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Construction and classification of discrete kinetic models without spurious invariants (**)

Contents

١.	· Introduction	4
2 .	Discrete kinetic models and conservation laws	4
	2.1 - Introduction and preliminaries	4
	2.2 - How to find the actual number of conservation laws for a given model?	į
	2.3 - Inductive method (1-extension)	(
	2.4 - Discrete kinetic models	
	2.5 - Normal DKMs with given conservation laws	
	2.6 - Classification problem. General algorithm for the construction of DKMs	1
	2.7 - DVMs for Inelastic Collisions	
	2.7.1 - Statement of the problem and geometrical interpretation	1
	2.7.2 - Classification and construction of normal models	1
	2.8 - DVMs of the Boltzmann Equation	
	2.8.1 - Statement of the problem and geometrical inter-	1

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2.8.2 - Algorithm for the construction of elastic DVMs	21
2.9 - Classification and construction of normal plane elastic models with	
small numbers of velocities	23
2.9.1 - Starting point $(n=6)$ and 1-extension	23
2.9.2 - Classification results for $n \in \{7,8\}$	30
2.9.3 - Algorithm for normal plane elastic models with	
small numbers of velocities	34
2.9.4 - Computer results for the cases $n=8$ and $n=9$	41
3 - Symmetric extensions of normal discrete velocity models	44
3.1 - More geometry of plane DVMs	44
3.2 - Symmetric extensions of normal models	47
3.3 - Rank of the extended matrix	50
3.4 - Invariant sets with three or four points	52
4 - Supernormal discrete velocity models for gas mixtures	62
4.1 - Introduction and preliminaries	62
4.2 - Geometrical interpretation of DVMs for mixtures. Definition and properties of SNMs	63
4.3 - General method for the construction of plane SNMs	66
4.4 - SNMs up to 20 velocities. Spectrum of the mass ratio	77

1 - Introduction

The Boltzmann equation (BE) is the fundamental mathematical model of the kinetic theory of gases, describing the time-evolution of the one-particle distribution function of a simple rarefied gas, $f = f(\mathbf{x}, \mathbf{v}, t)$, where $\mathbf{x} \in \mathbb{R}^d$, $\mathbf{v} \in \mathbb{R}^d$, $\mathbf{t} \in \mathbb{R}_+$ are the position, the particle velocity and the time respectively, in the phase-space $\mathbb{R}^d \times \mathbb{R}^d$.

Discretization methods have been developed on the idea of replacing the original BE by a finite set of non-linear hyperbolic PDEs (the so-called discrete BE, [7]) corresponding to the densities linked to a suitable finite set of velocities. This discrete model is relatively simple with respect to the continuous BE, easier to analyse from both mathematical and numerical point of view, also useful to describe gas mixtures or equations with multiple collisions. The concept of discrete velocity models (DVMs) was first considered by Carleman [8], but the real development of this theory began after Broadwell (1964) introduced his first models [6]. An important role in the development of the mathematical theory of DVMs had Gatignol [16] and Cabannes [7]. After their pioneering work, a considerable amount of research was devoted to DVMs. In particular, we mention the papers [3], [19] where it was proved that BE can be approximated by DVMs with any given accuracy. This

result was generalized to mixtures in [4]. A relatively recent review on DVMs can be found in the book [2]. More information on DVMs can be also found in the following books [17], [1], [18], [10].

It became clear already in 1975 [16] that the velocity discretization can lead to equations with spurious conservation laws (not linear combinations of the physical conservation laws). In many papers on DVMs authors postulate from the beginning that a finite velocity space with such "good" properties is given, and 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 spaces (sets) satisfying this type of "good" restrictions (Cercignani called such models "normal" in [9]).

This paper consists of three main parts presented in sections 2, 3 and 4.

Section 2 is devoted to the general method for the construction and classification of discrete kinetic models (DKMs) and its applications in the particular cases of inelastic and elastic BE. In 2.1 – 2.3 we present the general DVM of the BE and some preliminary results [5], [21], [13]. We introduce in 2.4 the most general class of DKMs in the spatially homogeneous case. We discuss the structure of invariant subspaces of such models and show that the number of invariant subspaces is always finite (Lemma 3). In sections 2.5, 2.6, the problem of the construction of all normal DKMs with given invariants is reduced to an equation for the phase set of the model (Theorem 1). We introduce the concept of universal invariants and use them to reduce the number of equations we need to solve. By using all these results, we classify all normal DKMs and give a general algorithm for their construction. Section 2.7 is devoted to DVMs with inelastic collisions. In this case, all normal models can be described explicitly (Proposition 1). Applications of the general theory to DVMs of the elastic BE are given in 2.8, 2.9, where we classify all models with up to 9 velocities and construct them. By our method, we find new classes of normal DVMs that can not be obtained by the inductive method [5].

In section 3 we develop a new method for the construction of normal DVMs, based on the idea of symmetric extensions. This is an inductive procedure, similar, in some sense, to the 1-extension method [5], that can lead from a given normal DVM to an extended DVM. The main result of this part is given in Theorem 3, where conditions for an extended model to be normal are stated. Many new normal models can be constructed in this way, and we give some examples to illustrate this.

Section 4 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 in section 4.2 a geometrical interpretation of plane DVMs for mixtures. Then, we give the definition of SNMs and derive a general method for the

construction of such models. We applied in [22] this method and obtained SNMs up to 20 velocities and their spectrum of mass ratio. In this paper we give some examples.

2 - Discrete kinetic models and conservation laws

2.1 - Introduction and preliminaries

The general discrete velocity model (DVM) of the Boltzmann equation reads [16]

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

where $\mathbf{x} \in \mathbb{R}^d$ and $t \in \mathbb{R}_+$ denote the position and the time respectively, and $V = \{\mathbf{v}_1, \dots, \mathbf{v}_n\} \subset \mathbb{R}^d$ 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

(2)
$$Q_{i}(f) = \sum_{i k l=1}^{n} \Gamma_{ij}^{kl}(f_{k}f_{l} - f_{i}f_{j}) \text{ for } i = 1, \dots, n,$$

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

(3)
$$\Gamma^{kl}_{ij} = \Gamma^{kl}_{ji} = \Gamma^{ij}_{kl} \ge 0,$$

with equality unless the conservation laws (momentum and energy)

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

are satisfied. A DVM (1), (2) is called *normal* [9] if any solution of the equations

(5)
$$\Psi(\mathbf{v}_i) + \Psi(\mathbf{v}_i) = \Psi(\mathbf{v}_k) + \Psi(\mathbf{v}_l)$$

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

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

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

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 Eq. (6). This problem appeared already at the early stage of the development of the mathematical theory of DVMs [16] and still remains, generally speaking, unsolved. One can easily find an actual number of invariants for any given DVM by using the method proposed in [21]. 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, before this work, there was just one particular method to do this. The method was proposed in [5] (see also [20]). Many new DVMs were obtained by the inductive method in the last years [20] [14]. 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 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*, in this case, means the absence of other (spurious) conservation laws.

2.2 - How to find the actual number of conservation laws for a given model?

We start by discussing a simple idea of Vedenyapin and Orlov [21] that represents (together with the paper [5]) a starting point for our present work. They have considered an arbitrary (not necessarily normal) DVM with the collision term (2) and introduced a set of vectors

(7)
$$\mathbf{e}_{ij}^{kl} = (\ldots, \underbrace{1}_{(i)}, \ldots, \underbrace{1}_{(i)}, \ldots, \underbrace{-1}_{(k)}, \ldots, \underbrace{-1}_{(l)}, \ldots) \in \mathbb{R}^n, \Gamma_{ij}^{kl} > 0,$$

for any combination of indices (i,j;k,l) such that $\Gamma^{kl}_{ij} > 0$ (dots stand for zeros). The conservation law (5) can be rewritten as a set of orthogonality conditions

(8)
$$\boldsymbol{\Psi} \cdot \mathbf{e}_{ij}^{kl} = 0, \ \Gamma_{ij}^{kl} > 0,$$

where

(9)
$$\boldsymbol{\Psi} = (\boldsymbol{\Psi}(\mathbf{v}_1), \dots, \boldsymbol{\Psi}(\mathbf{v}_n)) \in \mathbb{R}^n.$$

The whole set of vectors (7) for all cases when $\Gamma^{kl}_{ij}>0$ can be written (one vector under another one, in an arbitrary order) in the form of a matrix \widetilde{A} with n columns. The rank p of this matrix cannot, by the construction of the DVM, exceed (n-(d+2)), since for $\mathbf{v}=(v_1,\ldots,v_d)$, the functions

(10)
$$\Psi_0(\mathbf{v}) = 1; \ \Psi_a(\mathbf{v}) = v_a, \ a = 1, ..., d; \ \Psi_{d+1}(\mathbf{v}) = |\mathbf{v}|^2$$

lead to (d+2) linearly independent (in the general case) vectors (9) of conservation laws. Hence, the DVM is normal if and only if

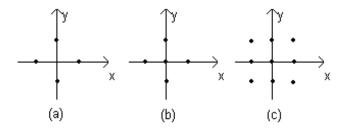
(11)
$$\operatorname{rank} \widetilde{\Lambda} = n - (d+2),$$

provided that the vectors (9), (10) are linearly independent.

This gives a simple *practical criterion of normality* for any given DVM: the number of linearly independent vectors (7) must be equal to (n-d-2). By using this technique, the authors of [21] proved that some DVMs for mixtures proposed in [4] had spurious invariants. This idea helps to reject some "bad" DVMs; however, it says nothing about the way to construct normal models. This question will be considered below for general discrete kinetic models (DKMs) and vectors of type (7) will play an important role in our approach.

2.3 - Inductive method (1-extension)

In [5] the authors introduced a method of constructing DVMs without non-physical invariants (normal models) using an inductive scheme of 1-extensions. The idea is that one can start with the simplest discrete model such as, for example, the modified Broadwell model for a simple gas. The Broadwell model with n=2d velocities is not (formally) normal since it has only d+1 conservation laws; to obtain a normal DVM, one adds one more velocity as in the following figure.



Here (a) represents the Broadwell model, (b) the modified Broadwell model and (c) the extended Broadwell model (the extended models (a) - (c) were first introduced in [4]). We explain below the general idea of [5].

Given a normal discrete model with the phase set

$$(12) X_n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subseteq \mathbb{R}^d$$

 $(X_n \text{ is a set of velocities for DVMs of BE})$ one constructs its extended version

(13)
$$X_{n+s} = \{\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}_{n+1}, \dots, \mathbf{x}_{n+s}\}, \ s \ge 1,$$

where all new states $\{n+1,...,n+s\}$ satisfy the conditions

$$(\forall) 1 \leq r \leq s \ (\exists) \ (i,j,k), 1 \leq i,j,k \leq n, \ \text{such that} \ \varGamma^{k,n+r}_{ij} > 0,$$

in other words, each new state (n+r) is a product of a certain reaction

$$(i) + (j) \rightarrow (k) + (n+r)$$

which includes three states $\{i, j, k\}$ present in the initial discrete model (12). The extended Broadwell model (c) corresponds to the case n = 5, s = 4.

Lemma 1 [5]. If the initial discrete model (12) is normal, then the same is true for the extended discrete model (13).

The proof is quite obvious, it is enough to consider the case s = 1, [5].

We shall use this approach in the case of DVMs for the classical Boltzmann equation. Let us look closely at the above figure. By using 1-extensions one can prove that such normal DVMs exist for any given $n \geq 6$ (we exclude DVMs with an isolated phase state, as in (b) for n=5). A straight forward continuation of the above described procedure, starting from the 9-velocity model (c), leads to an infinite hierarchy of normal DVMs whose velocities belong to the regular lattice in \mathbb{R}^2 [5]. On the other hand, it is clear that (at least for small numbers of velocities n=6,7) there are normal DVMs of different structure, with "rational" and "irrational" velocities. All normal DVMs obtained by 1-extensions are obviously "reducible" (by taking away one phase state after another) to some "irreducible" normal models. Can we reduce any normal model to the simplest 6-velocity one? If so, then the whole class of normal DVMs could be described in a simple way: just consider 6-velocity DVMs and make all possible 1-extensions.

We shall see in section 2.9 that the answer is negative: already in the case n=9 there are some normal models which can not be obtained by 1-extensions. Other examples, with more than 9 velocities, are given in Section 3.

2.4 - Discrete kinetic models

The most general spatially homogeneous 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 $\mathbf{z}_i \subset \mathbb{R}^d$, $i=1,\ldots,n$.

We fix the phase set

(14)
$$Z = \{\mathbf{z}_1, \dots, \mathbf{z}_n\} \subset \mathbb{R}^d$$

and describe the state of the N-particle system by a vector ρ of occupation numbers

(15)
$$\rho = (N_1, \dots, N_n), \quad N_1 + \dots + N_n = N,$$

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 ρ (15) to a new state $\rho^{(s)}(s = 1, \ldots, m)$

(16)
$$ho o
ho^{(s)} = \left(N_1^{(s)}, \dots, N_n^{(s)}\right), \ N_1^{(s)} + + N_n^{(s)} = N^{(s)},$$

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

It is convenient to introduce m vectors

(17)
$$\theta_s = \rho - \rho^{(s)} = (k_1^{(s)}, \dots, k_n^{(s)}), \quad s = 1, \dots, m,$$

with integer components $k_i^{(s)}$ and call them "vectors of reactions" (similar vectors were introduced in [21] for DVMs of the Boltzmann equation).

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

(18)
$$\Lambda = \{\theta_1, \dots, \theta_m\} \subset \Theta \subset \mathbb{Z}^n,$$

is fixed. Then it is clear that the Markovian dynamics of the model is uniquely defined by the set of reactions Λ (18) and the set of probabilities (frequencies) $\{p_1, \ldots, p_m\}$ of the reactions $\theta_1, \ldots, \theta_m$.

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

(19)
$$\rho(t) = (N_1(t), \dots, N_n(t)), t > 0.$$

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

It is easy to prove that there exists a unique vector $\mathbf{u} \in \mathbb{R}^n$ (called a *vector of conservation law*) such that

(20)
$$l[\boldsymbol{\rho}] = \mathbf{u} \cdot \boldsymbol{\rho} = \sum_{i=1}^{n} N_i u_i, \ \mathbf{u} = (u_1, \dots, u_n),$$

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

Lemma 2. A vector $\mathbf{u} \in \mathbb{R}^n$ is a vector of conservation law if and only if $\mathbf{u} \cdot \mathbf{\theta}_s = 0$, for all $\mathbf{\theta}_s \in \Lambda$.

Now we can easily describe the total set of linear (independent of ρ) conservation laws of a DKM with a given set of reactions Λ . We introduce a **space of reactions**

(21)
$$L = \operatorname{Span} \Lambda = \operatorname{Span} \{\theta_1, \dots, \theta_m\}$$

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

$$(22) U = L^{\perp}, L \oplus U = \mathbb{R}^n.$$

The following statement follows directly from Lemma 2 (a similar statement for DVMs of the Boltzmann equation was proved in [21]).

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 invariants is given by the equality

$$(23) p = \dim U = n - \dim L.$$

The important conclusion is that all the invariants of a given DKM are uniquely defined by its set of reactions Λ (18), 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 Eqs.(21), (22) is said to be the invariant subspace of the DKM (with given Λ). The number $p = \dim U$ 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 3. 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 (14) has a certain set Λ (18) of reactions containing exactly (n-p) linearly independent vectors $\boldsymbol{\theta}_1,\dots,\boldsymbol{\theta}_{n-p}\in\Theta$ (other vectors from Λ can be ignored since they do not influence the conservation laws). Then $U=L^\perp$, where $L=\operatorname{Span}\{\boldsymbol{\theta}_1,\dots,\boldsymbol{\theta}_{n-p}\}$ in accordance with Eqs. (21), (22). On the other hand, the set Θ is finite by the assumptions of the lemma, so it can not have more than a finite number of distinct subsets with (n-p) pairwise different elements. This completes the proof.

2.5 - Normal DKMs with given conservation laws

We assume below that the conditions of Lemma 3 are fulfilled and we fix two natural numbers n, p and a finite set $\Theta \subset \mathbb{Z}^n$.

Let us consider a d-dimensional DKM. Its phase set Z (14) is an element of the

space

$$Q = \underbrace{\mathbb{R}^d \times \cdots \times \mathbb{R}^d}_{n}.$$

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

We introduce p vector functions $\{\mathbf{u}_a:Q\to\mathbb{R}^n, a=1,\ldots,p\}$ and call them **given** invariants. Then the total set Λ (18) of reactions of the model is a subset $\Lambda(Z)$ of the set

(25)
$$\Lambda_*(Z) = \{ \theta \in \Theta : \theta \cdot \mathbf{u}_a(Z) = 0, \ a = 1, \dots, p \}.$$

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 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 $\Lambda_*(Z)$).

In the next step we exclude some phase sets that are not acceptable.

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

The following class of such models is particularly important for applications.

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)

(26)
$$U(Z) = \text{Span } \{\mathbf{u}_a(Z), a = 1, \dots, p\}, Z \in Q,$$

and partition all normal models into equivalent classes.

Definition 5. Two normal (as in Definition 4) DKMs $\{Z_i, \Lambda(Z_i)\}$, i = 1, 2, are said to be **equivalent** if $U(Z_1) = U(Z_2)$.

We can now formulate the result related to the **classification of normal DKMs** with given invariants.

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

- (A) three natural numbers (n, p, d), $n \ge p + 1$;
- (B) a maximal (finite) set of reactions $\Theta \subset \mathbb{Z}^n$;

11

(C) p linearly independent invariants $\{\mathbf{u}_a:Q\to\mathbb{R}^n, a=1,\ldots,p\}$ (Q from (24)). 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

$$(27) U(Z) = U,$$

for the phase set $Z \in Q$, where U is one of the N distinct invariant subspaces defined in Lemma 3, and U(Z) is defined in Eq. (26).

Proof. Two distinct classes of normal models can not have identical subspaces U(Z) (26) (see Definition 5). On the other hand, all $N(n, p; \Theta)$ possible (under conditions (A), (B)) p-dimensional invariant subspaces are defined in Lemma 3. Hence, we obtain the equation (27) and this completes the proof.

Remark 1. The Theorem 1 reduces the problem of the classification and construction of DKMs to a solution of Eq. (27).

By introducing a basis $\{\mathbf{e}_1, \dots, \mathbf{e}_p\}$ in the known subspace $U \subset \mathbb{R}^n$, one can rewrite the equation (27) as a set of equations

(28)
$$\mathbf{u}_{a}(\mathbf{z}_{1},\ldots,\mathbf{z}_{n})=a_{a\beta}\mathbf{e}_{\beta},\ a,\beta=1,\ldots,p.$$

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

Therefore, we obtain, in the most general case, pn scalar equations with $(dn + p^2)$ unknowns. Whether the equations (28) have a solution or not, depends on the specific functions $\mathbf{u}_a(Z)$ $(a=1,\ldots,p)$ and the subspace U.

This problem should be considered separately for any specific class of DKMs (some results for the case of DVMs of the Boltzmann equation are presented below). On the other hand, the equations (27)-(28) are universal for all non-degenerate normal DKMs with given invariants.

It is convenient to introduce the following definition.

Definition 6. A vector $\mathbf{w} \in \mathbb{R}^n$ is said to be a universal invariant for a set $\Theta \subset \mathbb{Z}^n$ if

(29)
$$\mathbf{w} \cdot \boldsymbol{\theta} = 0$$
, for all $\boldsymbol{\theta} \in \boldsymbol{\Theta}$.

If the set Θ has l linearly independent universal invariants $\{\mathbf{w}_i, i=1,\ldots,l\}$ then

the space

$$(30) W = \operatorname{Span} \{\mathbf{w}_1, \dots, \mathbf{w}_l\} \subset \mathbb{R}^n, \dim W = l < n - 1,$$

is called a universal invariant subspace.

In the case when the set Θ admits an l-dimensional universal invariant subspace W, the equations (27), (28) can be simplified (to skip some possible confusions, we stress that $W \subset \mathbb{R}^n$ is not a subspace of Θ , which is actually a finite set of reactions). In particular, all p-dimensional ($p \geq l+1$) subspaces U_1, \ldots, U_N , defined in Lemma 3 can be written as

(31)
$$U_{i} = W \oplus U'_{i}, \dim U'_{i} = p - l, i = 1, ..., N,$$

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

Similarly, the subspace U(Z) (26) is represented as

(32)
$$U(Z) = W \oplus U'(Z), \dim U'(Z) = p - l,$$

and finally we obtain, instead of Eq. (27), the equation

$$(33) U'(Z) = U',$$

where $U' = U'_{i}$, i = 1, ..., N.

A simplified version of Eqs. (28) 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

(34)
$$\{\mathbf{w}_1, \dots, \mathbf{w}_l; \mathbf{u}_a : Q \to \mathbb{R}^d, a = 1, \dots, q = p - l\}.$$

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

(35)
$$\mathbf{u}_{a}^{'}(Z) = a_{\alpha\beta}\mathbf{\omega}_{\beta}^{'}, \ a, \beta = 1, \dots, q,$$

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

If there exists $Z \in Q$ satisfying Eqs.(35) then

(36)
$$\mathbf{u}_{a}(Z) = a_{a\beta} \boldsymbol{\omega}_{\beta}' + \sum_{i=1}^{l} c_{ai} \mathbf{w}_{i} ,$$

for some coefficients c_{ai} , $a = 1, \ldots, q$.

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

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

form a basis of the subspace $U = W \oplus U'$. Then the equations (36) read

$$\mathbf{u}_a(Z) = a_{aeta} \mathbf{\omega}_{eta} + \sum_{i=1}^l b_{ai} \mathbf{w}_i,$$

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

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

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

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

then Eq. (28) can be reduced to the system of equations

(38)
$$\mathbf{u}_{a}(Z) = a_{a\beta}\omega_{\beta} + \sum_{i=1}^{l} b_{ai}\mathbf{w}_{i}, \ a, \beta = 1, \dots, q,$$

where $\{\omega_1, \ldots, \omega_q\}$ are vectors of any basis (37) in $U = W \oplus U'$ and $\{a_{a\beta}, a, \beta = 1, \ldots, q\}$ 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.

2.6 - Classification problem. General algorithm for the construction of DKMs

In applications we usually need to construct a DKM with a phase set

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

a set of reactions Λ (both Λ and Z are unknown) and with p given conservation laws

(39)
$$\sum_{k=1}^{n} N_k(t) \mathbf{u}_a(\mathbf{z}_k) = const., \ a = 1, \dots, p,$$

(or p given invariants $\mathbf{u}_a(Z) \in \mathbb{R}^n$).

The DKM $\{Z, \Lambda(Z)\}$ is assumed to be non-degenerate (Definition 3), i.e.

