General Methods of the Construction of Discrete Kinetic Models with Given Conservation Laws

A. V. Bobylev and M. C. Vinerean

Dept. of Mathematics, Karlstad University, Sweden

Abstract. In the present work 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 (not linear combinations of physical invariants). The problem has been addressed in the last decade by several authors, in particular by Cercignani, Bobylev, Vedenyapin, 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 develop such a general algorithm in the present work.

We introduce the most general class of discrete kinetic models and obtain a general method for the construction and classification of normal DKMs. In particular, it is proved that for any given dimension $d \geq 2$ and for any sufficiently large number N of velocities (for example, $N \geq 6$ for the planar case $d = 2$) there exists just a finite number of distinct (non-equivalent) classes of DKMs. We apply the general method in the particular cases of discrete velocity models (DVMs) of the inelastic BE and elastic BE. In the first case, we show that all normal models can be explicitly described. In the second case, we give a complete classification of normal models up to 9 velocities and show that the extension method does not lead to all 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 one-kind particles of the single gases involved in the mixture, the corresponding discrete models for a single gas are also normal models). We apply this method and obtain SNMs with up to 20 velocities and their spectrum of mass ratio.

Finally, we develop a new method that can lead, by symmetric transformations, from a given normal DVM to extended normal DVMs.

Keywords: Kinetic theory, discrete kinetic (velocity) models, conservation laws
PACS: 05.20.Dd, 51.10.+y, 47.45.Ab

INTRODUCTION

We consider in this paper the general problem of the construction of the discrete kinetic models with given invariants. This problem was first stated by R. Gatignol [1] in connection with discrete models of the Boltzmann equation. The general discrete velocity model (DVM) of the Boltzmann equation reads [1]

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

where $\mathbf{x}\in\mathbb{R}^d$ and $t\in\mathbb{R}_+$ denote the position and the time respectively, and $V=\{\mathbf{v}_1,\ldots,\mathbf{v}_n\}\subset\mathbb{R}^d$ denotes a set of velocities of the model. The functions $f_i(\mathbf{x},t)$ are understood as spatial densities of particles having velocities $\mathbf{v}_i\in\mathbb{R}^d$, usually $d=2,3$ in applications. The collision operators $Q_i(f)$ in (1) are given by

$$Q_i(f) = \sum_{j,k,l=1}^{n} \Gamma_{ij}^{kl}(f_k f_l - f_i f_j) \text{ for } i=1,\ldots,n, \tag{2}$$

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

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

with equality unless the conservation laws (momentum and energy)

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

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

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

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

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

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

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 [1] 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 [3]. 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 by Bobylev and Cercignani [4] in 1999 (see also [5]). Many new DVMs were obtained by the inductive method in the last years [5, 6]. 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 prove in this work that the answer is negative.

The main objective of this work 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.

DISCRETE KINETIC MODELS

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

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

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

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

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

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

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

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

It is convenient to introduce m vectors

$$\theta_s=\rho-\rho^{(s)}=\left(k_1^{(s)},\ldots,k_n^{(s)}\right),\quad s=1,\ldots,m, \tag{10}$$

with integer components $k_i^{(s)}$ and call them "vectors of reactions" (similar vectors were introduced in [3] for DVMs of the Boltzmann equation).
Let us assume that the total "set of reactions" of the model

$$\Lambda=\{\theta_1,\ldots,\theta_m\}\subseteq\Theta\subseteq\mathbb{Z}^n, \tag{11}$$

is fixed. Then it is clear that the Markovian dynamics of the model is uniquely defined by the set of reactions Λ (11) and the set of probabilities (frequencies) $\{p_1,\dots,p_m\}$ of the reactions $\theta_1,\dots,\theta_m$.

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

$$\rho(t) = (N_1(t),\dots,N_n(t)), t > 0\,. \tag{12}$$

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

$$l[\rho] = \mathbf{u}\cdot\rho = \sum_{i=1}^{n} N_i u_i,\ \mathbf{u} = (u_1,\dots,u_n), \tag{13}$$

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

Lemma 1 *A vector $\mathbf{u} \in \mathbb{R}^n$ is a vector of conservation law if and only if $\mathbf{u}\cdot\theta_s = 0$, for all $\theta_s \in \Lambda$.*

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***

$$L = \text{Span}\,\Lambda = \text{Span}\,\{\theta_1,\dots,\theta_m\} \tag{14}$$

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

$$U = L^{\perp},\ L \oplus U = \mathbb{R}^n. \tag{15}$$

The following statement follows directly from Lemma 1 (a similar statement for DVMs of the Boltzmann equation was proved in [3]).

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*

$$p = \dim U = n - \dim L. \tag{16}$$

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

Definition 2 *The subspace U defined by Eqs.(14), (15) 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 2 *If two numbers $n \geq 2$, $1 \leq p \leq n-1$, and the maximal set Θ of reactions (a finite subset of $\mathbb{Z}^n$) are given, then there exists at most finitely many distinct p-dimensional invariant subspaces $\{U_i, i = 1,\dots,N(n,p;\Theta)\}$ of corresponding DKMs having exactly p linearly independent invariants.*

NORMAL DKMS WITH GIVEN CONSERVATION LAWS

We assume below that the conditions of Lemma 2 are fulfilled and we fix two natural numbers n, p and a finite set $\Theta \subset \mathbb{Z}^n$.

