Boltzmann Equation and Discrete Velocity Models

A discrete velocity model for polyatomic molecules

Boltzmannekvationen och diskreta hastighetsmodeller
En diskret hastighetsmodell för polyatomiska molekyler

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Abstract

In the study of kinetic theory and especially in the study of rarefied gas dynamics one often turns to the Boltzmann equation. The mathematical theory developed by Ludwig Boltzmann was at first sight applicable in aerospace engineering and fluid mechanics. As of today, the methods in kinetic theory are extended to other fields, for instance, molecular biology and socioeconomics, which makes the need of finding efficient solution methods still important. In this thesis, we study the underlying theory of the continuous and discrete Boltzmann equation for monatomic gases. We extend the theory where needed, such that, we cover the case of colliding molecules that possess different levels of internal energy. Mainly, we discuss discrete velocity models and present explicit calculations for a model of a gas consisting of polyatomic molecules modelled with two levels of internal energy.

Sammanfattning

I studiet av kinetisk teori och speciellt i studiet av dynamik för tunna gaser vänds man sig ofta till Boltzmannekvationen. Den matematiska teorien utvecklad av Ludwig Boltzmann var vid första anblicken tillämpbar i flyg- och rymdteknik och strömningsmekanik. Idag generaliseras metoder i kinetisk teori till andra områden, till exempel inom molekylärbiologi och socioekonomi, vilket gör att vi har ett fortsatt behov av att finna effektiva lösningsmetoder. Vi studerar i denna uppsats den underliggande teorin av den kontinuerliga och diskreta Boltzmannekvationen för monatomiska gaser. Vi utvidgar teorin där det behövs för att täcka fallet då kolliderande molekyler innehar olika nivåer av intern energi. Vi diskuterar huvudsakligen diskreta hastighetsmodeller och presenterar explicita beräkningar för en modell av en gas bestående av polyatomiska molekyler modellerad med två lägen av intern energi.

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Chapter 1

Introduction

In kinetic theory, studying rarefied gas dynamics, we consider the flow of a dilute gas. In the general case it requires the consideration of the molecular structure of the gas and of the statistical ideas proposed by Ludwig Boltzmann in 1872 [16]. At an early stage of application of rarefied gas dynamics, the Boltzmann equation (BE) became a practical tool for the aerospace engineers facing the problem of flight in the upper atmosphere. Today with an increasing awareness of environmental problems such as local and global emission of particles from chemical plants, vehicles etc., understanding rarefied gas dynamics is useful [12]. Also, the kinetic theory seems to be applicable in some unexpected areas such as socio-economic problems. For instance, in [19] the authors proposed a kinetic model of economy involving both exchanges between agents and speculative trading.

In this work, we study the BE via discrete velocity models (DVMs), i.e. models where the velocity variable can only take a finite number of values. We consider single species gases and discuss both monatomic and polyatomic molecules where in the latter case the molecules can possess different levels of internal energy. Under suitable assumptions, the BE can be approximated by DVMs up to any order, and these discrete approximations can be used for numerical methods [2].

This thesis with its intuitive approach to the BE can be seen as an introduction to rarefied gas dynamics and DVMs. In Chapter 2, we motivate and derive the continuous BE and present the concept of binary elastic and inelastic collisions. We continue the discussion with a more detailed description regarding collisions and we introduce the collision operator for the discrete equation. In Chapter 3, a brief review of functions called collision invariants and some properties that follows in the discrete case is presented. Also, we introduce the equilibrium distribution called Maxwell distribution, and a linearization of the collision operator. These are concepts that we need later on in finding an approximation of the BE. In Chapter 4, we discuss DVMs generalized to include gases consisting of polyatomic molecules and continue the discussion with collisions from a geometric point of view. The chapter is concluded with some underlying theory and definitions needed to determine the level of normality for the DVM presented in Chapter
5, which contains our main new contribution. In Chapter 5, theory and ideas from earlier chapters are used together as we investigate, with explicit calculations, a 9-velocity Broadwell model for polyatomic molecules. This is a new model, yet unexplored in the literature (Doc. N. Bernhoff, pers. comm.). In the concluding part of the chapter we use the calculations of the DVM to approximate the solution to a Cauchy problem for the spatially homogeneous BE. In Chapter 6, we summarize our work and present further ideas of application of the DVM.
Chapter 2