(40)
$$\sum_{a=1}^{p} \lambda_a \mathbf{u}_a(\mathbf{z}_k) = 0, \ k = 1, \dots, n$$

implies that all $\lambda_a = 0$, $\alpha = 1, \dots, p$.

The model is normal if it has no other conservation laws except (39) (we discussed already in section 2.1 the example of DVMs).

By the *classification of normal DKMs* we mean the description of all distinct classes of normal DKMs (Definitions 4 and 5), i.e.the phase sets Z and the sets Λ of reactions, for given numbers n (the order of the model), d (the dimension of the model), p (the number of conservation laws), given invariants $\mathbf{u}_a(Z) \in \mathbb{R}^n$ (a = 1, ..., p) and given maximal set Θ of reactions.

It is clear in advance (see Theorem 1), that there exists at most a finite number (perhaps zero) of distinct equivalent classes of normal DKMs, each of them uniquely determined by the Eqs. (28), or equivalently (see Lemma 4) Eqs. (38).

The solvability of these equations is not enough in order to construct a "good" normal DKM. We need the extra condition that the model has exactly n distinct phase points. For this we introduce the following definition.

Definition 7. A set of reactions Λ is said to be well-defined if

$$\mathbf{e}_k - \mathbf{e}_l \notin \text{Span } \Lambda, 1 \leq k < l \leq n,$$

for any pair of standard unit vectors in \mathbb{R}^n ,

$$\mathbf{e}_i = (\ldots, \underbrace{1}_i, \ldots), i = 1, \ldots, n,$$

where dots denote zeros.

We get the following result.

Lemma 5. The condition $\mathbf{z}_k \neq \mathbf{z}_l$ for $k \neq l$ is fulfilled for all $\mathbf{z}_i \in Z$, i = 1, ..., 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 $\mathbf{u}_a(\mathbf{z}_k) = \mathbf{u}_a(\mathbf{z}_l)$ for all $a = 1, \dots, p$ and moreover

$$\mathbf{u}_a(Z) \cdot (\mathbf{e}_k - \mathbf{e}_l) = 0, \ a = 1, \dots, p,$$

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

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

and the supposition is false. This completes the proof.

Now we are able to give a general algorithm for the construction of all distinct normal DKMs $\{Z, \Lambda(Z)\}$ with given numbers (n, d, p), given invariants $\mathbf{u}_a(Z) \in \mathbb{R}^n$, $a = 1, \ldots, p$ and given maximal set of reactions Θ .

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 3), $N = N(n, p; \Theta)$.

Step 3. Fix $U = U_i$, $i \in \{1, ..., N\}$ and verify the solvability of Eqs. (28) (or equivalently Eqs. (38)).

If these equations are solvable, we compute the phase set $Z^{(i)}$ and construct the model $\{Z^{(i)}, \varLambda(Z^{(i)})\}$, where Span $\{\varLambda(Z^{(i)})\} = U_i^{\perp}$.

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

The algorithm is finished in N+2 total steps. It is clear that the algorithm can be modified in some specific cases (see below) in order to simplify and accelerate the procedure.

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 (28) 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 $n\geq 1$ and $p\geq 1$ provided that $p\leq d$. This means that, under certain conditions, the equations (28) are solvable for any admissible set of reactions A. This solves the classification problem in the case $p\leq d$.

Hence, the only time when we really need the above-described algorithm is in the case (c) p>d (the number of conservation laws is greater than the dimension of the phase space). This explains the difficulty of constructing normal DVMs for the classical Boltzmann equation with p=d+2 (conservation of mass, momentum and energy).

2.7 - DVMs for inelastic collisions

2.7.1 - Statement of the problem and geometrical interpretation

We consider the particular case of DVMs (identical particles with pair collisions) with mass and momentum conservation (granular gases, for example). The phase set Z (14) is the set of n distinct velocities (the numeration is fixed)

(41)
$$V = \{\mathbf{v}_1, \dots, \mathbf{v}_n\} \subset \mathbb{R}^d, d \in \{2, 3, \dots\}.$$

The reactions (inelastic pair collisions)

(42)
$$(\mathbf{v}_i) + (\mathbf{v}_i) \rightarrow (\mathbf{v}_k) + (\mathbf{v}_l), \{i, j, k, l\}$$
 all distinct,

correspond to the vectors of reaction

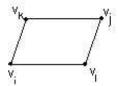
(43)
$$\theta = (\ldots, \underbrace{1}_{i}, \ldots, \underbrace{1}_{i}, \ldots, \underbrace{-1}_{k}, \ldots, \underbrace{-1}_{l}, \ldots),$$

where dots stand for zeros. Thus, the maximal set $\Theta \subset \mathbb{Z}^n$ of reactions consists of vectors (43) with all possible combinations of indices (i,j;k,l), all distinct.

The inelastic collision (42) satisfies (d+1) conservation laws (mass and momentum). The only non-trivial conservation laws are

$$(44) v_i^a + v_i^a = v_k^a + v_l^a, a = 1, \dots, d,$$

geometrically represented by a parallelogram in \mathbb{R}^d .



The model has p = d + 1 basic invariants (34)

$$\begin{cases} \mathbf{u}_a = (v_1^a, \dots, v_n^a), \ a = 1, \dots, d \\ \mathbf{w} = (1, \dots, 1) \text{ (universal invariant for } \boldsymbol{\Theta}). \end{cases}$$

In the general theory for DKMs we mentioned that we are in general looking only for non-degenerate models. The Definition 3 can be rewritten for this particular problem.

Definition 8. The set (41) is said to be non-degenerate provided the equalities

$$\mathbf{a} \cdot \mathbf{v}_k = const., \ \mathbf{a} \in \mathbb{R}^d, \ k = 1, \dots, n,$$

imply $\mathbf{a} = 0$. Otherwise, the set is said to be **degenerate**. The same terminology is used for DVMs with the phase set (41) and given invariants (45).

The meaning of degeneracy is obvious: a degenerate model has a real dimension $d_1 \leq d-1$ and should be considered after corresponding change of coordinates. It is clear that any set (41) with n < d is degenerate. From now on we consider only non-degenerate models.

The problem of the classification of all normal DVMs for inelastic collisions has an interesting geometrical interpretation. Consider a set V (41) 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 parallelogram in \mathbb{R}^d (the numeration of the points can be chosen arbitrarily). Then consider all such parallelograms with vertices $\mathbf{v} \in V$ and prescribe to each parallelogram a corresponding vector $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ (for example, the vector $\boldsymbol{\pm} \boldsymbol{\theta}$ from (43) corresponds to the parallelogram represented in the above figure). The sign of $\boldsymbol{\theta}$ plays no

role in the problem of the construction of normal models. In the case of inelastic collisions with energy dissipation, the sign of θ can be "almost always" defined uniquely by the condition

$$|\mathbf{v}_i|^2 + |\mathbf{v}_j|^2 \ge |\mathbf{v}_k|^2 + |\mathbf{v}_l|^2$$
.

The whole set $\Lambda = \{\theta_i, i = 1, ..., m\}$ of such vectors coincides with the set $\Lambda_*(V)$ (25), where p = d + 1, $\mathbf{u}_a(Z) = \mathbf{u}_a$ (a = 1, ..., d) from (45) and $\mathbf{u}_{d+1}(Z) = \mathbf{w}$ from (45). Thus the set $\Lambda = \Lambda_*(V)$ contains at most (n - d - 1) linearly independent vectors of reactions (or geometrically, parallelograms). Therefore, the set V (41) of velocities of a normal non-degenerate DVM for inelastic collisions is geometrically equivalent to such a configuration of n points in \mathbb{R}^d that contain exactly (n - d - 1) independent (in the sense of the following definition) parallelograms.

Definition 9. The parallelograms of a model are said to be **independent** if the corresponding vectors of reactions are linearly independent in \mathbb{R}^n .

It is clear that any DVM for inelastic collisions can not have more than (n-d-1) independent parallelograms (otherwise the model would have less than (d+1) conservation laws). Therefore the normal models have a simple geometrical meaning: they maximize (for given n and d) the number of independent parallelograms.

We briefly describe, in the next section, how to construct all such models.

2.7.2 - Classification and construction of normal models

Since we are studying a particular case of DKMs, we are going to follow the general theory for the classification and the construction of normal models, described in section 2.6. We consider a normal non-degenerate DVM for inelastic collisions, with given numbers $n \geq 4$ (order) and $d \geq 2$ (dimension), given set of invariants $\{\mathbf{w}, \mathbf{u}_a(V), a = 1, \ldots, d\}$ (45), and let V (41) be the velocity set.

The normal DVM has exactly p = d + 1 conservation laws

(46)
$$\sum_{k=1}^{n} N_k(t) \mathbf{v}_k = const. \in \mathbb{R}^d, \ \sum_{k=1}^{n} N_k(t) = const. \in \mathbb{R}_+$$

The set Θ of all possible vectors of reactions consists of vectors (43) and the set Λ of reactions must have (n-(d+1)) linearly independent vectors $\{\theta_1,...,\theta_{n-d-1}\}\subset\Theta$. The number of conservation laws p=d+1 relates formally to the "difficult" case (c) in the general algorithm (section 2.6). The models exist and we are able to construct them if Eqs.(28) are solvable. The solvability can sometimes be difficult to check.

Fortunately, in this particular case, the algorithm can be simplified, due to the existence of the universal invariant

$$\mathbf{w} = (1, \dots, 1) \in \mathbb{R}^n$$

(orthogonal to all vectors of the maximal set Θ). This allows us to apply Lemma 4, reduce the number of equations and solve, instead of Eqs. (28), the simplified Eqs. (38), i.e.

(47)
$$v_i^a = a_{a\beta} \omega_i^{\beta} + b_a, \ a, \beta = 1, \dots, d, \ i = 1, \dots, n,$$

where the vectors $\omega_1, \ldots, \omega_d$ of the basis (37) in the invariant subspace $U = W \oplus U'$ (note that l = 1 and $\mathbf{w}_1 = (1, \ldots, 1) \in \mathbb{R}^n$) have the form

(48)
$$\boldsymbol{\omega}_{\beta} = (\omega_{1}^{\beta}, \dots, \omega_{n}^{\beta}), \, \beta = 1, \dots, d$$

and $b_a = b_{a1}$, a = 1, ..., d (in the notations of Eqs. (38)).

The system (47) has $N_1=nd$ equations and $N_2=nd+d^2$ unknowns. Hence $N_2>N_1$ and Eqs.(47) are solvable for any invariant subspace

$$U = U_i, i = 1, ..., N, \dim U = d + 1,$$

defined in Lemma 3.

The solution (the velocity set of the normal DVM for inelastic collisions)

$$(49) V = \{\mathbf{v}_1, \dots, \mathbf{v}_n\} \subset \mathbb{R}^d$$

is determined by Eqs.(47) with accuracy up to any non-singular linear non-homogeneous transformation.

The construction of normal DVMs for inelastic collisions follows the general algorithm of classification and construction of DKMs, presented in section 2.6. We should remind that, in order to have distinct phase states, the sets Λ of reactions should be well-defined (see Step 1 of the general algorithm). In the particular case of the inelastic BE, the equations (38) in Step 3 of the general algorithm, read (47), and are always solvable. The solution is the velocity set V (49) of the normal inelastic model $\{V, \Lambda(V)\}$. We have the following result.

Proposition 1. Any well-defined set Λ of reactions

(50)
$$\Lambda = \{\theta_1, \dots, \theta_{n-d-1}\} \subset \Theta \subset \mathbb{Z}^n$$

generates through Eqs.(47) a velocity set

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

of a normal inelastic DVM.

Conversely, the total set Θ of reactions of any such DVM contains a certain well-defined set (50).

The above result solves, in principle, the problem of classification and construction of all normal DVMs for inelastic collisions.

Remark 2. Geometrically, any such model admits the 1-extension scheme (described in section 2.3), since one can always find three vertices (not all belonging to the same parallelogram of the model) and construct a new parallelogram with a new-added fourth vertex. The extended model is also normal (its parallelograms are independent).

We shall see below, when we discuss the elastic case for DVMs, that the problem of classification and construction becomes, by adding one more conservation law (energy conservation), more difficult to solve. We shall study in detail some properties of admissible (well-defined) sets of reactions and try to modify, using these properties, the algorithm of classification and construction of DVMs of the Boltzmann equation, in order to implement it.

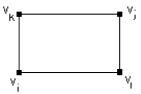
2.8 - DVMs of the Boltzmann equation

2.8.1 - Statement of the problem and geometrical interpretation

We consider the problem posed in section 2.7 with an additional restriction: any collision (reaction) (42) satisfies, besides the mass and momentum conservation, the energy conservation

(51)
$$|\mathbf{v}_i|^2 + |\mathbf{v}_j|^2 = |\mathbf{v}_k|^2 + |\mathbf{v}_l|^2$$
.

The collision (42) is, in such a case, elastic (satisfying (d+2) scalar conservation laws) and has as geometrical interpretation a rectangle in \mathbb{R}^d .



This justifies our assumptions that all indices i, j, k, l 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 (34)

(52)
$$\begin{cases} \mathbf{u}_a = (v_1^a, \dots, v_n^a), \ a = 1, \dots, d \\ \mathbf{u}_{d+1} = (|\mathbf{v}_1|^2, \dots |\mathbf{v}_n|^2) \\ \mathbf{w} = (1, \dots, 1) \text{ (universal invariant for } \boldsymbol{\Theta}). \end{cases}$$

Definition 9 of independence is the same for the case of rectangles. However, Definition 8 of non-degeneracy needs to be modified.

Definition 10. The phase set V (41) of an elastic DVM is said to be **non-degenerate** provided that the equalities

(53)
$$a + \mathbf{b} \cdot \mathbf{v}_k + c|\mathbf{v}_k|^2 = 0, \, \mathbf{b} \in \mathbb{R}^d, \, a, c \in \mathbb{R}, \, k = 1, \dots, n,$$

imply a = c = 0, $\mathbf{b} = 0$. Otherwise the set is said to be **degenerate**.

This means that we exclude two cases: (1) all velocities lying on a hyperplane $\mathbf{b} \cdot \mathbf{v} = const.$; (2) all velocities lying on a sphere $|\mathbf{v}|^2 = const.$ The case (1) can be reduced to the same problem, but in \mathbb{R}^{d-1} . For the case (2), it can be shown that the only class of normal elastic models on the sphere $S^{\widetilde{d}-1}$ (its radius can always be made 1) is the class of Broadwell-type models with $2\widetilde{d}$ velocities, $2 \leq \widetilde{d} \leq d$.

From now on we consider only non-degenerate models. Similarly to the inelastic case, we note that the normal DVMs of the Boltzmann equation represent sets of n points in \mathbb{R}^d which correspond to the maximal possible number (n-d-2) of independent rectangles. All such configurations are invariant under rotation, translation and scaling transformations (we obtain equivalent models). The DVMs with $n \in \{6,7\}$ velocities on the plane have some additional invariant transformations.

Hence, all normal DVMs of the Boltzmann equation can be geometrically described by certain configurations of n points in \mathbb{R}^d together with (n-d-2) independent rectangles connecting the points. In the inelastic case, one could always construct a new normal model by using the 1-extension scheme. This is not true in the elastic case (where parallelograms are replaced by rectangles). This means that we can not conclude automatically (as in the inelastic case, Proposition 1) that we have a one-to-one correspondence between well-defined sets of reactions and normal models. Moreover, as we shall see later, there are well-defined sets of reactions for which we can not construct a normal elastic model. Even if until now all known normal elastic models could be obtained by the 1-extension method, we wonder if we can not find normal models that are not 1-extentions. We shall try to do this by using a modified version of the general algorithm for DKMs (from section 2.6).

2.8.2 - Algorithm for the construction of elastic DVMs

Our goal is to describe and construct (if possible) all distinct non-degenerate normal DVMs for elastic collisions $\{V, \Lambda(V)\}$, where V (41) is the velocity set and $\Lambda(V)$ represents the set of reactions of the model, when the order $n \geq 4$, the dimension $d \geq 2$, the set of invariants (52) $\{\mathbf{w}, \mathbf{u}_a(V) : a = 1, \ldots, d+1\}$ and the maximal set Θ of reactions, are given.

The normal DVM has exactly p = d + 2 conservation laws

(54)
$$\begin{cases} \sum\limits_{k=1}^{n}N_{k}(t)=const.\in\mathbb{R}_{+}\\ \sum\limits_{k=1}^{n}N_{k}(t)\mathbf{v}_{k}=const.\in\mathbb{R}^{d}\\ \sum\limits_{k=1}^{n}N_{k}(t)|\mathbf{v}_{k}|^{2}=const.\in\mathbb{R}_{+}. \end{cases}$$

The set Θ of all possible vectors of reactions consists of vectors (43) and a set $\Lambda(V)$ of reactions must have (n-d-2) linearly independent vectors $\{\theta_1, \dots, \theta_{n-d-2}\} \subset \Theta$.

Following the general algorithm for the classification and construction of DKMs, we first consider the whole set of well-defined sets of reactions

(55)
$$\Lambda(V) = \{ \theta_i \subset \Theta, i = 1, \dots, n - d - 2 \}.$$

Then we construct all corresponding distinct subspaces of invariants U_1, \ldots, U_N (see Lemma 4) and, by taking them one by one, try to solve Eqs.(38) (with **w** (52) the universal invariant for Θ). If these equations have a solution, then we can construct our normal model. Otherwise we reject the subspace U_i and move further.

This theoretical algorithm needs to be slightly modified in order to implement it. That is why we are going to use, instead of the sets of reactions $\Lambda(V)$, the corresponding \widetilde{A} -matrices of reactions

(56)
$$\widetilde{\Lambda} = \begin{pmatrix} \theta_1(1) & \dots & \theta_1(n) \\ \dots & \dots & \dots \\ \theta_{n-d-2}(1) & \dots & \theta_{n-d-2}(n) \end{pmatrix}.$$

We need to introduce the following definition.

Definition 11. A matrix $\widetilde{\Lambda}$ (56) is said to be **well-defined** if the corresponding set of reactions Λ (55) is well-defined (as in Definition 7).

We can now rewrite the general algorithm in the following way.

Step 1. Generate all $(n-d-2) \times n$ $\widetilde{\Lambda}$ -matrices (56) having as rows (n-d-2) linearly independent vectors of type

$$(57) \quad \theta_a = (\ldots, \underbrace{1}_{i_a}, \ldots, \underbrace{1}_{j_a}, \ldots, \underbrace{-1}_{k_a}, \ldots, \underbrace{-1}_{l_a}, \ldots) \in \Theta, \ a = 1, \ldots, n - d - 2.$$

In addition, these matrices should be well-defined. To get such matrices, we add to \widetilde{A} a new row, containing one element 1, one element (-1) and the rest of the elements zero (all possible combinations), and then check if the new matrices have the rank equal to (n-d-1). For positive answer, we store the starting matrix \widetilde{A} .

The set $\widetilde{\Theta} = \left\{ \widetilde{\Lambda}_1, ..., \widetilde{\Lambda}_N \right\}$, of all generated matrices $\widetilde{\Lambda}$, is finite, since the set Θ is a finite set.

Step 2. For j = 1, ..., N do:

- $\circ \text{ Take } \widetilde{\Lambda} = \widetilde{\Lambda}_i \in \widetilde{\Theta};$
- $\circ\,$ Suppose that there exists a normal discrete DVM with the matrix $\widetilde{\varLambda}$ of reactions and denote by

(58)
$$X = (\mathbf{x}_1, ..., \mathbf{x}_n), \mathbf{x}_k \subseteq \mathbb{R}^d, k = 1, ..., n,$$

the vector of phase points of the model;

- Denote $\widetilde{X} = (|\mathbf{x}_1|^2, ..., |\mathbf{x}_n|^2);$
- o Check the solvability of the system

(59)
$$\begin{cases} \widetilde{\Lambda}X = \mathcal{O}_{(n-d-2)\times d} \\ \widetilde{\Lambda}\widetilde{X} = \mathcal{O}_{(n-d-2)\times 1} ,\end{cases}$$

where $\mathcal{O}_{i\times j}$ is the $(i\times j)$ null-matrix. The first equation has as motivation the momentum conservation, the second one, the energy conservation. Since the vector $\mathbf{w} = (1, ..., 1)$ is a universal invariant, orthogonal to every matrix of reactions \widetilde{A} , we do not need an extra equation for the mass conservation.

One way to check the solvability of the system (59) is the following.

From the equation $\widetilde{A}X = \mathcal{O}_{(n-d-2)\times d}$, where rank $\widetilde{A} = n-d-2$, we can express (n-d-2) variables through (d+2) parameters. Under certain numeration we obtain

(60)
$$\mathbf{x}_{k} = \sum_{a=n-d-1}^{n} a_{ka} \mathbf{x}_{a}, k = 1, \dots, n-d-2,$$

where a_{ka} are uniquely defined by the matrix $\widetilde{\Lambda}$, choice of *independent* variables $\{\mathbf{x}_{n-d-1},...,\mathbf{x}_n\}$ and given numeration.

Since we supposed that the model exists, we have that $|\mathbf{x}_i|^2$, i = 1, ..., n, satisfy Eqs. (60). Hence,

(61)
$$|\mathbf{x}_k|^2 = \sum_{a=n-d-1}^n a_{ka} |\mathbf{x}_a|^2, \ k = 1, \dots, n-d-2.$$

We know that

(62)
$$\sum_{a=n-d-1}^{n} a_{ka} = 1, k = 1, \dots, n-d-2,$$

since $\mathbf{w} = (1, ..., 1)$ is a solution to the system (60). We obtain the system of (n-d-2) equations

(63)
$$\left(\sum_{a=n-d-1}^{n} a_{ka} \mathbf{x}_{a}\right)^{2} = \sum_{a=n-d-1}^{n} a_{ka} |\mathbf{x}_{a}|^{2}, k = 1, \dots, n-d-2,$$

for (d+2)d scalar variables (components of the d-dimensional vectors $\{\mathbf{x}_{n-d-1},\ldots,\mathbf{x}_n\}\subseteq\mathbb{R}^d$). If the Eqs. (63) have a non-trivial solution, then we compute the vector of phase points (58) by Eqs. (60) and construct the normal model $(V, \Lambda(V))$, where

(64)
$$V = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subseteq \mathbb{R}^d \text{ with } X = (\mathbf{x}_1, \dots, \mathbf{x}_n), \mathbf{x}_k \subseteq \mathbb{R}^d, k = 1, \dots, n$$

and $\Lambda(V)$ is the set of reactions corresponding to the matrix $\widetilde{\Lambda}_j$. Otherwise, we reject the matrix $\widetilde{\Lambda}_j$.

