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Construction of Discrete Kinetic Models with Given Invariants

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Abstract We consider the general problem of the construction of discrete kinetic models (DKMs) with given conservation laws. This problem was first stated by Gatignol in connection with discrete models of the Boltzmann equation (BE) and it has been addressed in the last decade by several authors. Even though a practical criterion for the non-existence of spurious conservation laws has been devised, and a method for enlarging existing physical models by new velocity points without adding non-physical invariants has been proposed, a general algorithm for the construction of all normal (physical) discrete models with assigned conservation laws, in any dimension and for any number of points, is still lacking in the literature. We introduce the most general class of discrete kinetic models and obtain a general method for the construction and classification of normal DKMs. In particular, it is proved that for any given dimension $d \geq 2$ and for any sufficiently large number N of velocities (for example, $N \geq 6$ for the planar case $d = 2$) there exists just a finite number of distinct classes of DKMs. We apply the general method in the particular cases of discrete velocity models (DVMs) of the inelastic BE and elastic BE. Using our general approach to DKMs and our results on normal DVMs for a single gas, we develop a method for the construction of the most natural (from physical point of view) subclass of normal DVMs for binary gas mixtures. We call such models supernormal models (SNMs) (they have the property that by isolating the velocities of single gases involved in the mixture, we also obtain normal DVMs).

Keywords Boltzmann equation · Discrete kinetic models · Conservation laws · Collision invariants

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1 Introduction

The main objective of this paper is to develop a very general approach to the problem of the description of *all* distinct classes of normal discrete kinetic models with given conservation laws. The word *normal*, introduced by Cercignani in [8], means the absence of other (spurious) conservation laws.

This problem was first stated by Gatignol [13] in connection with discrete models of the Boltzmann equation (BE), when it became clear that the velocity discretization can lead to equations with spurious conservation laws (non-physical conservation laws). In many papers on DVMs authors postulate from the beginning that a finite velocity space with "good" properties (representing a normal model) is given, and only after this step they study the discrete BE. Our aim is not to study the equations for DVMs, but to discuss all possible choices of finite sets satisfying this type of "good" restrictions.

Even though a practical criterion for the non-existence of spurious conservation laws has been devised [17], and a method for enlarging existing physical models by new velocity points without adding non-physical invariants has been proposed [5], a general algorithm for the construction of all normal (physical) discrete models with assigned conservation laws, in any dimension and for any number of points, is still lacking in the literature. We introduce in this paper the most general class of discrete kinetic models and obtain a general method for the construction and classification of normal DKMs and apply the general method in the particular cases of discrete velocity models (DVMs) of the inelastic BE and elastic BE. We also develop a method for the construction of the most natural (from physical point of view) subclass of normal DVMs for binary gas mixtures, which we call supernormal models (SNMs).

The general discrete velocity model (DVM) of the Boltzmann equation reads [6, 13]

$$\left(\frac{\partial}{\partial t}+\mathbf{v}_i\cdot\frac{\partial}{\partial \mathbf{x}}\right) f_i(\mathbf{x},t)=Q_i(f)=Q_i(f_1,\ldots,f_n),\quad i=1,\ldots,n, \tag{1}$$

where $\mathbf{x}\in\mathbb{R}^d$ and $t\in\mathbb{R}_+$ denote the position and the time respectively, and $\{\mathbf{v}_1,\ldots,\mathbf{v}_n\}\subset\mathbb{R}^d$ denotes a set of velocities of the model.

The functions $f_i(\mathbf{x},t)$ are understood as spatial densities of particles having velocities $\mathbf{v}_i\in\mathbb{R}^d$, usually $d=2,3$ in applications.

The collision operators $Q_i(f)$ in (1) are given by

$$Q_i(f)=\sum_{j,k,l=1}^{n}\Gamma_{ij}^{kl}(f_kf_l-f_if_j)\quad\text{for } i=1,\ldots,n, \tag{2}$$

such that the collision coefficients Γ_{ij}^{kl}, $1\le i,j,k,l\le n$, satisfy the relations

$$\Gamma_{ij}^{kl}=\Gamma_{ji}^{kl}=\Gamma_{kl}^{ij}\ge 0, \tag{3}$$

with equality unless the conservation laws

$$\mathbf{v}_i+\mathbf{v}_j=\mathbf{v}_k+\mathbf{v}_l,\qquad |\mathbf{v}_i|^2+|\mathbf{v}_j|^2=|\mathbf{v}_k|^2+|\mathbf{v}_l|^2 \tag{4}$$

are satisfied. DVM (1), (2) is called "normal" if any solution of the equations

$$\boldsymbol{\Psi}(\mathbf{v}_i)+\boldsymbol{\Psi}(\mathbf{v}_j)=\boldsymbol{\Psi}(\mathbf{v}_k)+\boldsymbol{\Psi}(\mathbf{v}_l), \tag{5}$$

where indexes $(i, j; k, l)$ take all possible values satisfying (4), is given by

$$\Psi(\mathbf{v}) = a + \mathbf{b} \cdot \mathbf{v} + c|\mathbf{v}|^2 \tag{6}$$

for some constants $a, c \in \mathbb{R}$ and $\mathbf{b} \in \mathbb{R}^d$.

The "*normality*" of DVMs is a very important condition (similar to the condition of uniqueness of collision invariants for the Boltzmann equation [1, 2, 7]). Such a condition is usually assumed in most of the mathematical papers on DVMs (see for review [6, 15]).

On the other hand, it is not easy to construct a normal d-dimensional DVM (to be more precise, its set of velocities $\{\mathbf{v}_1, \ldots, \mathbf{v}_n\} \subset \mathbb{R}^d$, such that any conservation law (5) is given by (6). This problem appeared already at the early stage of the development of the mathematical theory of DVMs [13] and still remains, generally speaking, unsolved. One can easily find an actual number of invariants (vectors of conservation laws) for any given DVM by using the method proposed in [17]. However the general problem "*How to construct DVMs without non-physical invariants?*" remains open (especially for more general discrete kinetic models related to gases with internal degrees of freedom, mixtures, chemically reacting gases, etc.). To our knowledge there was just one particular method to do this. The method was proposed in [5] (see also [16]). Many new DVMs were obtained by the inductive method in the last years [11, 16]. On the other hand, this is just a particular method that does not answer many questions. For example, before this work it was still unclear whether or not the conjecture that all normal DVMs with a given number n of velocities can be obtained by the inductive approach is true. We shall see below that the answer is negative.

The paper is organized as follows. We introduce in Sect. 2 the most general class of discrete kinetic models (in the spatially homogeneous case that is sufficient for our goals). Then we discuss the structure of invariant subspaces of such models and show that the number of invariant subspaces is always finite (Lemma 2). The problem of the construction of all models with given conservation laws is reduced to an equation for the phase set of the model in Sect. 3 (Theorem 1). Applications of the general theory to DVMs of the Boltzmann equation are given in Sect. 4. We describe all normal plane DVMs with small number $n \leq 9$ of velocities (Figs. 2–6). Section 5 is devoted to DVMs with inelastic collisions (without energy conservation). In this case all normal DVMs can be described explicitly. Section 6 is devoted to normal DVMs for mixtures. Using our general approach to DKMs and our results on normal DVMs for a single gas, we develop a method for the construction of the most natural (from physical point of view) subclass of normal DVMs for binary gas mixtures. We call such models supernormal (SNMs). We discuss in detail a geometrical interpretation of plane DVMs for mixtures. Then, we give the definition of SNMs. In Sect. 7 we derive a general method for the construction of such models and give some examples.