Derivation of the Boltzmann Equation

2.1 Motivation

It is suitable to start with a motivation for the Boltzmann equation. As one tries to comprehend, describe, and draw conclusions of how a gas acts in a medium, it is not obvious where to begin. The dynamical system is tracking the evolution in time of an extremely large number of molecules. For instance, one cubic centimeter at atmospheric air at ground level contains approximately $2.5 \times 10^{19}$ molecules [12, p. xv]. We assume that our dynamical system consists of $N$ molecules, that we can apply classical mechanics, and that the molecules are subject to Newton’s second law [11]. Moreover, we assume that the state of each molecule, with label $i \in \{1, ..., N\}$, is fully determined by its position and velocity. Then, the state of the system, for $t \in [0, T]$ and $x_i, \xi_i \in C^1(0, T)$, is described completely by

$$\begin{cases}
\dot{x}_i(t) = \xi_i(t) \\
\dot{\xi}_i(t) = X_i(t),
\end{cases} \quad (2.1)$$

where $x_i$ is the three-component position vector of the $i$th molecule, a function of time, and $\xi_i$ its three-component velocity vector, also a function of time. In general, $X_i$ will denote the sum of external forces acting on the molecule. To specify the microscopic state of the system we must solve the $6N$ differential equations given in (2.1). Also, it requires that the initial state at $t = 0$ is known, i.e. $x(0) = x_0 \in \mathbb{R}^{3N}$, and $\xi(0) = \xi_0 \in \mathbb{R}^{3N}$. Given the large number of molecules, it seems to be an impossible task to draw (from a microscopic point of view) any macroscopic conclusions. As one turn to statistical mechanics, where one, instead of speaking of certain positions and velocities for given particles, speaks of their probability to take different positions and velocities, one will see that this is not the case.
2.2 The evolution equation

In this section we discuss, in a certain sense, a direct and intuitive derivation of the evolution equation of a dilute gas of $N$ molecules. At first, we consider a gas where no collisions occur to describe the motion of the system. Then we discuss some properties of elastic and inelastic collisions, but leave the details of what happens in the situation of colliding molecules to Section 2.4. For more details in deriving the equation see [15, 16]. An alternative and more detailed derivation of the evolution equation or the so-called Liouville’s equation can be found in [11].

The derivation

Considering the large number of molecules, we cannot draw any conclusions from the microscopic state of the system, i.e. from (2.1). Therefore, we decide to use a probabilistic description, and we consider a density distribution function $f = f(x, \xi, t) \geq 0$. We define $f : \Omega \to \mathbb{R}_+$, where $\Omega \subset \mathbb{R}^3 \times \mathbb{R}^3$ and $\mathbb{R}_+ = [0, \infty)$, such that $f(x, \xi, t)dxd\xi$ describes, at time $t$, the probable number of molecules within the volume elements $dx$ and $d\xi$ surrounding the three component position vector $x$ and the three component velocity vector $\xi$.

It is helpful to think of the system of $N$ particles in terms of a six dimensional phase space, i.e as a system with three position axis and three velocity axis. We call this space the $\mu$-space, and we define $\mu = \{(x, \xi) \mid (x, \xi) \in \mathbb{R}^3 \times \mathbb{R}^3\}$. We partition the $\mu$-space and choose these phase-cells (volume elements), such that they contain a large number of molecules, but also small enough such that, as a result of a collision, the molecules will leave the phase-cell. Now, to describe the system of $N$ particles in terms of the distribution function, at some time $t$ we fixate a cell $dx_jd\xi_j$ to each molecule $i \in \{1, \ldots, N\}$. We can choose a subset of these cells, such that they are disjoint (almost everywhere) and cover the $\mu$-space. Without loss of generality (after a possible renumbering) we can assume that the subset consists of the cells $1, \ldots, \tilde{N}$. Then, the expected number of particles $(x, \xi)$ in the cell with label $j$ (with $j \in \{1, \ldots, \tilde{N}\}$) is given by

$$f(x, \xi, t)dx_jd\xi_j.$$

Due to the large number of molecules in each cell, and since one can assume that the density of molecules does not vary rapidly in neighbouring cells, the distribution function $f(x, \xi, t)$ can be regarded as a continuous function of its arguments [15, p.53]. Therefore, if we consider the distribution function over the subset of cells in $\mu$-space, and sum them up, we get the following approximation

$$\sum_{j=1}^{\tilde{N}} f(x, \xi, t)dx_jd\xi_j \approx \int_{\mu} f(x, \xi, t)dxd\xi.$$
Assuming no collisions between molecules and that the system changes with time, each cell will gain and lose some molecules. Therefore, a molecule in some surrounding to \((x, \xi)\) at time \(t\), will move to a neighbouring cell at time \(t+\delta t\) surrounding \((x+\xi \delta t, \xi+(X_0/m)\delta t)\) where \(X_0\) is the external force acting on a molecule. In the absence of collisions, and as \(\delta t \to 0\), we have

\[
f(x + \xi \delta t, \xi + (X_0/m)\delta t, t + \delta t)dx'd\xi' = f(x, \xi, t)dxd\xi,
\]

and it is possible to show that the volume elements \(dxd\xi = dx'd\xi'\) (in \(\mu\)-space) are invariant with respect to the evolution of the system. Therefore, by cancellation, and if we move everything to the left-hand side and expand, we have derived the evolution equation

\[
\frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial x} + \frac{X_0}{m} \cdot \frac{\partial f}{\partial \xi} = 0.
\]

In the proceeding sections we assume that the external force \(X_0\) acting on a molecule is zero, and therefore, the third term in the above equation will be excluded.