 ${f 2.9}$ - Classification and construction of normal plane elastic models with small numbers of velocities

2.9.1 - Starting point
$$(n = 6)$$
 and 1-extension

We are going to study the particular case of plane elastic models with small numbers of velocities. It is already known that all quadratic DVMs are normal and that they can be obtained by the 1-extension method. We are now especially interested in the case of "reducible" non-quadratic models. Using geometrical arguments, we shall obtain all models up to 10 velocities, which are results of the 1-extension scheme. As we have seen before, from the geometrical point of view, we can represent a normal plane elastic model as a lattice of rectangles. The simplest model has six vertices (velocities) and two independent rectangles; for normal models, the number p of independent rectangles is given by the equality

$$p = n - d - 2$$
.

where n is the number of points and d is the dimension.

Definition 12. By a neighbour of a rectangle in a normal plane DVM, we understand any other independent rectangle in the model having at least a vertex in common with the initial rectangle.

Lemma 6. For any given rectangle in a normal model with n=6 velocities there exists only one neighbour of it; in a model with n=7 velocities there exist two neighbours of the given rectangle; in a normal model with $n \geq 8$ velocities there exist at least three neighbours of a given rectangle, except the case of a quadratic 8-velocity model of type (E) (see below) where there exist at least two neighbours.

Proof. We denote by

- $X_n = {\mathbf{x}_1, \dots \mathbf{x}_n} \subset \mathbb{R}^2$, the phase set of the model;
- $A = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\} \subset X_n$, the set of phase points that are vertices of some fixed rectangle belonging to the model with phase set X_n ;
 - o $B = X_n \setminus A$, the rest of the s = (n 4) vertices of the model;
- \circ R(B), the number of independent rectangles having as vertices only elements of B;
 - \circ R(AB), the number of neighbours of the fixed rectangle.

Since the model is normal, the total number of independent rectangles is

$$1 + R(B) + R(AB) = n - 4 = s$$
.

We need to evaluate the number R(AB) in order to prove our lemma. We have from the above relations

(65)
$$R(AB) = s - 1 - R(B) = n - 5 - R(B).$$

We study the following possible cases: (i) $s \le 3$; (ii) s = 4; (iii) $s \ge 5$.

Case (i). We have $n-4=s\leq 3$, which implies $n\in\{6,7\}$. Since $s\leq 3$ we have automatically that R(B)=0. Using the relation (65) we obtain R(AB)=n-5 and hence, R(AB)=1 if n=6 and R(AB)=2 if n=7.

Case (ii). Since s = 4, we obtain the necessary condition $R(B) \le 1$.

If R(B) = 0 then from (65) R(AB) = 3 and the result for n = 8 is proved.

Suppose now that R(B) = 1. This means that the 8 vertices of the model can be seen as two groups belonging to two different circles (if the circles are the same, the energy conservation is automatically fulfilled and we have degeneracy). Since s = 4 and R(B) = 1 we have in the model two independent rectangles: the set of vertices of rectangle(1) is A and for rectangle(2) is B. A normal model of order n = 8 has four independent rectangles and hence R(AB) = 2 (two independent rectangles neigh-

bours to the fixed rectangle(1)). It is clear that both these independent rectangles contain two velocities from the rectangle(1) and two velocities from the rectangle(2). Both these new rectangles can be constructed having as parallel sides:

- (a) one side of rectangle(1) and one side of rectangle(2);
- (b) one diagonal of rectangle(1) and one diagonal of rectangle(2);
- (c) one side of rectangle(1) and one diagonal of rectangle(2) (or vice versa).

Geometrically, all these cases can be rejected, except the last case side-diagonal which gives a normal quadratic model of type (E) (see below in Section 5.3.1, Fig. 3).

Hence, R(AB) = 3 for n = 8, except the particular case of the quadratic model (E).

Case (iii). To this case belong the models with $n \geq 9$ velocities, since $s \geq 5$. We rewrite Eq. (65) as

$$R(AB) = 3 + (s - 4 - R(B)).$$

If $R(B) \le 1$, then $R(AB) \ge 3 + (s - 5) \ge 3$ and the lemma is proved.

Suppose now that $R(B) \geq 2$. Then the model has at least two independent rectangles with all vertices in B. Since the set B contains s vertices, the number of independent rectangles we can construct with vertices from B is less or equal to (s-4), if B is non-degenerate. In this case, we obtain the necessary condition $(s-4) \geq R(B) \geq 2$, which implies that $(s-4-R(B)) \geq 0$. Hence, $R(AB) \geq 3$ and the lemma is proved.

We study now the case when $R(B) \geq 2$ and B is degenerate (all points are lying on a line or a circle). The case when the points are lying on a line is impossible, since then we have two independent reactions on a straight line.

Let us study the case when all s points of B are lying on a circle. Assume that there exist q free points (not participating in any reaction) in B. It is clear that the number of the other points in B must be even (every rectangle has as diagonals diameters of the circle). We fix a rectangle on the circle. One can prove that to get N more independent reactions, one need to add 2N particles. We fix one reaction on the circle. If we want one more reaction we need to add two more particles (the number of new reactions N=1, the number of added particles 2N=2); if we now add two more particles we get formally three rectangles, but only two of them are independent (the number of new reactions is N=2, the number of added particles is 2N=4); by induction one can prove that this is true for any N.

We have the total number of reactions in B given by R(B)=N+1, with $N\geq 1$ (because $R(B)\geq 2$). The number of particles in B is s=4+2N+q. Hence, $(s-4-R(B))=N-1+q\geq 0$ and from Eq. (65), $R(AB)\geq 3$.

The lemma is proved.

Lemma 7. All 6-velocity normal models contain two independent rectangles having two vertices in common.

Proof. Suppose the contrary. We know that a 6-velocity normal model has p=6-4=2 independent rectangles. From Lemma 6 we know that a given rectangle in a 6-velocity normal model has exactly one neighbour. This means that the two independent rectangles have at least one vertex and at most two vertices in common. From our supposition they can have only one common vertex. Then the $\widetilde{\Lambda}$ -matrix corresponding to the model can be arranged in the following form

where the first line represents a fixed reaction (\blacksquare -symbol is a non-zero element of the row, belonging to the set $\{\pm 1\}$; every row is a vector of type θ^{\perp} from (57)). In the second row we can take a non-zero element in one of the first four positions (so we get a vertex in common): for example in the first column. Since there can not be two vertices in common, we are forced to put zeros in the next three columns. This leaves only two free places for the other three non-zeros of the second row, so the model is impossible to construct. Our supposition is false and the lemma is proved.

This result leads to all possibilities for plane 6-velocity normal models:

- (a) two rectangles that share one side;
- (b) two rectangles such that one diagonal in the first rectangle is a side in the second one;
 - (c) two rectangles that share one diagonal.

The last case (common diagonal) is forbidden since all velocities lie on a circle $(1,\mathbf{v},|\mathbf{v}|^2)$ are linearly dependent) and the conservation of energy is automatically fulfilled. Hence, the only possible cases for n=6 are illustrated in Fig. 1. All other possibilities are obtained by translation, rotation or scaling. The models have, as free parameters, the angles t and s, 0 < t, $s < \frac{\pi}{2}$ (to be able to plot, we fix these parameters in Fig. 1).

Definition 13. Two Λ -matrices are said to be **equivalent** if they correspond to two equivalent normal models (in the sense of Definition 5).

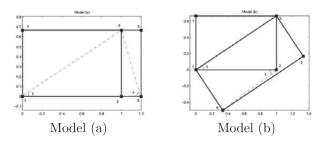


Fig. 1. All 6-velocity normal models.

To a normal DVM it can be put in correspondence a class of equivalent $\widetilde{\Lambda}$ -matrices. The corresponding $\widetilde{\Lambda}$ -matrices for the above two cases are

$$\begin{split} \widetilde{\varLambda}_{(a)} &= \begin{pmatrix} 1 & -1 & 1 & -1 & 0 & 0 \\ 1 & 0 & 0 & -1 & 1 & -1 \end{pmatrix}, \\ \widetilde{\varLambda}_{(b)} &= \begin{pmatrix} 1 & -1 & 1 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 & 1 & -1 \end{pmatrix}, \end{split}$$

and all matrices equivalent with $\widetilde{\Lambda}_{(a)}$ and $\widetilde{\Lambda}_{(b)}$, in the sense of Definition 13.

Using the 1-extension method for the construction of normal models (section 2.3), we can start with the simplest normal model (in our case with n=6) and add one more velocity such that the new point is a vertex of some new independent rectangle. By Lemma 1, we obtain a new normal model. If we approach the problem in this way, using only geometrical arguments and checking the rule for the number of independent rectangles, we get the complete results for 1-extensions.

We start from a 6-velocity model, given in the above figures, (a) or (b), with the angles t and s as free parameters. We add a new velocity such that the new model is normal (a 7-velocity model with 3 independent rectangles). The only possible cases for n=7 are illustrated in Fig. 2 (we fix the parameter t, to be able to plot).

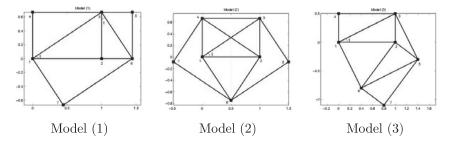


Fig. 2. All 7-velocity normal models.

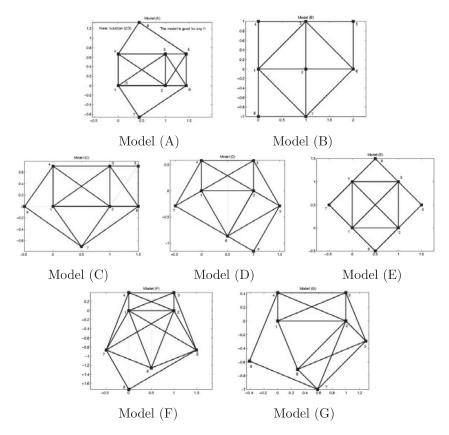


Fig. 3. All 8-velocity normal models.

Knowing all 7-velocity models obtained by the 1-extension method, we try to add a new velocity in order to get 8-velocity normal models (with 4 independent rectangles). We have 7 possible cases for n=8 (illustrated in Fig. 3). Model (A) has a free parameter t (to plot the model we fix the free parameter $t=\arctan 2/3$). The other models do not have free parameters. Model (B) and (E) have $t=\frac{\pi}{4}$. Model (C)

$$\text{has } t = \arctan \frac{1}{\sqrt{2}}, \text{model } (D) \text{ has } t = \frac{\pi}{6}, \text{model } (F) \text{ has } t = \arctan \left(\frac{\sqrt{11}-\sqrt{3}}{4}\right) \text{ and } \\ \text{model } (G) \text{ has } t = \frac{\pi}{8}.$$

The next natural step is to find all 9-velocity models obtained by 1-extensions. We try to add one new velocity to the 8-velocity models obtained above. This time, we construct models with five independent rectangles. All 6 possible models (illustrated in Fig. 4) do not have free parameters. Model (i) and (ii) have $t=\frac{\pi}{4}$, model (iii) and

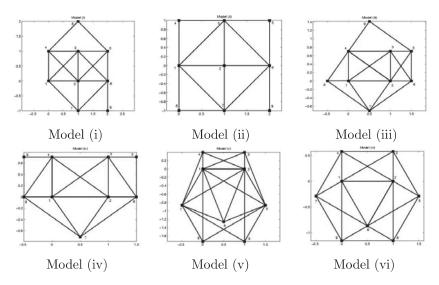


Fig. 4. All 9-velocity normal models: 1-extensions.

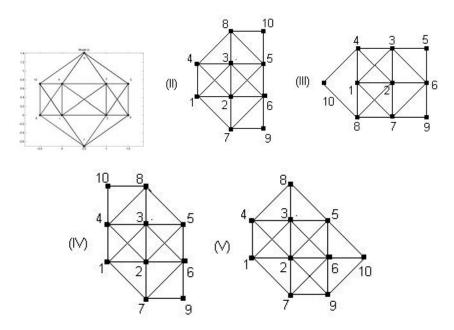


Fig. 5. All 10-velocity normal models: 1-extensions.

$$\begin{array}{l} (iv) \text{ has } t = \arctan \frac{1}{\sqrt{2}}, \text{ model } (v) \text{ has } t = \arctan \left(\frac{\sqrt{11}-\sqrt{3}}{4}\right) \text{ and model } (vi) \text{ has } t = \frac{\pi}{6}. \end{array}$$

The only left 9-velocity models which admit 1-extension are the models (i), (ii), (iii) and (iv). Their extensions are given in Fig. 5. Model (I) does not admit further 1-extension, but the quadratic models admit 1-extensions in infinitely many steps.

2.9.2 - Classification results for $n \in \{7,8\}$

We have described in the previous section all reducible normal models with n=7 and n=8 (results of the 1-extension scheme). We wonder now, if there exist other normal models with n=7 and n=8 which are irreducible.

We can arrange the corresponding $\widetilde{\Lambda}$ -matrix of any normal model in the special equivalent table-form, described below.

	1					0		0
	- 1		*	*	*	*		*
(67)		0		*	*	*		*
(01)		0	0		*	*		*
	- (0	0	0		*		*
	- (0	0	0	0	*		*

- first we rearrange the matrix \widetilde{A} (if needed) in order to obtain a row that has all its four non-zeros in the first four columns: denote the new matrix by \overline{A} (we can always interchange columns and get an equivalent matrix);
- every line of the above table can contain more than one row of the matrix $\overline{\Lambda}$ (vectors of type θ^{\perp} (43));
 - every column of the table contains exactly one column of the matrix $\overline{\Lambda}$;
- first line contains only one row of the matrix \overline{A} having in the first four columns all its non-zeros $\{1, 1, -1, -1\}$ (because of the first step, this row exists);
- the " \blacksquare "-symbol is a non-zero element of the row, belonging to the set $\{\pm 1\}$ (or a vector of non-zeros, if the line of the table contains more then one row of the matrix);
- the "*"-symbol stands for the elements of a line left after we filled the positions we know; it can contain an element belonging to the set $\{0,\pm 1\}$ (or a vector of such elements).
- the second line contains all $k_1 \geq 0$ rows of $\overline{\Lambda}$, left after we wrote the first line, having a non-zero element in the first column;
- the third line contains all $k_2 \ge 0$ rows of \overline{A} , left after we wrote the two first lines of the table, having a non-zero element in the second column;

- the fourth line contains all $k_3 \geq 0$ rows of \overline{A} , left after we wrote the first three lines of the table, having a non-zero element in the third column;
- the fifth line contains all $k_4 \geq 0$ rows of $\overline{\Lambda}$, left after we wrote the first four lines of the table, having a non-zero element in the fourth column;
- the last line of the table contains all left $m_1 \ge 0$ rows (these rows will have only zeros in the first four columns);
- we have $1 + (k_1 + k_2 + k_3 + k_4) + m_1 = n 4$ (if the model has order n and dimension d = 2).

Remark 3. The rectangles given by the rows k_1, k_2, k_3, k_4 represent all the neighbours of the rectangle given in the first line of the table and because of Lemma 7 we have that for n > 8

$$k_1 + k_2 + k_3 + k_4 \ge 3$$
,

except for the particular case of the quadratic 8-velocity normal model (E), Fig. 3.

Lemma 8. All normal models of order n = 7 or n = 8 contain a 6-velocity normal model (in other words, two independent rectangles having two vertices in common).

Proof. (a) n = 7: We suppose the contrary. We can arrange the corresponding $\tilde{\Lambda}$ -matrix of the model using the special form (67) as

We are forced, because of our supposition (not two vertices in common), to replace "*" in the columns 2,3,4 of (67) by zeros. Since we have four non-zero elements in each row, we need to fill the rest of the columns, with non-zero elements.

The matrix Λ has only three rows (n=7), so it fulfills the condition

$$(69) k_1 + k_2 + k_3 + k_4 + m_1 = 2.$$

From the table (68) we notice that $m_1 = 0$ is a necessary condition (we get only three non-zero elements in a reaction). Then $k_1 + k_2 + k_3 + k_4 = 2$, so there are two rows having three common non-zero elements (in other words they describe the same reaction). This is a contradiction since all rows should describe linearly independent reactions. Hence, our supposition for n = 7 was false and the lemma is proved in this case.

(b) n=8: For the quadratic models it is known that all 8-velocity normal model contain a 6-velocity normal model. Thus, it only remains to prove the lemma for the non-quadratic models.

We suppose the contrary. Then we can write the corresponding $\widetilde{\Lambda}$ -matrix of the model, using the special form (67), as

To obtain (70) we used the assumption that there are not two vertices in common. Since the matrix $\widetilde{\Lambda}$ has only four rows (n=8), it fulfills the condition

$$k_1 + k_2 + k_3 + k_4 + m_1 = 3.$$

But we have that $k_1 + k_2 + k_3 + k_4 \ge 3$ (Remark 3).

Hence,
$$m_1 = 0$$
 and $k_1 + k_2 + k_3 + k_4 = 3$.

In the last three rows, all possible combinations for arranging the left non-zeros, lead to at least two non-zeros in common for two different rows. Hence, our supposition is false and the lemma is proved.

With the help of Lemma 8 we can now prove the following theorem.

Theorem 2. All normal models of order n = 7 and n = 8 are 1-extensions of models of order n = 6 and n = 7, respectively.

Proof. We treat the two cases separately.

- (a) n = 7: We proved that all normal models with n = 7 velocities contain a 6-velocity normal model. Hence they are all 1-extensions.
- (b) n=8: We proved that all normal models with n=8 velocities contain a 6-velocity normal model. If they all contain a 7-velocity normal model, then the theorem is true.

Suppose that there exist normal models with n=8 velocities, obtained as 2-extensions of a 6-velocity normal model. Then the corresponding \widetilde{A} -matrix of the model has at least two non-zero elements in all columns (otherwise the model is reducible to a 7-velocity normal model).

Case 1. The model contains a 6-velocity model of type (a). The corresponding \widetilde{A} -matrix is given by

$$\begin{pmatrix} 1 & -1 & 1 & -1 & 0 & 0 \\ 1 & 0 & 0 & -1 & 1 & -1 \end{pmatrix},$$

(all other models of this type lead to matrices which are equivalent with $\widetilde{\Lambda}$, in the sense of Definition 13).

Then the matrix corresponding to the 8-velocity model has the form (we now use the normal way to write a matrix)

$$\begin{pmatrix}
1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & -1 & 1 & -1 & 0 & 0 \\
0 & * & * & 0 & * & * & \blacksquare & \blacksquare \\
0 & * & * & 0 & * & * & \blacksquare & \blacksquare
\end{pmatrix}$$

Since we (by our supposition) cannot have a column with only one non-zero, we are forced to put non-zeros in the last two columns (last two rows). We also need to have at least one more non-zero in columns 2,3,5 and 6. Since for each of the last two rows we have available only two more non-zeros, we need to put zero in columns 1 and 4, in the last two rows. These arguments explain the form (71). Noting that by interchanging two rows or multiplying them with (-1) or interchanging two columns in the matrix of reactions, we obtain the same model, we have the following possible matrices for the 8-velocity normal model in **Case 1**.

/	1	-1	1	-1	0	0	0	0	Λ	
(79)	1	0	0	-1	1	-1	0	0		
(72)	0	0		0		0				,
(0		0	0	0				V	

or

/	1	-1	1	-1	0	0	0	0	1	
(73)	1	0	0	-1	1	-1	0	0	П	
(19)	0			0	0	0			П	,
/	0	0	0	0					/	

or

1	1	-1	1	-1	0	0	0	0	Λ	
(74)	1	0	0	-1	1	-1	0	0		
(14)	0		0	0		0				•
/	0	0		0	0				/	

Using geometrical arguments, one can prove that all these three cases are impossible (we remember the reader that " \blacksquare " symbolizes a non-zero element belonging to the set $\{\pm 1\}$).

Case (72): If we denote by (i,j,k,l) a reaction of the model (where i,j,k,l are the positions, in the vector of reaction, containing the non-zeros), then the last two reactions are (3,5,7,8) and (2,6,7,8) and the first two reactions are given in the 6-velocity model of type (a). Suppose that the last two reactions are possible. Then (3,5) and (2,6) are either both sides or diagonals or one is a diagonal and the other one is a side of their corresponding rectangles (by (i,j)) we mean the segment connecting the vertices i and j). In the first situation, we can construct two such rectangles, but the 8-velocity models will not be normal since they will contain only three independent rectangles, instead of four. In the second situation, if both are diagonals they intersect the diagonal (7,8) in its middle point and hence, they have a point in common, which is false, since they are parallel (see Model (a)). The last possibility is not working either (we have (3,5) and (2,6) parallel, and (7,8) is parallel with one of them and intersect the other one).

Case (73): The last two reactions are (2,3,7,8) and (5,6,7,8). We can easily prove, using similar arguments as for case (72), that they are impossible.

Case (74): The last two reactions are (2,5,7,8) and (3,6,7,8). The segments (2,5) and (3,6) are diagonals in the rectangle (2,3,5,6). This means that they cannot be both sides in the rectangles (2,5,7,8) and (3,6,7,8), since this leads to that (2,5) is parallel with (3,6). They cannot both be diagonals in these two rectangles since then the model will have only three independent rectangles instead of four. If one of (2,5) and (3,6) is a diagonal in the new rectangles, then it intersects (7,8) in the middle point and hence, (7,8) intersects the other one also in the middle point, so the case when one is a diagonal and the other one is a side is excluded.

Case 2. Can be treated in a similar way as Case 1 (see for details [22]).

Since we proved that all normal models of order n=7 and n=8 are 1-extensions and in the previous section we described all these models, we have now a complete image over the case of normal plane elastic models of order n=7 and n=8.

2.9.3 - Algorithm for normal plane elastic models with small numbers of velocities

We start by proving a result that will enable us to give a more explicit algorithm for the construction of elastic plane normal discrete models, based on the general algorithm, given in section 2.8.

Lemma 9. Let (1) + (2) = (3) + (4) be one reaction (a rectangle, geometrically) of a normal model $\{V, \Lambda(V)\}$, with V from (64). Then there exists $\delta \in \mathbb{N}$, $5 \leq \delta \leq n$, such that

(75)
$$\mathbf{x}_k = (a_{k1}\mathbf{x}_1 + a_{k2}\mathbf{x}_2 + a_{k3}\mathbf{x}_3 + a_{k\delta}\mathbf{x}_{\delta}) \in \mathbb{R}^2, \text{ for all } k = 1, ..., n,$$
where

(76)
$$\begin{cases} a_{ka} = \delta_{ka}, a = 1, 2, 3, \delta \\ a_{4\delta} = 0 \\ a_{41} = a_{42} = -a_{43} = 1 \end{cases}$$

(we remind that $\delta_{ka} = \begin{cases} 1 & \text{if } k = a \\ 0, & \text{otherwise} \end{cases}$; we have used for the last coefficients the fact that $\mathbf{x}_1 + \mathbf{x}_2 = \mathbf{x}_3 + \mathbf{x}_4$); i.e. all velocities of a model can be expressed by a linear combination of three velocities belonging to a fixed reaction, and a fourth velocity from a different reaction.

