, \qquad \mathbf{v}_{2,4} = \{0, \pm M\} \qquad \text{(light particles)} \\ &\mathbf{w}_{1,3} = \{\pm m, 0\}, \qquad \mathbf{w}_{2,4} = \{0, \pm m\} \qquad \text{(heavy particles)} \end{aligned} \tag{3.1}$$

The next model has $8+8$ velocities and has the same drawback. The velocities are defined as follows: we take the previous $4+4$ velocities and add another set of $4+4$ velocities:

$$\begin{aligned} &\mathbf{v}_{5,6,7,8} = \{\pm M, \pm M\}, \qquad \text{(light particles)} \\ &\mathbf{w}_{5,6,7,8} = \{\pm m, \pm m\}, \qquad \text{(heavy particles)} \end{aligned} \tag{3.2}$$

where, of course, all the possible combinations of signs have to be taken. The velocities of this model are shown in Fig. 1.

In order to obtain less trivial models, we must increase the number of velocities. Hence we shall introduce two new models with $5+8$ and $9+16$ velocities, respectively. The first of these models will still have a drawback, as we shall see.

The first model is defined as follows:

(a) The heavy particles, having mass M, can possess one out of five velocities:

$$\mathbf{w}_0 = 0, \qquad \mathbf{w}_{1,3} = \{\pm 2m, 0\}, \qquad \mathbf{w}_{2,4} = \{0, \pm 2m\} \tag{3.3}$$

(b) The light particles, having mass m, can possess one out of eight velocities:

$$\begin{aligned} \mathbf{v}_{1,3} &= \{\pm(M-m), 0\}, \qquad \mathbf{v}_{2,4} = \{0, \pm(M-m)\} \\ \mathbf{v}_{5,7} &= \{\pm(M+m), 0\}, \qquad \mathbf{v}_{6,8} = \{0, \pm(M+m)\} \end{aligned} \tag{3.4}$$

The model is illustrated in Fig. 2. All the Broadwell-type collisions between identical particles with the same speed are permitted. Moreover, the following nontrivial collisions (with the scattering angle $\Theta = \pi$) are possible:

$$\begin{aligned} (\mathbf{w}_0, \mathbf{v}_5) &\leftrightarrow (\mathbf{w}_1, \mathbf{v}_3), \qquad (\mathbf{w}_0, \mathbf{v}_6) \leftrightarrow (\mathbf{w}_2, \mathbf{v}_4) \\ (\mathbf{w}_0, \mathbf{v}_7) &\leftrightarrow (\mathbf{w}_3, \mathbf{v}_1), \qquad (\mathbf{w}_0, \mathbf{v}_8) \leftrightarrow (\mathbf{w}_4, \mathbf{v}_2) \end{aligned} \tag{3.5}$$

A clear drawback of this model is that it becomes "unreasonable" in the limiting case of two non-interacting species. In this limit one expects the model to tend to two independent "reasonable" DVM for each component of the binary mixture. Yet these DVM are unsatisfactory because we obtain two independent Broadwell models (with velocities $\{\mathbf{v}_i\}$ and $\{\mathbf{v}_{i+4}\}$, $i = 1,..., 4$) for light particles, and the Broadwell model (with velocities $\{\mathbf{w}_i\}$, $i = 1,..., 4$, plus the non-interacting particles with velocity $\{\mathbf{w}_0\}$) for heavy particles.

Because of the above unsatisfactory feature, we introduce a second nontrivial model, which is free from this drawback. The main idea behind it is to allow some new collisions between the identical particles of the previous model, with the consequence of constructing a "reasonable" model for each component of the mixture even in the limiting case discussed

