# Discrete Velocity Models for Multicomponent Mixtures and Polyatomic Molecules without Nonphysical Collision Invariants and Shock Profiles

Niclas Bernhoff

*Department of Mathematics and Computer Science, Karlstad University, 651 88 Karlstad, Sweden*

Corresponding author: niclas.bernhoff@kau.se

**Abstract.** An important aspect of constructing discrete velocity models (DVMs) for the Boltzmann equation is to obtain the right number of collision invariants. It is a well-known fact that, in difference to in the continuous case, DVMs can have extra collision invariants, so called spurious collision invariants, in plus to the physical ones. A DVM with only physical collision invariants, and so without spurious ones, is called normal. The construction of such normal DVMs has been studied a lot in the literature for single species as well as for binary mixtures. For binary mixtures also the concept of supernormal DVMs has been introduced by Bobylev and Vinerean. Supernormal DVMs are defined as normal DVMs such that both restrictions to the different species are normal as DVMs for single species.

In this presentation we extend the concept of supernormal DVMs to the case of multicomponent mixtures and introduce it for polyatomic molecules. By polyatomic molecules we mean here that each molecule has one of a finite number of different internal energies, which can change, or not, during a collision. We will present some general algorithms for constructing such models, but also give some concrete examples of such constructions.

The two different approaches above can be combined to obtain multicomponent mixtures with a finite number of different internal energies, and then be extended in a natural way to chemical reactions.

The DVMs are constructed in such a way that we for the shock-wave problem obtain similar structures as for the classical discrete Boltzmann equation (DBE) for one species, and therefore will be able to apply previously obtained results for the DBE. In fact the DBE becomes a system of ordinary differential equations (dynamical system) and the shock profiles can be seen as heteroclinic orbits connecting two singular points (Maxwellians). The previous results for the DBE then give us the existence of shock profiles for shock speeds close to a typical speed, corresponding to the sound speed in the continuous case. For binary mixtures this extension has already been addressed before by the author.

## INTRODUCTION

We consider the Boltzmann equation for a mixture with polyatomic molecules [1], here represented by that each molecule has one of finitely many internal energies that can change (or not) during collisions. In particular we will study discrete velocity models (DVMs), i.e. we assume that the velocity variable can take only a finite number of different given (vector) values. The Boltzmann equation can be approximated by DVMs up to any order [2, 3], and these discrete approximations can be used for numerical methods, see e.g. [4] and references therein. However, in the construction of DVMs there is a classical question of having the correct number of collision invariants [5]. In difference to in the continuous case there can be additional collision invariants to the physical ones; mass, momentum, and energy, for DVMs. DVMs, without additional collision invariants, for which the collision invariants are linearly independent are called normal. The construction of normal DVMs for single species as well as for binary mixtures has been well studied, see for example [6, 7, 8] (and references therein), and recently also for multicomponent mixtures [9] and (single species of) polyatomic molecules [10].

Even if a DVM for a binary mixture is normal, the restrictions of the DVM to the two single species, might not be normal. The concept of supernormal DVMs for binary mixtures, was introduced in [7] for normal DVMs, such that both the restrictions to the single species also are normal. Later this concept was generalized to the case of multicomponent mixtures in [9] and introduced for polyatomic molecules in [10]. A supernormal DVM for a mixture

with polyatomic molecules is a normal DVM, such that also the restriction to any collection of species with any collection of (belonging) internal energies is normal.

We present an algorithm for constructing such DVMs. Actually, to check whether a DVM for a mixture with polyatomic molecules is supernormal or not, we just have to consider the restrictions to all possible binary mixtures (with any combination of fixed internal energies) and all possible pairs of internal energies for each species, and check whether they are supernormal or not. We also conclude that for any finite number of species and any combinations of rational mass ratios and any given (finite number of) multiples of an internal "basic" energy we can construct a supernormal DVM. Our constructed DVMs can always be extended to larger DVMs by the method of one-extensions [11, 6, 7]. The method of one-extensions is an effective way of creating new normal DVMs out of already existing ones. A one-extension is obtained by, having three velocities from a possible collision, but not the fourth, in the velocity set, adding the fourth velocity from the collision to the velocity set to obtain a new linearly independent collision with respect to previously existing collisions (i.e. a collision that can't be obtained by combining previously existing collisions and/or their inverse collisions). Furthermore, it is always possible to extend the constructed DVMs to DVMs that are symmetric with respect to the axes by this method.

Here we consider the problem of constructing DVMs for mixtures of polyatomic molecules with the right number of collision invariants. Another important issue is the one of approximating the full Boltzmann equation by DVMs, which has been addressed for mixtures of monatomic molecules in [11], and for single species of polyatomic molecules in [12]. For simulations it is important to have the right number of collision invariants. Our results concerning the number of collision invariants are independent of the modeling of the collision coefficients as long as the collision coefficients for a maximal set of linearly independent collisions (i.e. collisions that can't be obtained by combining the other collisions, including corresponding inverse collisions, in the set) are nonzero, which we implicitly assume below. We also stress that the symmetry relations (see Eq.(3) below) are fulfilled for the proposed models in [11] (with the weights $g_1^1 = ... = g_s^1 = 1$, cf. (1) below), and in [12] (with $g_1^j = \left(E_1^j\right)^{\delta/2-1}$, where $\delta$ stands for the number of "internal degrees of freedom").

An applicable result for the analytically difficult problem of existence of shock profiles [13, 14] is also presented. The shock profiles can for DVMs be seen as heteroclinic orbits between two stationary points (Maxwellians) [15]. The result is stated without proof, since the proof is exactly the same as for DVMs for monatomic single species, which can be found in [15]. We also present characteristic speeds ("speed of sound") that was calculated in [16] for mixtures with monatomic molecules and single species with polyatomic molecules. To our knowledge no similar result exist, neither in the continuous case.