In [18] we applied this method and obtained SNMs up to 20 velocities and their spectrum of mass ratio.

2 Discrete Kinetic Models

The most general spatially homogeneous Discrete Kinetic Model (DKM) can be described in the following way. We consider an asymptotically large number N of particles and assume that each particle occupies one of n distinct phase states $\mathbf{z}_i \in \mathbb{R}^d$, $i = 1, \ldots, n$.

We fix the phase set

$$Z = \{\mathbf{z}_1, \ldots, \mathbf{z}_n\} \subset \mathbb{R}^d \tag{7}$$

and describe the state of the N-particle system by a vector $\boldsymbol{\rho}$ of *occupation numbers*.

$$\boldsymbol{\rho} = (N_1, \ldots, N_n), \quad N_1 + \cdots + N_n = N, \tag{8}$$

such that N_i is the number of particles occupying the phase state $\mathbf{z}_i$ $(i = 1, \ldots, n)$. We do not assume that all particles are identical. Therefore the numeration of the phase states is fixed.

A stochastic dynamics of the multi-particle system is defined as follows: at any time instant $t \geq 0$ the system may undergo, with certain probability $dW_s(t) = p_s dt, s = 1, \ldots, m$, one of m elementary reactions ("jumps"). This can be written as a transition from a pre-reaction state $\boldsymbol{\rho}$ (8) to a new state $\boldsymbol{\rho}^{(s)} (s = 1, \ldots, m)$

$$\boldsymbol{\rho} \to \boldsymbol{\rho}^{(s)} = (N_1^{(s)}, \ldots, N_n^{(s)}), \quad N_1^{(s)} + \cdots + N_n^{(s)} = N^{(s)}, \tag{9}$$

where, generally speaking, $N^{(s)} \neq N$.

It is convenient to introduce m vectors

$$\boldsymbol{\theta}_s = \boldsymbol{\rho} - \boldsymbol{\rho}^{(s)} = (k_1^{(s)}, \ldots, k_n^{(s)}), \quad s = 1, \ldots, m, \tag{10}$$

with integer components $k_i^{(s)}$ and call them "vectors of reactions" (similar vectors were introduced in [17] for DVMs of the Boltzmann equation).

Let us assume that the total "set of reactions" of the model

$$\Lambda = \{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_m\} \subseteq \Theta \subseteq \mathbb{Z}^n \tag{11}$$

is fixed. Then it is clear that the Markovian dynamics of the model is uniquely defined by the set of reactions Λ (11) and the set of probabilities (frequencies) $\{p_1, \ldots, p_m\}$ of the reactions $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_m$.

The time-dependent state of the multi-particle system is given by

$$\boldsymbol{\rho}(t) = (N_1(t), \ldots, N_n(t)), \quad t \geq 0. \tag{12}$$

Definition 1 A *linear conservation law* of a DKM is defined by a linear functional $l[\boldsymbol{\rho}]$ $(l : \mathbb{R}^n \to \mathbb{R})$, such that $l[\boldsymbol{\rho}] = \text{const.}$ (independent of t).

Then there exists a unique vector $\mathbf{u} \in \mathbb{R}^n$ (a *vector of conservation law* or equivalently, an *invariant*) such that

$$l[\boldsymbol{\rho}] = \mathbf{u} \cdot \boldsymbol{\rho} = \sum_{i=1}^{n} N_i u_i, \quad \mathbf{u} = (u_1, \ldots, u_n),$$

where "$\cdot$" denotes the usual scalar product in $\mathbb{R}^n$. Assuming that the set Λ (11) is given, we obtain the following result.

Lemma 1 *A vector* $\mathbf{u} \in \mathbb{R}^n$ *is a vector of a conservation law* (*an invariant*) *if and only if* $\mathbf{u} \cdot \boldsymbol{\theta}_s = 0$ *for all* $\boldsymbol{\theta}_s \in \Lambda$.

Now we can easily describe the total set of linear (independent of $\boldsymbol{\rho}$) conservation laws of a DKM with a given set of reactions Λ. We introduce a *space of reactions*

$$L = \text{Span}\, \Lambda = \text{Span}\{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_m\} \tag{13}$$

and its orthogonal complement in $\mathbb{R}^n$

$$U = L^{\perp}, \quad L \oplus U = \mathbb{R}^n. \tag{14}$$

The following statement follows directly from Lemma 1.

Corollary 1 *Any vector* $\mathbf{u} \in U$ *is a vector of conservation law for a DKM with a given set of reactions* Λ. *The number* p *of linearly independent conservation laws is given by the equality*

$$p = \dim U = n - \dim L. \tag{15}$$

The important conclusion is that all conservation laws of a given DKM are uniquely defined by its set of reactions (11) and form a linear subspace $U \subset \mathbb{R}^n$ (an orthogonal complement to the space of reactions $L = \operatorname{Span} \Lambda$).

Definition 2 The subspace U defined by (13), (14) is said to be the *invariant subspace* of the DKM (with given Λ). The number $p = \dim \Lambda$ is called the *number of conservation laws*.

In applications we usually know in advance the maximal set $\Theta \subset \mathbb{Z}^n$ of reactions (consider, for example, pair collisions that preserve the total number of particles). Moreover, the set Θ is finite for finite n. Then we can prove the following.

Lemma 2 *If two numbers* $n \geq 2$, $1 \leq p \leq n-1$, *and the maximal set* Θ *of reactions* (*a finite subset of* $\mathbb{Z}^n$) *are given, then there exists at most finitely many distinct* p*-dimensional invariant subspaces* $\{U_i, i = 1, \ldots, N(n, p; \Theta)\}$ *of corresponding DKMs having exactly* p *linearly independent invariants.*

Proof Any such DKM with the phase set (7) has a certain set Λ (11) of reactions containing exactly $(n-p)$ linearly independent vectors $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_{n-p} \in \Theta$. Then $U = L^{\perp}$, where $L = \operatorname{Span}\{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_{n-p}\}$ in accordance with (13), (14). On the other hand, the set Θ is finite by the assumptions of the lemma. Therefore it can not have more than a finite number of distinct subsets with $(n-p)$ pairwise different elements. This completes the proof. □

3 Normal DKMs with Given Invariants

We assume below that the conditions of Lemma 2 are fulfilled and we fix two natural numbers n, p and a finite set $\Theta \subset \mathbb{Z}^n$. Then we consider a d-dimensional DKM. Its phase set Z (7) is an element of the space

$$Q = \underbrace{\mathbb{R}^d \times \ldots \times \mathbb{R}^d}_{n}. \tag{16}$$

The basic conservation laws of the model (as functions of Z) are assumed to be known in advance.

We introduce p vector functions $\{\mathbf{u}_\alpha : Q \to \mathbb{R}^n, \alpha = 1, \ldots, p\}$ and call them *given invariants*. Then the total set Λ (11) of reactions of the model is a subset $\Lambda(Z)$ of the set

$$\Lambda_*(Z) = \{\boldsymbol{\theta} \in \Theta : \boldsymbol{\theta} \cdot \mathbf{u}_\alpha(Z) = 0, \ \alpha = 1, \ldots, p\}. \tag{17}$$

This means that only the reactions satisfying the basic conservation laws are allowed. We do not assume that $\Lambda(Z) = \Lambda_*(Z)$ since there can also be other restrictions on $\Lambda(Z)$ (not related to the conservation laws).