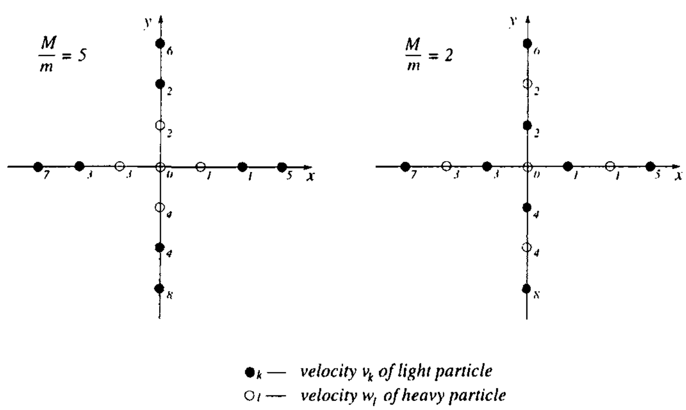

Fig. 2. The discrete velocities for the first nontrivial model.

above. A price to be paid for this improvement is that the new model has $9+16$ velocities.

The new model is defined as follows:

(a) The heavy particles, having mass M, can possess one out of nine velocities, 5 of which are the five velocities of the previous model. The new velocities are:

$$\mathbf{w}_{5,7} = \pm\{m, m\}, \qquad \mathbf{w}_{6,8} = \pm\{-m, m\} \tag{3.6}$$

The new velocities are the result of the following collisions (with scattering angle $\Theta = \pi/2$):

$$(\mathbf{w}_0, \mathbf{w}_1) \leftrightarrow (\mathbf{w}_5, \mathbf{w}_8), \ldots \tag{3.7}$$

(b) The light particles, having mass m, can possess one out of sixteen velocities, 5 of which are the five velocities of the previous model. The new velocities are:

$$\begin{aligned} \mathbf{v}_{9,11} &= \pm\{M, m\}, \qquad & \mathbf{v}_{10,12} &= \pm\{-m, M\} \\ \mathbf{v}_{13,15} &= \pm\{M, -m\}, \qquad & \mathbf{v}_{14,16} &= \pm\{m, M\} \end{aligned} \tag{3.8}$$

The new velocities are the result of the following collisions (with scattering angle $\Theta = \pi/2$):

$$(\mathbf{v}_1, \mathbf{v}_5) \leftrightarrow (\mathbf{v}_9, \mathbf{v}_{13}), \ldots \tag{3.9}$$

The model is illustrated in Fig. 3. This model is more complicated, but rather rich (many collisions are possible) and much mote realistic. The following nontrivial collisions between non-identical particles are possible:

$$\begin{aligned} &(\mathbf{w}_0, \mathbf{v}_5) \leftrightarrow (\mathbf{w}_1, \mathbf{v}_3) \leftrightarrow (\mathbf{w}_5, \mathbf{v}_{12}) \leftrightarrow (\mathbf{w}_8, \mathbf{v}_{14}) \\ &(\mathbf{w}_0, \mathbf{v}_6) \leftrightarrow (\mathbf{w}_2, \mathbf{v}_4) \leftrightarrow (\mathbf{w}_5, \mathbf{v}_{15}) \leftrightarrow (\mathbf{w}_6, \mathbf{v}_9) \\ &(\mathbf{w}_0, \mathbf{v}_7) \leftrightarrow (\mathbf{w}_3, \mathbf{v}_1) \leftrightarrow (\mathbf{w}_7, \mathbf{v}_{10}) \leftrightarrow (\mathbf{w}_6, \mathbf{v}_{16}) \\ &(\mathbf{w}_0, \mathbf{v}_8) \leftrightarrow (\mathbf{w}_4, \mathbf{v}_2) \leftrightarrow (\mathbf{w}_7, \mathbf{v}_{13}) \leftrightarrow (\mathbf{w}_8, \mathbf{v}_{11}) \end{aligned} \tag{3.10}$$

Remark. A general rule for selecting these collisions is very simple: two non-identical particles with velocities $\mathbf{v}$ (light species) and $\mathbf{w}$ (heavy species) can collide if and only if

$$\mathbf{u} = \mathbf{v} - \mathbf{w} = \pm(M+m, 0) \qquad \text{or} \qquad \mathbf{u} = \pm(0, M+m) \tag{3.11}$$