The construction of the DVMs is such that also for half-space problems [17], as the Milne and Kramers problems [18], but also nonlinear ones [19], one obtain similar structures as for the classical discrete Boltzmann equation for one species [20, 21, 22, 16].

## DVMs FOR MIXTURES WITH POLYATOMIC MOLECULES

Assume that we have $s$ different species, labelled with $\alpha_1, ..., \alpha_s$, with the masses $m_{\alpha_1}, ..., m_{\alpha_s}$. Also, assume that we for each species $\alpha_i$ have $r_i$ different internal energies $E_i^1, ..., E_i^{r_i}$.

For each species $\alpha_i$ and internal energy $E_i^j$ we fix a set of velocity vectors $\mathrm{V}_i^j = \left\{\xi_1^{ij}, ..., \xi_{n_{ij}}^{ij}\right\} \subset \mathbb{R}^d$ and assign the label $\alpha_i$ and the internal energy $E_i^j$ to each velocity vector in $\mathrm{V}_i^j$. We obtain a set of $n = \sum_{i=1}^{s} \sum_{j=1}^{r_i} n_{ij}$ triples (each triple being composed of a velocity vector, a label, and an internal energy)

$$\mathcal{V} = \{\left(\xi_1^{1,1}, \alpha_1, E_1^1\right), ..., \left(\xi_{n_{1,1}}^{1,1}, \alpha_1, E_1^1\right), ..., \left(\xi_1^{sr_s}, \alpha_s, E_s^{r_s}\right), ..., \left(\xi_{n_{sr_s}}^{sr_s}, \alpha_s, E_s^{r_s}\right)\} = \{(\mathbf{v}_1, \alpha(1), E_1), ..., (\mathbf{v}_n, \alpha(n), E_n)\}.$$

Obviously, the same velocity can be repeated many times, but only for different species and/or internal energies; the triples are unique. We may need to scale the distribution functions to be able to obtain the symmetry relations (3) below for the collision coefficients (assuming a convenient reciprocity relation [1, p.9], cf. [10])

$$f_r' = \frac{f_r}{g_i^j} \text{ if } E_r = E_i^j,\ r = 1, ..., n, \text{ for some numbers } g_i^j,\ 1 \le i \le s, 1 \le j \le r_i. \tag{1}$$

We consider the general DVM, or the discrete Boltzmann equation (DBE) [5, 23], which reads

$$\frac{\partial f_i}{\partial t} + \mathbf{v}_i \cdot \nabla_{\mathbf{x}} f_i = Q_i(f, f), \, i = 1, ..., n, \tag{2}$$

where $f_i = f_i(\mathbf{x}, t) = f(\mathbf{x}, t, \mathbf{v}_i, \alpha(i), E_i)$ represents the microscopic density of particles (of species $\alpha(i)$ and with internal energy $E_i$) with velocity $\mathbf{v}_i$ at time $t \in \mathbb{R}_+$ and position $\mathbf{x} \in \mathbb{R}^d$. Note that, if we have made the scaling (1) then the left-hand side in Eq.(2) will be multiplied with the different scaling factors $g_i^j$, cf. Eq.(10) below. However, when the scaling factors will have no significant effect on the structure of the results, we will for brevity, as in Eq.(2), leave them out.

For a function $h = h(\mathbf{v})$ (possibly depending on more variables than $\mathbf{v}$), we identify $h$ with its restrictions to the points $\mathbf{v}$, i.e.

$$h = (h_1, ..., h_n), \text{ with } h_i = h(\mathbf{v}_i), \, i = 1, ..., n.$$

Then $f = (f_1, ..., f_n)$ in Eq.(2).

The collision operators $Q_i(f, f)$ in (2) are given by

$$Q_i(f, f) = \sum_{j,k,l=1}^{n} \Gamma_{ij}^{kl} \left( f_k f_l - f_i f_j \right), \, i = 1, ..., n,$$

where it is assumed that the collision coefficients $\Gamma_{ij}^{kl}$, $1 \leq i, j, k, l \leq n$, satisfy the relations

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

with equality unless we have conservation of mass for each species, momentum, and total energy:

$$\{\alpha(i), \alpha(j)\} = \{\alpha(k), \alpha(l)\},$$
$$m_{\alpha(i)} \mathbf{v}_i + m_{\alpha(j)} \mathbf{v}_j = m_{\alpha(k)} \mathbf{v}_k + m_{\alpha(l)} \mathbf{v}_l,$$
$$\frac{m_{\alpha(i)} |\mathbf{v}_i|^2}{2} + \frac{m_{\alpha(j)} \left| \mathbf{v}_j \right|^2}{2} + E_i + E_j = \frac{m_{\alpha(k)} |\mathbf{v}_k|^2}{2} + \frac{m_{\alpha(l)} |\mathbf{v}_l|^2}{2} + E_k + E_l.$$