We denote such DKMs by $\{Z, \Lambda(Z)\}$. The model is uniquely determined by its phase set $Z \in Q$ (in the case when $\Lambda(Z) \neq \Lambda_*(Z)$, one uses the given "other restrictions" to determine $\Lambda(Z)$ from $\Lambda_*(Z)$).

Definition 3 A DKM $\{Z, \Lambda(Z)\}$ with given invariants $\{\mathbf{u}_\alpha : Q \to \mathbb{R}^n, \alpha = 1, \ldots, p\}$ is said to be *non-degenerate* if the vectors $\{\mathbf{u}_\alpha(Z), \alpha = 1, \ldots, p\}$ are linearly independent. Otherwise it is called *degenerate*.

Definition 4 A non-degenerate DKM $\{Z, \Lambda(Z)\}$ is said to be *normal* if it has exactly p linearly independent invariants.

We introduce the space of invariants (see Definition 2)

$$U(Z) = \mathrm{Span}\{\mathbf{u}_\alpha(Z),\ \alpha = 1, \ldots, p\}, \quad Z \in Q, \tag{18}$$

and partition all normal models into equivalent classes.

Definition 5 Two normal models $\{Z_i, \Lambda(Z_i)\}$, $i = 1, 2$ are said to be *equivalent* if $U(Z_1) = U(Z_2)$.

We can now formulate the final result related to the *classification of normal DKMs with given invariants (conservation laws)*.

Theorem 1 *We assume that the following data are given*:

(A) *three natural numbers* (n, p, d), $n \geq p + 1$;
(B) *a maximal (finite) set of reactions* $\Theta \subset \mathbb{Z}^n$;
(C) p *linearly independent invariants* $\{\mathbf{u}_\alpha : Q \to \mathbb{R}^n,\ \alpha = 1, \ldots, p\}$, *with* Q *from* (16).

Then there exists at most a finite number of distinct equivalent classes of normal DKMs with given invariants. Each such class is uniquely determined by the equation for the phase set $Z \in Q$

$$U(Z) = U, \tag{19}$$

where U *is one of the* N *distinct invariant subspaces defined in Lemma* 2, *and* $U(Z)$ *is defined in* (18).

Proof Two distinct classes of normal models can not have identical subspaces $U(Z)$ (18). On the other hand, all $N(n, p; \Theta)$ possible (under conditions (A), (B)) p-dimensional invariant subspaces are defined in Lemma 2. Hence, we obtain (19) and this completes the proof. □

The theorem reduces the problem of the construction and the classification of all normal DKMs to a solution of (19). The solvability of this equation is not enough in order to construct a normal DKM. We need the extra condition that the model has exactly n distinct phase points. For this we introduce the following definition.

Definition 6 The set Λ of m linearly independent vectors is said to be *well-defined* if $\mathbf{e}_k - \mathbf{e}_l \notin \operatorname{Span}\Lambda$, $1 \le k < l \le n$, for any pair of standard unit vectors in $\mathbb{R}^n$,

$$e_i = (0, \ldots, \underbrace{1}_{i}, \ldots, 0), \quad i = 1, \ldots, n.$$

Lemma 3 *The condition $\mathbf{z}_k \neq \mathbf{z}_l$ for $k \neq l$ is fulfilled for all $\mathbf{z}_i \in Z$, $i = 1, \ldots, n$, if the set of reaction Λ is well-defined.*

Proof Suppose that Λ is well-defined and let $\mathbf{z}_k = \mathbf{z}_l$, for $k \neq l$. Then $\mathbf{u}_\alpha(\mathbf{z}_k) = \mathbf{u}_\alpha(\mathbf{z}_l)$ for all $\alpha = 1, \ldots, p$ and moreover

$$\mathbf{u}_\alpha(Z) \cdot (\mathbf{e}_k - \mathbf{e}_l) = 0, \quad \alpha = 1, \ldots, p,$$

where dot denotes the usual scalar product in $\mathbb{R}^n$. Hence,

$$\mathbf{e}_k - \mathbf{e}_l \in L = \operatorname{Span}\Lambda, \qquad L^\perp = U(Z)$$

and the supposition is false. This completes the proof. □

The *general algorithm for the construction of all distinct normal DKMs* $\{Z, \Lambda(Z)\}$ with given numbers (n, d, p), given invariants $\mathbf{u}_\alpha(Z) \in \mathbb{R}^n$, $\alpha = 1, \ldots, p$ and given maximal set of reactions Θ, is described by the following steps.

Step 1. Consider the whole set of well-defined sets of reactions $\Lambda_1, \ldots, \Lambda_N$.

Step 2. Construct all corresponding distinct subspaces $U_1, \ldots, U_N$ (from Lemma 2), $N = N(n, p; \Theta)$.

Step 3. Fix $U = U_i$, $i \in \{1, \ldots, N\}$ and verify the solvability of (19).
If this equation is solvable, compute the phase set $Z^{(i)}$ and construct the model $\{Z^{(i)}, \Lambda(Z^{(i)})\}$, where $\operatorname{Span}\{\Lambda(Z^{(i)})\} = U_i^\perp$.

Step 4. Return to *Step 3* and take the next space of invariants $U = U_{i+1}$, etc.

There are three possible cases: (a) $p = d$; (b) $p < d$; (c) $p > d$. The cases (a) and (b) are relatively simple since the number of equations in the system (19) is equal to $N_1 = np$ and the number of unknowns is equal to $N_2 = nd + p^2$. Hence $N_1 < N_2$ for any $n \ge 1$ and $p \ge 1$ provided that $p \le d$. This means that, under certain conditions, the system (19) is solvable for any admissible set of reactions Λ. This solves the classification problem in the case $p \le d$.

By introducing a basis $\{\mathbf{e}_1, \ldots, \mathbf{e}_p\}$ in the known subspace $U \subset \mathbb{R}^n$, one can rewrite (19) as the set of equations

$$\mathbf{u}_\alpha(\mathbf{z}_1, \ldots, \mathbf{z}_n) = a_{\alpha\beta}\mathbf{e}_\beta, \quad \alpha, \beta = 1, \ldots, p. \tag{20}$$

Here and below the summation over repeating Greek indices is assumed. The non-singular matrix $\{a_{\alpha\beta}, \quad \alpha, \beta = 1, \ldots, p\}$ and the points (phase states) $\mathbf{z}_i \in \mathbb{R}^n$, $i = 1, \ldots, n$, are unknown, whereas the functions $\mathbf{u}_\alpha(Z) \in \mathbb{R}^n$ and the vectors $\mathbf{e}_\alpha \in \mathbb{R}^n$ $(\alpha = 1, \ldots, p)$ are given.

Therefore we obtain, in the most general case, pn scalar equations for $(dn + p^2)$ unknowns. Whether (20) have a solution or not, depends on the specific functions $\mathbf{u}_\alpha(Z)$ and on the subspace U. This problem should be considered separately for any specific class of

DKMs (some results for DVMs of the Boltzmann equation are presented below). On the other hand, (19), (20) are universal for all non-degenerate normal DKMs with given invariants.