Let us consider a d-dimensional DKM. Its phase set Z (7) is an element of the space

$$Q = \underbrace{\mathbb{R}^d \times \cdots \times \mathbb{R}^d}_{n}. \tag{17}$$

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

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

$$\Lambda_*(Z) = \{\theta \in \Theta : \theta \cdot \mathbf{u}_\alpha(Z) = 0,\ \alpha = 1,\dots,p\}. \tag{18}$$

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 $\Lambda_*(Z)$).

Not all the phase sets are acceptable. In the next step we exclude some *"bad"* phase sets.

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

$$U(Z) = \text{Span}\,\{\mathbf{u}_\alpha(Z), \alpha = 1,\dots,p\},\ Z \in Q, \tag{19}$$

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), $n \geq p+1$;

(B) a maximal (finite) set of reactions $\Theta \subset \mathbb{Z}^n$;

(C) p linearly independent invariants $\{\mathbf{u}_\alpha : Q \to \mathbb{R}^n,\ \alpha = 1,\dots,p\}$ (Q from (17)).

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

$$U(Z) = U, \tag{20}$$

for the phase set $Z \in Q$, where U is one of the N distinct invariant subspaces defined in Lemma 2, and $U(Z)$ is defined in Eq.(19).

Remark 1 *The Theorem 1 reduces the problem of the classification and construction of DKMs to a solution of Eq.(20).*

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

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

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

Step 3. Fix $U = U_i$, $i \in \{1,\dots N\}$ and verify the solvability of Eq.(20).

If this equation is solvable, compute the phase set $Z^{(i)}$ and construct the model $\{Z^{(i)}, \Lambda(Z^{(i)})\}$, where Span $\{\Lambda(Z^{(i)})\} = U_i^\perp$.

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

There are three possible cases: (a) $p = d$; (b) $p < d$; (c) $p > d$. The cases (a) and (b) are relatively simple since the number of equations in the system (20) 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 system (20) is solvable for any admissible set of reactions Λ. 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).

DVMS OF THE BOLTZMANN EQUATION

The general method described above can be applied in the particular cases of discrete velocity models (DVMs) of the inelastic BE and elastic BE. In the first case, we show [7, 8] that all normal models can be explicitly described. In the second case, we give [7, 8] a complete classification of normal models up to 9 velocities and show that the extension method does not lead to all normal DVMs.

We consider now the particular case of usual DVMs [1] of the Boltzmann equation, presented in Introduction. The phase set $Z\ (7)$ is the set of n distinct velocities (the numeration is fixed)

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

It can be shown [8] that, in the plane case $d = 2$, all normal models with $n \in \{7, 8\}$ velocities can be obtained from two 6-velocity models by the method of 1-extentions [4]. This is not true, however, for $n \geq 9$. The computer implementation of the above described general algorithm in this particular case, lead to 6 not 1-extensions models with $n = 9$.

In [8] is presented in detail the classification and construction of all normal plane elastic models with small number of velocities. We present below only the 9-velocity normal models that are not 1-extensions.

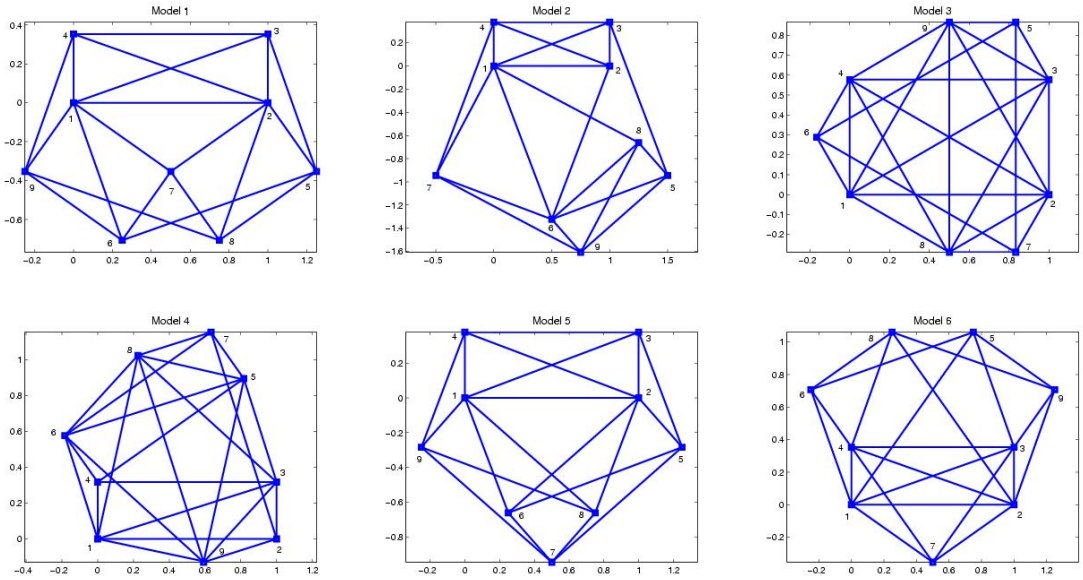

FIGURE 1. All 9-velocity normal DVMs: not 1-extensions

SUPERNORMAL DVMS FOR BINARY GAS MIXTURES

The general method of construction and classification of normal DKMs with given invariants can be applied without any changes to normal DVMs for binary gas 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 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.