A collision is obtained by the exchange of velocities and/or internal energies

$$\left\{ (\mathbf{v}_i, \alpha(i), E_i), (\mathbf{v}_j, \alpha(j), E_j) \right\} \leftrightarrows \{ (\mathbf{v}_k, \alpha(k), E_k), (\mathbf{v}_l, \alpha(l), E_l) \}, \tag{4}$$

and can occur if and only if $\Gamma_{ij}^{kl} \neq 0$. Geometrically, a collision obtained by (4) is represented by an isosceles trapezoid in $\mathbb{R}^d$, if $\left\{ E_i, E_j \right\} = \{E_k, E_l\}$ (a rectangle if additionally $\alpha(i) = \alpha(j)$, or more generally if and only if $m_{\alpha(i)} = m_{\alpha(j)}$), with the corners in $\left\{ \mathbf{v}_i, \mathbf{v}_j, \mathbf{v}_k, \mathbf{v}_l \right\}$, where $\mathbf{v}_i$ and $\mathbf{v}_j$ (and therefore, also $\mathbf{v}_k$ and $\mathbf{v}_l$) are diagonal corners, and

$$m_{\alpha(i)} |\mathbf{v}_i - \mathbf{v}_k| = m_{\alpha(j)} \left| \mathbf{v}_j - \mathbf{v}_l \right|, \tag{5}$$

if $\alpha(i) = \alpha(k)$, and with $k$ and $l$ interchanged in (5), otherwise. However, if $\left\{ E_i, E_j \right\} \neq \{E_k, E_l\}$, the geometrical interpretation is not clear.

A function $\phi = \phi(\mathbf{v})$, is a collision invariant, if and only if

$$\phi_i + \phi_j = \phi_k + \phi_l,$$

for all indices such that $\Gamma_{ij}^{kl} \neq 0$. The trivial collision invariants (or physical collision invariants) are

$$1_{\alpha_1}, ..., 1_{\alpha_s}, m v^1, ..., m v^d, m |\mathbf{v}|^2 + 2E \tag{6}$$

(including all possible linear combinations), where $m = m(\mathbf{v}) = (m_{\alpha(1)}, ..., m_{\alpha(n)})$, $v^i = (v_1^i, ..., v_n^i)$ (with $\mathbf{v}_j = \left( v_j^1, ..., v_j^d \right)$), $|\mathbf{v}|^2 = (|\mathbf{v}_1|^2, ..., |\mathbf{v}_n|^2)$, $E = E(\mathbf{v}) = (E_1, ..., E_n)$, and

$$1_{\alpha_j} = \left( \left( 1_{\alpha_j} \right)_1, ..., \left( 1_{\alpha_j} \right)_n \right), \text{ with } \left( 1_{\alpha_j} \right)_i = \delta_{\alpha_j \alpha(i)} = \begin{cases} 1 \text{ if } \alpha(i) = \alpha_j \\ 0 \text{ if } \alpha(i) \neq \alpha_j \end{cases}.$$

These are the only collision invariants in the continuous case. However, for DVMs there can also be extra, so called spurious, collision invariants. DVMs without spurious collision invariants are called normal, if the $s + d + 1$ collision invariants (6) are linearly independent. A DVM such that the collision invariants (6) are linearly dependent are called degenerate, and otherwise non-degenerate. Typical examples of degenerate DVMs for monatomic single species are the Broadwell models [24]. For normal DVMs the collision invariants are of the form

$$\phi = (\phi_1, ..., \phi_n), \text{ with } \phi_i = a_{\alpha(i)} + m_{\alpha(i)}\mathbf{b} \cdot \mathbf{v}_i + c\left(m_{\alpha(i)} |\mathbf{v}_i|^2 + 2E_i\right) \tag{7}$$

for some constant $a_{\alpha_1}, ..., a_{\alpha_s}, c \in \mathbb{R}$ and $\mathbf{b} \in \mathbb{R}^d$. Methods of construction of normal DVMs for monatomic single species and mixtures can be found in e.g. [6, 7]. We stress that for normal DVMs we will have exactly $s + d + 1$ linearly independent collision invariants.

A Maxwellian distribution (or just a Maxwellian) is a function $M = M(\mathbf{v})$, such that $Q(M, M) = 0$ and $M \geq 0$, and are for normal DVMs of the form

$$M = e^{\phi}, \tag{8}$$

where $\phi$ is given by Eq.(7).

## Supernormal DVMs

A DVM

$$\mathcal{V} = \left\{\left\{\mathrm{V}_1^1, \alpha_1, E_1^1\right\}, ..., \left\{\mathrm{V}_1^{r_1}, \alpha_1, E_1^{r_1}\right\}, ..., \left\{\mathrm{V}_s^1, \alpha_s, E_s^1\right\}, ..., \left\{\mathrm{V}_s^{r_s}, \alpha_s, E_s^{r_s}\right\}\right\}, \tag{9}$$

with internal energies $\left\{E_j^i : 1 \leq i \leq s, 1 \leq j \leq r_i\right\}$, is called normal if it is non-degenerate and has exactly $s + d + 1$ linearly independent collision invariants. Furthermore, A DVM $\mathcal{V}$ (9) is called supernormal if the restriction to each non-empty subset of $\mathcal{V}$ constitutes a normal DVM, which can be proven to be equivalent to that the restriction to each pair of sets in $\mathcal{V}$ constitutes a supernormal DVM (cf. [9, 10]).

**Theorem 1** *For any given number $s$ of species with given rational masses $m_{\alpha_1}, ..., m_{\alpha_s}$, and with given internal energies $\{p_{i1}E, ..., p_{ir_i}E\}$ for a fixed $E \in \mathbb{R}_+$ and rational numbers $p_{i1}, ..., p_{ir_i}$, $i = 1, ..., s$, there is a supernormal DVM for the mixture of polyatomic molecules.*

The proof of Theorem 1 can be obtained by combining the proofs of the corresponding results in the particular cases $r_1 = ... = r_s = 1$ (mixture with monatomic molecules) in [9] and $s = 1$ (single species with polyatomic molecules) in [10].