Proof. From the system

(77)
$$\theta_a X = 0 , a = 1, \dots, n-4,$$

with θ_a $(a=1,\ldots,n-4)$ from (57), linearly independent, and X from (58), there exist $1 \le a, \beta, \gamma, \delta \le n$ all different such that

$$\mathbf{x}_k = A_{ka}\mathbf{x}_a + A_{k\beta}\mathbf{x}_\beta + A_{k\nu}\mathbf{x}_\nu + A_{k\delta}\mathbf{x}_\delta , k = 1, \dots, n.$$

 (a_1) If $1 \in \{a, \beta, \gamma, \delta\}$, and (without loss of generality we can let) a = 1, then

$$\mathbf{x}_k = A_{k1}\mathbf{x}_1 + A_{k\beta}\mathbf{x}_{\beta} + A_{k\gamma}\mathbf{x}_{\gamma} + A_{k\delta}\mathbf{x}_{\delta}, k = 1, ..., n.$$

 (a_2) Else

$$\mathbf{x}_1 = A_{1a}\mathbf{x}_a + A_{1\beta}\mathbf{x}_{\beta} + A_{1\gamma}\mathbf{x}_{\gamma} + A_{1\delta}\mathbf{x}_{\delta},$$

with at least two coefficients from $A_{1a}, A_{1\beta}, A_{1\gamma}, A_{1\delta}$ different of zero, since $A_{1a} + A_{1\beta} + A_{1\gamma} + A_{1\delta} = 1$ from Eq. (62) and since, if we consider for example only $A_{1a} \neq 0$, then $\mathbf{x}_1 = A_{1a}\mathbf{x}_a$ implies $A_{1a} = 1$, and $\mathbf{x}_1 = \mathbf{x}_a$. This contradicts our supposition that all numbers a, β, γ, δ are different of 1. Without loss of generality, we can assume that $A_{1a} \neq 0$. Then \mathbf{x}_a can be expressed as

$$\mathbf{x}_{a} = A_{a1}^{'} \mathbf{x}_{1} + A_{a\beta}^{'} \mathbf{x}_{\beta} + A_{a\gamma}^{'} \mathbf{x}_{\gamma} + A_{a\delta}^{'} \mathbf{x}_{\delta}.$$

Hence,

$$\mathbf{x}_k = A_{k1}^{''}\mathbf{x}_1 + A_{k\beta}^{''}\mathbf{x}_\beta + A_{k\gamma}^{''}\mathbf{x}_\gamma + A_{k\delta}^{''}\mathbf{x}_\delta , \ k = 1,\ldots,n.$$

In both cases (a_1) and (a_2) we have $\mathbf{x}_k \in \text{Span } \{\mathbf{x}_1, \mathbf{x}_{\beta}, \mathbf{x}_{\gamma}, \mathbf{x}_{\delta}\}$ for all $k = 1, \ldots, n$. We denote by B_{kj} , the coefficients A_{kj} or A''_{kj} , $j \in \{1, \beta, \gamma, \delta\}$, from the cases (a_1) or (a_2) , respectively.

 (b_1) If $2 \in \{\beta, \gamma, \delta\}$, for example $\beta = 2$, then

$$\mathbf{x}_k = B_{k1}\mathbf{x}_1 + B_{k2}\mathbf{x}_2 + B_{k\nu}\mathbf{x}_{\nu} + B_{k\delta}\mathbf{x}_{\delta} , k = 1, \dots, n.$$

 (b_2) If $2 \notin \{\beta, \gamma, \delta\}$), then

$$\mathbf{x}_2 = B_{21}\mathbf{x}_1 + B_{2\beta}\mathbf{x}_{\beta} + B_{2\gamma}\mathbf{x}_{\gamma} + B_{2\delta}\mathbf{x}_{\delta}.$$

Suppose that $B_{2\beta}=B_{2\gamma}=B_{2\delta}=0$. From $B_{21}+B_{2\beta}+B_{2\gamma}+B_{2\delta}=1$ (see Eq. (62)), we get $B_{21}=1$ and hence, $\mathbf{x}_1=\mathbf{x}_2$ (contradiction to the supposition that $\mathbf{x}_1,\mathbf{x}_2$ belong to the same reaction). This means that at least one of $B_{2\beta},B_{2\gamma},B_{2\delta}$ is non-zero, for example $B_{2\beta}\neq 0$. We can now express \mathbf{x}_β as a linear combination of $\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_\gamma,\mathbf{x}_\delta$. Hence, we can write

$$\mathbf{x}_{k} = B'_{k1}\mathbf{x}_{1} + B'_{k2}\mathbf{x}_{2} + B'_{k\gamma}\mathbf{x}_{\gamma} + B'_{k\delta}\mathbf{x}_{\delta}, k = 1, \dots, n.$$

In both cases (b_1) and (b_2) we have $\mathbf{x}_k \in \text{Span } \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_{\gamma}, \mathbf{x}_{\delta}\}$ for all k = 1, ..., n. We denote by C_{kj} , $j \in \{1, 2, \gamma, \delta\}$ the coefficients B_{kj} or B'_{kj} , from the cases (b_1) or (b_2) , respectively.

 (c_1) If $3 \in {\gamma, \delta}$, for example $\gamma = 3$, then

$$\mathbf{x}_k = C_{k1}\mathbf{x}_1 + C_{k2}\mathbf{x}_2 + C_{k3}\mathbf{x}_3 + C_{k\delta}\mathbf{x}_{\delta}, \ k = 1, \dots, n.$$

 (c_2) Else

$$\mathbf{x}_3 = C_{31}\mathbf{x}_1 + C_{32}\mathbf{x}_2 + C_{3\nu}\mathbf{x}_3 + C_{3\delta}\mathbf{x}_{\delta}.$$

If $C_{3\gamma} = C_{3\delta} = 0$ we obtain using (62)

$$C_{31} + C_{32} = 1 \stackrel{C_{31} = a}{\Longrightarrow} C_{32} = 1 - a$$

and in this case

$$\mathbf{x}_3 = a\mathbf{x}_1 + (1-a)\mathbf{x}_2.$$

We get $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ collinear. But these velocities belong to a reaction of the model (which, from geometrical point of view is a rectangle) and thus, this case is impossible. Hence, at least one of the coefficients $C_{3\gamma}, C_{3\delta}$ is different of zero. We can take, for example, $C_{3\gamma} \neq 0$. We express \mathbf{x}_{γ} as a linear combination of $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_{\delta}$ and obtain

$$\mathbf{x}_{k} = C'_{k1}\mathbf{x}_{1} + C'_{k2}\mathbf{x}_{2} + C'_{k3}\mathbf{x}_{3} + C'_{k\delta}\mathbf{x}_{\delta}, k = 1, \dots, n.$$

In both cases (c_1) and (c_2) we have $\mathbf{x}_k \in \text{Span } \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_\delta\}$ for all k = 1, ..., n. We denote the coefficients C_{kj} (or C'_{kj}), $j \in \{1, 2, 3, \delta\}$ by $a_{k1}, a_{k2}, a_{k3}, a_{k\delta}$, respectively. Then

(78)
$$\mathbf{x}_{k} = a_{k1}\mathbf{x}_{1} + a_{k2}\mathbf{x}_{2} + a_{k3}\mathbf{x}_{3} + a_{k\delta}\mathbf{x}_{\delta}, k = 1, \dots, n,$$

with

$$(79) a_{k1} + a_{k2} + a_{k3} + a_{k\delta} = 1$$

and x_1, x_2, x_3 belonging to the same reaction and x_δ to another one (if $x_\delta = x_4$, since $x_4 \in \text{Span } \{x_1, x_2, x_3\}$ we get

$$\mathbf{x}_{k} = a'_{k1}\mathbf{x}_{1} + a'_{k2}\mathbf{x}_{2} + a'_{k3}\mathbf{x}_{3}, \ k = 1, \dots, n,$$

which contradicts the fact that the system (77) has four free parameters) and the lemma is proved.

From Lemma 9 we have that the solution of the system $\widetilde{A}X = 0$ can be written in the form (78), with coefficients fulfilling (79).

Because of the invariance under translation, rotation and scaling transformations, we can take

(80)
$$\begin{cases} \mathbf{x}_{1} = (0,0) \\ \mathbf{x}_{2} = (1,0) = \mathbf{e}_{1} \\ \mathbf{x}_{3} = (1,\theta) \\ \mathbf{x}_{4} = (0,\theta) = \theta \mathbf{e}_{2}, \theta \in \mathbb{R}_{+} \\ \mathbf{x}_{\delta} = (x,y) \notin \{\mathbf{x}_{1}, \mathbf{x}_{2}, \mathbf{x}_{3}\} \end{cases}$$

Hence, the solution has the general form

(81)
$$\mathbf{x}_k = a_k \mathbf{e}_1 + b_k \theta \mathbf{e}_2 + c_k \mathbf{x}_{\delta}, \ k = 1, \dots, n,$$

where a_k, b_k, c_k are real constants. One can prove that $\mathbf{x}_{\delta} = (x, y)$ fulfills an additional restriction

(82)
$$\left(x - \frac{1}{2}\right)^2 + \left(y - \frac{\theta}{2}\right)^2 \neq \frac{1 + \theta^2}{4},$$

i.e. it does not lie on the circle circumscribing the triangle having as vertices the points $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ from (80).

The system (59) given in the general algorithm in section 2.8, will be replaced,

using the Eq. (63) by

$$\begin{cases} \mathbf{x}_{1} = (0,0) \\ \mathbf{x}_{2} = (1,0) = \mathbf{e}_{1} \\ \mathbf{x}_{3} = (0,\theta) = \theta \mathbf{e}_{2}, \theta \in \mathbb{R}_{+} \\ \mathbf{x}_{4} = (1,\theta) \\ \mathbf{x}_{\delta} = (x,y) \notin \{\mathbf{x}_{1},\mathbf{x}_{2},\mathbf{x}_{3}\}; \ \mathbf{x}_{\delta} \text{fulfills (82)} \\ \mathbf{x}_{k} = a_{k}\mathbf{e}_{1} + b_{k}\theta\mathbf{e}_{2} + c_{k}\mathbf{x}_{\delta}, \ k \in \{5,\dots,n\} \setminus \{\delta\} \\ \widetilde{A}X = 0 \\ (a_{k}^{2} - a_{k}) + (b_{k}^{2} - b_{k})\theta^{2} + (c_{k}^{2} - c_{k})(x^{2} + y^{2}) + 2a_{k}c_{k}x + 2b_{k}c_{k}\theta y = 0 \\ \text{for all } k \in \{5,\dots,n\} \setminus \{\delta\} \end{cases}$$

If this system admits a non-trivial solution $(\theta, x, y, a_k, b_k, c_k : k \ge 6)$, then we can find the normal model $\{V, \Lambda(V)\}$, with

$$V = {\mathbf{x}_1, ..., \mathbf{x}_n} \subseteq \mathbb{R}^2$$

and we can construct it.

We try to improve the form of the system (83) by proving the following lemma.

Lemma 10. All normal models of order $n \in \{9,10\}$ contain a 6-velocity normal model (in other words, two independent rectangles having two vertices in common).

Proof. (a)We suppose that the normal models of order n=9 do not contain two independent rectangles having two vertices in common. In this case, using the special representation (67), we can write the corresponding matrix of reactions of the model as

We know that for a normal model with n = 9 velocities we have

$$1 + (k_1 + k_2 + k_3 + k_4) + m_1 = 5$$

and we proved in Lemma 7 (see Remark 3) that $(k_1 + k_2 + k_3 + k_4) \ge 3$. Hence,

 $m_1 \leq 1$. We have the following possibilities:

$$(a_1) m_1 = 1 \Longrightarrow k_1 + k_2 + k_3 + k_4 = 3.$$

In this case, the last row has four non-zero elements on the last five free positions. The above three rows have three non-zero elements in the last five free positions. We cannot arrange the non-zero elements such that, in two different rows, there are not two columns with non-zero elements (in both rows). Hence, we get two vertices in common in two different independent rectangles.

$$(a_2) m_1 = 0 \Longrightarrow k_1 + k_2 + k_3 + k_4 = 4.$$

In each of last four rows there are three non-zero elements, arranged in the last five free positions of the rows. All possibilities to arrange the non-zero elements lead to contradictions of our supposition. Hence, the lemma is true for n = 9.

(b)
$$n = 10$$
: similar proof as in the case $n = 9$ (see for details [22])

Lemma 8 and Lemma 10 imply that, for the cases $n \in \{8, 9, 10\}$, in the system (83) the vector $\mathbf{x}_{\delta} = (x, y)$ can be taken as a vertex in a rectangle, neighbour to the initial rectangle (with vertices $(0, 0), (1, 0), (1, \theta), (0, \theta)$), such that it has as first common vertex (0, 0) and as a second common vertex

- (i) $(0, \theta)$: in this case $\mathbf{x}_{\delta} = (y, 0) = (\mu, 0)$ (the model contains a 6-velocity model of type (a));
- (ii) $(1,\theta)$: in this case $\mathbf{x}_{\delta} = (-y\theta,y) = (-\mu\theta,\mu)$ (the model contains a 6-velocity model of type (b)).

If we take as the second common vertex (1,0), then $\mathbf{x}_{\delta} = (0,y)$, and we obtain an equivalent model to the one in case (i), due to the invariance under rotation and scaling. The point \mathbf{x}_{δ} fulfills in both cases the condition (82).

The system (83) will now have the following two forms

Case
$$(i)$$
:

(85)
$$\begin{cases} \mathbf{x}_{1} = (0,0) \\ \mathbf{x}_{2} = (1,0) = \mathbf{e}_{1} \\ \mathbf{x}_{3} = (1,\theta) \\ \mathbf{x}_{4} = (0,\theta) = \theta \mathbf{e}_{2}, \theta \in \mathbb{R}_{+} \\ \mathbf{x}_{5} = (\mu,\theta) \\ \mathbf{x}_{6} = (\mu,0), \mu \in \mathbb{R} \setminus \{0,1\} \\ \mathbf{x}_{k} = a_{k} \mathbf{e}_{1} + b_{k} \theta \mathbf{e}_{2} + c_{k}(\mu,0), \ k = 7, \dots, n \\ \widetilde{A}X = 0, \ X = (\mathbf{x}_{1}, \dots, \mathbf{x}_{n}), \ \mathbf{x}_{k} \in \mathbb{R}^{2}, \ k = 1, \dots, n \\ (a_{k}^{2} - a_{k}) + (b_{k}^{2} - b_{k})\theta^{2} + (c_{k}^{2} - c_{k})\mu^{2} + 2a_{k}c_{k}\mu = 0, \\ \text{for all } k = 7, \dots, n. \end{cases}$$

Case (ii):

(86)
$$\begin{cases} \mathbf{x}_{1} = (0,0) \\ \mathbf{x}_{2} = (1,0) = \mathbf{e}_{1} \\ \mathbf{x}_{3} = (1,\theta) \\ \mathbf{x}_{4} = (0,\theta) = \theta \mathbf{e}_{2}, \theta \in \mathbb{R}_{+} \\ \mathbf{x}_{5} = (1 - \mu\theta, \theta + \mu) \notin \{x_{i}, i < 6\} \\ \mathbf{x}_{6} = (-\mu\theta, \mu) \notin \{x_{i}, i < 5\}, \mu \in \mathbb{R} \setminus \{0\} \\ \mathbf{x}_{k} = a_{k}\mathbf{e}_{1} + b_{k}\theta\mathbf{e}_{2} + c_{k}(-\mu\theta, \mu), \ k = 7, \dots, n \\ \widetilde{A}X = 0, \ X = (\mathbf{x}_{1}, \dots, \mathbf{x}_{n}), \ \mathbf{x}_{k} \in \mathbb{R}^{2}, \ k = 1, \dots, n \\ (a_{k}^{2} - a_{k}) + (b_{k}^{2} - b_{k})\theta^{2} + (c_{k}^{2} - c_{k})\mu^{2}(1 + \theta^{2}) + 2c_{k}(b_{k} - a_{k})\mu\theta = 0, \\ \text{for all } k = 7, \dots, n. \end{cases}$$
Trying to implement the algorithm, using the above systems, we realize that easier to use the systems (85) and (86) in the equivalent forms given below

Trying to implement the algorithm, using the above systems, we realize that it is easier to use the systems (85) and (86) in the equivalent forms given below.

Case (i):

(87)
$$\begin{cases} \mathbf{x}_{1} = (0,0) \\ \mathbf{x}_{2} = (1,0) = \mathbf{e}_{1} \\ \mathbf{x}_{3} = (1,\theta) \\ \mathbf{x}_{4} = (0,\theta) = \theta \mathbf{e}_{2}, \theta \in \mathbb{R}_{+} \\ \mathbf{x}_{5} = (\mu,\theta) \\ \mathbf{x}_{6} = (\mu,0), \mu \in \mathbb{R} \setminus \{0,1\} \\ \mathbf{x}_{k} = (a'_{k},b'_{k}), k = 7, \dots, n \\ \widetilde{A}X = 0, X = (\mathbf{x}_{1},\dots,\mathbf{x}_{n}), \mathbf{x}_{k} \in \mathbb{R}^{2}, k = 1,\dots, n \\ \widetilde{A}\widetilde{X} = 0, \widetilde{X} = (|\mathbf{x}_{1}|^{2},\dots,|\mathbf{x}_{n}|^{2}). \end{cases}$$

Case (ii): system (87) with modified $\mathbf{x}_5 = (1 - \mu\theta, \theta + \mu), \ \mathbf{x}_6 = (-\mu\theta, \mu), \mu \in$ $\mathbb{R}\setminus\{0\}.$

Since for $n \in \{7, 8, 9, 10\}$ all normal models have a corresponding $((n-4) \times n)$ matrix Λ which contains a 6-velocity model (of type (a) or type (b)), and since by interchanging rows or columns, we get an equivalent matrix to the initial one, we can state that all matrices corresponding to normal models of order n have one of the following two forms

(88)
$$\widetilde{\Lambda} = \begin{pmatrix} 1 & -1 & 1 & -1 & 0 & 0 & \dots & 0 \\ 1 & 0 & 0 & -1 & 1 & -1 & 0 & \dots & 0 \\ * & * & \dots & \ddots & \ddots & \ddots & * \\ * & * & \dots & \dots & \ddots & \ddots & * \end{pmatrix}$$

or

(89)
$$\widetilde{\Lambda} = \begin{pmatrix} 1 & -1 & 1 & -1 & 0 & 0 & \dots & 0 \\ 1 & 0 & -1 & 0 & 1 & -1 & 0 & \dots & 0 \\ * & * & \dots & \ddots & \ddots & \ddots & \ddots & * \\ * & * & \dots & \ddots & \dots & \ddots & \ddots & * \end{pmatrix},$$

where the rows with "*" contain vectors of type

$$oldsymbol{ heta}_{i,j;k,l} = (\ldots, rac{1}{i}, \ldots, rac{-1}{k}, \ldots, rac{1}{j}, \ldots, rac{-1}{l}, \ldots) \in \mathbb{R}^n,$$

such that rank $\tilde{\Lambda} = n - 4$ (dots stand for zeros).

Note also that a matrix (88) corresponds to the above case (i) and a matrix (89) corresponds to the above case (ii).

Lemma 10 for $n \in \{8, 9, 10\}$ allows us to consider only matrices of the forms (88) and (89), having the first two rows fixed. This is a big advantage in the process of generating the matrices (the number decreases considerable) and also in the implementation of the algorithm, for small number of velocities.

The **algorithm** follows the next steps

Step 1. Generate all $((n-4)\times n)$ $\widetilde{\varLambda}$ matrices (of type (88) and (89)), with rank $\widetilde{\varLambda}=n-4$, fulfilling the "3 corners rule" (in two different rows there are not three columns having non-zero elements in both rows) since three vertices define completely a rectangle. Moreover, by adding to $\widetilde{\varLambda}$ a new row, containing one element 1, one element (-1) and the rest of elements zero (all possible combinations), we should obtain new matrices having rank equal to (n-3) (then $\widetilde{\varLambda}$ is well-defined). The sets $\Theta_1=\{\widetilde{\varLambda}_1,\ldots,\widetilde{\varLambda}_N\}$ of all generated matrices of type (88) and $\Theta_2=\{\widetilde{\varLambda}_1',\ldots,\widetilde{\varLambda}_M'\}$ of all generated matrices of type (89) , will be finite.

Step 2. Consider first the set Θ_1 . For $j=1,\ldots,N$, take $\widetilde{A}=\widetilde{A}_j$ in the system (87) and check if the system is solvable. In the affirmative case, save the matrix and use the non-trivial solution $(\theta,\mu,,a_k',b_k',:k\geq 7)$ to compute the phase set

$$V = {\mathbf{x}_1, \dots, \mathbf{x}_n} \subseteq \mathbb{R}^2$$

and construct the normal model by plotting the phase points. In the negative case, simply reject the matrix \widetilde{A}_i .

Step 3. Repeat **Step 2**, for the set Θ_2 , by checking, this time, the solvability of the system from case (ii).

2.9.4 - Computer results for the cases n = 8 and n = 9

For the particular cases n=8 and n=9, we obtained in advance all 1-extension normal models (see above). We also proved analytically that all normal models with n=8 are "reducible" (results of 1-extension scheme), but it is still not answered what happens in the case n=9. Are all 9-velocity normal models "reducible", like all

normal models with n < 9? An analytical approach is almost impossible in this case and the only solution is to use the above algorithm and the help of computer.

A necessary condition for a model to be "irreducible" is that its corresponding matrix of reactions \widetilde{A} contains in all its columns at least two non-zero elements (otherwise, one can remove the column and the row corresponding to the non-zero element and obtain a normal model). We denote this condition with (*), so we can refer to it later. Condition (*) is not sufficient, in general.

We modify **Step 1** in the above algorithm and generate instead all matrices $\tilde{\Lambda}$ having in all columns at least two non-zero elements and fulfilling all initial conditions of **Step 1**. Then we follow **Step 2** and **Step 3** and check all these matrices.

In the case n=8, the result is the expected one: the algorithm rejects all generated matrices. Hence, the property that all 8-velocity normal models are 1-extentions, is verified. As we proved analytically, in this case, the condition (*) is not only necessary, but also sufficient.