We consider now such DVMs for binary mixtures (we call them ***supernormal***). In [8] we present a computer algorithm for the construction of SNMs on the basis of our results for normal DVMs for single gases. The detailed numerical results (i.e. SNMs with up to 20 velocities) are also presented in [8]. We also construct large planar SNMs and give (see [8]) 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 one with irrational mass ratio).

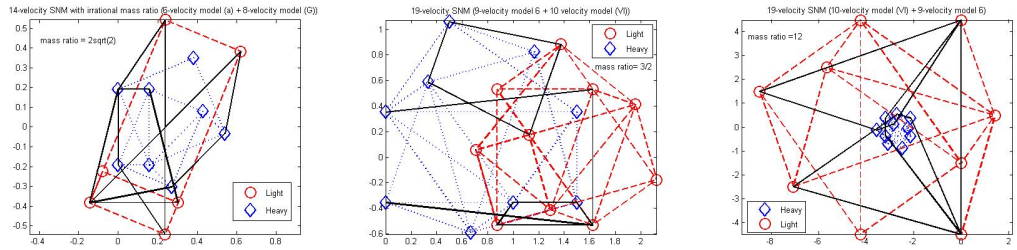

FIGURE 2. Examples of supernormal DVMs for binary mixtures

SYMMETRIC EXTENSIONS OF NORMAL DVMS

It is remarkable that many of our normal DVMs appear to be axially symmetric. A connection between elementary symmetric transformations and normal DVMs is considered in this part.

We find with the help of symmetric transformations (see [8]) a new method that can lead from a given normal DVM to an extended normal DVM. The main result is given in Theorem 3 ([8], p.130), where conditions under which an extended model is normal, are stated.

This method can produce many new normal DVMs. We give below, for illustration, a concrete example where we extend a normal DVM with 9 velocities. In just three steps we get a normal DVM with 22 velocities. The process of extension can be continued until the model is completly symmetric.

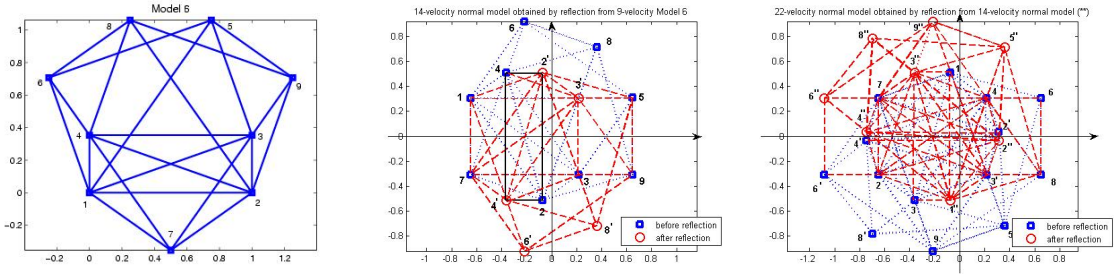

FIGURE 3. Symmetric extensions of a 9-velocity Model6

ACKNOWLEDGEMENTS

The support by the grant 2003-5357 from Swedish Research Council for both authors is gratefully acknowledged.

REFERENCES

1. R. Gatignol, *Théorie Cinétique des Gaz à Répartition Discrète de Vitesses*, Springer-Verlag, New York, 1975.
2. C. Cercignani, *C. R. Acad. Sc. Paris* **301**, 89–92 (1985).
3. V. V. Vedenyapin, and Y. N. Orlov, *Teoret. and Math. Phys.* **121**, 1516–1523 (1999).
4. A. V. Bobylev, and C. Cercignani, *J. Statist. Phys.* **97**, 677–686 (1999).
5. V. V. Vedenyapin, *Transport Theory and Statist. Phys.* **28**, 727–742 (1999).
6. H. Cornille, and C. Cercignani, *J. Statist. Phys.* **99**, 967–991 (2000).
7. A. V. Bobylev, and M. C. Vinerean, "Discrete kinetic models and conservation laws," in *Modelling and Numerics of Kinetic Dissipative Systems*, edited by L. Pareschi, G. Russo, and G. Toscani, Nova Science, 2005, pp. 159–174.
8. M. C. Vinerean, *Discrete Kinetic Models and Conservation Laws*, Karlstad University Studies, 2005, thesis for the degree of doctor of philosophy.