### *Algorithm For Construction of Supernormal DVMs*

1. (a) Choose a set of velocities $\mathrm{V}_1^1$ such that it corresponds to a normal DVM for a monatomic single species. Here, and in all the steps below, the set should be chosen in such a way, that we can obtain normal models for any mass ratio and/or energy levels we intend to consider, otherwise we might also be able to extend the set(s) later, as we realize that it is needed.
   (b) For $j = 2, \ldots, r_1$ : choose a set of velocities $\mathrm{V}_1^j$ corresponding to a normal DVM such that $\left\{\left\{\mathrm{V}_1^k, E_1^k\right\}, \left\{\mathrm{V}_1^j, E_1^j\right\}\right\}$ is a normal DVM for each $1 \leq k < j$.
2. For $i = 2, \ldots, s$ :
   (a) Choose a normal set of velocities $\mathrm{V}_i^1$ such that it, together with each of $\mathrm{V}_1^1, \ldots, \mathrm{V}_1^{r_1}, ..., \mathrm{V}_{i-1}^1, ..., \mathrm{V}_{i-1}^{r_{i-1}}$, corresponds to a supernormal DVM for binary mixtures.
   (b) For $j = 2, \ldots, r_i$ : choose a set of velocities $\mathrm{V}_i^j$ such that
      i. $\mathrm{V}_i^1$ together with each of $\mathrm{V}_1^1, \ldots, \mathrm{V}_1^{r_1}, ..., \mathrm{V}_{i-1}^1, ..., \mathrm{V}_{i-1}^{r_{i-1}}$ corresponds to a supernormal DVM for binary mixtures;
      ii. $\left\{\left\{\mathrm{V}_i^k, E_i^k\right\}, \left\{\mathrm{V}_i^j, E_i^j\right\}\right\}$ is a normal DVM for each $1 \leq k < j$.

We will call a set of collisions for linearly dependent if one of them can be obtained by a combination of (some of) the other collisions (including corresponding inverse collisions), and correspondingly linearly independent otherwise.

**Remark 1** *In each case, if we don't allow any collisions between the two species or levels of internal energies, we will have $2d + 4$ linearly independent collision invariants. However, we would like to have $d + 3$ or $d + 2$ linearly independent collision invariants for two species or levels of internal energies, respectively. Hence, cf. [7], we need to have $d+1$ and $d+2$ linearly independent (also with respect to the collisions inside the two species or levels of internal energies) collisions between the two species or levels of internal energies, respectively.*

## Examples of Supernormal DVMs

We will use an odd-integer grid as our basic universe, instead of the usual integer grid, since in some applications (e.g. boundary layers [20, 21, 22, 25]) it is preferable that the first component of the velocity is non-zero. However, the integer grid and the odd-integer grid are the same up to a shift and a scaling, and we could also use the integer grid as our basic universe. If desirable, it is also possible to find "larger" normal (and symmetric) DVMs that contains the velocity sets for all of the species and different energy levels and hence, can be used as a common velocity set for all species and levels of internal energies. We are here concerned with having $d+1$ and $d+2$ linearly independent (also with respect to the collisions inside the different species/energy levels) collisions between each two species and energy levels, respectively. These collisions are not the only ones between each two species/energy levels, but all collisions between each species/energy levels can be obtained by combining (one or more of) those linearly independent collisions (including corresponding reverse collisions) with the collisions inside the species/energy levels.

We start with a normal DVM V, which contains the normal DVM with the 6 velocities $\{(\pm 1, \pm 1), (3, \pm 1)\}$ for $d = 2$ or the normal DVM with the 10 velocities $\{(\pm 1, \pm 1, \pm 1), (3, \pm 1, 1)\}$ for $d = 3$. Extensions to larger normal models (of any finite size) can be obtained by the so-called one-extension method [11, 6, 7]. The smallest "symmetric" normal extensions of the minimal DVMs (under our assumption) are the 12-velocity DVM $\{(\pm 1, \pm 1), (\pm 3, \pm 1), (\pm 1, \pm 3)\}$ for $d = 2$ and the 32-velocity DVM $\{(\pm 1, \pm 1, \pm 1), (\pm 3, \pm 1, \pm 1), (\pm 1, \pm 3, \pm 1), (\pm 1, \pm 1, \pm 3)\}$ for $d = 3$.

We let

$$\mathrm{V}_i^j = \frac{\sqrt{E}}{2m_{\alpha_i}}\mathrm{V},\ i = 1, ..., s.$$

Our minimal models are normal DVMs, which easily can be checked by methods in [7]. Note that the minimal models only allow mass ratio 1, and that the maximal total change of internal energies under a collision is $E$, i.e. except the elastic collisions, only collisions such that $E_i + E_j - E_k - E_l = E$ are possible. Instead of using the same V for all species, we can also use different subsets of V for different species.

In all examples below we consider, for brevity, the case $d = 2$. We also denote

$$\begin{aligned}\mathrm{V}_1 &= \{(\pm 1, \pm 1), (3, \pm 1)\},\ \mathrm{V}_2 = \{(\pm 1, \pm 1), (3, \pm 1), (1, 3), (3, 3)\},\\ \mathrm{V}_3 &= \{(\pm 1, \pm 1), (3, 1), (1, 3), (3, 3)\},\ \mathrm{V}_4 = \{(\pm 1, \pm 1), (3, \pm 1), (1, 3), (3, 3), (5, 1)\},\end{aligned}$$

which all constitutes normal DVMs.