We are going to describe how we implemented the algorithm for the case n=9 and present the results. We split the problem in two cases (by M(i:j,k:l)) we mean the matrix containing the rows from i to j and the columns from k to l of a matrix M):

```
(1) \det \tilde{\Lambda}(3:5,7:9) \neq 0
(2) \det \tilde{\Lambda}(3:5,7:9) = 0.
```

By generating the matrices, we get $|\Theta_{(1)}| = 7779$ and $|\Theta_{(2)}| = 4271$, where by |A| we denote the number of elements in the set A.

Denote by $\Theta_{(k)(j)}$ the set of all matrices belonging to the above cases (j) where j=1,2, and (k), k=i, ii, from (88) and (89). We have $\left|\Theta_{(i)(1)}\right|=3486, \left|\Theta_{(i)(2)}\right|=1806, \left|\Theta_{(i)(1)}\right|=4293, \left|\Theta_{(ii)(2)}\right|=2465.$

We start to study the case (1).

To check the matrices in $\Theta_{(i)(1)}$, we use the system (87) in the equivalent form

```
\begin{cases} \mathbf{x}_{1} = (0,0); \ \mathbf{x}_{2} = (1,0); \ \mathbf{x}_{3} = (1,\theta) \\ \mathbf{x}_{4} = (0,\theta), \theta \in (0,1] \subset \mathbb{R} \\ \mathbf{x}_{5} = (\mu,\theta); \ \mathbf{x}_{6} = (\mu,0), \mu \in \mathbb{R} \setminus \{0,1\} \\ \mathbf{x}_{k} = (a'_{k},b'_{k}), k = 7, 8, 9 \\ X = (\mathbf{x}_{1},\ldots,\mathbf{x}_{9}); \ X_{1} = X(1:6,1:2) \\ A = \widetilde{A}(3:5,7:9); \ N = \widetilde{A}(3:5,1:6); \\ B = A^{-1}; \ Y = -B \cdot N \cdot X_{1}; \\ \mathbf{x}_{7} = (Y(1,1),Y(1,2)); \\ \mathbf{x}_{8} = (Y(2,1),Y(2,2)); \\ \mathbf{x}_{9} = (Y(3,1),Y(3,2)); \\ \widetilde{X} = (\mathbf{x}_{1} \cdot \mathbf{x}_{1}^{t},\ldots,\mathbf{x}_{9} \cdot \mathbf{x}_{9}^{t}); \ \overline{A} = \widetilde{A} \cdot \widetilde{X}; \\ \begin{cases} \overline{A}(3) = 0 \\ \overline{A}(4) = 0 \\ \overline{A}(5) = 0, \end{cases} \end{cases}
```

where \mathbf{x}^t is the transposed vector \mathbf{x} and Y(i,j) is the element in row i and column j of matrix Y. The vector $\overline{A} \in \mathbb{R}^5$, but because of the form of $\mathbf{x}_1, ..., \mathbf{x}_6$, the first two components are zero and just the last three components are interesting for us. The initial system

(90) has a solution if the new formed system of equations (perhaps non-linear) $\begin{cases} \overline{\underline{A}}(3) = 0\\ \overline{\underline{A}}(4) = 0\\ \overline{\underline{A}}(5) = 0 \end{cases}$ with unknowns θ , μ has solution.

The restrictions on θ and μ are: $\theta \in (0,1]$, $\mu \notin \{0,1\}$, because $\theta = \tan t, t \in \left(0,\frac{\pi}{4}\right]$, where t is the free parameter in 6-velocity models (Section 5.3.1) and $\mathbf{x}_6 \notin \{\mathbf{x}_1,\mathbf{x}_2\}$.

We checked all 3486 matrices in $\Theta_{(i)(1)}$ and we obtained three different models (all known from before, as 1-extensions, from models of type (iv), (v) and (vi)). We found, in this way, our first examples of matrices \widetilde{A} for which the condition (*) is not sufficient.

To check the matrices in $\Theta_{(ii)(1)}$ we use the system (90), with the corresponding changes for $\mathbf{x}_5, \mathbf{x}_6$: $\mathbf{x}_5 = (1 - \mu\theta, \theta + \mu)$ and $\mathbf{x}_6 = (-\mu\theta, \mu)$ (see case (ii) above). We have the restrictions $\theta \in (0,1]$ (as before) and $\mu \notin \{0\}$, from $\mathbf{x}_6 \neq \mathbf{x}_1$. We checked all 4293 matrices in $\Theta_{(ii)(1)}$ and we found 7 different models (one already known, representing the 1-extension normal model (iv)). The other six normal models are new and more important they are "irreducible".

We present the models in Fig. 6. If we denote by t_i the angle $\widehat{213}$ for Model $i=1,\ldots,6$, then we have: $t_1=\arctan\left(\frac{1}{2\sqrt{2}}\right),\ t_2=\arctan\left(\frac{1}{\sqrt{7}}\right),\ t_3=\frac{\pi}{6},\ t_4=\arctan\left(\sqrt{3}-\sqrt{2}\right),\ t_5=\arctan\left(\frac{1}{\sqrt{7}}\right),\ t_6=\arctan\left(\frac{1}{2\sqrt{2}}\right).$

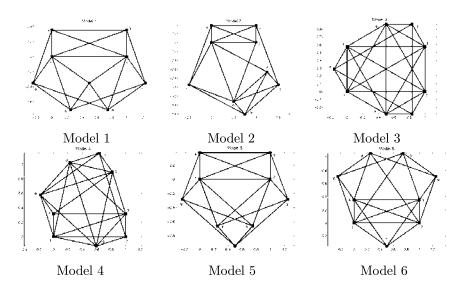


Fig. 6. All 9-velocity normal models: not 1-extensions.

Model 1 and Model 6 are 3-extensions of a 6-velocity normal model of type (b); Model 2 and Model 3 are 2-extensions of a 7-velocity normal model of type (2); Model 4 and Model 5 are 2-extensions of a 7-velocity normal model of type (3).

We checked, by now, only matrices belonging to the case (1). We can now proceed with the case (2), in a similar way.

To check the matrices in $\Theta_{(i)(2)}$ we use the system (87) in the equivalent form (as above). We checked all 1806 matrices in $\Theta_{(i)(2)}$ and all 2464 matrices in $\Theta_{(ii)(2)}$. None of these matrices lead to a solvable system, and hence, to a normal model. The conclusion is that we have six different 9-velocity models that are not 1-extentions (irreducible) and all of them contain a 6-velocity model of type (b).

Many of the normal DVMs constructed in above appear to be axially symmetric. In section 3, we prove that by symmetric transformations, one can obtain new normal DVMs with greater numbers of velocities.

3 - Symmetric extensions of normal discrete velocity models

It is remarkable that many of our normal DVMs (section 2) appear to be axially symmetric. We consider now a connection between elementary symmetric transformations and normal DVMs. We try to find, with the help of symmetric transformations, a new method that can lead from a given normal DVM to an extended normal DVM. The main result is given in Theorem 3, where conditions under which an extended model is normal, are stated. This method can produce many new normal DVMs. We give, for illustration, some concrete examples, in the end of this section.

3.1 - More geometry of plane DVMs

Definition 14. Singular lines in \mathbb{R}^2 are straight lines or circles defined by the equation

(91)
$$\phi(\mathbf{x}) = a + \mathbf{b} \cdot \mathbf{x} + c|\mathbf{x}|^2 = 0,$$

where $a, c \in \mathbb{R}$ and $\mathbf{b} \in \mathbb{R}^2$ are constants.

The set $X_n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subset \mathbb{R}^2$ of $n \geq 4$ points is said to be **non-degenerate** if not all its points lie on a singular line. Otherwise, the set is **degenerate**.

Remark 4. All points $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^2$ are assumed to be distinct ($\mathbf{x}_i \neq \mathbf{x}_k$ if $i \neq k$). We omit below the word "distinct" for brevity.

We can easily prove the following

Lemma 11. (i) Any three points $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3 \in \mathbb{R}^2$ lie on a singular line and uniquely define the line.

(ii) The set X_n , $n \geq 4$, is non-degenerate if and only if it contains a 4-point non-degenerate set.

Proof. Part (i) is a well-known fact of elementary plane geometry. Part (ii) follows directly from (i) and Definition 14.

Definition 15. A **plane DVM** $\{X, \Lambda(X)\}$ is a non-degenerate set $X \subset \mathbb{R}^2$ of $n \geq 4$ points and a corresponding set of vectors of reactions $\Lambda(X)$ (it is always assumed below that $\Lambda(X) \neq \emptyset$).

We choose any numeration of the points $\mathbf{x}_1,\ldots,\mathbf{x}_n$ and vectors of reactions θ_1,\ldots,θ_m $(n\geq 4,\,m\geq 1)$. Then the corresponding $(m\times n)$ $\widetilde{\Lambda}$ -matrix of reactions-reads

(92)
$$\widetilde{\Lambda}(X) = \{\theta_i(k); i = 1, ..., m \text{ and } k = 1, ..., n\},\$$

where (i, k) correspond to the rows and columns, respectively.

It is convenient to consider $\Lambda(X)$ as an n-vector of columns

(93)
$$\widetilde{\Lambda}(X) = (P(\mathbf{x}_1) \dots P(\mathbf{x}_n)),$$

where

(94)
$$X = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \text{ and } P(\mathbf{x}_k) = \begin{pmatrix} \theta_1(k) \\ \vdots \\ \theta_n(k) \end{pmatrix}, k = 1, \dots, n.$$

It was already shown in Lemma 2 that

(95)
$$\sum_{\mathbf{x} \in X} \phi(\mathbf{x}) P(\mathbf{x}) = \sum_{k=1}^{n} \phi(\mathbf{x}_k) P(\mathbf{x}_k) = 0,$$
 for any $\phi(\mathbf{x}) = a + \mathbf{b} \cdot \mathbf{x} + c|\mathbf{x}|^2$.

Let us consider any singular line

(96)
$$C = \{ \mathbf{x} \in \mathbb{R}^2 : \phi_C(\mathbf{x}) = 0 \}$$

that contains some points of X, i.e. $X \cap C \neq \emptyset$.

We denote

$$(97) X_C = X \cap C.$$

Then the identity

(98)
$$\sum_{\mathbf{x} \in X \setminus X_C} \phi_C(\mathbf{x}) P(\mathbf{x}) = 0$$

follows directly from Eqs.(95), (96).

Definition 16. A set $X_C = X \cap C$, where C is a singular line, is called a **singular subset** of X (the trivial case when $X_C = \emptyset$), is also included).

It is now easy to prove some properties of the columns of the matrix of reactions $\widetilde{\Lambda}(X)$ (93), corresponding to the DVM $\{X, \Lambda(X)\}$.

Let us choose any numeration of the points of X, such that the set

 $\Omega = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$ is non-degenerate (such set exists for any plane DVM, see Definition 15). We define four singular lines C_{ijk} , $1 \le i < j < k \le 4$, such that

$$\{\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k\} \subset C_{ijk}.$$

The equation of the singular line C_{ijk} reads

(100)
$$\phi_{ijk}(\mathbf{x}) = 0, \ \phi_{ijk}(\mathbf{x}_i) = \phi_{ijk}(\mathbf{x}_j) = \phi_{ijk}(\mathbf{x}_k) = 0.$$

Moreover $\phi_{ijk}(\mathbf{x}_l) \neq 0$ for the fourth point \mathbf{x}_l , $l \notin \{i, j, k\}$, of the set S.

Hence, Eq. (98) leads to the following equations

(101)
$$\begin{cases} P(\mathbf{x}_1) + \sum_{a=5}^{n} \Psi_{234}(\mathbf{x}_a) P(\mathbf{x}_a) = 0 \\ P(\mathbf{x}_2) + \sum_{a=5}^{n} \Psi_{134}(\mathbf{x}_a) P(\mathbf{x}_a) = 0 \\ P(\mathbf{x}_3) + \sum_{a=5}^{n} \Psi_{124}(\mathbf{x}_a) P(\mathbf{x}_a) = 0 \\ P(\mathbf{x}_4) + \sum_{a=5}^{n} \Psi_{123}(\mathbf{x}_a) P(\mathbf{x}_a) = 0 \end{cases}$$

where

(102)
$$\Psi_{ijk}(\mathbf{x}) = \frac{\phi_{ijk}(\mathbf{x})}{\phi_{ijk}(\mathbf{x}_l)}, \ 1 \le i, j, k, l \le 4, \ i < j < k, \ l \notin \{i, j, k\}.$$

If the points $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ are fixed, then \mathbf{x}_4 can be changed to any point $\mathbf{x} \in X \setminus X_{C_{123}}$, and the last equality in (101) can be written as

(103)
$$P(\mathbf{x}) + \sum_{\mathbf{x}' \in X \setminus X_{C_{123}}}^{n} \Psi_{123}(\mathbf{x}') P(\mathbf{x}') = 0,$$

where

$$\Psi_{123}(\mathbf{x}^{'}) = \frac{\phi_{123}(\mathbf{x}^{'})}{\phi_{123}(\mathbf{x})}, \ \mathbf{x} \in X \setminus X_{C_{123}}.$$

The identities (101) - (103) will be used below for the construction of extended normal models.

We note that, for any plane DVM without isolated points (i.e. each point participates in at least one reaction), its maximal singular subset X_C contains not more than (n-2) points. Otherwise the identity (103) with $P(\mathbf{x}) \neq 0$ cannot be satisfied.

It follows from Eqs.(101) that for any plane DVM, $\{X, \Lambda(X)\}$, and for any non-degenerate subset $\Omega = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\} \subset X$, there exist four linearly independent vectors

$$\mathbf{u}_a = (u_a(\mathbf{x}_1), \dots, u_a(\mathbf{x}_n)) \in \mathbb{R}^n, \ a = 1, 2, 3, 4,$$

such that

(104)
$$\sum_{k=1}^{n} u_a(\mathbf{x}_k) P(\mathbf{x}_k) = 0$$

and

$$u_a(\mathbf{x}_{\beta}) = \delta_{a\beta}, \ a, \beta = 1, 2, 3, 4;$$

(such vectors are constructed above, in explicit form: $\mathbf{u}_1(\mathbf{x}) = \Psi_{234}(\mathbf{x})$, $\mathbf{u}_2(\mathbf{x}) = \Psi_{134}(\mathbf{x})$, $\mathbf{u}_3(\mathbf{x}) = \Psi_{124}(\mathbf{x})$, $\mathbf{u}_4(\mathbf{x}) = \Psi_{123}(\mathbf{x})$).

If the model is normal, then any other vector $\mathbf{u}' = (u'(\mathbf{x}_1), \dots, u'(\mathbf{x}_n))$ satisfying Eqs.(104) is a linear combination of \mathbf{u}_a , a = 1, 2, 3, 4. By taking $\mathbf{u}' = (1, \dots, 1)$ (\mathbf{u}' satisfies Eqs.(104), see Eqs.(95)), we therefore obtain the identity

(105)
$$\Psi_{234}(\mathbf{x}_k) + \Psi_{134}(\mathbf{x}_k) + \Psi_{124}(\mathbf{x}_k) + \Psi_{123}(\mathbf{x}_k) = 1, 5 \le k \le n,$$

(with the notation from (102)) for any normal DVM.

3.2 - Symmetric extensions of normal models

Our aim in this section is to introduce another inductive procedure, similar, in some sense, to the 1-extension method [5], that can lead from a given normal DVM to an extended normal DVM.

We assume that we have given a normal DVM $\{X, \Lambda(X)\}$ (as in Definition 4) with fixed numeration, such that

$$(106) X = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subset \mathbb{R}^2,$$

and the corresponding $\widetilde{\varLambda}(X)$ matrix of reactions reads

(107)
$$\widetilde{\Lambda}(X) = \{\theta_i(k); i = 1, \dots, n - 4; k = 1, \dots, n\}, r(\widetilde{\Lambda}(X)) = n - 4,$$

where we denote by r(A) the rank of any matrix A.

We shall use the following simple idea of a symmetric extension: suppose that we transform the set X to another set

(108)
$$X' = \{\mathbf{x}'_{1}, \dots, \mathbf{x}'_{n}\} \subset \mathbb{R}^{2},$$

in such a way that any rectangle with vertices $\{\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k, \mathbf{x}_l\}$ from the initial model, is transformed to a rectangle with vertices $\{\mathbf{x}_i', \mathbf{x}_j', \mathbf{x}_k', \mathbf{x}_l'\}$.

Obvious examples of such transformations are rotations, translations and reflections in \mathbb{R}^2 (the group of motions of the plane).

The extended model is defined as the pair $\{X_1, \Lambda_1(X_1)\}$, where $X_1 = X \cup X'$. The new model includes all reactions (rectangles) from its components $\{X, \Lambda(X)\}$ and $\{X', \Lambda(X')\}$ and perhaps some new reactions between points from X and X'.

Let us, for the moment, forget about the new reactions and consider just the old ones. We try, in this way, to answer the key question: *How many new (independent) reactions do we need in order to make the extended model to be normal?*

If $X \cap X' = \emptyset$ (the simplest case) then the new phase set

(109)
$$X_{1} = \{\mathbf{x}_{1}, \dots, \mathbf{x}_{n}; \mathbf{x}_{1}^{'}, \dots, \mathbf{x}_{n}^{'}\}$$

contains 2n points. The extended matrix, without the possible new reactions, $\widetilde{A}_*(X_1)$, obviously reads

(110)
$$\widetilde{\varLambda}_*(X_1) = \begin{pmatrix} \widetilde{\varLambda}(X) & \mathcal{O}_{(n-4)\times n} \\ \mathcal{O}_{(n-4)\times n} & \widetilde{\varLambda}(X') \end{pmatrix}$$

where $\mathcal{O}_{a \times \beta}$ is the null-matrix with a rows and β columns. All the rows of $\widetilde{\Lambda}_*(X_1)$ are linearly independent and therefore $r(\widetilde{\Lambda}_*(X)) = 2n - 8$. Hence, such model, with N = 2n velocities, can be normal if we can find four new independent reactions (this does not look promising).

The situation, however, becomes much better, if we assume that $X \cap X' \neq \emptyset$. Let us assume that there exists a set of p points in X which is invariant under the above transformation. Without loss of generality, we can assume that the maximal invariant set consists of the points $\{\mathbf{x}_i; i=1,\ldots,p\}$.

The case p=n means that the model is invariant under our transformation and therefore its extension is trivial: $X_1=X$, with accuracy up to numeration. Therefore, we assume below that $1 \le p \le n-1$.

We now represent the matrix of reactions $\widetilde{\Lambda}(X)$ in the following form

(111)
$$\widetilde{\Lambda}(X) = (\underbrace{R}_{p} \underbrace{S}_{n-p}),$$

where the $(m \times p)$ -matrix R consists of the first p columns of $\widetilde{\Lambda}(X)$, corresponding to the maximal invariant set (here m = n - 4).

It should be pointed out that the invariance of $\{\mathbf{x}_1,\ldots,\mathbf{x}_p\}$ does not mean that $\mathbf{x}_a'=\mathbf{x}_a, a=1,\ldots,p$. It means instead that $\mathbf{x}_a'=\mathbf{x}_{a'}, a=1,\ldots,p$, where $\{1',\ldots,p'\}$ is any permutation of the numbers $\{1,\ldots,p\}$. Having this in mind, we can easily construct the extended matrix, without the possible new reactions, $\widetilde{A}_*(X_1)$, in the following form

$$\widetilde{\varLambda}_*(X_1) = \begin{pmatrix} R & S & \mathcal{O}_{m \times (n-p)} \\ R^{'} & \mathcal{O}_{m \times (n-p)} & S \end{pmatrix}, \, m = n-4,$$

where R' is obtained from R by a permutation of its columns, R and S are the $(m \times p)$ -matrix and the $(m \times (n-p))$ -matrix from (111), respectively. The matrix $\widetilde{\Lambda}_*(X_1)$ in (112), is a matrix of reactions, perhaps with some linearly dependent and some missing new independent reactions, of a DVM with (2n-p) points (velocities) in \mathbb{R}^2 . Therefore

$$(113) r(\widetilde{\Lambda}_*(X_1)) \le 2n - p - 4.$$

Our goal now is to obtain a lower estimate for $r(\widetilde{\varLambda}_*(X_1))$.

The following statement holds for any matrix $\widetilde{A}(X)$ of the form (111) with $n \geq m$ (we do not assume that m = n - 4, as in (111) and (112)).

Lemma 12. If $r(\widetilde{\Lambda}(X)) = m$ then for any decomposition (111) of $\widetilde{\Lambda}(X)$ with $1 \leq p \leq n-1$, the following inequality holds for the extended matrix $\widetilde{\Lambda}_*(X_1)$:

(114)
$$r(\widetilde{\Lambda}_*(X_1)) \ge m + r(S).$$

Proof. From the assumptions of the lemma we have $r(\widetilde{\Lambda}(X)) = m$, where $\widetilde{\Lambda}(X)$ is of the form (111). Using the form (112) for the matrix $\widetilde{\Lambda}_*(X_1)$, we obtain

$$r(\widetilde{\Lambda}_*(X_1)) \ge r(\widetilde{\Lambda}(X)) + r(S),$$

since the rank is given by the number of linearly independent rows. This completes the proof.

We note that

$$r(\widetilde{\Lambda}_*(X_1)) \le \min(2m, 2n - p)$$

since the rank of a matrix is always less than or equal to its number of rows (columns). Therefore,

(115)
$$m + r(S) \le r(\widetilde{\Lambda}_*(X_1)) \le \min(2m, 2n - p), 1 \le p \le n - 1, m \le n.$$

In particular,

$$r(\widetilde{\Lambda}_*(X_1)) = 2m \text{ if } r(S) = m.$$

In the next section, we are going to apply these inequalities to the matrix (112) of the extended model.

3.3 - Rank of the extended matrix

Let us consider a matrix of reactions $\widetilde{\Lambda}(X)$ (107) (and its equivalent forms (93), (94)) of a normal DVM $\{X, \Lambda(X)\}$. We decompose then the matrix $\widetilde{\Lambda}(X)$ in accordance with Eq. (112). We first try to answer the following question:

What can be said about r(S) in the general case $1 \le p \le n-1$?

We recall the identities (101)-(103), from Section 11.1, and note that the model is normal if and only if the columns $\{P(\mathbf{x}_5)\dots P(\mathbf{x}_n)\}$ in Eqs. (101) are linearly independent (otherwise $r(\widetilde{A}(X)) \leq n-5$). On the other hand, the points $\{\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3\}$ can be chosen arbitrarily and then the point \mathbf{x}_4 can be replaced by any other point $\mathbf{x} \in X$ such that $\mathbf{x} \notin C_{123}$ (see Eq. (103)).

Hence, any three columns of $\varLambda(X)$ are linear combinations of the other columns, and therefore

(116)
$$r(S) = m = n - 4 \text{ if } 1 \le p \le 3,$$

in the decomposition (111).