Definition 7 A vector $\mathbf{w} \in \mathbb{R}^n$ is said to be a *universal invariant* for a set $\Theta \subset \mathbb{Z}^n$ if $\mathbf{w} \cdot \boldsymbol{\theta} = 0$, for all $\boldsymbol{\theta} \in \Theta$. If the set Θ has l linearly independent universal invariants $\{\mathbf{w}_i,\, i = 1, \ldots, l\}$ then the space

$$W = \mathrm{Span}\{\mathbf{w}_1, \ldots, \mathbf{w}_l\} \subset \mathbb{R}^n, \qquad \dim W = l \le n - 1, \tag{21}$$

is called a *universal invariant subspace*.

In the case when the set Θ admits an l-dimensional universal invariant subspace W (19), (20) can be simplified. In particular, all p-dimensional ($p \ge l + 1$) subspaces $U_1, \ldots, U_N$, defined in Lemma 2 can be written as

$$U_i = W \oplus U_i', \qquad \dim U_i' = p - l, \quad i = 1, \ldots, N,$$

where $\oplus$ denotes the direct sum in $\mathbb{R}^n$.

Similarly, the subspace $U(Z)$ (18) is represented as

$$U(Z) = W \oplus U'(Z), \qquad \dim U'(Z) = p - l,$$

and finally we obtain, instead of (19), the equation

$$U'(Z) = U', \tag{22}$$

where $U' = U_i'$, $i = 1, \ldots, N$.

A simplified version of (20) can be obtained in such cases in the following way. We assume that the invariants (condition (C) in Theorem 1) are given in the form

$$\{\mathbf{w}_1, \ldots, \mathbf{w}_l;\ \mathbf{u}_\alpha : Q \to \mathbb{R}^d,\ \alpha = 1, \ldots,\ q = p - l\}.$$

Then we introduce a basis $\{\boldsymbol{\omega}_1', \ldots, \boldsymbol{\omega}_q'\}$ in the known space U' and obtain

$$\mathbf{u}_\alpha'(Z) = a_{\alpha\beta}\boldsymbol{\omega}_\beta', \quad \alpha, \beta = 1, \ldots, q, \tag{23}$$

where $\mathbf{u}_\alpha'(Z)$ are the orthogonal projections of $\mathbf{u}_\alpha(Z)$ onto $\mathbb{R}^n \backslash W$ and $\{a_{\alpha\beta}, \alpha, \beta = 1, \ldots, q\}$ is a non-singular matrix, $q = p - l$.

If there exists $Z \in Q$ satisfying (23) then

$$\mathbf{u}_\alpha(Z) = a_{\alpha\beta}\boldsymbol{\omega}_\beta' + \sum_{i=1}^{l} c_{\alpha i}\mathbf{w}_i, \tag{24}$$

for some coefficients $c_{\alpha i}$, $\alpha = 1, \ldots, q$.

On the other hand, it is clear that $\{\boldsymbol{\omega}_\beta'$, $\beta = 1, \ldots, q\}$ can be changed to any set $\{\boldsymbol{\omega}_\beta$, $\beta = 1, \ldots, q\}$ provided that the p vectors

$$\{\mathbf{w}_1, \ldots, \mathbf{w}_l;\ \boldsymbol{\omega}_1, \ldots, \boldsymbol{\omega}_q\} \tag{25}$$

form a basis of the subspace $U = W \oplus U'$. Then (24) read

$$\mathbf{u}_\alpha(Z) = a_{\alpha\beta}\boldsymbol{\omega}_\beta + \sum_{i=1}^{l} b_{\alpha i}\mathbf{w}_i,$$

for some coefficients $b_{\alpha i}$, $\alpha = 1, \ldots, q$. This proves the following lemma.

Lemma 4 *If the conditions of Theorem 1 are satisfied and*

(1) *the set Θ has $l \le p-1$ universal invariants $\mathbf{w}_i \in \mathbb{R}^n$, $i = 1, \ldots, l$;*
(2) *a set of given invariants (condition (C), Theorem 1) reads*

$$\{\mathbf{w}_1, \ldots, \mathbf{w}_l;\ \mathbf{u}_\alpha : Q \to \mathbb{R}^d,\ \alpha = 1, \ldots, q\},$$

then (20) can be reduced to the system of equations

$$\mathbf{u}_\alpha(Z) = a_{\alpha\beta}\boldsymbol{\omega}_\beta + \sum_{i=1}^{l} b_{\alpha i}\mathbf{w}_i, \quad \alpha, \beta = 1, \ldots, q, \tag{26}$$

where $\{\boldsymbol{\omega}_1, \ldots, \boldsymbol{\omega}_q\}$ are vectors of any basis (25) in $U = W \oplus U'$ and $\{a_{\alpha\beta},\ \alpha, \beta = 1, \ldots, q\}$ is a non-singular matrix.

Thus, the number of equations to be solved, in the process of the construction of DKMs, can be reduced if the maximal set of reactions Θ has universal invariants.

4 Discrete Velocity Models (DVMs) of the Boltzmann Equation

We consider a particular case of usual DVMs [6, 13] of the Boltzmann equation. The phase set Z (7) is the set of n distinct velocities

$$V = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\} \subset \mathbb{R}^d, \quad d = 2, 3, \ldots. \tag{27}$$

The reactions (elastic pair collisions)

$$(\mathbf{v}_i) + (\mathbf{v}_j) \to (\mathbf{v}_k) + (\mathbf{v}_l), \quad i \ne j \ne k \ne l \tag{28}$$

correspond to the vectors

$$\theta = (\ldots, \underbrace{1}_{i}, \ldots, \underbrace{1}_{j}, \ldots, \underbrace{-1}_{k}, \ldots, \underbrace{-1}_{l}, \ldots) \in \mathbb{Z}^n, \tag{29}$$

where dots stand for zeroes. Thus, the maximal set $\Theta \subset \mathbb{Z}^n$ of reactions consists of vectors (29) with all possible combinations of indexes $(i, j|k, l)$ (i, j, k, l all distinct).

The elastic collision (28) satisfies $(d+1)$ scalar conservation laws

$$\begin{cases} \mathbf{v}_i + \mathbf{v}_j = \mathbf{v}_k + \mathbf{v}_l, \\ |\mathbf{v}_i|^2 + |\mathbf{v}_j|^2 = |\mathbf{v}_k|^2 + |\mathbf{v}_l|^2, \end{cases} \tag{30}$$

and therefore the four velocities form a rectangle in $\mathbb{R}^d$ (as in Fig. 1).

This justifies our assumptions that all indexes i, j, l, k are distinct (exchange of velocities $\mathbf{v}_i = \mathbf{v}_j$, $\mathbf{v}_k = \mathbf{v}_l$ is irrelevant for identical particles).

The model has $p = d + 2$ basic invariants

$$\begin{cases} \mathbf{w} = (1, \dots, 1) \\ \mathbf{u}_\alpha = (v_1^{(\alpha)}, \dots, v_n^{(\alpha)}), \quad \alpha = 1, \dots, d\ . \\ \mathbf{u}_{d+1} = (|\mathbf{v}_1|^2, \dots, |\mathbf{v}_n|^2) \end{cases} \tag{31}$$

The model is non-degenerate (Definition 3) if not all velocities $\mathbf{v}_1, \dots, \mathbf{v}_n$ lie on a plane or on a sphere in $\mathbb{R}^d$. Thus all assumptions of Theorem 1 are fulfilled.