**Example 1** *Assume that $s = 1$ and $r_1 = 3$, with the internal energies $E$, $2E$, and $3E$, and mass $m$. Then*

$$\mathrm{V}_1^1 = \frac{\sqrt{E}}{2\sqrt{m}}\mathrm{V}_2;\ \mathrm{V}_1^2 = \mathrm{V}_1^3 = \frac{\sqrt{E}}{2\sqrt{m}}\mathrm{V}_1,$$

*constitutes a supernormal DVM, see Fig.*1.

**Example 2** *Assume that $s = 3$ and $r_1 = r_2 = r_3 = 1$, with the masses $2m$, $3m$, and $6m$. Then*

$$\mathrm{V}_1^1 = 3\mathrm{V}_3;\ \mathrm{V}_2^1 = 2\mathrm{V}_3^1 = \mathrm{V}_4,$$

*constitutes a supernormal DVM, see Fig.*1.

**Example 3** *Assume that $s = 2$ and $r_1 = r_2 = 2$, with the masses $m$ and $2m$, and the internal energies $E$ and $2E$. Then*

$$\mathrm{V}_1^1 = \mathrm{V}_1^2 = 2\mathrm{V}_1;\ \mathrm{V}_2^1 = \mathrm{V}_2^2 = \mathrm{V}_2,$$

*constitutes a supernormal DVM, see Fig.*2*. However, the same sets also constitutes a supernormal DVM, see Fig.*2*, for the case with mass $m$, and internal energies $2E$ and $4E$, and mass $2m$, and internal energies $E$ and $2E$, respectively.*

## Bimolecular Chemical Reactions.

We can also add bimolecular reactive collisions (by changing corresponding collision coefficients to be nonzero) to DVMs for mixtures of polyatomic molecules and by that extend to DVMs for bimolecular chemical reactions. For each linearly independent (also with respect to all other collisions) reactive collision we obtain one new relation on the masses. Note that the maximal number of linearly independent bimolecular reactive collisions are $d - 1$, since the total number of particles will still be conserved.

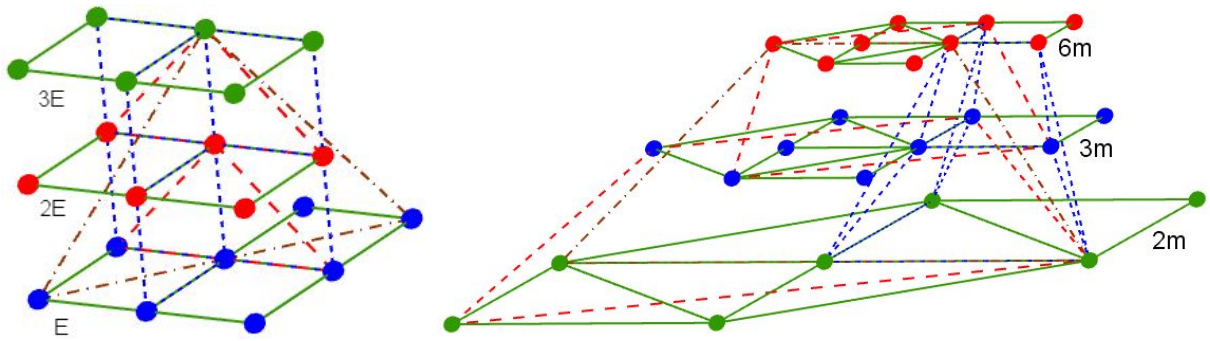


**FIGURE 1.** a) Single species with polyatomic molecules; internal energies $E$, $2E$, and $3E$ (to the left); b) Mixture of three species with monatomic molecules; mass ratios $3/2$, 2, and 3 (to the right).

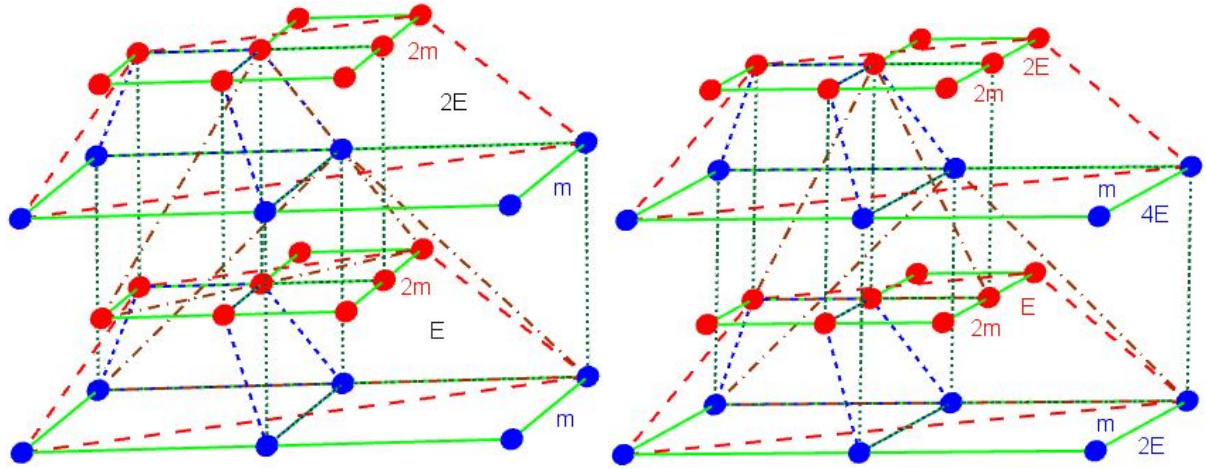


**FIGURE 2.** Binary mixtures with polyatomic molecules (two energy levels). The same velocity sets for two different cases, with one (brown/chained) "essential" collision changed. a) Mass ratio 2 and internal energies $E$ and $2E$ (to the left); b) Mass ratio 2 and internal energies $E$ and $2E$ (heavy species), and $2E$ and $4E$ (light species), respectively (to the right).