The case $p \ge 4$ is less trivial. In such a case, we fix the points $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ and define a corresponding singular line $C = C_{123}$. Two alternatives are possible:

- $(a) \{\mathbf{x}_4, \dots, \mathbf{x}_p\} \subset C$ or
- (b) there exists at least one point \mathbf{x}_k , $4 \le k \le p$, such that $\mathbf{x}_k \notin C$.

In the case (a) (for a degenerate set $\{\mathbf{x}_1,\ldots,\mathbf{x}_p\}$, $p\geq 4$) there is exactly one column, say, $P(\mathbf{x}_k)$, $p+1\leq k\leq n$ that can be represented as a linear combination of the other columns of $\widetilde{A}(X)$. According to Eq. (103), $\mathbf{x}_k\notin C$ and $P(\mathbf{x}_k)$ is a linear combination of columns $P(\mathbf{x}_j)$ with $\mathbf{x}_j\notin C$. This means automatically that $k,j\geq p+1$, i.e. exactly one of the columns of the matrix S (in the decomposition (111)) is a linear combination of the other columns of S. Therefore

(117)
$$r(S) = n - p - 1,$$

if the set $\{\mathbf{x}_1, \dots, \mathbf{x}_p\}$ is degenerate.

In the case (b) we can assume without loss of generality that k = 4, then the columns $\{P(\mathbf{x}_5), \dots, P(\mathbf{x}_n)\}$ are linearly independent and therefore

$$r(S) = n - p$$
,

if the set $\{\mathbf{x}_1, \dots, \mathbf{x}_p\}$ is non-degenerate (we note that this automatically gives $p \geq 4$). Finally we note that any set of $1 \leq p \leq 3$ points is degenerate and collect the

Finally we note that any set of $1 \le p \le 3$ points is degenerate and collect the above results in the following statement (its proof is already given above).

Lemma 13. If $\widetilde{\Lambda}(X)$ is a matrix of reactions of a normal DVM $\{X, \Lambda(X)\}$, decomposed in accordance with Eq. (111), then

[i] $r(S) = \min(n-4, n-p-1)$ if the set $\{\mathbf{x}_1, \dots, \mathbf{x}_p; 1 \le p \le n-2\}$ is degenerate:

[ii]
$$r(S) = n - p$$
 if the set $\{\mathbf{x}_1, \dots, \mathbf{x}_p; 4 \le p \le n - 1\}$ is non-degenerate.

Now, we can combine Lemma 12 with Lemma 13 and estimate the rank of the extended matrix (without new possible reactions) $\widetilde{A}_*(X_1)$ (112). We recall that the matrix $\widetilde{A}_*(X_1)$ corresponds to the extended model with the phase set

$$X_{1} = X \cup X^{'} = \{\mathbf{x}_{1}, \dots, \mathbf{x}_{n}; \mathbf{x}_{n+1}^{'}, \dots, \mathbf{x}_{n}^{'}\}$$

obtained under the assumption that the transformation $X \to X'$ preserves the set

(118)
$$\Pi = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}.$$

We wonder how close our new model is to a normal one?

The new model contains $n_1=2n-p$ points. Its full matrix of reactions $\widetilde{A}_1(X_1)$ contains the extended matrix $\widetilde{A}_*(X_1)$ (112). Therefore

(119)
$$r(\widetilde{\Lambda}_*(X_1)) \le r(\widetilde{\Lambda}_1(X_1)) \le 2n - p - 4,$$

where $r(\widetilde{\Lambda}_*(X_1))$ satisfies the inequality (114), with m=n-4. Hence,

$$(120) (n-4) + r(S) \le r(\tilde{\Lambda}_1(X_1)) \le 2n - p - 4.$$

We can now use Lemma 13.

We consider first, the case [i] with a degenerate invariant set Π (118) and obtain

$$\min{(2n-8,2n-p-5)} \leq r(\widetilde{\varLambda}_1(X_1)) \leq 2n-p-4, \text{ if } 1 \leq p \leq n-2.$$

In the second case [ii] for a non-degenerate invariant set Π (118), we obtain the exact equality

$$r(\widetilde{\Lambda}_1(X_1)) = 2n - p - 4$$
, if $4 \le p \le n - 1$.

Hence, the following statement is proved.

Theorem 3. Let $\{X_1 = X \cup X^{'}, \Lambda_1(X_1)\}$ be the extended DVM obtained from a given normal DVM $\{X, \Lambda(X)\}$ by the procedure described in the Section 11.2. Let Π be the p-point maximal invariant set of the transformation $X \to X^{'}$, $1 \le p \le n-1$. Then

[1] if $1 \le p \le n-2$ and the set Π is degenerate, then the following estimate holds for the rank $r(\widetilde{\Lambda}_1(X_1))$ of the matrix of reactions corresponding to the extended DVM

(121)
$$\min(2n-8,2n-p-5) \le r(\widetilde{\Lambda}_1(X_1)) \le 2n-p-4;$$

[2] if $4 \le p \le n-1$ and the set Π is non-degenerate, then the extended DVM is normal.

Corollary 2. If $p \geq 3$ and the set Π is degenerate, then not more than one linearly independent reaction (rectangle) between "old" and "new" points (velocities) is needed to make sure that the extended model is normal.

Hence, such an extension with an invariant set of more than two points, leads automatically to a normal, or at least, almost normal (just one more independent reaction is needed) models with a greater number of velocities. We consider some specific examples of such transformations in the next section.

3.4 - Invariant sets with three or four points

In the previous section we proved (see Theorem 3) that an extended DVM $\{X_1 = X \cup X^{'}, \varLambda_1(X_1)\}$ obtained from a given normal DVM $\{X, \varLambda(X)\}$ by a symmetric transformation $X \to X^{'}$, preserving a p-point set Π (118), with $1 \le p \le n-1$, is normal if $4 \le p \le n-1$ and the set Π is non-degenerate. In the same theorem, we also proved that, if $p \ge 3$ and the set Π is degenerate, then the extended model is normal if and only if there exists one independent reaction between "old" (belonging to X) and "new" (belonging to $X^{'}$) velocities (points).

By checking the normal DVMs constructed in section 2 we can find some models that can be extended by symmetric transformations (reflection with respect to a fixed axis is typical), preserving a p-point non-degenerate set Π , with $p \geq 4$, and hence, leading directly to a new normal model, having more velocities. On the other hand, some normal models also admit symmetric transformations that preserve a p-point degenerate set Π , with p=3 or p=4, in the following way.

Case (a) p = 3: (with an invariant set of three colinear points)

The set X of velocities of the model contains three points that lie on the same straight line (no other points of X are colinear with them or symmetric with respect

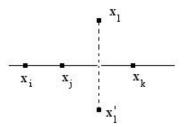


Fig. 7.

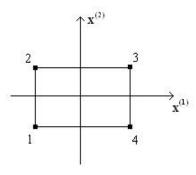


Fig. 8.

to this straight line). Then the reflection with respect to this line preserves a 3-point degenerate set Π (see Fig. 7). The extended model $\{X_1 = X \cup X', \varLambda_1(X_1)\}$, obtained by this transformation, has N = 2n - 3 velocities and the extended matrix $\widetilde{\varLambda}_*(X_1)$ contains M = 2n - 8 independent rows (reactions). The new model is normal if and only if there exists a linearly independent reaction between old and new velocities, i.e. $r(\widetilde{\varLambda}_1(X_1)) = 2n - 7$.

Case (b) p = 4 (with an invariant rectangle):

For any DVM, we can always choose the coordinate system and the numeration such that the first rectangle with vertices $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$ have the form as in Fig. 8.

We consider reflections with respect to the coordinate axes. The total number of rectangles (n-4) of the initial normal model, multiplied by 2, yields the number of such transformations (some of them can coincide, in some special cases, but this is not typical).

We assume that the model has no other points (except the vertices of its first rectangle) symmetric with respect to the axis chosen for reflection. Therefore, the transformation has a 4-point degenerate set $\Pi = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$. The extended

model $\{X_1 = X \cup X^{'}, \Lambda_1(X_1)\}$ has N = 2n-4 velocities and the extended matrix $\widetilde{\Lambda}_*(X_1)$ contains M = 2n-9 independent rows (the explanation is given below, when we study in more detail the case (b)). The new model is normal if and only if there exists a linearly independent reaction between old and new velocities, i.e. $r(\widetilde{\Lambda}_1(X_1)) = 2n-8$.

More general estimates for the rank of the extended matrix $\widetilde{\varLambda}_*(X_1)$ are given below.

Lemma 14. If $p \geq 3$ and the invariant set Π is degenerate, then

(122)
$$r(\widetilde{\Lambda}_*(X_1)) = 2n - 8 \text{ if } p = 3$$

and

(123)
$$2n - p - 5 \le r(\widetilde{\Lambda}_*(X_1)) \le 2n - p - 4$$
 if $p \ge 4$.

Proof. Eq. (122) was already explained in the above case (a). The second result follows from the proof of Theorem 3, where Eq. (121) is valid not only for $\widetilde{\Lambda}_1(X_1)$, but also for $\widetilde{\Lambda}_*(X_1)$ (see Eqs. (115), (119) and Lemma 13, [i]). Hence,

(124)
$$\min(2n-8, 2n-p-5) \le r(\widetilde{\Lambda}_*(X_1)) \le 2n-p-4$$
, if Π is degenerate.

For $p \ge 4$ the relations (124) yield the inequalities (123), and the lemma is proved.

Remark 5. In both cases (a) and (b), one needs to find out if there exists a linearly independent reaction between old and new velocities. In the affirmative case, the extended model is normal. A direct way would be to take all such possible reactions and verify their linearly independence. But this is not an easy or economic way. That is why we shall try below to find out more about these transformations, in order to decrease the number of new reactions (between old and new velocities) that we need to check, when we verify the normality of an extended model.

We start with the case (b), since this type of extension is possible for almost every DVM from Section 1.

Case (b) for p = 4 (with an invariant rectangle, Fig. 8).

Let us choose, for example, to do a reflection with respect to the $x^{(1)}$ -axis. Then the transformation $X \to X^{'}$ reads (see Fig. 8)

(125)
$$\mathbf{x}_{k} = (x_{k}^{(1)}, x_{k}^{(2)}) \to \mathbf{x}_{k}^{'} = (x_{k}^{(1)}, -x_{k}^{(2)}), k = 1, \dots, n.$$

The transformation $X \to X'$ has a 4-point degenerate set $\Pi = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$ and (see Fig. 8)

(126)
$$\mathbf{x}_{1}^{'} = \mathbf{x}_{2}, \ \mathbf{x}_{2}^{'} = \mathbf{x}_{1}, \ \mathbf{x}_{3}^{'} = \mathbf{x}_{4} \ \text{and} \ \mathbf{x}_{4}^{'} = \mathbf{x}_{3}.$$

The extended matrix reads

$$(127) \qquad \widetilde{\varLambda}_*(X_1) = \begin{pmatrix} P_1 & P_2 & P_3 & P_4 & P_5 & \dots & P_n & \mathcal{O} \\ P_2 & P_1 & P_4 & P_3 & \mathcal{O} & P_5 & \dots & P_n \end{pmatrix},$$

where $\mathcal{O} = \mathcal{O}_{(n-4)\times(n-4)}$, $P_k \in \mathbb{R}^{n-4}$, $k = 1, \ldots, n$, are the vector columns in the initial matrix of reactions $\widetilde{A}(X)$: $P_k = P(\mathbf{x}_k)$ in the notations of Eq. (93) or, equivalently,

(128)
$$P_k = (\theta_1(k), \dots, \theta_{n-4}(k)), k = 1, \dots, n,$$

in terms of the vectors of reactions of $\widetilde{\Lambda}(X)$

(129)
$$\theta_i = (\theta_i(1), \dots, \theta_i(n)), i = 1, \dots, n-4$$

 $(\boldsymbol{\theta}_i^{\top} \text{ are rows of the matrix } \widetilde{\varLambda}(X)).$

The matrix $\widetilde{\Lambda}_*(X_1)$ has 2(n-4) rows and (2n-4) columns. In accordance with Lemma 14, $2n-9 \le r(\widetilde{\Lambda}_*(X_1)) \le 2n-8$. In this case, it is easy to see that

$$(130) r(\widetilde{\Lambda}_*(X_1)) = 2n - 9,$$

since two rows of $\widetilde{\Lambda}_*(X_1)$,

(131)
$$\mathbf{g}_{1}^{\top} = (1 \quad -1 \quad 1 \quad -1 \quad 0 \quad \dots \quad 0)$$
$$\mathbf{g}_{n-2}^{\top} = (-1 \quad 1 \quad -1 \quad 1 \quad 0 \quad \dots \quad 0)$$

are identical with accuracy up to the sign (we denote by \mathbf{g}_i^{\top} , $i=1,\ldots,2n-8$, the rows of the matrix $\widetilde{A}_*(X_1)$).

Hence, the extended matrix $A_*(X_1)$ has exactly (2n-9) linearly independent rows (reactions). Therefore the extended model can be normal if and only if it admits one more independent reaction (between old and new velocities).

Let us consider a typical case when the initial model has, in addition to the rectangle shown in Fig. 8, a pair of points, say \mathbf{x}_5 and \mathbf{x}_6 , such that $x_5^{(2)} = x_6^{(2)}$ as in Fig. 9 (not necessary symmetric with respect to the $x^{(2)}$ -axis; however, note that such pairs, with $x_5^{(2)} = x_6^{(2)}$ and $x_5^{(1)} = -x_6^{(1)}$, always exist for models symmetric with respect to the $x^{(2)}$ -axis).

We obtain a new reaction for the extended model

$$\mathbf{x}_{5} + \mathbf{x}_{6}^{'} \rightleftarrows \mathbf{x}_{6} + \mathbf{x}_{5}^{'},$$

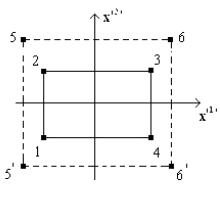


Fig. 9.

where (see Fig. 9)

$$\mathbf{x}_{5}^{'} = \mathbf{x}_{5'} \text{ and } \mathbf{x}_{6}^{'} = \mathbf{x}_{6'}.$$

The corresponding vector of reaction reads

(133)
$$\theta = (\underbrace{0, 0, 0, 0, 1, -1, 0, \dots, 0}_{n}, \underbrace{-1, 1, 0, \dots, 0}_{n-4}),$$

and the matrix $\widetilde{\Lambda}_1(X_1)$ reads

(134)
$$\widetilde{\Lambda}_1(X_1) = \begin{pmatrix} \widetilde{\Lambda}_*(X_1) \\ \boldsymbol{\theta}^\top \end{pmatrix}.$$

We can prove the following result

Proposition 2. The vector of reaction θ (133) is linearly independent of the vectors of reactions corresponding to the rows of the extended matrix $\widetilde{\Lambda}_*(X_1)$, and therefore $r(\widetilde{\Lambda}_1(X_1)) = 2n - 8$ (i.e. the extended model $\{X_1 = X \cup X', \Lambda_1(X_1)\}$, with the corresponding matrix of reactions $\widetilde{\Lambda}_1(X_1)$ given in (134), is normal), if and only if $x_5^{(1)} + x_6^{(1)} \neq 0$ provided that $|\mathbf{x}_5| \neq |\mathbf{x}_1|$ (see Fig. 9).

Proof. Let us consider (2n-7) numbers

(135)
$$v; \lambda_i, i = 1, ..., n-4; \mu_i, j = 1, ..., n-4$$

such that

(136)
$$\sum_{i=1}^{n-4} \lambda_i g_i(k) + \sum_{j=1}^{n-4} \mu_j g_{n-4+j}(k) + v g_{2n-7}(k) = 0, \ k = 1, \dots, 2n-4,$$

where

(137)
$$\mathbf{g}_{i}^{\top} = (g_{i}(1) \dots g_{i}(2n-4)), i = 1, \dots, 2n-7,$$

are the rows of the matrix $\widetilde{\Lambda}_1(X_1)$ (134).

Our goal is to find necessary and sufficient conditions such that the system (136) does not admit a non-trivial solution (135) with $v \neq 0$. In the contrary case, $r(\tilde{\Lambda}_1(X_1)) = 2n - 9$, and we need to replace (if possible) in (134), the vector of reaction θ (133), with another vector of reaction between old and new velocities, such that $r(\tilde{\Lambda}_1(X_1)) = 2n - 8$ (the extended model is normal).

We introduce the notations

(138)
$$\lambda = (\lambda_1, \dots, \lambda_{n-4}) \in \mathbb{R}^{n-4}, \, \mu = (\mu_1, \dots, \mu_{n-4}) \in \mathbb{R}^{n-4}.$$

By using the standard scalar product in \mathbb{R}^{n-4} , we transform (using the forms (127) and (134) of the matrices $\widetilde{\Lambda}_*(X_1)$ and $\widetilde{\Lambda}_1(X_1)$) Eqs. (136) into

(139)
$$\begin{cases} \lambda \cdot P_1 + \mu \cdot P_2 = 0, \ \lambda \cdot P_2 + \mu \cdot P_1 = 0 \\ \lambda \cdot P_3 + \mu \cdot P_4 = 0, \ \lambda \cdot P_4 + \mu \cdot P_3 = 0, \end{cases}$$

(140)
$$\begin{cases} \lambda \cdot P_5 + v = 0, \ \lambda \cdot P_6 - v = 0 \\ \mu \cdot P_5 - v = 0, \ \mu \cdot P_6 + v = 0 \\ \lambda \cdot P_k = \mu \cdot P_k = 0, \ k = 7, \dots, n \end{cases}$$

To simplify the computations we introduce an additional assumption (see Fig. 9)

$$|\mathbf{x}_5| \neq |\mathbf{x}_1|.$$

This means that the 4-point set $\Omega = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_5\}$ is non-degenerate. Therefore (see Eqs.(101) where \mathbf{x}_4 is replaced by \mathbf{x}_5) there exist numbers

$$A, B, C, \{a_k, b_k, c_k, d_k; k = 6, \dots, n\}$$

such that

(142)
$$\begin{cases} P_1 + AP_4 + \langle \mathbf{a}, \mathbf{P} \rangle = 0, P_2 + BP_4 + \langle \mathbf{b}, \mathbf{P} \rangle = 0 \\ P_3 + CP_4 + \langle \mathbf{c}, \mathbf{P} \rangle = 0, P_5 + \langle \mathbf{d}, \mathbf{P} \rangle = 0, \end{cases}$$

where

$$\langle \mathbf{a}, \mathbf{P} \rangle = \sum_{k=6}^{n} a_k P_k,$$

and similar notations for $\langle \mathbf{b}, \mathbf{P} \rangle$, $\langle \mathbf{c}, \mathbf{P} \rangle$, $\langle \mathbf{d}, \mathbf{P} \rangle$ are used.

From Eq. (105) we obtain that

(143)
$$A + B + C = 1; a_k + b_k + c_k + d_k = 1; k = 6, \dots, n,$$

for any choice of the non-degenerate set $\Omega = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_5\}$, provided that the extended model is normal.

The column P_4 is separated from the other columns in (142), since the coefficients A, B, C can be easily found. We recall the definition (128) of the column P_k and the first row \mathbf{g}_1^{\top} of the matrix $\widetilde{A}_1(X_1)$, given in (131). By writing the system (142) only for the first components of the vectors, we obtain the new system

(144)
$$\begin{cases} g_1(1) + Ag_1(4) = 0 \\ g_1(2) + Bg_1(4) = 0 \\ g_1(3) + Cg_1(4) = 0 \end{cases}$$

with $g_1(1) = 1$, $g_1(2) = -1$, $g_1(3) = 1$, $g_1(4) = -1$, and therefore

$$(145) A = 1, B = -1, C = 1.$$

From Eqs.(140) it follows that

(146)
$$\lambda \cdot \langle \mathbf{a}, \mathbf{P} \rangle = \langle \mathbf{a}, \lambda \cdot \mathbf{P} \rangle = va_6; \ \mu \cdot \langle \mathbf{a}, \mathbf{P} \rangle = -va_6; \\ \lambda \cdot \langle \mathbf{b}, \mathbf{P} \rangle = vb_6; \ \lambda \cdot \langle \mathbf{c}, \mathbf{P} \rangle = vc_6; \ \lambda \cdot \langle \mathbf{d}, \mathbf{P} \rangle = vd_6; \\ \mu \cdot \langle \mathbf{b}, \mathbf{P} \rangle = -vb_6; \ \mu \cdot \langle \mathbf{c}, \mathbf{P} \rangle = -vc_6; \ \mu \cdot \langle \mathbf{d}, \mathbf{P} \rangle = -vd_6.$$

We substitute Eq. (142) for P_5 into Eqs.(140) and obtain

$$\lambda \cdot P_5 + v = 0 \iff -vd_6 + v = 0;$$

 $u \cdot P_5 - v = 0 \iff vd_6 - v = 0.$

Since we assume $v \neq 0$, we get

$$(147)$$
 $d_6 = 1,$

and this is the first necessary condition for the solvability of Eqs.(139)-(140).

We assume that this condition is fulfilled and therefore Eqs.(140) can be reduced to the equations

(148)
$$\lambda \cdot P_k + v \delta_{k6} = 0, \ \mu \cdot P_k - v \delta_{k6} = 0, \ k = 6, \dots, n.$$

We substitute Eqs.(145), (146) into Eqs.(142) and obtain

$$\lambda \cdot P_{1} = -\lambda \cdot P_{4} - va_{6};$$

$$\lambda \cdot P_{2} = \lambda \cdot P_{4} - vb_{6};$$

$$\lambda \cdot P_{3} = -\lambda \cdot P_{4} - vc_{6};$$

$$\mu \cdot P_{1} = -\mu \cdot P_{4} + va_{6};$$

$$\mu \cdot P_{2} = \mu \cdot P_{4} + vb_{6};$$

$$\mu \cdot P_{3} = -\mu \cdot P_{4} + vc_{6}.$$

Hence, Eqs.(139) are reduced to

(149)
$$\begin{cases} (\mu - \lambda) \cdot P_4 + v(b_6 - a_6) = 0; \\ (\mu - \lambda) \cdot P_4 - vc_6 = 0. \end{cases}$$

These equations can be satisfied for $v \neq 0$ only if

$$(150) a_6 = b_6 + c_6,$$

i.e. the second necessary condition for the solvability of Eqs. (139) -(140).