### 2.3 Two types of collisions

In this section we discuss two types of collisions: elastic collisions and inelastic collisions. To fully understand the derivation of the collision operator, one must at first understand the actual collision. We assume that the gas is rarefied, and hence, the probability for non-binary collisions is negligible. In other words, we have \(P(Y \geq 3) \approx 0\), where \(Y\) := number of colliding particles, for all collisions at any time \(t \in \mathbb{R}_+\). The molecules of the gas are modelled as identical hard spheres, i.e. with the same mass and radius.

It is worth mentioning that the theory presented in Section 2.4 is built on the foundation of binary elastic collisions [10, p.4].

**Elastic collisions**

At first, we only consider monatomic gases, i.e. molecules with no internal degree of freedom. In other words, we consider elastic collisions, which means that in each collision we have conservation of mass, momentum, and of kinetic energy. Let \(\xi_1\) denote the velocity corresponding to the first particle and \(\xi_2\) denote the velocity corresponding to the second particle. We denote by \(\xi'_1\) and \(\xi'_2\), respectively, the corresponding velocities after the collision, and by \(|\cdot|\), the Euclidean norm in \(\mathbb{R}^3\). Then, we have that the conservation of momentum in a collision is given by

\[
\xi_1 + \xi_2 = \xi'_1 + \xi'_2,
\]

and that the conservation of kinetic energy in a collision is given by

\[
|\xi_1|^2 + |\xi_2|^2 = |\xi'_1|^2 + |\xi'_2|^2.
\]
We aim to express $\xi'_1$ and $\xi'_2$ in terms of $\xi_1$ and $\xi_2$, and we introduce a unit vector $n$ along $\xi'_1 - \xi_1$, such that $\xi'_1 - \xi_1 = nC$, where $C \in \mathbb{R}$ and $|n| = 1$. Then, with respect to (2.2), we can write

\[
\begin{cases}
\xi'_1 = \xi_1 + nC \\
\xi'_2 = \xi_2 - nC.
\end{cases}
\] (2.4)

If we insert the equations given in (2.4) in (2.3) we get $-n \cdot V C + C^2 = 0$, where we denote by $V = \xi_2 - \xi_1$, the relative velocity. We dismiss the trivial solution $C = 0$, which otherwise would give no interaction. This implies $C = n \cdot V$, which yields

\[
\begin{cases}
\xi'_1 = \xi_1 + n \cdot (\xi_2 - \xi_1)n \\
\xi'_2 = \xi_2 - n \cdot (\xi_2 - \xi_1)n.
\end{cases}
\] (2.5)

This parametrization based on the collision mechanism of perfectly elastic rigid spheres, plays an important role in deriving the collision operator for the continuous Boltzmann equation. The details can be found in [12, p.5]. Subtracting the former equation from the latter one in (2.5) we get $V' = V - 2n(n \cdot V)$, where $V' = \xi'_2 - \xi'_1$. That is, the relative velocity undergoes a specular reflection$^1$ at the instant moment of a collision. It also follows that the relative speed is the same before and after the interaction, i.e.

$$|V|^2 = |V'|^2.$$ (2.6)

An elastic collision is illustrated in Figure 2.1. The velocity components of the particles along $n$ will be exchanged, and the velocity components perpendicular to $n$ will remain the same. In other words, we have $\xi'_1 \cdot n = \xi_2 \cdot n$ and $\xi'_2 \cdot n = \xi_1 \cdot n$.

Figure 2.1: Collision mechanism of perfectly elastic rigid spheres

**Inelastic collisions**

Now, we consider a polyatomic gas and examine the binary collisions. A polyatomic molecule have additional degrees of freedom (other than the translational ones) associated

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$^1$In this case, the collision of molecules behaves like the mirror-like reflection of waves. That is, the angle before and after the collision are the same, but on opposing sides of the surface normal.
to their internal energy states, in particular, the rotational and vibrational states [14]. One way to model the polyatomicity is well described in [12, p.209]: "The molecule is a mechanical system, which differs from a point mass by having a sequence of internal states, which can be identified by a label, assuming integral values. In the simplest cases these states differ from each other because the molecule have, besides kinetic energy, an internal energy taking different values $E_i$ in each of the different states. A collision between two molecules, besides changing the velocities, can also change the internal states of the molecules and, as a consequence, the internal energy enters in the energy balance."