## SHOCK PROFILES

In this section we consider the problem of existence of shock profiles for the DBE for mixtures with polyatomic molecules, assuming the symmetry relation (3).

We denote, after having made the scaling (1) of the distribution functions,

$$B = \mathrm{diag}(v_1^1, ..., v_n^1),\ D = \mathrm{diag}(g_1^1, ..., g_1^1, ..., g_1^{r_1}, ..., g_1^{r_1}, ..., g_s^1, ..., g_s^1, ..., g_s^{r_s}, ..., g_s^{r_s}), \tag{10}$$

(we remind the notation $\mathbf{v}_j = \left(v_j^1, ..., v_j^d\right)$) and consider the system

$$D(B - cI)\frac{df}{dy} = Q(f, f),\ c \in \mathbb{R}, \text{ where } f \to M_\pm \text{ as } y \to \pm\infty. \tag{11}$$

Here $M_\pm$ are two Maxwellians and $f = (f_1, ..., f_n)$, with $f_i = f_i(y) = f(y, \mathbf{v}_i, \alpha(i), E_i)$, $i = 1, ..., n$.

We denote by $\left\{\phi_1, ..., \phi_p\right\}$ ($p = d + 2$ for normal DVMs) a basis for the vector space of collision invariants. In a standard way, we obtain that the Maxwellians $M_-$ and $M_+$ must fulfill the Rankine-Hugoniot conditions (here and below, we denote by $\langle \cdot, \cdot \rangle$ the Euclidean scalar product in $\mathbb{R}^n$)

$$\langle D(B - cI) M_+, \phi_i \rangle = \langle D(B - cI) M_-, \phi_i \rangle,\ i = 1, ..., p.$$

We make the following assumptions on our DVMs:

1. There is a number $c_0$, with the following properties:
   [i] $\text{rank}(K) = p-1$, where $K$ is the $p\times p$ matrix with the elements $k_{ij} = \left\langle D\left(B - c_0 I\right) M_+\phi_i, \phi_j\right\rangle$. Note that the rank of $K$ is independent of the choice of the basis $\left\{\phi_1, ..., \phi_p\right\}$. In other words, there is a unique (up to its sign) vector $\phi_\perp$ in $\text{span}(\phi_1, ..., \phi_p)$, such that $\langle M_+\phi_\perp, \phi_\perp\rangle = 1$ and $\langle D\left(B - c_0 I\right) M_+\phi_\perp, \phi\rangle = 0$ for all $\phi \in \text{span}(\phi_1, ..., \phi_p)$.
   [ii] $c_0 \neq v_i^1$ for $i = 1, ..., n$, or, equivalently, $\det(B - c_0 I) \neq 0$.
2. The vector(s) $\phi_\perp$ in [i] above, also satisfies $\left\langle D\left(B - c_0 I\right) M_+\phi_\perp, \phi_\perp^2\right\rangle \neq 0$. We choose the sign of the vector $\phi_\perp$, such that $\left\langle D\left(B - c_0 I\right) M_+\phi_\perp, \phi_\perp^2\right\rangle > 0$.

We assume that assumptions 1 and 2 are fulfilled and denote $\|h\| = \|h(y)\| = \sup_{y\in\mathbb{R}} |h(y)|$ for any bounded (vector or scalar) function $h(y) : \mathbb{R} \to \mathbb{R}^k$, where $k$ is a positive integer.

**Theorem 2** *For any given positive Maxwellian $M_+$, there exists a family of Maxwellians $M_- = M_-(\varepsilon)$ and shock speeds $c = c(\varepsilon) = c_0 + \varepsilon$, such that the shock wave problem* (11) *has a non-negative locally unique (with respect to the norm $\|\cdot\|$ and up to a shift in the independent variable) non-trivial bounded solution for each sufficiently small $\varepsilon > 0$. Furthermore, $M_-$ is determined by $M_+$ and $c$.*

The proof of Theorem 2 is identical with the proof in [15] for the case of one species with monatomic molecules, see also [25] for the case of binary mixtures with monatomic molecules.

## Characteristic Speed

In this section we study such symmetric sets V, such that

$$\text{if } \xi = (\xi^1, ..., \xi^d) \in \text{V}, \text{ then } (\pm\xi^1, ..., \pm\xi^d) \in \text{V}. \tag{12}$$

We will also assume that the Maxwellian $M_+$ is non-drifting (i.e. we have $\mathbf{b} = \mathbf{0}$ in Eq.(7), (8)).

*Mixtures*

Let $r_1 = ... = r_s = 1$, i.e. that we have monatomic molecules. We assume that the set $\mathcal{V}$ consists of $s$ symmetric (in the sense of Eq.(12)) sets of $2N_{\alpha_i}$, $i = 1, ..., s$, velocities respectively, which constitute normal DVMs for single species, but also a normal DVM as a mixture (cf. semi-supernormal DVMs in [9]) and that $g_1^1 = ... = g_s^1 = 1$ (we denote $\xi_j^{i1} = \xi_j^{\alpha_i} = (\xi_j^{\alpha_i,1}, ..., \xi_j^{\alpha_i,d})$). Then