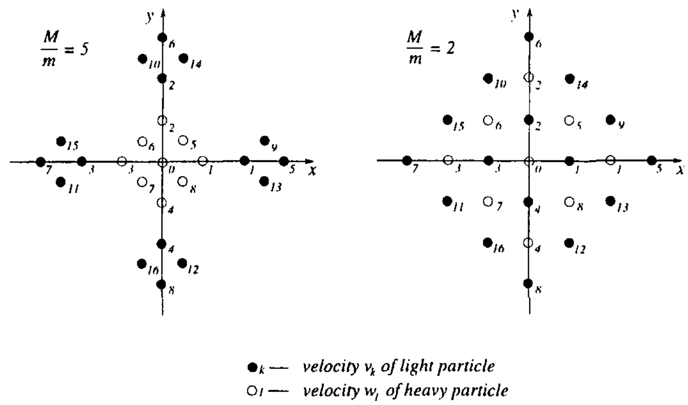

Fig. 3. The discrete velocities for the second nontrivial model.

It is clear from Fig. 3 that for each $\mathbf{v}$ there is one and only one value $\mathbf{w}$ which can permit a collision. As for heavy particles with velocity $\mathbf{w}_i$ ($i = 1,\ldots, 8$), there exists just one possibility for $i = 1, 2, 3, 4$, two possibilities for $i = 5, 6, 7, 8$ and four possibilities for $i = 0$.

We remark that there are two kinds of collisions between non-identical particles. Thus $(\mathbf{w}_0, \mathbf{v}_5) \leftrightarrow (\mathbf{w}_1, \mathbf{v}_3)$ corresponds to the scattering angle $\Theta = \pi$, whilst $(\mathbf{w}_0, \mathbf{v}_5) \leftrightarrow (\mathbf{w}_5, \mathbf{v}_{12})$ and $(\mathbf{w}_0, \mathbf{v}_5) \leftrightarrow (\mathbf{w}_8, \mathbf{v}_{14})$ correspond to $\Theta = \pi/2$. Generally speaking, we should prescribe two different cross sections, say $\sigma_{\parallel}$ $(\Theta = \pi)$ and $\sigma_{\perp}$ $(\Theta = \pi/2)$, to the two kinds of collisions. As we already mentioned, $|\mathbf{v}_i - \mathbf{w}_k| = M + m = \text{const.}$ for any colliding pair $(\mathbf{v}_i, \mathbf{w}_k)$; hence the two constants $\sigma_{\parallel}$ and $\sigma_{\perp}$ define completely the DVM related to collisions between different species.

There are also many new possible collisions (in comparison with the previous model) between identical particles. All these collisions correspond to $\Theta = \pi/2$ ($\Theta = \pi$ is equivalent to $\Theta = 0$ for identical particles). Hence the cross sections may only depend on the relative speed. We shall now briefly list all the possible collisions between identical particles. As before we denote by $|\mathbf{u}| = |\mathbf{v}_i - \mathbf{v}_k|$ (light particles) and $|\mathbf{u}| = |\mathbf{w}_i - \mathbf{w}_k|$ (heavy particles) the relative speed. We assume, of course that the corresponding cross-sections $\sigma_{mm}(|\mathbf{u}|)$ and $\sigma_{MM}(|\mathbf{u}|)$ are given. Here is the list:

1. Light particles.

   (a) Collisions of the Broadwell-type:

$$
\begin{aligned}
|\mathbf{u}| &= 2(M - m), \qquad (\mathbf{v}_1, \mathbf{v}_3) \leftrightarrow (\mathbf{v}_2, \mathbf{v}_4) \\
|\mathbf{u}| &= 2(M + m), \qquad (\mathbf{v}_5, \mathbf{v}_7) \leftrightarrow (\mathbf{v}_6, \mathbf{v}_8)
\end{aligned}
\tag{3.12}
$$

(b)

$$|\mathbf{u}| = 2m, \quad (\mathbf{v}_1, \mathbf{v}_5) \leftrightarrow (\mathbf{v}_9, \mathbf{v}_{13}), \quad (\mathbf{v}_2, \mathbf{v}_6) \leftrightarrow (\mathbf{v}_{10}, \mathbf{v}_{14})$$
$$(\mathbf{v}_3, \mathbf{v}_7) \leftrightarrow (\mathbf{v}_{11}, \mathbf{v}_{15}), \quad (\mathbf{v}_4, \mathbf{v}_8) \leftrightarrow (\mathbf{v}_{12}, \mathbf{v}_{16}) \tag{3.13}$$