First of all we construct all distinct subspaces $U_1, \dots, U_N$ (Lemma 2) by taking, one after another, all possible collections of $(n-d-2)$ linearly independent vectors (29) $\{\theta_i \in \Theta, i = 1, \dots, n-d-2\}$.

Then we consider (19) with $U = U_i$, $i = 1, \dots, N$, and represent it in the form (26) (note that w is a universal invariant of the set Θ). We omit details of the investigation of the solvability of the corresponding (26) (see for details [18]). In this case we can obviously reduce the number of distinct equivalent classes (Definition 5) by changing the numeration of velocities.

It should be pointed out that the problem of the classification of all normal DVMs of the Boltzmann equation has an interesting geometric interpretation. Consider a set V (27) of n points in $\mathbb{R}^d$ and assume that each point $\mathbf{v}_i \in V$, together with three other points $\mathbf{v}_{j,k,l} \in V$, forms a rectangle in $\mathbb{R}^d$ (the numeration of the points can be chosen arbitrarily). Then we consider all such rectangles with vertices $\mathbf{v} \in V$ and prescribe to each rectangle a corresponding vector $\theta \in \Theta$ (for example, the vector $\pm\theta$ in (29) corresponds to the rectangle in Fig. 1, the sign of θ does not play any role). The whole set $\Lambda = \{\theta_i, i = 1, \dots, m\}$ of such vectors coincides with the set $\Lambda_*(V)$ (17), under given invariants (31) and $p = d+2$. Hence, the set $\Lambda = \Lambda_*(V)$ contains at most $(n-d-2)$ linearly independent vectors (rectangles). Thus, the set V (27) of velocities of a normal non-degenerate DVM is geometrically equivalent to such a configuration of n points in $\mathbb{R}^d$ that contains exactly $(n-d-2)$ "independent rectangles" (in the above described sense). All such configurations are obviously invariant under rotation, translation and scaling transformations (the configurations with minimal numbers $n = 6, 7$ of velocities on the plane have some additional invariant transformations). Hence, all normal models can be described by certain configurations of n points in $\mathbb{R}^d$, together with $(n-d-2)$ independent rectangles connecting the points.

The method of 1-extensions [5] is geometrically equivalent to the following procedure. Let $V_n = \{\mathbf{v}_1, \dots, \mathbf{v}_n\} \in \mathbb{R}^d$ be a phase set of normal DVM. If there exists a point $v_{n+1} \notin V_n$, such that v_{n+1} forms a rectangle together with certain three points $\mathbf{v}_{i,j,k} \in V_n$, then $V_{n+1} = \{\mathbf{v}_1, \dots, \mathbf{v}_n, \mathbf{v}_{n+1}\}$ is also a set of normal DVM. It can be shown [18] that, in the plane case $d = 2$, all normal models with $n \in \{7, 8\}$ velocities can be obtained from two 6-velocity models by 1-extensions. This is not true, however, for $n \geq 9$. The computer implementation of the above described scheme led to 6 "irreducible" models with $n = 9$ (the models that can not be obtained by 1-extensions; see Fig. 6). The results (all normal plane DVMs with $n \leq 9$) are presented below in the above explained geometrical form. This way of presenting our models helps us to find a general algorithm for the construction of normal

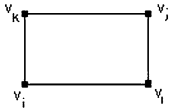

Fig. 1 Geometrical representation of an elastic collision

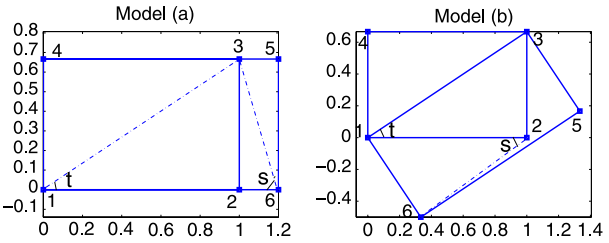

Fig. 2 (Color online) All 6-velocity normal DVMs

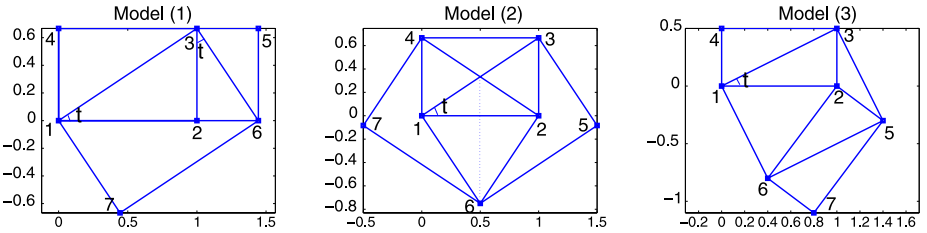

Fig. 3 (Color online) All 7-velocity normal DVMs

DVMs for gas mixtures (Sect. 6). In the same time it is remarkable that many of our normal DVMs are axially symmetric. With the help of symmetric transformations we found a new method that can lead from a given normal DVM to an extended normal DVM (the number of velocities increases fast and we get many normal DVMs). This method is presented in [18]. We mention it here in order to justify the reason we present all our normal models in geometrical form.

5 DVMs for Inelastic Collisions

In this section we consider the problem posed in Sect. 6, however without the assumption that the collisions are elastic (granular gases, for example). This means that the only non-trivial conservation law is the momentum conservation (geometrically this means that the rectangle in Fig. 1 is replaced by any parallelogram).

Let V (27) be the velocity set of such model and $\{\mathbf{w}, \mathbf{u}_\alpha(V); \alpha = 1, \ldots, d\}$ given in (31), be its invariants (note that $\mathbf{u}_{d+1}(V)$ (31) is absent now!). Then we apply Lemma 4 and obtain (see (26))

$$v_i^\alpha = a_{\alpha\beta}\omega_i^\beta + b_\alpha, \quad \alpha = 1, \ldots, d;\ i = 1, \ldots, n, \tag{32}$$

where the vectors $\omega_1, \ldots, \omega_d$ of the basis (25) in the invariant subspace $U = W \oplus U'$ (note that $l = 1$ and $\mathbf{w}_1 = (1, \ldots, 1)$) have the form

$$\omega_\alpha = (\omega_1^\alpha, \ldots, \omega_n^\alpha), \quad \alpha = 1, \ldots, d,$$

and $b_\alpha = b_{\alpha 1}$ ($\alpha = 1, \ldots, d$) in the notation of (26).