Therefore we have

$$m|\xi_1|^2 + 2E_1 + m|\xi_2|^2 + 2E_2 = m|\xi_1'|^2 + 2E_1' + m|\xi_2'|^2 + 2E_2',$$

(2.7)

where $E_1, E_2$ and $E_1', E_2'$ denote the corresponding internal energies of the molecules, before and after the collision, respectively. We denote by $m$ the mass of the molecules. Observe that if $E_1 + E_2 = E_1' + E_2'$, then, the internal energies bring no contribution to (2.7). If we consider a polyatomic gas consisting of molecules with only two levels of internal energy, then, this type of collision behaves like an elastic collision. Therefore, later on in this thesis we consider collisions where $E_1 + E_2 = E_1' + E_2'$ to be of elastic type, but if instead we have $E_1 + E_2 \neq E_1' + E_2'$, then the collisions are considered to be of inelastic type.

As we saw in (2.6), the relative velocities before and after an elastic collision are equal up to a sign. We apply this idea in Section 2.4 where we consider a more detailed discussion of the collisions. Also, we discuss the concept of "micro-reversibility", which means that the "inverse" collisions are obtained with the same probability. Though, it is important to mention that in a polyatomic gas there is no guarantee that a collision have a specular reflection and that one can correlate an inverse collision with the same probability [12, p.210].

### 2.4 A derivation of the discrete Boltzmann equation

The discrete Boltzmann equation is a nonlinear mathematical model of kinetic theory of gases, which describes the evolution of a gas of particles allowed to move with a finite number of velocities [1, p.9]. In other words, we discretize the continuous velocity variable and model the Boltzmann equation, such that we only have a finite set of velocities $\mathcal{V} = \{\xi_1, ..., \xi_n\} \subset \mathbb{R}^3$ at our disposal. The density distribution function $f_i : \mathbb{R}^3 \times \mathbb{R}_+ \rightarrow \mathbb{R}_+$, such that $f_i = f(x, \xi_i, t) \in C^1(\mathbb{R}^3 \times \mathbb{R}_+)$ for $i \in \{1, ..., n\}$, is a function of time and position. The molecules do not interact with each other during most of the time. Therefore, we consider a distribution that corresponds to the one-particle distribution function [16, p.34]. Since $f_1, ..., f_n$ satisfy the evolution equation, we can write the discrete Boltzmann equation as a system of partial differential equations (PDEs), which is given
by
\[ \frac{\partial f_i}{\partial t} + \xi_i \cdot \nabla_x f_i = Q_i(f,f), \quad i = 1, \ldots, n, \]
where we denote by \( Q_i(f,f) \) the collision operators (see details below).

Even though we continue the discussion in ordinary physical space, it is worth mentioning that the discrete models of the Boltzmann equation are extendable to any finite dimension. That is, \( \mathbf{x}, \xi \in \mathbb{R}^d \), with \( d \in \mathbb{N} \).

**Transition probabilities**

We aim to discuss the collision operator from a viewpoint where we have a discrete set of velocities \( \mathcal{V} \). As in Section 2.2, where we derived the continuous Boltzmann equation, we consider here the case of a monatomic ideal gas (see description below). We denote, in the ordinary physical space the position vector by \( \mathbf{x} \in \mathbb{R}^3 \), and time by \( t \in \mathbb{R}_+ \). We consider binary elastic collisions, and hence, momentum and kinetic energy are conserved in each collision. Therefore, we have

\[
\begin{align*}
\xi_i + \xi_j &= \xi_k + \xi_l, \\
|\xi_i|^2 + |\xi_j|^2 &= |\xi_k|^2 + |\xi_l|^2,
\end{align*}
\]

where \( \xi_i \) and \( \xi_j \) denote the velocities before the collision, and \( \xi_k \) and \( \xi_l \) denote the velocities after the collision, such that \( i, j, k, l \in \{1, \ldots, n\} \). We denote a collision by \( (\xi_i, \xi_j) \rightarrow (\xi_k, \xi_l) \), or, in other words, by indicating the change of velocities. Given two velocities \( (\xi_i, \xi_j) \), we only allow the possible pairs of velocities \( (\xi_k, \xi_l) \) such that (2.8) is satisfied, as a result of the collision.