$$c_0 = \sqrt{\frac{\mathcal{X}}{\chi_2\left(\sum\limits_{i=1}^{s}\frac{(\chi_3^{\alpha_i})^2}{\chi_1^{\alpha_i}} - \chi_5\right)}}, \text{ with } \mathcal{X} = \chi_4^2 + \chi_5\sum_{i=1}^{s}\frac{(\chi_2^{\alpha_i})^2}{\chi_1^{\alpha_i}} - 2\chi_4\sum_{i=1}^{s}\frac{\chi_2^{\alpha_i}\chi_3^{\alpha_i}}{\chi_1^{\alpha_i}} - \sum_{i=1}^{s}\frac{(\chi_2^{\alpha_i}\chi_3^{\alpha_j} - \chi_2^{\alpha_j}\chi_3^{\alpha_i})^2}{\chi_1^{\alpha_i}\chi_1^{\alpha_j}}, \tag{13}$$

where $\chi_1^{\alpha_i} = \left\langle\phi_1^{\alpha_i}, \phi_1^{\alpha_i}\right\rangle, \chi_2^{\alpha_i} = \left\langle\phi_1^{\alpha_i}, B\phi_2\right\rangle = m_{\alpha_i}\left\langle\phi_2^{\alpha_i}, \phi_2^{\alpha_i}\right\rangle, \chi_2 = \langle\phi_2, \phi_2\rangle, \chi_3^{\alpha_i} = \left\langle\phi_1^{\alpha_i}, \phi_3\right\rangle = m_{\alpha_i}\left\langle\phi_1^{\alpha_i}, \phi_3^{\alpha_i}\right\rangle, \chi_4 = \langle\phi_2, B\phi_3\rangle$, and $\chi_5 = \langle\phi_3, \phi_3\rangle$, with $\phi_1^{\alpha_i} = M_+^{1/2}\cdot(\underbrace{0, ..., 0}_{2\sum_{j=1}^{i-1}N_{\alpha_j}}, \underbrace{1, ..., 1}_{2N_{\alpha_i}}, \underbrace{0, ..., 0}_{2\sum_{j=i+1}^{s}N_{\alpha_j}})$ for $i = 1, ..., s$, $\phi_2 = M_+^{1/2}\cdot(m_{\alpha_1}\phi_2^{\alpha_1}, ..., m_{\alpha_s}\phi_2^{\alpha_s})$, where $\phi_2^\alpha = (\xi_1^{\alpha,1}, ..., \xi_{N_\alpha}^{\alpha,1}, -\xi_1^{\alpha,1}, ..., -\xi_{N_\alpha}^{\alpha,1})$, and $\phi_3 = M_+^{1/2}\cdot(m_{\alpha_1}\phi_3^{\alpha_1}, ..., m_{\alpha_s}\phi_3^{\alpha_s})$, where $\phi_3^\alpha = (\left|\xi_1^\alpha\right|^2, ..., \left|\xi_{N_\alpha}^\alpha\right|^2, \left|\xi_1^\alpha\right|^2, ..., \left|\xi_{N_\alpha}^\alpha\right|^2)$ fulfills (at least) assumption 1 [i] [16].

In the continuous limit, for the full Boltzmann equation, with $d = 3$, [16]

$$\chi_1^{\alpha_i} = n_{\alpha_i}, \chi_2^{\alpha_i} = n_{\alpha_i}T, \chi_2 = \sum_{i=1}^{s} m_{\alpha_i}n_{\alpha_i}T, \chi_3^{\alpha_i} = 3n_{\alpha_i}T, \chi_4 = 5\sum_{i=1}^{s} n_{\alpha_i}T^2, \chi_5 = 15\sum_{i=1}^{s} n_{\alpha_i}T^2,$$

(where $n_{\alpha_1}, ..., n_{\alpha_s}$, and $T$ denote the number densities of the species $\alpha_1, ..., \alpha_s$ and the temperature respectively), if the Maxwellian is non-drifting of the type $M_+ = (M_{\alpha_1}, ..., M_{\alpha_s})$, with $M_{\alpha_i} = \frac{n_{\alpha_i}}{(2\pi T)^{3/2}}e^{-m_{\alpha_i}|\xi|^2/2T}$. Therefore, for the continuous Boltzmann equation, with $d = 3$, for a mixture of $s$ species the characteristic speed (13) is

$$c_0 = \sqrt{\frac{\sum_{i=1}^{s} n_{\alpha_i}}{\sum_{i=1}^{s} m_{\alpha_i}n_{\alpha_i}}}\sqrt{\frac{5T}{3}}.$$

*Polyatomic Molecules*

Let $s = 1$ and $r_1 = r$, i.e. we consider a single species with polyatomic molecules. We assume that the set $\mathcal{V}$ contains $r$ copies of the same symmetric (cf. Eq.(12)) set V of $2N$ velocities (we denote $\xi_j^{1,1} = ... = \xi_j^{1,r} = \xi_j = (\xi_j^1, ..., \xi_j^d)$), which constitutes a normal model, with corresponding internal energies $E^1, ..., E^r$, and that we have made the change of variables (1). Then

$$c_0 = \sqrt{\frac{\chi_1\chi_4^2 + \chi_2^2\chi_5 - 2\chi_2\chi_3\chi_4}{\chi_2(\chi_1\chi_5 - \chi_3^2)}}, \tag{14}$$

where $\chi_1 = \langle\phi_1, D\phi_1\rangle$, $\chi_2 = \langle\phi_2, D\phi_2\rangle$, $\chi_3 = \langle\phi_1, D\phi_3\rangle$, $\chi_4 = \langle\phi_2, DB\phi_3\rangle$, and $\chi_5 = \langle\phi_3, D\phi_3\rangle$, with $\phi_1 = M_+^{1/2} \cdot (1, ..., 1)$, $\phi_2 = M_+^{1/2} \cdot (\widetilde{\phi}_2, ..., \widetilde{\phi}_2)$, where $\widetilde{\phi}_2 = (\xi_1^1, ..., \xi_N^1, -\xi_1^1, ..., -\xi_N^1)$, and $\phi_3 = M_+^{1/2} \cdot (\phi_3^1, ..., \phi_3^r)$, where $\phi_3^i = (m|\xi_1|^2 + 2E^i, ..., m|\xi_N|^2 + 2E^i, m|\xi_1|^2 + 2E^i, ..., m|\xi_N|^2 + 2E^i)$ fulfills (at least) assumption 1 [i] [16].