Hence, (26) (or, equivalently, (32)) are solvable for any invariant subspace U_i, $i = 1, \ldots, N$, $\dim U_i = d + 1$, defined in Lemma 2 (with $p = d + 1$). Moreover, the solution

$$V = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\} \subset \mathbb{R}^d$$

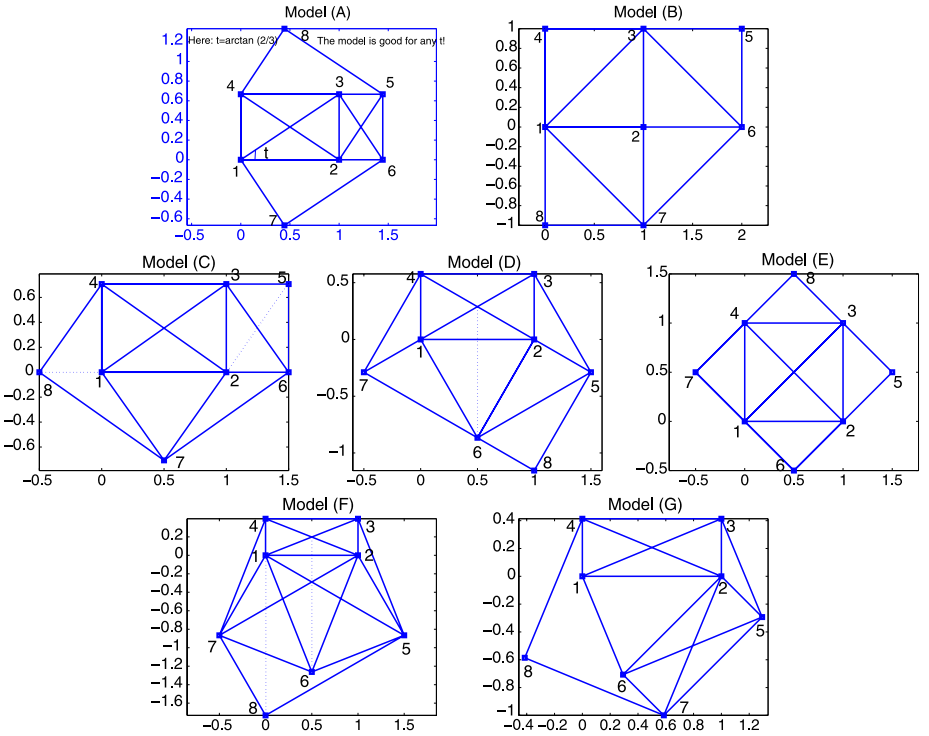

Fig. 4 (Color online) All 8-velocity normal DVMs

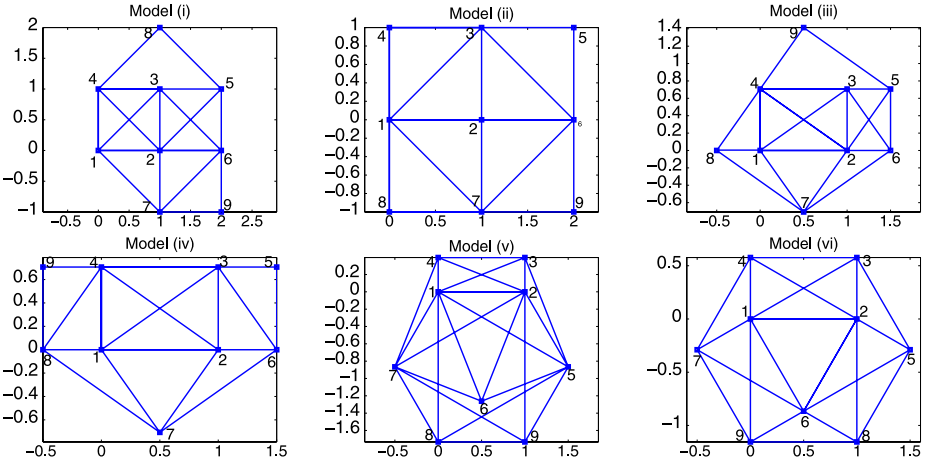

Fig. 5 (Color online) All 9-velocity normal DVMs: 1-extensions

(the velocity set of the normal DVM for inelastic collisions) is determined by (32) with accuracy to any non-singular linear nonhomogeneous transformation.

The final step is to impose some conditions which guarantee that all n velocities in V are distinct. In order to do this we remind the reader how to construct all invariant subspaces

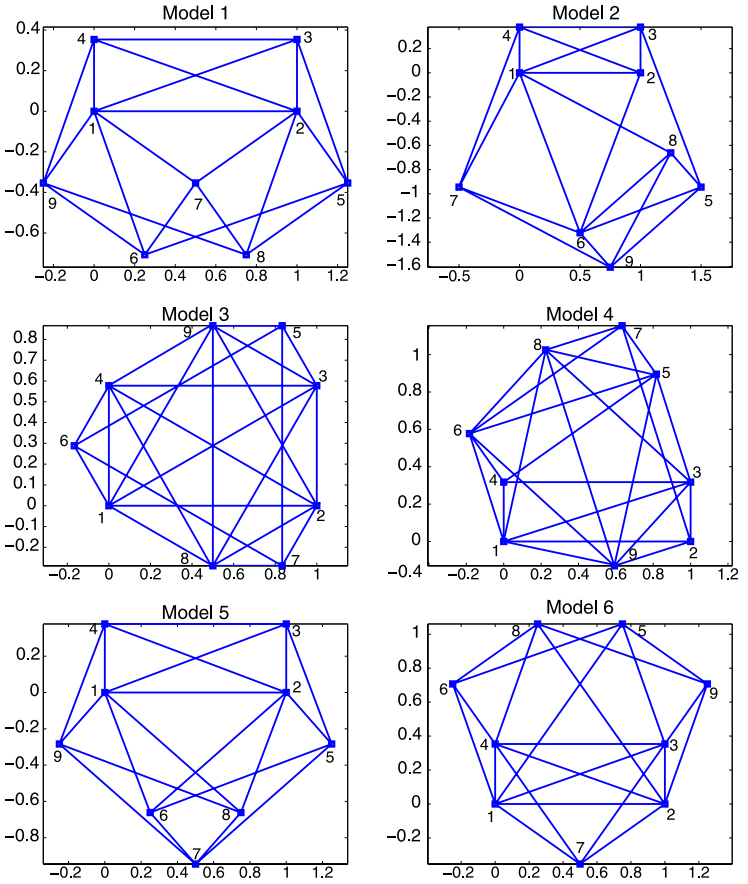

Fig. 6 (Color online) All 9-velocity normal DVMs: not 1-extensions

$U_1, \ldots, U_N$ (Lemma 2). We take an arbitrarily collection of $(n-d-1)$ linearly independent vectors of the form (29) and consider the set

$$\Lambda = \{\theta_1, \ldots, \theta_m\}, \quad m = n - d - 1. \tag{33}$$

Then we have $U = L^{\perp}$, where $L = \operatorname{Span} \Lambda$, and we obtain in such a way all distinct subspaces $U_1, \ldots, U_N$ (Lemma 2).

It can be proved (see [18]) that (32) lead to n distinct velocities $V = \{v_1, \ldots, v_n\}$ if and only if $U = (\operatorname{Span} \Lambda)^{\perp}$, where Λ is a well-defined set. Thus, any well-defined set (33) generates, through (32), a velocity set V of a normal "inelastic" DVM. Conversely, the total set of reactions of any such DVM contains a certain well-defined set (33). This solves, in principle, the problem of the construction of all normal "inelastic" DVMs.