Let us consider a gas where the time of flight between collisions is much greater than the actual collision time. This condition is satisfied by rarefied gases [16, p.16]. We also consider an ideal gas, i.e. a gas in which the volume occupied by the molecules is small compared to the volume available to the gas. We call an ideal gas a Boltzmann gas, if the ratio of the mean free path (the average distance travelled by a moving molecule between successive collisions) of the molecules in the gas to a characteristic flow dimension is finite (details can be seen in [16, p.34]). Now, if we consider a Boltzmann gas, it follows that the expected number of collisions of type \( (\xi_i, \xi_j) \rightarrow (\xi_k, \xi_l) \), during the time \( (t, t + dt) \), in a cell \( d\mathbf{x} \) in \( \mathbb{R}^3 \) surrounding \( \mathbf{x} \) is given by

\[ \Gamma_{ij}^{kl} f_i f_j dt |d\mathbf{x}|, \]  

where \( \Gamma_{ij}^{kl} \) is called the transition probability of the collision. Here, we consider a regular grid (in space) and denote by \( |d\mathbf{x}| \), the volume of the cell \( d\mathbf{x} \) [10, p.5].

To fully understand the nature of the transition probability, we imagine a picture where one of the molecules, let us assume the molecule with velocity \( i \), is seen as a fixed point at the center of the action sphere \( \sigma \) with the radius two times the actual
molecule radius $r$. We let the other molecule with velocity $j$, that may be regarded as a point mass, collide with the action sphere $\sigma$ with the relative velocity $|\xi_i - \xi_j|$. As the point mass with velocity $j$ reach the sphere, the collision takes place in a cylinder with cross sectional area $S$ and with height $|\xi_i - \xi_j|dt$. The fixed point picture, and also the specular reflection of the relative velocity before and after a collision, are illustrated in Figure (2.2). Observe that in the illustration, we denote by the fixed point $x_i$ the center of mass of the molecule with velocity $\xi_i$, and by $x_j$, the point mass that corresponds to the molecule with velocity $\xi_j$.

The probability that a collision of two molecules with the velocity couple $(\xi_i, \xi_j)$ results in the new velocity couple $(\xi_k, \xi_l)$ is denoted by $a^{kl}_{ij}$. Since the possible outcomes are mutually exclusive, the sum of the probabilities of the events must be one, i.e.

$$\sum_{(k,l)} a^{kl}_{ij} = 1,$$

where summation is performed over all possible couples $(k,l)$. Therefore, the expected number of collisions given by (2.9) is more explicitly given by

$$S |\xi_i - \xi_j| f_i f_j a^{kl}_{ij} dt |dx|,$$

where $\Gamma^{kl}_{ij} = S |\xi_i - \xi_j| a^{kl}_{ij}$. (2.10)

Let us observe two things:

Observation 1. As a consequence of (2.8), the magnitude of the relative velocity of the molecules is identical before and after the collision, i.e. $|V| = |\xi_i - \xi_j| = |\xi_k - \xi_l| = |V'|$.

Observation 2. In implementations one often assume that all possible couples of velocities after a collision are obtained with the same probability. That is, if the molecules with velocity couple $(\xi_i, \xi_j)$ and $(\xi_k, \xi_l)$ collide, respectively, then the number of possible velocity couples $(\xi_p, \xi_q)$ after the collision are equal, for some $p, q \in \{1, \ldots, n\}$. Also, as a consequence of the discrete model, we have $a^{kl}_{ij} = a^{ij}_{kl}$ [10, p.6].

We apply the two observations above in expression (2.10), which confirms the assumption that the transition probabilities $\Gamma^{kl}_{ij}$ are non-negative and symmetric with respect to the velocities. In other words, we assume the transition probabilities satisfy the symmetry
relations
\[ \Gamma_{ij}^{kl} = \Gamma_{ji}^{kl} = \Gamma_{kl}^{ij} \geq 0, \quad \text{where } i, j, k, l \in \{1, ..., n\}. \]  
(2.11)

The transition probabilities in (2.11) are equal to zero unless the conservation laws in (2.8) are satisfied. This means that the collision and the "reversed collision" are obtained with the same probability, which we denote by \((\xi_i, \xi_j) \leftrightarrow (\xi_k, \xi_l)\). We call this property the relation of micro-reversibility.