We now collect all conditions on a_6 , b_6 , c_6 and d_6 (Eqs. (143), (147), (150))

(151)
$$\begin{cases} a_6 + b_6 + c_6 + d_6 = 1 \\ d_6 = 1 \\ a_6 = b_6 + c_6 \end{cases}$$

Hence, we obtain

$$(152) a_6 = 0, d_6 = 1, b_6 + c_6 = 0.$$

Let us recall that all coefficients in the expansion (142) for the normal extended model, are uniquely defined by the functions $\Psi_{ikj}(\mathbf{x})$ (102). In particular, $a_6=0$ means that $\Psi_{235}(\mathbf{x}_6)=0$, in the notations (101), (102) with \mathbf{x}_5 instead of \mathbf{x}_4 . In other words, there exists a function

$$\phi_{235}(\mathbf{x}) = a + \boldsymbol{\beta} \cdot \mathbf{x} + \gamma |\mathbf{x}|^2, \ a, \gamma \in \mathbb{R}, \ \boldsymbol{\beta} \in \mathbb{R}^2$$

such that

$$\phi_{235}(\mathbf{x}_2) = \phi_{235}(\mathbf{x}_3) = \phi_{235}(\mathbf{x}_5) = 0 \text{ and } \phi_{235}(\mathbf{x}_6) = 0.$$

Geometrically (see Fig. 9 and the condition (141)), this means that \mathbf{x}_6 lies on a singular line through the points \mathbf{x}_2 , \mathbf{x}_3 , \mathbf{x}_5 .

On the other hand, the condition $d_6=1$ means (see (101), (102) with \mathbf{x}_5 instead of \mathbf{x}_4) that $\phi_{123}(\mathbf{x}_5)=\phi_{123}(\mathbf{x}_6)$. But (see Fig. 9) we have

$$\phi_{123}(\mathbf{x}) = |\mathbf{x}|^2 - |\mathbf{x}_1|^2$$

which implies, in the condition (141), $|\mathbf{x}_5| = |\mathbf{x}_6|$.

Both conditions on \mathbf{x}_6 are automatically satisfied if $x_5^{(1)} = -x_6^{(1)}$, i.e. the points \mathbf{x}_5 , \mathbf{x}_6 are symmetric with respect to the $x^{(2)}$ -axis on Fig. 9.

The condition $b_6 + c_6 = 0$ is always satisfied if $a_6 = 0$, $d_6 = 1$ (see (151)). From Eqs.(149), (148) we obtain

(153)
$$\begin{cases} (\lambda - \mu) \cdot P_4 = vb_6; \\ \lambda \cdot P_k = -v\delta_{k6}, k = 6, \dots, n; \\ \mu \cdot P_k = v\delta_{k6}, k = 6, \dots, n. \end{cases}$$

Hence,

(154)
$$(\lambda - \mu) = v\mathbf{u}, \ \mathbf{u} = (u_1, \dots, u_{n-4}) \in \mathbb{R}^{n-4},$$

$$\mathbf{u} \cdot P_4 = b_6, \ \mathbf{u} \cdot P_k = \delta_{k6}, \ k = 6, \dots, n.$$

Thus we have (n-4) equations for (n-4) unknowns $\{u_1, \ldots, u_{n-4}\}$. All vector columns $\{P_4, P_6, P_7, \ldots, P_n\} \subset \mathbb{R}^{n-4}$ are linearly independent and therefore there exists a unique non-zero solution $\mathbf{u} \in \mathbb{R}^{n-4}$ of Eqs.(154).

If we denote $\lambda + \mu = \mathbf{w}$, then $\mathbf{w} \cdot P_k = 0$, $k = 6, \dots, n$. Even the simplest choice of $\mathbf{w} = 0$ leads to non-trivial solutions

$$\lambda = \frac{1}{2}v\mathbf{u}$$
 and $\mu = -\frac{1}{2}v\mathbf{u}$

of the Eqs.(139)-(140).

Hence, the new reaction θ (132) is independent if and only if $x_5^{^{(1)}} + x_6^{^{(1)}} \neq 0$ ($\mathbf{x}_5, \mathbf{x}_6$ are not symmetric with respect to the $x^{(2)}$ -axis), provided $|\mathbf{x}_5| \neq |\mathbf{x}_1|$, and the proof is completed.

The symmetric extension, discussed in the above case (b), is often possible for the normal DVMs constructed in section 1. Many of the new reactions between old and new velocities have, unfortunately, the form discussed in Proposition 2, with their corresponding vertices, \mathbf{x}_5 and \mathbf{x}_6 , symmetric with respect to the $x^{(2)}$ -axis, and hence, they are linearly dependent. Such reactions can be directly eliminated, because of Proposition 2. Sometimes this leaves almost no "new" reactions to be checked, implying that the extended model has small (often none) chances to be normal. Still, there are examples of normal extended models with an invariant degenerate set with p=4.

Similar studies can be done for the case of an invariant set with three elements (see for details [22]).

One can do similar studies for other types of new reactions that appear in extended models (obtained by the symmetric transformations discussed in the above cases (a) and (b)). We chose to analyse only some cases that seem to be typical for the symmetric extensions with a degenerate invariant set. We use the above results to eliminate the new reactions that are not linearly independent. We find, in this way, that many extended models, obtained by symmetric transformations, are not normal. We also find examples of extensions that lead to normal models.

We present in Fig. 10 some of our results. Using the above discussed methods, we extend the 9-velocity Model 5 (see section 2) and obtain the 11-velocity model (*) and 15-velocity model(*!). The process of extension is not finished (but we give here just some examples). Similar extensions of the 9-velocity Model 6 lead us to the below given models 14-velocity model (**) and 22-velocity model (**!). Finally the 9-velocity

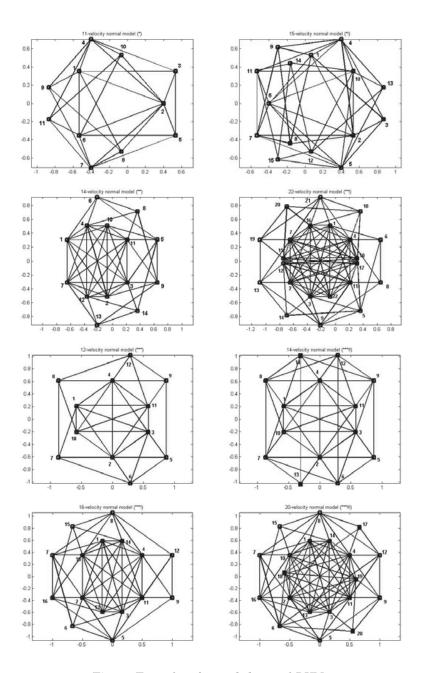


Fig. 10. Examples of extended normal DVMs.

model (iii) takes us to the 12-velocity model (***), 14-velocity model (***!!), 16-velocity model (***!) and 20-velocity model (***!!!) (see Fig. 10). The steps we did in order to obtain all these models are given in detail in [22]. We observe that by such extensions the normal models become more and more symmetric.

4 - Supernormal discrete velocity models for gas mixtures

4.1 - Introduction and preliminaries

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], [19] 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 $\gamma=2$, [14]) spurious invariants (this fact was mentioned in papers like [21], [5]). The simplest example of a binary mixture, with 6+5=11 velocities and arbitrary mass ratio, was first constructed by Cercignani and Cornille [11].

The inductive method (1-extensions) of construction of normal DKMs [5] (see section 2.3) was also applied in [5] to mixtures. Several examples constructed by this method were presented in papers like [4], [12], [14], [15], [20]. It was also shown in [12], that the method of 1-extensions allows the construction of normal models with arbitrarily large number of velocities ("large size DVMs") for some integer values of mass ratio ($\gamma = 2, 3, 4, 5$).

All the above results for mixtures were, in fact, obtained for binary mixtures in the planar (d=2) case.

It is clear that the general methods of construction and classification of normal DKMs with given invariants (section 2) 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, studied in 1.9. Such DVMs for binary mixtures (we call them *supernormal*) are considered below. The supernormality obviously implies that $n, m \ge 6$.

4.2 - Geometrical interpretation of DVMs for mixtures. Definition and properties of SNMs.

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

(155)
$$V = \{\mathbf{v}_1, \dots, \mathbf{v}_n\} \subset \mathbb{R}^d \text{ and } W = \{\mathbf{w}_1, \dots, \mathbf{w}_m\} \subset \mathbb{R}^d.$$

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

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

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

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

such that the conservation laws

(156)
$$\begin{cases} \mathbf{v}_{i} + \mathbf{v}_{j} = \mathbf{v}_{k} + \mathbf{v}_{l} \text{ and } |\mathbf{v}_{i}|^{2} + |\mathbf{v}_{j}|^{2} = |\mathbf{v}_{k}|^{2} + |\mathbf{v}_{l}|^{2}, \ 1 \leq i, j, k, l \leq n \\ \mathbf{w}_{i} + \mathbf{w}_{j} = \mathbf{w}_{k} + \mathbf{w}_{l} \text{ and } |\mathbf{w}_{i}|^{2} + |\mathbf{w}_{j}|^{2} = |\mathbf{w}_{k}|^{2} + |\mathbf{w}_{l}|^{2}, \ 1 \leq i, j, k, l \leq m \\ m_{A}\mathbf{v}_{i} + m_{B}\mathbf{w}_{j} = m_{A}\mathbf{v}_{k} + m_{B}\mathbf{w}_{l} \text{ and } \\ m_{A}|\mathbf{v}_{i}|^{2} + m_{B}|\mathbf{w}_{j}|^{2} = m_{A}|\mathbf{v}_{k}|^{2} + m_{B}|\mathbf{w}_{l}|^{2}, \ 1 \leq i, k \leq n \text{ och } 1 \leq j, l \leq m \end{cases}$$

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.

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

(157)
$$\begin{cases} \mathbf{v}_i + \frac{1}{\gamma} \mathbf{w}_j = \mathbf{v}_k + \frac{1}{\gamma} \mathbf{w}_l \\ |\mathbf{v}_i|^2 + \frac{1}{\gamma} |\mathbf{w}_j|^2 = |\mathbf{v}_k|^2 + \frac{1}{\gamma} |\mathbf{w}_l|^2. \end{cases}$$

By (157) the vectors $(\mathbf{v}_i - \mathbf{v}_k)$ and $(\mathbf{w}_l - \mathbf{w}_j)$ are parallel, $|\mathbf{v}_i - \mathbf{v}_k| = \frac{1}{\gamma} |\mathbf{w}_l - \mathbf{w}_j|$ and $(\mathbf{v}_i + \mathbf{v}_k) \cdot \mathbf{a} = (\mathbf{w}_l + \mathbf{w}_j) \cdot \mathbf{a}$, with $\mathbf{a} = (\mathbf{v}_i - \mathbf{v}_k)$. Then the vector $(\mathbf{v}_i + \mathbf{v}_k - \mathbf{w}_l - \mathbf{w}_j)/2$ which connects the middle points of the segments $(\mathbf{v}_i, \mathbf{v}_k)$ and $(\mathbf{w}_l, \mathbf{w}_j)$ is perpendicular

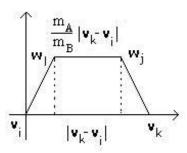


Fig. 11. Geometrical interpretation of a mixture reaction (c).

to the vector **a** and hence, the geometrical figure, having as vertices \mathbf{v}_i , \mathbf{v}_k , \mathbf{w}_j , \mathbf{w}_l , is an isosceles trapezoid. Eqs.(157) are invariant under translation, rotation and scaling. This implies that geometrically we can represent the reaction (c) as in Fig. 11.

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. 11). 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

(158)
$$(a) \theta_{ij}^{kl} = (\underbrace{\dots, \underbrace{1}_{(i)}, \dots, \underbrace{-1}_{(k)}, \dots, \underbrace{-1}_{(l)}, \dots, \underbrace{\dots}_{m}}_{n})$$

$$(b) \theta_{ij}^{kl} = (\underbrace{\dots, \underbrace{1}_{(i)}, \dots, \underbrace{1}_{(j)}, \dots, \underbrace{-1}_{(k)}, \dots, \underbrace{-1}_{(l)}, \dots)}_{m})$$

$$(c) \theta_{ij}^{kl} = (\underbrace{\dots, \underbrace{1}_{(i)}, \dots -1}_{(k)}, \dots, \underbrace{\dots, \underbrace{1}_{(j)}, \dots, \underbrace{-1}_{(l)}, \dots)}_{m})$$

where dots denote zeros.

Definition 17. 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).

The above given definition explains why we do not know by now so many normal DVMs for mixtures. It is not so easy to construct sets of velocities with such geometrical properties. But this geometrical construction can be simplified if we consider an (n+m) mixture of the gases A and B having the set of velocities $\{V,W\}$, such that the corresponding DVMs for the single gases, (V,n) and (W,m), are normal. Geometrically, we start with (n-d-2) linearly independent rectangles with vertices which are velocities in V and (m-d-2) linearly independent rectangles with vertices which are velocities in W. The DVM for gas mixtures is normal if we can find (d+1) linearly independent isosceles trapezoids (i.e. vectors of reactions of type (c) Eq. (158) with two vertices in V and the other two in W as in Fig. 11, such that the rank of the matrix of reactions is (n+m-d-3).

This idea gives a new method for the construction of a special type of normal DVMs for mixtures that we shall call *supernormal models* (with the property that by removing the linearly independent reactions corresponding to mixtures, i.e. reactions of type (c), we obtain two normal DVMs for the single gases involved in the mixture).

Definition 18. 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

(159)
$$\widetilde{\boldsymbol{\Lambda}} = \begin{pmatrix} N & \mathcal{O}_{(n-d-2)\times m} \\ \mathcal{O}_{(m-d-2)\times n} & \boldsymbol{M} \\ \boldsymbol{\theta}_1^\top \\ & \ddots \\ \boldsymbol{\theta}_{d+1}^\top \end{pmatrix},$$

where $\mathcal{O}_{a\times\beta}$ is a null-matrix with a rows and β columns, θ_k , k=1,2,3, represent three linearly independent vectors of type (c) in (158), 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 (158), respectively, and

(160)
$$\operatorname{rank} \widetilde{\Lambda} = n + m - d - 3.$$

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.

4.3 - 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 Eq. (155) with d=2. We assume that the DVMs for the single gases, (V,n) and (W,m), are normal models.

The DVM for the mixture is a SNM (as in Definition 18) if we can find three linearly independent isosceles trapezoids with two vertices in V and the other two in W, as in Fig. 11, such that Eq. (160) is fulfilled. Such a geometrical structure might not exist and, in this case, the "combination" (mixture) of the two normal DVMs, for the gases A and B, does not result into a normal DVM for mixtures.

We shall present an algorithm that allows us to tell if the combination is a good one (has a SNM as result) and, in the affirmative cases, to find the spectrum for the mass ratio γ .

From now on we shall denote by \mathbf{v}_a (or \mathbf{w}_a) pre-collision velocities and by \mathbf{v}_a' (or \mathbf{w}_a') post-collision velocities corresponding to the particles of the gas A (or B).

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

Given two 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. 12 (γ fixed and $l = \|\mathbf{v}_a' - \mathbf{v}_a\|$), such that Eq. (160) is fulfilled.

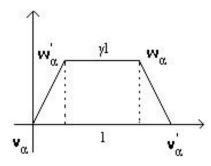


Fig. 12.

We shall denote these three reactions (if they exist) by $(\mathbf{v}_a, \mathbf{v}'_a | \mathbf{w}_a, \mathbf{w}'_a)$ and the parallel vectors in the corresponding trapezoids by

(161)
$$\mathbf{x}_{a} = \mathbf{v}_{a}^{'} - \mathbf{v}_{a} \text{ and } \mathbf{y}_{a} = \mathbf{w}_{a}^{'} - \mathbf{w}_{a}, \ a = 0, 1, 2.$$

By introducing the notations

(162)
$$X_a = \frac{\mathbf{v}_a + \mathbf{v}_a'}{2}$$
$$Y_a = \frac{\mathbf{w}_a + \mathbf{w}_a'}{2}$$

we can rewrite the conservations laws (157) for the reaction $(\mathbf{v}_a, \mathbf{v}_a^{'} | \mathbf{w}_a, \mathbf{w}_a^{'})$, on an easier form

$$\begin{cases} \mathbf{x}_a + \frac{1}{\gamma} \mathbf{y}_a = 0 \text{ (conservation of momentum)} \\ \mathbf{x}_a \cdot (Y_a - X_a) = 0 \text{ (conservation of energy)}. \end{cases}$$

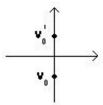
In the process of finding a solution to the stated problem, we follow the next steps.

Step 1. Choose two pairs $(\mathbf{v}_0, \mathbf{v}_0')$ and $(\mathbf{w}_0, \mathbf{w}_0')$, where $\mathbf{v}_0 = \mathbf{v}_{i_0} \in V$, $\mathbf{v}_0' = \mathbf{v}_{k_0} \in V$, $\mathbf{w}_0 = \mathbf{w}_{j_0} \in W$ and $\mathbf{w}_0' = \mathbf{w}_{l_0} \in W$, as candidate vertices for the first isosceles trapezoid and change the scaling such that

(164)
$$W \to \lambda W, \text{ where } \lambda = \frac{\|\mathbf{v}_0' - \mathbf{v}_0\|}{\|\mathbf{w}_0' - \mathbf{w}_0\|} \stackrel{\text{denote}}{=} \frac{\|\mathbf{x}_0\|}{\|\mathbf{v}_0\|}.$$

It is obvious that $\mathbf{v}_0 \neq \mathbf{v}_0'$ and $\mathbf{w}_0 \neq \mathbf{w}_0'$ (they are velocities belonging to the phase sets of normal models for a single gas) and therefore, Eq. (164) is well-defined.

Step 2. Perform the appropriate rotation and translation on the set V, such that $\mathbf{v}_0 + \mathbf{v}_0' = 0$ and $\mathbf{v}_{0x} = \mathbf{v}_{0x}' = 0$ as in the following figure.



We denote for this, $d = \frac{\|\mathbf{x}_0\|}{2}$ and $\mathbf{v}\mathbf{n} = (0, -d)$.

We first perform the translation

$$\mathbf{v}_i = \mathbf{v}_i + (\mathbf{v}\mathbf{n} - \mathbf{v}_0), \ \mathbf{v}_i \in V, \ i = 1, \dots, n.$$

Denote

$$\begin{cases} a(i) = \mathbf{v}_i(1) \\ b(i) = \mathbf{v}_i(2) + d \end{cases}, \quad i = 1, \dots, n.$$

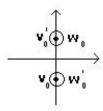
We now perform the rotation

$$\begin{cases} \mathbf{v}_i(1) = a(i)\cos\theta - b(i)\sin\theta \\ \mathbf{v}_i(2) = a(i)\sin\theta + b(i)\cos\theta - d \end{cases}, i = 1, \dots, n,$$

where

$$\theta = \left\{ \begin{aligned} & \arccos\left(\frac{\langle \mathbf{x}_0, \mathbf{u} \rangle}{2d}\right), \text{ if } (\mathbf{x}_0, 0) \times (\mathbf{u}, 0) \geq 0 \text{ , where } \mathbf{u} = (0, 1) \\ & -\arccos\left(\frac{\langle \mathbf{x}_0, \mathbf{u} \rangle}{2d}\right), \text{ otherwise .} \end{aligned} \right.$$

Step 3. Perform the appropriate rotation and translation on the set W such that $\mathbf{v}_0' = \mathbf{w}_0$ and $\mathbf{v}_0 = \mathbf{w}_0'$, as in the following figure.



For this, we first perform the translation and scaling with λ from Step 1,

$$\mathbf{w}_i = \lambda \mathbf{w}_i + \mathbf{v}_0' - \lambda \mathbf{w}_0, \ \mathbf{w}_i \in W, \ i = 1, \dots, m.$$

We denote

$$\begin{cases} a(i) = \mathbf{w}_{i}(1) - \mathbf{v}_{0}^{'}(1) \\ b(i) = \mathbf{w}_{i}(2) - \mathbf{v}_{0}^{'}(2) \end{cases}, \quad i = 1, \dots, m$$

and compute the angle

$$au = rccos\left(rac{\langle -\mathbf{x}_0, \mathbf{y}_0
angle}{\|\mathbf{x}_0\|\|\mathbf{y}_0\|}
ight).$$

Then we perform the rotation

$$\begin{cases} \mathbf{w}_i(1) = a(i)\cos\beta - b(i)\sin\beta + \mathbf{v}_0'(1) \\ \mathbf{w}_i(2) = a(i)\sin\beta + b(i)\cos\beta + \mathbf{v}_0'(2) \end{cases}, i = 1, \dots, m,$$

where

$$\beta = \begin{cases} \tau, & \text{if } (\mathbf{x}_0, 0) \times (\mathbf{y}_0, 0) \ge 0 \\ -\tau, & \text{otherwise} . \end{cases}$$

Step 4. Construct two tables

$$X = \{ \mathbf{x}_{ik} = \mathbf{v}_k - \mathbf{v}_i : i \neq k \in \{1, \dots, n\} \}$$
 and $Y = \{ \mathbf{y}_{il} = \mathbf{w}_l - \mathbf{w}_i : j \neq l \in \{1, \dots, m\} \}$

and find all possible indices $(i_a, k_a; j_a, l_a)$, with $a \neq 0$, such that

$$\mathbf{x}_{ik} + \mathbf{y}_{il} = 0.$$

We numerate by a = 1, ..., r, the pairs of indices $(i_a, k_a; j_a, l_a)$ that satisfy the relation (165). Then the vectors

$${\bf v}_a={\bf v}_{i_a},\,{\bf v}_a^{'}={\bf v}_{k_a},\,{\bf w}_a={\bf w}_{i_a},\,{\bf w}_a^{'}={\bf w}_{l_a},\,a=0,\ldots r$$

satisfy the equality

$$\mathbf{v}_a + \mathbf{w}_a = \mathbf{v}'_a + \mathbf{w}'_a, \ a = 0, \dots r$$

or equivalently,

$$\mathbf{x}_a + \mathbf{y}_a = 0, \, a = 0, \dots r.$$

We can include here the case a = 0 because of Step 3.

Remark 6. In the steps 3 and 4, we try to find pairs of parallel vectors which later on can be bases in the linearly independent isosceles trapezoids we are looking for.

In Step 5 we shall find all possible triplets of such pairs of vectors $(\mathbf{x}_a, \mathbf{y}_a)$, having fixed the first pair $(\mathbf{x}_0, \mathbf{y}_0)$, with the property that the corresponding vectors of reactions are linearly independent and such that the matrix of reaction of the model has the rank (n+m-5). In this way, the isosceles trapezoids (if they exist) will be linearly independent.