6 Supernormal Discrete Velocity Models for Gas Mixtures

We consider below DVMs of the classical (elastic) Boltzmann equation for gas mixtures. A systematic study of DVMs for mixtures began with the paper [4] in 1998. It was shown

in [4] that the known results from [3, 14] on approximation of the Boltzmann equation for a single gas by DVMs, can be easily generalized to mixtures. On the other hand, the two specific examples of symmetric DVMs for binary mixtures presented in [4] had (except for the special case of the mass ratio $\gamma = 2$, [11]) spurious invariants (this fact was mentioned in papers like [5, 17]). The simplest example of a binary mixture, with $6 + 5 = 11$ velocities and arbitrary mass ratio, was first constructed by Cercignani and Cornille [9]. The inductive method (1-extensions) of construction of normal DKMs [5] was also applied in [5] to mixtures. Several examples constructed by this method were presented in papers like [4, 10–12, 16]. It was also shown in [10], that the method of 1-extensions allows the construction of normal models with arbitrarily large number of velocities for some integer values of mass ratio ($\gamma = 2, 3, 4, 5$). All the above results for mixtures were obtained for binary mixtures in the planar case.

It is clear that the general methods of construction and classification of normal DKMs with given invariants (Sect. 3) can be applied without any changes to binary mixtures. In this case, we have the same set Θ of pair reactions (with conservation of number of particles of each kind) and $p = d + 3$ (d is the dimension of the model) given invariants: momentum, kinetic energy, and two universal invariants corresponding to the number of particles of each kind. On the other hand, the physical meaning of a gas mixture suggests something more than the formal "normality" (in the above discussed sense). Let us assume that the interaction between two species of a binary mixture is very weak. Then, in the limit of zero interaction, we obtain two separate DVMs (say with n and m velocities, respectively) for one-component gases. It is natural to demand that such DVMs must be also normal. Then the velocity space of the binary DVM must be a union of velocity spaces of two normal DVMs for single gases (section 4). Such DVMs for binary mixtures (we call them *supernormal*) are considered below.

We consider below a binary gas mixture of the gases A and B. We denote now the corresponding sets of velocities as

$$\begin{aligned} V &= \{\mathbf{v}_1, \ldots, \mathbf{v}_n\} \subset \mathbb{R}^d \quad \text{and} \\ W &= \{\mathbf{w}_1, \ldots, \mathbf{w}_m\} \subset \mathbb{R}^d. \end{aligned} \tag{34}$$

We denote by $\gamma = \frac{m_A}{m_B}$ the ratio of masses of the model.

In a binary mixture the possible reactions between particles are of the type

(a) $(\mathbf{v}_i) + (\mathbf{v}_j) \to (\mathbf{v}_k) + (\mathbf{v}_l)$ (collision between particles of gas A)

(b) $(\mathbf{w}_i) + (\mathbf{w}_j) \to (\mathbf{w}_k) + (\mathbf{w}_l)$ (collision between particles of gas B)

(c) $(\mathbf{v}_i) + (\mathbf{w}_j) \to (\mathbf{v}_k) + (\mathbf{w}_l)$ (collision between particles of gas A and B)

such that the conservation laws

$$\begin{cases} \mathbf{v}_i + \mathbf{v}_j = \mathbf{v}_k + \mathbf{v}_l \quad \text{and} \quad |\mathbf{v}_i|^2 + |\mathbf{v}_j|^2 = |\mathbf{v}_k|^2 + |\mathbf{v}_l|^2, \quad 1 \le i, j, k, l \le n, \\ \mathbf{w}_i + \mathbf{w}_j = \mathbf{w}_k + \mathbf{w}_l \quad \text{and} \quad |\mathbf{w}_i|^2 + |\mathbf{w}_j|^2 = |\mathbf{w}_k|^2 + |\mathbf{w}_l|^2, \quad 1 \le i, j, k, l \le m, \\ m_A \mathbf{v}_i + m_B \mathbf{w}_j = m_A \mathbf{v}_k + m_B \mathbf{w}_l \quad \text{and} \\ m_A |\mathbf{v}_i|^2 + m_B |\mathbf{w}_j|^2 = m_A |\mathbf{v}_k|^2 + m_B |\mathbf{w}_l|^2, \quad 1 \le i, k \le n \text{ och } 1 \le j, l \le m \end{cases} \tag{35}$$

are satisfied.

Geometrically, the cases (a) and (b) are represented by rectangles (see DVMs with mass, momentum and energy for a single gas, in 2.8) and the case (c) by an isosceles trapezoid.

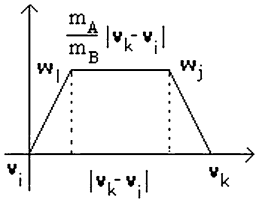

Fig. 7 Geometrical interpretation of a mixture reaction (c)

The corresponding conservation laws (momentum and energy) for mixtures read

$$\begin{cases} \mathbf{v}_i + \dfrac{1}{\gamma}\mathbf{w}_j = \mathbf{v}_k + \dfrac{1}{\gamma}\mathbf{w}_l, \\ |\mathbf{v}_i|^2 + \dfrac{1}{\gamma}|\mathbf{w}_j|^2 = |\mathbf{v}_k|^2 + \dfrac{1}{\gamma}|\mathbf{w}_l|^2. \end{cases} \tag{36}$$

Equations (36) are invariant under translation, rotation and scaling. This implies that geometrically we can represent the reaction (c) as in Fig. 7.

Hence, an $(n+m)$ DVM for a binary mixture is a set of points (velocities) $V_{n+m} = \{V, W\}$ such that each point belonging to V or W respectively, is a vertex of one or several parallelograms whose other vertices also belong to V or W respectively, or/and a vertex of one or several isosceles trapezoids having one more vertex in the same set V or W respectively, and the other two vertices in W or V, respectively (as in Fig. 7). The ratio of parallel sides in the trapezoids must be the same for all of them.

The set of reactions for an $(n+m)$ DVM for mixtures contains vectors of the following three types

$$\begin{aligned}
&\text{(a)} \quad \boldsymbol{\theta}_{ij}^{kl} = (\underbrace{\ldots, \underset{(i)}{1}, \ldots, \underset{(j)}{1}, \ldots, \underset{(k)}{-1}, \ldots, \underset{(l)}{-1}, \ldots}_{n}, \underbrace{\ldots}_{m}), \\
&\text{(b)} \quad \boldsymbol{\theta}_{ij}^{kl} = (\underbrace{\ldots}_{n}, \ldots, \underset{(i)}{1}, \ldots, \underset{(j)}{1}, \ldots, \underset{(k)}{-1}, \ldots, \underset{(l)}{-1}, \ldots), \\
&\text{(c)} \quad \boldsymbol{\theta}_{ij}^{kl} = (\underbrace{\ldots, \underset{(i)}{1}, \ldots, \underset{(k)}{-1}, \ldots}_{n}, \underbrace{\ldots, \underset{(j)}{1}, \ldots, \underset{(l)}{-1}, \ldots}_{m})
\end{aligned} \tag{37}$$

where dots denote zeros.

Definition 8 An $(n+m)$ DVM for mixtures with the set of velocities in $\mathbb{R}^d$ is a *normal* model if it can be represented geometrically by $(n+m-d-3)$ linearly independent rectangles and isosceles trapezoids, in the way described above, i.e. the corresponding vectors of reactions are linearly independent and the rank of the matrix of reactions is $(n+m-d-3)$.

Definition 9 An $(n+m)$ *supernormal model (SNM)* is a normal DVM for an $(n+m)$ mixture of two gases A and B with the set of velocities $\{V, W\}$ such that the DVMs for the single gases, (V, n) and (W, m), are normal.