The collision operator

We define the collision operator \(Q_i : (C^1(\mathbb{R}^3 \times \mathbb{R}_+))^n \times (C^1(\mathbb{R}^3 \times \mathbb{R}_+))^n \to (C^1(\mathbb{R}^3 \times \mathbb{R}_+))^n\), such that for \(f = [f_1, ..., f_n]\), \(Q_i(f, f) = G_i - L_i\), where \(G_i\) and \(L_i\) represents the gain and loss of molecules in the cell \(d\mathbf{x}\) with velocity \(\xi_i\) during time \((t, t + dt)\). We assume that the cell of interaction is small enough, such that due to a non-trivial collision \((\xi_i, \xi_j) \to (\xi_k, \xi_l)\), with \(i \neq j\), and \((\xi_k, \xi_l) \neq (\xi_i, \xi_j)\), the molecules leave the cell \(d\mathbf{x}\), and the molecule with velocity \(\xi_i\) takes a new velocity \(\xi_k\) for some \(k \in \{1, ..., n\}\). Similarly, due to some other collision in some neighboring cell \(d\mathbf{x}'\), during time \((t, t + dt)\), a particle with velocity \(\xi_i\) may enter the cell \(d\mathbf{x}\). We obtain

\[ G_i - L_i = \sum_{j=1}^{n} \sum_{(k,l)} \left( \Gamma_{ij}^{kl} f_k f_l - \Gamma_{kl}^{ij} f_i f_j \right), \]

where the summation is made over all possible couples \((k, l)\) [10, p.7]. If we instead do the summation over the indices \(j, k, l\) and apply (2.11) we have derived the coupled system of PDEs, or as we call it, the discrete Boltzmann equation:

\[ \frac{\partial f_i}{\partial t} + \xi_i \cdot \nabla_x f_i = \frac{1}{2} \sum_{j,k,l=1}^{n} \Gamma_{ij}^{kl} (f_k f_l - f_i f_j), \quad i = 1, ..., n, \]  
(2.12)

where the right-hand side is the explicit form of \(Q_i(f, f)\). Sometimes it is more convenient to study the more general bilinear expression associated with the collision operator [3, 12], which is given by

\[ Q_i(f, g) = \frac{1}{4} \sum_{j,k,l=1}^{n} \Gamma_{ij}^{kl} (f_k g_l + g_k f_l - f_i g_j - g_i f_j), \quad i \in \{1, ..., n\}, \]  
(2.13)

where \(f_i = f_i(\mathbf{x}, t), \ g_i = g_i(\mathbf{x}, t) \in C^1(\mathbb{R}^3 \times \mathbb{R}_+)\).

In the study of the Boltzmann equation introduced in (2.12), it should be clear that the left-hand side and the right-hand side are completely different in nature, from both a mathematical and a physical standpoint [11, p.40]. The part to the left is a linear differential operator acting on the distribution function describing the evolution of the gas, meanwhile, the part to the right consists of quadratic terms of possible binary collisions.
Chapter 3

Collision Invariants, Maxwellians, and the Linearized Collision Operator

In this chapter we introduce three concepts related to the Boltzmann equation, namely: the special type of functions called collision invariants, equilibrium distribution functions called the Maxwell distributions, and a linearization of the collision operator. In Chapter 5, as we make use of these concepts, we will see the great importance of them.

3.1 Collision invariants

Now, we study how the collision operator $Q_i(f, f)$ acts on the functions $\phi_i = \phi(\xi_i)$, where for generality we let $\xi_i \in \mathbb{R}^d$. By multiplying $\phi = [\phi_1, ..., \phi_n]$ with $Q(f, f) = [Q_1(f, f), ..., Q_n(f, f)]$ we obtain

$$\langle \phi, Q(f, f) \rangle = \frac{1}{2} \sum_{i,j,k,l=1}^{n} \Gamma_{ij}^{kl} \phi_i (f_k f_l - f_i f_j),$$  \hspace{1cm} (3.1)

where $\langle \cdot, \cdot \rangle$ denotes the Euclidean scalar product in $\mathbb{R}^n$. We apply the symmetry relations (2.11) and interchange the indices $i, j, k, l$ systematically. Then, we obtain four different ways to express the left-hand side of (3.1) [10, p.8], and if expressed as a linear combination, it follows that

$$\langle \phi, Q(f, f) \rangle = \frac{1}{8} \sum_{i,j,k,l=1}^{n} \Gamma_{ij}^{kl} (\phi_i + \phi_j - \phi_k - \phi_l)(f_k f_l - f_i f_j).$$  \hspace{1cm} (3.2)
The function $\phi$ is called a collision invariant if and only if
\[
\phi_i + \phi_j = \phi_k + \phi_l, \text{ for all } i, j, k, l \in \{1, ..., n\}, \text{ such that } \Gamma_{ij}^{kl} \neq 0. \tag{3.3}
\]
Observe that the expression (3.2) is equal to zero independently of the choice of $f$ if $\phi$ is a collision invariant. In other words, the collision operator is orthogonal to the set of collision invariants. It can be shown that (3.3) is satisfied if the collision invariants take the following form [12, p.14]:
\[
\phi(\xi_i) = a + b \cdot \xi_i + c|\xi_i|^2, \text{ where } a, c \in \mathbb{R}, \ b \in \mathbb{R}^d. \tag{3.4}
\]
We can interpret the collision invariants $\phi$ as linear combinations of the conservation of mass, momentum, and the kinetic energy. In the continuous case, the only possible collision invariants are the physical ones, but in the discrete case there could be additional non-physical so-called spurious collision invariants. At this moment it is worth mentioning that a DVM without spurious collision invariants is said to be normal, if the collision invariants are linearly independent.