(c)

$$|\mathbf{u}| = 2M, \quad (\mathbf{v}_1, \mathbf{v}_7) \leftrightarrow (\mathbf{v}_{10}, \mathbf{v}_{16}), \quad (\mathbf{v}_3, \mathbf{v}_5) \leftrightarrow (\mathbf{v}_{12}, \mathbf{v}_{14})$$
$$(\mathbf{v}_9, \mathbf{v}_{15}) \leftrightarrow (\mathbf{v}_4, \mathbf{v}_6), \quad (\mathbf{v}_2, \mathbf{v}_8) \leftrightarrow (\mathbf{v}_{11}, \mathbf{v}_{13}) \tag{3.14}$$

1. Heavy particles.

(a) Collisions of the Broadwell-type:

$$|\mathbf{u}| = 2\sqrt{2}\, m, \quad (\mathbf{w}_5, \mathbf{w}_7) \leftrightarrow (\mathbf{w}_6, \mathbf{w}_8)$$
$$|\mathbf{u}| = 4m, \quad (\mathbf{w}_1, \mathbf{w}_3) \leftrightarrow (\mathbf{w}_2, \mathbf{w}_4) \tag{3.15}$$

(b)

$$|\mathbf{u}| = 2m, \quad (\mathbf{w}_0, \mathbf{w}_1) \leftrightarrow (\mathbf{w}_5, \mathbf{w}_8), \quad (\mathbf{w}_0, \mathbf{w}_2) \leftrightarrow (\mathbf{w}_5, \mathbf{w}_6)$$
$$(\mathbf{w}_0, \mathbf{w}_3) \leftrightarrow (\mathbf{w}_6, \mathbf{w}_7), \quad (\mathbf{w}_0, \mathbf{w}_4) \leftrightarrow (\mathbf{w}_7, \mathbf{w}_8) \tag{3.16}$$

4. KINETIC EQUATIONS AND COLLISION TERMS

In this section we shall briefly describe the equations for the second non-trivial model (which includes the first one as a limiting case). Let f_i ($i = 1,..., 16$) and F_k ($k = 0, 1,..., 9$) denote the distribution functions of the light and heavy particles, respectively.

Then we can write the Boltzmann equations for a binary mixture in the following form:

$$\partial f_i/\partial t + \mathbf{v}_i \cdot \partial f_i/\partial \mathbf{x} = I_i + S_i, \qquad i = 1,..., 16$$
$$\partial F_k/\partial t + \mathbf{v}_k \cdot \partial F_k/\partial \mathbf{x} = Q_k + R_k, \qquad k = 0,..., 8 \tag{3.17}$$

where I_i, Q_k and S_i, R_k correspond to collisions of identical and non-identical particles, respectively. First, we put:

$$g_{\|} = (M + m)\,\sigma_{\|}, \qquad g_{\perp} = (M + m)\,\sigma_{\perp} \tag{3.18}$$

and discuss the structure of the "mixed" collision terms S_i and R_k. Our models are obviously symmetric under the symmetry transformations

$$(x, y) \Leftrightarrow (y, x), \qquad (x, y) \Leftrightarrow (-x, y), \qquad (x, y) \Leftrightarrow (x, -y) \tag{3.19}$$

with corresponding permutations of indices i and k (see Figs. 2 and 3). Therefore, it is sufficient to consider just a few essentially different cases, say $i = 1, 5, 9$ and $k = 0, 1, 5$ (see Figs. 2 and 3). In all cases we can write:

$$S_i = g_{\|} S_i^{(1)} + g_{\perp} S_i^{(2)}, \qquad R_k = g_{\|} R_k^{(1)} + g_{\perp} R_k^{(2)} \tag{3.20}$$