If we denote by N and M the matrices of reactions for the normal DVMs (V, n) for the gas A and (W, m) for the gas B, respectively, then the matrix of reactions for the SNM

$(\{V, W\}, n+m)$ has the following form

$$\widetilde{\Lambda} = \begin{pmatrix} N & \mathcal{O}_{(n-d-2)\times m} \\ \mathcal{O}_{(m-d-2)\times n} & M \\ \boldsymbol{\theta}_1^{\mathsf{T}} & \\ \cdots & \\ \boldsymbol{\theta}_{d+1}^{\mathsf{T}} & \end{pmatrix}, \tag{38}$$

where $\mathcal{O}_{\alpha\times\beta}$ is a null-matrix with α rows and β columns, $\boldsymbol{\theta}_k$, $k = 1, 2, 3$, represent three linearly independent vectors of type (c) in (37), M and N contain $(n-d-2)$ and $(m-d-2)$ linearly independent rows corresponding to vectors of reactions of the type (a) and (b) in (37), respectively,and

$$\operatorname{rank} \widetilde{\Lambda} = n + m - d - 3. \tag{39}$$

Questions that arise now are: *How to construct such SNMs? Is it possible to do this for any combination of two given normal DVMs for single gases? For which mass ratio is this possible to do?* These are problems we are concerned with in the next sections.

7 General Method for the Construction of Plane SNMs

We consider a mixture of n particles of a gas A and m particles of a gas B and denote by γ the mass ratio of the mixture. The particles from the gases A and B are moving with velocities from V and W respectively, given in (34) with $d = 2$. We assume that the DVMs for the single gases, (V, n) and (W, m), are normal models.

The problem of construction of a SNM can be formulated as follows.

Given two normal DVMs, (V, n) and (W, m) (geometrically represented by $(n-4)$ and $(m-4)$, linearly independent rectangles, respectively) for simple gases, find (if possible) three linearly independent reactions of type (c), geometrically represented by isosceles trapezoids of the form given in Fig. 7, such that (39) is fulfilled.

We develop in this way a *general method of construction of SNMs* (see for details [18]). Given two DVMs (V, n) and (W, m) for simple gases, the method leads to the following two situations

- there is no SNM that contains the normal DVMs for simple gases, or
- we obtain all possible SNMs $(\{V, W\}, n+m)$ and the spectrum of the mass ratio.

All our results ([18]) have a finite spectrum for the mass ratio and, except one model (14-velocity SNM, Fig. 8), the spectrum has rational values.

In [18] we present a computer algorithm for the construction of SNMs on the basis of our results for normal DVMs for single gases and the general method for the construction of plane SNMs given above. The detailed numerical results (i.e. all SNMs with up to 20 velocities) are also presented in [18]. We also construct large planar SNMs (see example in Fig. 8) and give (see [18]) the whole spectrum of the mass ratio for SNMs with up to 20 velocities. We present below just some examples of normal SNMs (the first model in Fig. 8 is with irrational mass ratio $\gamma = 2\sqrt{2}$).

It is clear that the class of SNMs is the most natural (from physical point of view) subclass of the general class of normal DVMs for mixtures. We proved (details in [18]) that there exists a large number of such SNMs for binary mixtures with various values of mass ratio $\gamma > 1$, even for relatively small total number $(n \leq 20)$ of velocities. A non-trivial result of our computations is the following: for any $(n_1 + n_2)$-velocity SNM for binary mixture, with

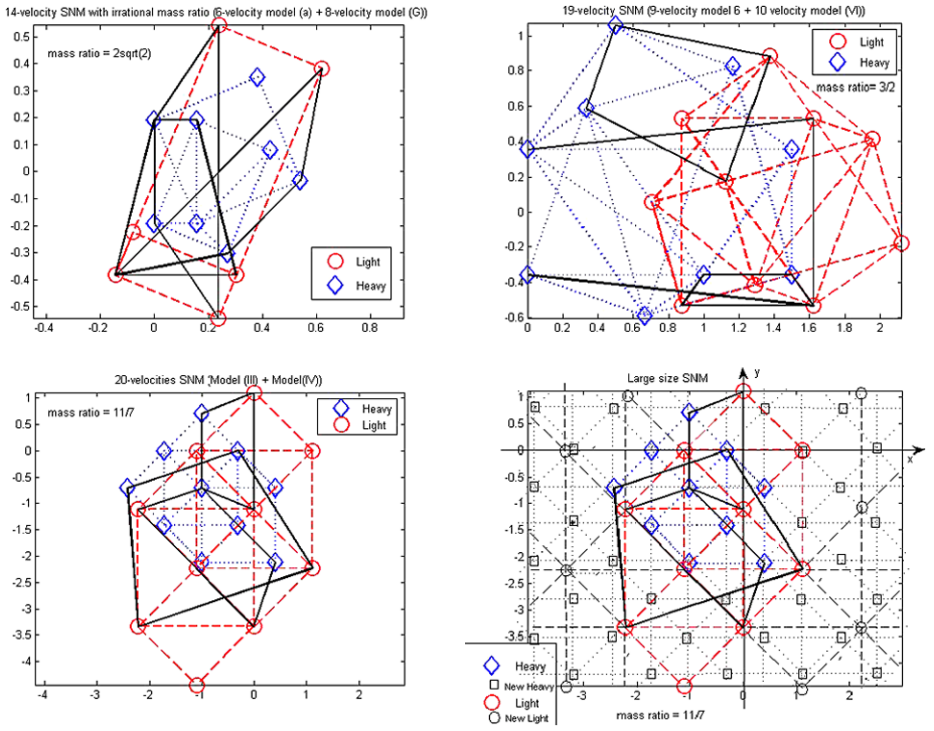

Fig. 8 (Color online) Examples of SNMs

$8 \le n_{1,2} \le 9$ (except for the case of 8-velocity model (A) with one free parameter) there exists a finite number of admissible values (spectrum) of mass ratio $\gamma > 1$. All the values of γ appear to be rational in this case. On the other hand, the general method of construction of SNMs admits, in principle, the existence of universal SNMs with arbitrary mass ratio. After applying our algorithm, we can only say that universal models with $8 \le n_{1,2} \le 9$ (except for the case of 8-velocity model (A) with one free parameter) do not exist.

These facts clarify, to some extent, the problem of existence of normal DVMs for binary mixtures with irrational mass ratio (raised in [4], where the authors questioned the extension of DVMs to mixtures when the ratio of masses is irrational). Such models do exist, the first example of a SNM with irrational mass ratio $\gamma = 2\sqrt{2}$ is 14-velocity SNM presented in Fig. 8. From our results (see the complete spectrum for mass ratio in [18]), we can deduce that irrational values of γ for SNMs with $n_{1,2} \le 9$ are possible only if at least one value of $n_{1,2}$ is small enough ($n_1 = 6, 7$ or $n_2 = 6, 7$). The probable reason for this is that the normal DVMs with $n = 6, 7$ for a single gas contain free parameters and one can play with these parameters in order to obtain any given value of γ (in some interval). This gives us a hope to construct universal SNMs with small numbers of velocities. On the other hand, it may happen that SNMs with large numbers of velocities $n_{1,2} \ge 9$ and irrational γ, do not exist.

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