### 3.2 Maxwellian distributions

A Maxwell distribution, or a Maxwellian $M = [M_1, ..., M_n]$, is an equilibrium distribution function, in other words, it describes a gas in a statistical equilibrium state. We define $M : \mathcal{U} \subset \mathbb{R}^d \to \mathbb{R}^+$, such that $M_i = M(\xi_i)$. A gas in an equilibrium state does not exchange mass and energy with other bodies, and its state does not change with time [12, p.24]. Therefore, the collisions in this state does not bring any contribution to the equation, and hence, the distribution yields a vanishing collision operator, i.e. $Q(M, M) = 0$. It can be shown that all Maxwellians $M$ are Gaussians, and for normal DVMs, take the form [5]:
\[
M_i = M(\xi_i) = e^{\phi_i} = e^{a + b \cdot \xi_i + c|\xi_i|^2}, \quad i \in \{1, ..., n\}. \tag{3.5}
\]

To see this, let $\phi_i = \log f_i$ and by insertion in (3.2) we have
\[
\langle \log f, Q(f, f) \rangle = \frac{1}{8} \sum_{i,j,k,l=1}^{n} \Gamma_{ij}^{kl}(f_k f_l - f_i f_j) \log \frac{f_i f_j}{f_k f_l} \leq 0. \tag{3.6}
\]

The equality holds in (3.6) if and only if
\[
f_i f_j = f_k f_l, \text{ for all } i, j, k, l \in \{1, ..., n\}, \text{ such that } \Gamma_{ij}^{kl} \neq 0. \tag{3.7}
\]
This follows from the fact that
\[
(y - x) \log \frac{x}{y} \leq 0, \tag{3.8}
\]
for every \( x, y \in \mathbb{R}_+ \), with equality if and only if \( x = y \).

**Proof of (3.8).** Let \( x, y \in \mathbb{R}_+ \). First, if \( x = y \), then equality in (3.8) is trivial. Secondly, we assume \( x > y \). Then, \( y - x < 0 \) and \( \log \frac{x}{y} = \log x - \log y > 0 \), from where it follows that (3.8) is satisfied. In a similar fashion one can show that (3.8) holds for \( y > x \). \( \square \)

Then, we take the logarithm of (3.7) and we see that \( f \) is a Maxwellian if and only if \( \log f \) is a collision invariant [3].

### 3.3 The linearized collision operator

If we make an expansion around a Maxwellian \( M \), we obtain a linear part, called the linearized collision operator, and a quadratic part [3]. Let

\[
f_i = M_i + M_i^{1/2} h_i, \quad i \in \{1, ..., n\},
\]

where \( h_i : \mathbb{R}^d \times \mathbb{R}_+ \to \mathbb{R} \), such that, \( h_i = h(x, \xi_i, t) \in C^1(\mathbb{R}^d \times \mathbb{R}_+) \), and \( M_i = M(\xi_i) \) are given in (3.5). If we insert the distribution function \( f = [f_1, ..., f_n] \) given by (3.9) in (2.12) – (2.13) we obtain the system

\[
\frac{\partial h_i}{\partial t} + \xi_i \cdot \nabla_x h_i = -(Lh)_i + S_i(h), \quad i = 1, ..., n,
\]

where \( L \) is the linearized collision operator \((n \times n)\) matrix given by

\[
Lh = -2M^{-1/2}Q(M, M^{1/2}h),
\]

and \( S \) is the quadratic part given by

\[
S(h) = M^{-1/2}Q(M^{1/2}h, M^{1/2}h).
\]

By (3.3) and (3.5), we have

\[
M_iM_j = M_kM_l \quad \text{for} \quad i, j, k, l \in \{1, ..., n\}.
\]

By (3.13), we obtain the following equivalent expressions

\[
\frac{M_j^{1/2}}{M_k^{1/2}} = \frac{M_i^{1/2}}{M_l^{1/2}} \quad \text{and} \quad \frac{M_j^{1/2}}{M_i^{1/2}} = \frac{M_k^{1/2}}{M_l^{1/2}}.
\]