- Step 5. (i) If r<2, then we reject the candidate pairs of velocities from Step 1, pick up new ones and repeat the algorithm.
 - (ii) If r2, then we construct the vectors

$$egin{aligned} \mathbf{e}_a = &(\ldots, rac{1}{(i_a)}, \ldots, rac{-1}{(k_a)}, \ldots) \ oldsymbol{\sigma}_a = &(\ldots, rac{1}{(j_a)}, \ldots, rac{-1}{(l_a)}, \ldots), \ a = 1, \ldots r. \end{aligned}$$

We find all triplets $(0, \beta, \delta)$, with $1 \le \beta \le r$ and $1 \le \delta \le r$, such that

$$\operatorname{rank} egin{pmatrix} N \ \mathbf{e}_0 \ \mathbf{e}_{eta} \ \mathbf{e}_{\delta} \end{pmatrix} = n-1 \,\, ext{and}$$

$$\operatorname{rank}egin{pmatrix} M \ oldsymbol{\sigma}_0 \ oldsymbol{\sigma}_eta \ oldsymbol{\sigma}_\delta \end{pmatrix} = m-1,$$

where N and M are the corresponding matrices of reactions for the DVMs (V, n) and (W, m) for single gases, respectively.

Then the corresponding matrix of reactions for the DVM for mixtures,

$$\widetilde{ec{ec{A}}}_{eta\delta} = egin{pmatrix} N & \mathcal{O}_{(n-4) imes m} \ \mathcal{O}_{(m-4) imes n} & M \ \mathbf{e}_0 & \mathbf{\sigma}_0 \ \mathbf{e}_eta & \mathbf{\sigma}_eta \ \mathbf{e}_\delta & \mathbf{\sigma}_\delta \end{pmatrix},$$

has rank $\widetilde{\Lambda}_{\beta\delta} = (m+n) - 5$.

- If there are no triples with such property, then we reject the candidate pairs of velocities from Step 1, pick up new ones and repeat the algorithm.
- \circ Otherwise we take each case, one by one, and go to Step 6, where we check if the vectors of reactions in the last three rows of the matrix \widetilde{A} , correspond to isosceles trapezoids. In the affirmative cases we will find the spectrum for the mass ratio γ and the matrix \widetilde{A} will be accepted as the matrix of reactions of the SNM $(\{V,W\},n+m)$. Obviously, the number of admissible (output of Step 5) matrices \widetilde{A} is finite.
- **Step 6.** In this moment the matrix \widetilde{A} is fixed. That is why we can refer to the vectors in the last two rows by indices 1, 2 and skip the notations with β and δ . We take the last three reactions (corresponding to mixtures) and try to find out if they lead to isosceles trapezoids. For this, we follow the next steps.
- The velocities involved in these reactions, $(\mathbf{v}_a, \mathbf{v}_a' | \mathbf{w}_a, \mathbf{w}_a')$, a = 0, 1, 2 have the property

$$\mathbf{x}_a + \mathbf{y}_a = 0, \ a = 0, 1, 2.$$

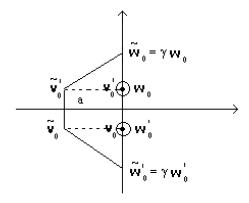
This means that the vectors $\mathbf{x}_a = \mathbf{v}_a^{'} - \mathbf{v}_a$ and $\mathbf{y}_a = \mathbf{w}_a^{'} - \mathbf{w}_a$ are parallel and of opposite directions.

■ We consider a scaling transformation of the set W with a parameter $\gamma > 0$ (which represents the mass ratio), and a parallel translation of the set V along the Ox axis, with a parameter $a \in \mathbb{R}$, that read

(166)
$$\begin{cases} \widetilde{W} = \gamma W \\ \widetilde{V} = V - a\omega, \ \omega = (1,0), \end{cases}$$

hoping that these transformations will lead to a SNM (i.e., we obtain isosceles trapezoids).

For a=0 these transformations can be illustrated geometrically by the following isosceles trapezoid.



■ After the transformations (166), the conservation of momentum (Eq. (163)) is satisfied and reads

$$\widetilde{\mathbf{x}}_a + \frac{1}{\gamma} \widetilde{\mathbf{y}}_a = 0, \ a = 0, 1, 2,$$

where $\widetilde{\mathbf{x}}_a = \mathbf{x}_a$ and $\widetilde{\mathbf{y}}_a = \gamma \mathbf{y}_a$, with \mathbf{x}_a , \mathbf{y}_a from Eq. (161).

■ The problem now is to find the parameter $a \in \mathbb{R}$ and the spectrum of possible values $\gamma > 0$ (mass ratio) such that the conservation of energy is also fulfilled, i.e.

$$\widetilde{\mathbf{x}}_a \cdot (\widetilde{Y}_a - \widetilde{X}_a) = 0, \ a = 0, 1, 2,$$

where $\widetilde{\mathbf{x}}_a = \mathbf{x}_a$, $\widetilde{X}_a = X_a - a\omega$ and $\widetilde{Y}_a = \gamma Y_a$, with X_a , Y_a from Eqs.(162).

In the initial variables $(\mathbf{x}_a, X_a; \mathbf{y}_a, Y_a)$ we have

(167)
$$\mathbf{x}_a \cdot (\gamma Y_a + a\omega - X_a) = 0, \ a = 0, 1, 2, \ \omega = (1, 0).$$

The vector \mathbf{x}_0 (see the figure in Step 2),

$$\mathbf{x}_{0} = \mathbf{v}_{0}^{'} - \mathbf{v}_{0} = 2 \|\mathbf{v}_{0}\| \mathbf{u}, \ \mathbf{u} = (0, 1),$$

is perpendicular to $\omega = (1,0)$. Moreover, $X_0 = Y_0 = 0$. Therefore Eq. (167) is automatically fulfilled for a = 0.

What remains is a set of two equations

(168)
$$\gamma \langle \mathbf{x}_a, Y_a \rangle + a \langle \mathbf{x}_a, \omega \rangle = \langle \mathbf{x}_a, X_a \rangle, \ a = 1, 2,$$

with unknowns $\{a, \gamma\}$, where $\langle \cdot, \cdot \rangle$ is the usual scalar product.

The determinant of the system (168) reads

$$\Delta = \langle \mathbf{x}_1, Y_1 \rangle \langle \mathbf{x}_2, \boldsymbol{\omega} \rangle - \langle \mathbf{x}_2, Y_2 \rangle \langle \mathbf{x}_1, \boldsymbol{\omega} \rangle.$$

We distinguish two cases.

Case 1. If $\Delta \neq 0$ then there is a unique solution

$$a = a_* = rac{\langle \mathbf{x}_2, X_2
angle \langle \mathbf{x}_1, Y_1
angle - \langle \mathbf{x}_1, X_1
angle \langle \mathbf{x}_2, Y_2
angle}{\Delta}$$
 and $\gamma = \gamma_* = rac{\langle \mathbf{x}_1, X_1
angle \langle \mathbf{x}_2, \omega
angle - \langle \mathbf{x}_2, X_2
angle \langle \mathbf{x}_1, \omega
angle}{\Delta}.$

If $\gamma \leq 0$, we reject the solutions. Otherwise, we accept the matrix $\widetilde{\Lambda}$ and we construct the corresponding SNM $(\{V,W\},n+m)$.

Then we go back to Step 5 and pick the next matrix Λ . After checking all possibilities, we obtain the hole spectrum for the mass ratio γ .

The spectrum is going to be finite, if all outputs are coming from the Case 1.

Case 2. If $\Delta = 0$, i.e.

$$\langle \mathbf{x}_1, Y_1 \rangle \langle \mathbf{x}_2, \boldsymbol{\omega} \rangle = \langle \mathbf{x}_2, Y_2 \rangle \langle \mathbf{x}_1, \boldsymbol{\omega} \rangle, \, \boldsymbol{\omega} = (1, 0).$$

We have the following possibilities.

- (i) $\langle \mathbf{x}_1, \boldsymbol{\omega} \rangle = \langle \mathbf{x}_2, \boldsymbol{\omega} \rangle = 0$;
- (ii) $\langle \mathbf{x}_1, \boldsymbol{\omega} \rangle \neq 0$ and $\langle \mathbf{x}_2, \boldsymbol{\omega} \rangle \neq 0$;
- (iii) $\langle \mathbf{x}_1, \boldsymbol{\omega} \rangle = 0$ and $\langle \mathbf{x}_2, \boldsymbol{\omega} \rangle \neq 0$;
- $(iv) \langle \mathbf{x}_1, \boldsymbol{\omega} \rangle \neq 0 \text{ and } \langle \mathbf{x}_2, \boldsymbol{\omega} \rangle = 0.$

The cases (iii) and (iv) are equivalent because the equation is symmetric, so it is enough to discuss only one of them.

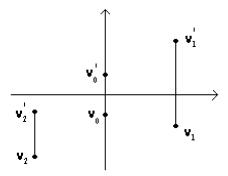
Case 2(i). If $\langle \mathbf{x}_1, \omega \rangle = \langle \mathbf{x}_2, \omega \rangle = 0$ then $\mathbf{x}_1 \perp \omega$ and $\mathbf{x}_2 \perp \omega$, which implies that $\mathbf{v}_{1x} = \mathbf{v}_{1x}^{'}$ and $\mathbf{v}_{2x} = \mathbf{v}_{2x}^{'}$. Moreover we have $\mathbf{v}_{0x} = \mathbf{v}_{0x}^{'}$.

Because of the momentum conservation we have

$$\sum_{i=1}^{n} N_i(t) \mathbf{v}_i + \frac{1}{\gamma} \sum_{i=1}^{m} \widetilde{N}_j(t) \mathbf{w}_i = const. \in \mathbb{R}^2,$$

where $N_i(t)$ ($\widetilde{N}_j(t)$ respectively) represents the number of particles moving with the velocity \mathbf{v}_i (\mathbf{w}_i respectively) at time t.

But \mathbf{v}_0 , \mathbf{v}_1 , \mathbf{v}_2 (indices 1 and 2 stand for β and δ from Step 5) are the only precollision velocities from the normal DVM for the gas A, (V,n), involved in the mixture and their corresponding post-collision velocities have the same x-component. The geometrical interpretation is illustrated in the following figure.



In this case we have

$$\begin{pmatrix} N & \mathcal{O}_{(n-4)\times m} \\ \mathcal{O}_{(m-4)\times n} & M \\ \mathbf{e}_0 & \boldsymbol{\sigma}_0 \\ \mathbf{e}_1 & \boldsymbol{\sigma}_1 \\ \mathbf{e}_2 & \boldsymbol{\sigma}_2 \end{pmatrix} \begin{pmatrix} 1 & 0 & \mathbf{v}_{1x} & \mathbf{v}_{1y} & \mathbf{v}_1^2 & \mathbf{v}_{1x} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & \mathbf{v}_{nx} & \mathbf{v}_{ny} & \mathbf{v}_n^2 & \mathbf{v}_{nx} \\ 0 & 1 & \frac{1}{\gamma} \mathbf{w}_{1x} & \frac{1}{\gamma} \mathbf{w}_{1y} & \frac{1}{\gamma} \mathbf{w}_1^2 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & \frac{1}{\gamma} \mathbf{w}_{mx} & \frac{1}{\gamma} \mathbf{w}_{my} & \frac{1}{\gamma} \mathbf{w}_m^2 & 0 \end{pmatrix} = 0$$

and $(\mathbf{v}_{1x},\ldots,\mathbf{v}_{nx},\underbrace{0,\ldots,0}_m)$ is a vector of conservation law for the model for gas mixture.

This implies that

$$\sum_{i=1}^{n} N_i(t) \mathbf{v}_{ix} = const \in \mathbb{R}$$

is a conservation law for the model. Moreover, it is linearly independent of the other five conservation laws (mass, momentum, energy).

Hence we obtained a spurious conservation law and the model is not normal. We reject the matrix $\widetilde{\Lambda}$, go back to Step 5 and pick up the next matrix $\widetilde{\Lambda}$.

Case 2(ii). We have $\langle \mathbf{x}_1, \boldsymbol{\omega} \rangle \neq 0$ and $\langle \mathbf{x}_2, \boldsymbol{\omega} \rangle \neq 0$. We can rewrite the system (168) as

$$\gamma \frac{\langle \mathbf{x}_a, Y_a \rangle}{\langle \mathbf{x}_a, \boldsymbol{\omega} \rangle} + a = \frac{\langle \mathbf{x}_a, X_a \rangle}{\langle \mathbf{x}_a, \boldsymbol{\omega} \rangle}, \ a = 1, 2.$$

From $\Delta = 0$ we have that

$$\frac{\langle \mathbf{x}_1, Y_1 \rangle}{\langle \mathbf{x}_1, \boldsymbol{\omega} \rangle} = \frac{\langle \mathbf{x}_2, Y_2 \rangle}{\langle \mathbf{x}_2, \boldsymbol{\omega} \rangle} = const.$$

But $\mathbf{x}_a + \mathbf{y}_a = 0$, a = 1, 2; hence,

$$\frac{\langle \mathbf{y}_1, Y_1 \rangle}{\langle \mathbf{y}_1, \boldsymbol{\omega} \rangle} = \frac{\langle \mathbf{y}_2, Y_2 \rangle}{\langle \mathbf{y}_2, \boldsymbol{\omega} \rangle} = \mu = const.$$

The system (167) is equivalent (since $\mathbf{x}_a = -\mathbf{y}_a$) with

$$\mathbf{y}_a \cdot (\gamma Y_a + a\omega - X_a) = 0, \ a = 0, 1, 2, \ \omega = (1, 0) \iff$$

$$\gamma \cdot \underbrace{\frac{\langle \mathbf{y}_a, Y_a \rangle}{\langle \mathbf{y}_a, \boldsymbol{\omega} \rangle}}_{\boldsymbol{\mu}} + a = \frac{\langle \mathbf{y}_a, X_a \rangle}{\langle \mathbf{y}_a, \boldsymbol{\omega} \rangle} \left(= \frac{\langle \mathbf{x}_a, X_a \rangle}{\langle \mathbf{x}_a, \boldsymbol{\omega} \rangle} \right) \Longrightarrow$$

$$\frac{\langle \mathbf{x}_a, X_a \rangle}{\langle \mathbf{x}_a, \boldsymbol{\omega} \rangle} = \mu \gamma + a = \rho = const.$$

Hence,

$$egin{aligned} \langle \mathbf{x}_a, X_a
angle -
ho \langle \mathbf{x}_a, oldsymbol{\omega}
angle &= 0 \Longrightarrow \ &rac{1}{2} \Big(\mathbf{v}_a^{'2} - \mathbf{v}_a^2 \Big) -
ho \omega \Big(\mathbf{v}_a^{'} - \mathbf{v}_a \Big) = 0 \Longleftrightarrow \ & \Big(\mathbf{v}_a^{'2} - \mathbf{v}_a^2 \Big) - 2
ho \omega \mathbf{v}_a^{'} + 2
ho \omega \mathbf{v}_a = 0 \Longleftrightarrow \ & \Big(\mathbf{v}_a^{'} -
ho \omega \Big)^2 - (\mathbf{v}_a -
ho \omega)^2 = 0 \;, \; a = 0, 1, 2. \end{aligned}$$

But $\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_2$ are the only pre-collision velocities from the normal DVM for the gas A, (V, n), involved in the mixture. Therefore

$$((\mathbf{v}_1 - \rho \boldsymbol{\omega})^2, \dots, (\mathbf{v}_n - \rho \boldsymbol{\omega})^2, \underbrace{0, \dots, 0}_{m})$$

is a vector of conservation laws linearly independent of the other five vectors of conservation laws (mass, momentum, energy).

This implies that

$$\sum_{i=1}^{n} N_i(t) (\mathbf{v}_i - \rho \omega)^2 = const \in \mathbb{R}$$

is a spurious conservation law for the model. We reject the matrix \widetilde{A} and go back to Step 5 and pick up the next matrix \widetilde{A} .

Case 2(iii). We have $\langle \mathbf{x}_1, \boldsymbol{\omega} \rangle = 0$ and $\langle \mathbf{x}_2, \boldsymbol{\omega} \rangle \neq 0$. Since $\Delta = 0$, we obtain that

$$\langle \mathbf{x}_{1}, Y_{1} \rangle = 0 \Longrightarrow \mathbf{x}_{1} \perp Y_{1}$$

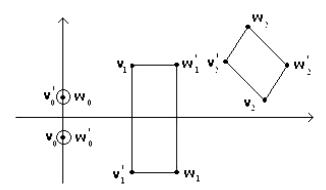
$$\text{But } \mathbf{x}_{1} \perp \boldsymbol{\omega}$$

$$\Rightarrow Y_{1} \parallel \boldsymbol{\omega} \Rightarrow (\mathbf{w}_{1} + \mathbf{w}_{1}^{'}) \parallel \boldsymbol{\omega}$$

$$\text{But } (-\mathbf{y}_{1} = \mathbf{x}_{1}) \perp \boldsymbol{\omega} \Rightarrow (\mathbf{w}_{1} - \mathbf{w}_{1}^{'}) \perp \boldsymbol{\omega}$$

$$\Longrightarrow \mathbf{w}_{1x} = \mathbf{w}_{1x}^{'} \text{ and } \mathbf{w}_{1y} = -\mathbf{w}_{1y}^{'}.$$

Moreover we have $\mathbf{x}_2 + \mathbf{y}_2 = 0$ with $\langle \mathbf{x}_2, \boldsymbol{\omega} \rangle \neq 0$. The geometrical interpretation is given in the following figure.



By the scaling of the set W with any parameter $\gamma>0$ and the parallel translation of the set V along the Ox axis with any parameter a, we obtain for sure two linearly independent isosceles trapezoids $(\mathbf{v}_a,\mathbf{v}_a^{'}|\mathbf{w}_a,\mathbf{w}_a^{'}),\ a=0,1.$ The problem is to find (if possible) the right transformations such that $(\mathbf{v}_2,\mathbf{v}_2^{'}|\mathbf{w}_2,\mathbf{w}_2^{'})$ is also an isosceles trapezoid.

The system (168) is replaced by the following equation with two unknowns (γ, a)

(169)
$$\gamma \langle \mathbf{x}_2, Y_2 \rangle + a \langle \mathbf{x}_2, \boldsymbol{\omega} \rangle = \langle \mathbf{x}_2, X_2 \rangle, \ \gamma > 0, \ a \in \mathbb{R}.$$

We distinguish the following cases.

(a) If $\langle \mathbf{x}_2, Y_2 \rangle = 0$ and $\langle \mathbf{x}_2, X_2 \rangle = 0$, then $(\mathbf{v}_2, \mathbf{v}_2' | \mathbf{w}_2, \mathbf{w}_2')$ is a rectangle before the transformations. From Eq. (169) we obtain a = 0 and the only possible scaling is

 $\gamma = 1$. This case is not of a big interest for us, since we are looking, in general, for mixtures with $\gamma \neq 1$.

(b) If $\langle \mathbf{x}_2, Y_2 \rangle = 0$ and $\langle \mathbf{x}_2, X_2 \rangle \neq 0$ then we have the solution

$$a = \frac{\langle \mathbf{x}_2, X_2 \rangle}{\langle \mathbf{x}_2, \boldsymbol{\omega} \rangle}; \, \forall \, \, \gamma > 0.$$

(c) If $\langle \mathbf{x}_2, Y_2 \rangle \neq 0$ then

$$\begin{cases} a = \frac{\langle \mathbf{x}_2, X_2 \rangle}{\langle \mathbf{x}_2, \boldsymbol{\omega} \rangle} - t \frac{\langle \mathbf{x}_2, Y_2 \rangle}{\langle \mathbf{x}_2, \boldsymbol{\omega} \rangle} \\ \gamma = t > 0. \end{cases}$$

In the cases (b) and (c), after the translation and scaling, we obtain three linearly independent isosceles trapezoids, as in the following figure.

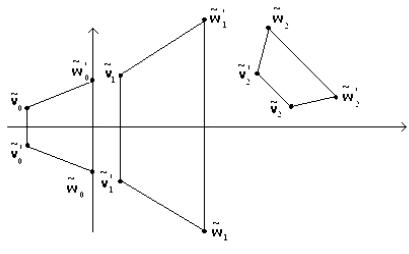


Fig. 13.

Moreover in the cases (b) and (c) we can construct the SNM for every mass ratio $\gamma > 0$. We shall call this type of model *universal model*.

After checking (in Step 6) all admissible matrices \widetilde{A} (output in Step 5) we go back in Step 1, pick up new pairs of velocities $(\mathbf{v}_0, \mathbf{v}_0')$ and $(\mathbf{w}_0, \mathbf{w}_0')$ as candidates, and repeat the algorithm.

Step 1 to Step 6 describe *the general method of construction of SNMs*: given two DVMs (V, n) and (W, m) for simple gases, there are two possible situations

 \circ there is no SNM that contains the two normal DVMs for simple gases, or

 \circ we obtain all possible SNMs ($\{V, W\}, n+m$) and the spectrum of the mass ratio.

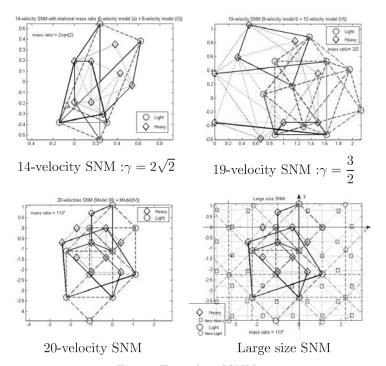


Fig. 14. Examples of SNMs.

Even though the cases 2(iii) (b) - (c), in the above algorithm, give us hope that we can construct normal DVMs for gas mixtures for every mass ratio, all the examples that we have managed to construct, do not belong to these cases. All our results have a finite spectrum for the mass ratio and, except one model (see 14-velocity SNM in Fig. 14), the spectrum has rational values.

4.4 - SNMs up to 20 velocities. Spectrum of the mass ratio

In [22] 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 [22]. We also construct large planar SNMs (see example in Fig. 14) and give (see [22]) 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. 14 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 [22]) 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 $(n \le 20)$ of velocities. A non-trivial result of our computations is the following: for any $(n_1 + n_2)$ -velocity SNM for binary mixture, with $8 \le n_{1,2} \le 9$ (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 (rased in [4], where the authors questioned the extension of DVMs to mixtures when the ratio of masses is irrational). Such models do exist, the universal normal model (though not a SNM) with 11 velocities from [11] is the simplest example. The first example of a SNM with irrational mass ratio $\gamma = 2\sqrt{2}$ is 14-velocity SNM presented in Fig. 14. From our results (see the complete spectrum for mass ratio in [22]), we can deduce that irrational values of γ for SNMs with $n_{1,2} \leq 9$ 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 $n_{1,2} \geq 9$ and irrational γ , do not exist.

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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 R. Gatignol 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. The problem has been

addressed in the last decade by several authors, in particular by Cercignani, Bobylev, Vedenyapin, Orlov and Cornille. 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 develop 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. We also develop a new method that can lead, by symmetric transformations, from a given normal DVM to extended normal DVMs. 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). We apply this method and obtain SNMs with up to 20 velocities and their spectrum of mass ratio.

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