Then, glancing at the list of possible collisions (Eq. (3.10)), we easily obtain:

$$\begin{aligned}
&S_1^{(1)} = f_7 F_0 - f_1 F_3, \qquad S_1^{(2)} = f_{10} F_7 + f_{16} F_6 - 2f_1 F_3 \\
&S_5^{(1)} = f_3 F_1 - f_5 F_0, \qquad S_5^{(2)} = f_{12} F_5 + f_{14} F_8 - 2f_5 F_0 \\
&S_9^{(1)} = f_{15} F_5 - f_9 F_6, \qquad S_9^{(2)} = f_6 F_0 + f_4 F_2 - 2f_9 F_6 \\
&R_0^{(1)} = f_3 F_1 + f_4 F_2 + f_1 F_3 + f_2 F_4 - (f_5 + f_6 + f_7 + f_8) F_0 \\
&R_0^{(2)} = f_{12} F_5 + f_{14} F_8 + f_{15} F_5 + f_9 F_6 + f_{10} F_7 + f_{16} F_6 + f_{13} F_7 \\
&\qquad + f_{11} F_8 - 2(f_5 + f_6 + f_7 + f_8) F_0 \\
&R_1^{(1)} = f_5 F_0 - f_3 F_1, \qquad R_1^{(2)} = f_{12} F_5 + f_{14} F_8 - 2f_3 F_1 \\
&R_5^{(1)} = f_{14} F_8 + f_9 F_6 - (f_{12} + f_{15}) F_5 \\
&R_5^{(2)} = f_5 F_0 + f_3 F_1 + f_6 F_0 + \bar{f}_4 F_2 - 2(f_{12} + f_{15}) F_5
\end{aligned} \tag{3.21}$$

Let us examine, now, the collision terms I_i and Q_k corresponding to the same values of i and k considered for the "mixed" collisions (i.e., $i = 1, 5, 9$ and $k = 0, 1, 5$). To this goal we introduce the following notations for the collision frequencies:

$$\begin{gathered}
a_{\pm} = 2(M \pm m)\, \sigma_{mm}(2(M \pm m)) \\
b = 2m\sigma_{mm}(2m), \qquad c = 2M\sigma_{mm}(2M) \\
A = 4m\sigma_{MM}(4m), \qquad B = 2\sqrt{2}\, m\sigma_{MM}(2\sqrt{2}\, m) \\
C = 2m\sigma_{MM}(2m)
\end{gathered} \tag{3.22}$$

Then we obtain

$$\begin{aligned} I_i &= a_+ I_i^+ + a_- I_i^- + b I_i^{(1)} + c I_i^{(2)} \qquad & i &= 1,\ldots, 16 \\ Q_k &= A Q_k^{(1)} + B Q_k^{(2)} + C Q_k^{(3)} & k &= 0,\ldots, 9 \end{aligned} \tag{3.23}$$

where (for $i = 1, 5, 9$ and $k = 0, 1, 5$)

$$\begin{gathered} I_1^+ = 0, \quad I_1^- = f_2 f_4 - f_1 f_3, \quad I_1^{(1)} = f_9 f_{13} - f_1 f_5, \quad I_1^{(2)} = f_{10} f_{16} - f_1 f_7 \\ I_5^+ = f_6 f_8 - f_5 f_7, \quad I_5^- = 0, \quad I_5^{(1)} = f_9 f_{13} - f_1 f_5, \quad I_5^{(2)} = f_{13} f_{14} - f_3 f_5 \\ I_9^+ = I_9^- = 0, \quad I_9^{(1)} = f_1 f_5 - f_9 f_{13}, \quad I_9^{(2)} = f_4 f_6 - f_9 f_{15} \\ Q_0^{(1)} = Q_0^{(2)} = 0, \quad Q_0^{(3)} = (F_6 + F_8)(F_5 + F_7) - F_0(F_5 + F_6 + F_7 + F_8) \\ Q_1^{(1)} = F_2 F_4 - F_1 F_3, \quad Q_1^{(2)} = 0, \quad Q_1^{(3)} = F_5 F_8 - F_0 F_1 \\ Q_5^{(1)} = 0, \quad Q_5^{(2)} = F_6 F_8 - F_5 F_7 \quad Q_5^{(3)} = F_0(F_1 + F_2) - F_5(F_6 + F_8) \end{gathered} \tag{3.24}$$

Any other collision term (for $i \neq 1, 5, 9$ and $k \neq 0, 1, 5$) in the system of Boltzmann equations can be easily obtained from the terms listed above through a symmetry transformation.