In the continuous limit, for the full Boltzmann equation, with $d = 3$, the numbers $\chi_1, ..., \chi_5$ are given by [16]

$$\chi_1 = n, \chi_2 = \frac{nT}{m}, \chi_3 = 3nT + \frac{2nQ_1}{Q_0}, \chi_4 = \frac{5nT^2}{m} + \frac{2nTQ_1}{mQ_0}, \chi_5 = 15nT^2 + \frac{12nTQ_1}{Q_0} + \frac{4nQ_2}{Q_0},$$

where $Q_j = \sum_{i=1}^r g_1^i \left(E^i\right)^j e^{-E^i/T}$ for $j = 0, 1, 2$, and $E^1, ..., E^r$, and $T$ denote the different internal energies and the temperature, respectively, if the Maxwellian is non-drifting of the type $M_+ = (M_1, ..., M_r)$, with $M_i = \frac{n}{(2\pi T)^{3/2} Q_0} e^{-\left(m|\xi|^2/2 + E^i\right)/T}$. Therefore, for the continuous Boltzmann equation, with $d = 3$, the characteristic speed (14) is (note: the constant $\gamma = \frac{5+\delta}{3+\delta}$, where $\delta$ is the number of "internal degrees of freedom" [12], is obtained under the second square root below by replacing the sums by integrals over the internal energy $E$ and the $g_1^i$ with $E^{\delta/2-1}$).

$$c_0 = \sqrt{\frac{T}{m}} \sqrt{\frac{5\left(Q_0 T\right)^2 + 2\left(Q_0 Q_2 - \left(Q_1\right)^2\right)}{3\left(Q_0 T\right)^2 + 2\left(Q_0 Q_2 - \left(Q_1\right)^2\right)}}, \text{ with } Q_j = \sum_{i=1}^r g_1^i \left(E^i\right)^j e^{-E^i/T},\ j = 0, 1, 2.$$

## REFERENCES


[1] A. Ern and V. Giovangigli, *Multicomponent Transport Algorithms* (Springer-Verlag, 1994).
[2] A. Palczewski, J. Schneider, and A. V. Bobylev, SIAM J. Numer. Anal. **34**, 1865–1883 (1997).
[3] L. Fainsilber, P. Kurlberg, and B. Wennberg, Siam J. Math. Anal. **37**, 1903–1922 (2006).
[4] C. Mouhot, L. Pareschi, and T. Ray, Math. Model. Numer. Anal. **47**, 1515–1531 (2013).
[5] R. Gatignol, *Théorie Cinétique des Gaz à Répartition Discrète de Vitesses* (Springer-Verlag, 1975).
[6] A. V. Bobylev and C. Cercignani, J. Stat. Phys. **97**, 677–686 (1999).
[7] A. V. Bobylev and M. C. Vinerean, J. Stat. Phys. **132**, 153–170 (2008).
[8] A. V. Bobylev, M. C. Vinerean, and A. Windfall, Kinet. Relat. Models **3**, 35–58 (2010).
[9] N. Bernhoff and M. Vinerean, J. Stat. Phys. (2016), Online First; DOI: 10.1007/s10955-016-1624-7.
[10] N. Bernhoff, Discrete velocity models for polyatomic molecules without nonphysical collision invariants, Preprint ( 2016).
[11] A. V. Bobylev and C. Cercignani, J. Stat. Phys. **91**, 327–341 (1998).
[12] C. Buet, Math. Mod. Meth. Appl. Sci. **7**, 165–192 (1997).
[13] R. E. Caflisch and B. Nicolaenko, Comm. Math. Phys. **86**, 161–194 (1982).
[14] T.-P. Liu and S.-H. Yu, Comm. Math. Phys. **246**, 133–179 (2004).
[15] N. Bernhoff and A. Bobylev, Commun. Math. Sci. **5**, 815–832 (2007).
[16] N. Bernhoff, Boundary layers for discrete kinetic models: multicomponent mixtures, polyatomic molecules, bimolecular reactions, and quantum kinetic equations, Preprint ( 2016).
[17] C. Bardos, F. Golse, and Y. Sone, J. Stat. Phys. **124**, 275–300 (2006).
[18] C. Bardos, R. E. Caflisch, and B. Nicolaenko, Comm. Pure Appl. Math. **39**, 323–352 (1986).
[19] S. Ukai, T. Yang, and S.-H. Yu, Comm. Math. Phys. **236**, 373–393 (2003).
[20] A. V. Bobylev and N. Bernhoff, in *Lecture Notes on the Discretization of the Boltzmann Equation*, edited by N. Bellomo and R. Gatignol (World Scientific, 2003), pp. 203–222.
[21] N. Bernhoff, Riv. Mat. Univ. Parma **9**, 73–124 (2008).
[22] N. Bernhoff, Kinet. Relat. Models **3**, 195–222 (2010).
[23] H. Cabannes, *The discrete Boltzmann Equation* (University of California, Berkeley, 1980 (rev. 2003)).
[24] J. E. Broadwell, Phys. Fluids **7**, 1243–1247 (1964).
[25] N. Bernhoff, Kinet. Relat. Models **5**, 1–19 (2012).