This concludes the discussion of the second non-trivial term introduced in this paper. The first, simpler model can be obtained as a limiting case by letting:

$$\begin{gathered} g_\perp = 0, \qquad b = c = B = C = 0 \\ f_i = 0 \quad \text{for } i = 9,\ldots, 16, \qquad F_k = 0 \quad \text{for } k = 5,\ldots, 8 \end{gathered} \tag{3.25}$$

It is clear that the second model can be extended by adding new velocities appearing as a result of new collisions between particles of this model (with scattering angle $\Theta = \pi$ and $\Theta = \pi/2$). Following this procedure, we can construct a sequence of DVM which consistently approach (the proof is very

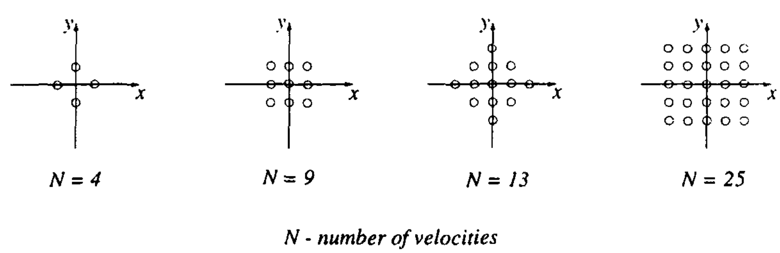

Fig. 4. Sequence of DVM for a simple gas.

easy in this case) a continuous model, i.e., a system of Boltzmann equations. The differential cross section will have the very particular form:

$$\sigma(u, \Theta) = \sigma_{\|}(u)\, \delta(\Theta - \pi) + \sigma_{\perp}(u)\, \delta(\Theta - \pi/2) \tag{3.26}$$

As an example of such sequence, we show in Fig. 4 the sequence of the sets of velocities corresponding to a single gas (in which case we can always put $\sigma_{\|}(u) = 0$).

5. CONCLUDING REMARKS

We have shown that the procedure used to approximate the Boltzmann equation for a simple gas by DVM can be extended to mixtures. In addition to giving a general procedure, we have studied in some detail a few models with a small number of velocities. This part of the paper may perhaps be looked upon as superfluous. This is not our opinion; in fact no models (except trivial ones) have appeared before and our detailed treatment shows that this lack of models in the literature is due to the fact that one must go as far as 25 ($= 9 + 16$) velocities in order to obtain a satisfactory, simple model. This model has clearly several limitations and should not be taken as typical of the large class of models which have been introduced in Section 2.

The renewed interest for DVM and their potential use as tools to produce approximate solutions to the Boltzmann equation makes it necessary to cover the area of mixtures as well. We remark that a byproduct of this paper is the possibility of showing that the coefficient of $|\mathbf{v}|^2$ in the exponent of the discrete Maxwellian must be a function of the absolute temperature multiplied by the molecular mass. In fact, we can introduce the "discrete Maxwellians," which are of the form $\exp(\psi)$ where ψ is any collision invariant. If the only collision invariants for a single gas are the classical ones (i.e., if the model is normal[17]), then the discrete Maxwellian are exponentials of a second degree polynomial in $\mathbf{v}$ and can be written as the usual Maxwellians. When we consider a nontrivial model for a mixture of normal discrete gases, then equilibrium can be attained if and only if the coefficients of the second and first degree terms in the Maxwellians of each gas are in the same ratio as their masses (because of conservation of mass and momentum). In particular if the mixture is at rest just the coefficients of the second degree terms count and the only macroscopic parameter which must be equal for the two gases is temperature and the statement above follows. Thus the proof of this basic fact can be carried out within discrete kinetic theory without the necessity of resorting to a general argument of equilibrium statistical mechanics as done in ref. 10.

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