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Then, by (2.13) and (3.14), we can obtain a more explicit form of the linearized operator (3.11). We have

\[
(Lh)_i = -2M_i^{-1/2} \frac{1}{4} \sum_{j,k,l=1}^{n} \Gamma_{ij}^{kl} \left( M_k M_i^{1/2} h_l + M_l M_i^{1/2} h_k - M_i M_j^{1/2} h_j - M_j M_i^{1/2} h_i \right)
\]

\[
= -\frac{1}{2} \sum_{j,k,l=1}^{n} \Gamma_{ij}^{kl} \left( M_k \frac{M_i^{1/2}}{M_i^{1/2}} h_l + M_l \frac{M_i^{1/2}}{M_i^{1/2}} h_k - M_i \frac{M_j^{1/2}}{M_i^{1/2}} h_j - M_j h_i \right)
\]

\[
= -\frac{1}{2} \sum_{j,k,l=1}^{n} \Gamma_{ij}^{kl} M_j^{1/2} \left( M_k^{1/2} h_l + M_l^{1/2} h_k - M_i^{1/2} h_j - M_j^{1/2} h_i \right),
\]

for \( i \in \{1, \ldots, n\} \). In a similar way one can obtain an explicit form of the quadratic part (3.12) given by

\[
S_i(h) = \frac{1}{2} \sum_{j,k,l=1}^{n} \Gamma_{ij}^{kl} M_j^{1/2} (h_k h_l - h_i h_j).
\]

Using similar arguments as for obtaining (3.2), but now with respect to (3.15) instead of \( Q(f, f) \), we obtain

\[
\langle g, Lh \rangle = \frac{1}{8} \sum_{i=1}^{n} \sum_{j,k,l=1}^{n} \Gamma_{ij}^{kl} \left( M_k^{1/2} g_l + M_l^{1/2} g_k - M_i^{1/2} g_j - M_j^{1/2} g_i \right)
\]

\[
\times \left( M_k^{1/2} h_l + M_l^{1/2} h_k - M_i^{1/2} h_j - M_j^{1/2} h_i \right),
\]

and can conclude that that the matrix \( L \) is symmetric [3, p.15], i.e.

\[
\langle g, Lh \rangle = \langle Lg, h \rangle,
\]

for all \( g = [g_1, \ldots, g_n] \) and \( h = [h_1, \ldots, h_n] \).

**Remark.** \( L \) is semi-positive. To see this, we insert \( h \) instead of \( g \) in (3.16), and obtain \( \langle h, Lh \rangle \geq 0 \) for all \( h = h(\xi) \), with equality if and only if

\[
M_k^{1/2} h_l + M_l^{1/2} h_k = M_i^{1/2} h_j + M_j^{1/2} h_i
\]

for all indices \( i, j, k, l \in \{1, \ldots, n\} \), such that \( \Gamma_{ij}^{kl} \neq 0 \). Therefore, it follows that if we insert \( h = M_i^{1/2} \phi \) in (3.18), by (3.13), we see that (3.3) is satisfied, and we have

\[
(Lh)_i = 0 \text{ if and only if } h_i = M_i^{1/2} \phi_i, \quad i \in \{1, \ldots, n\},
\]

where \((Lh)_i\) is given in (3.15), and \( \phi = [\phi_1, \ldots, \phi_n] \) is a collision invariant.
Chapter 4

Discrete Velocity Models for Polyatomic Molecules

The general discrete velocity model based on the Boltzmann equation is given by

$$\frac{\partial f_i}{\partial t} + \xi_i \cdot \nabla_x f_i = Q_i(f, f), \quad i = 1, \ldots, n,$$

where $\mathcal{V} = \{\xi_1, \ldots, \xi_n\} \subset \mathbb{R}^d$ is a finite set of velocities. The purpose and the idea of DVMs are well described in [20]: "The models generate systems of highly coupled semi-linear partial differential equations which approximate the Boltzmann equation, and are particularly useful for studying problems in rarefied gas dynamics, such as Couette flow, Rayleigh flow and shock structure, especially at high Mach number."

In [17], the authors analyze a certain class of models which are numerical approximations to the Boltzmann equation, and also, they prove the consistency of the approximation for the collision integral.\(^1\)

4.1 DVMs generalized for polyatomic gases

We consider the situation of a gas that consists of polyatomic molecules. The polyatomicity can be modelled such that each molecule is coupled with an internal energy $E$. We have $\mathcal{V}_{\text{pol}} = \{(\xi_1, E_1), \ldots, (\xi_n, E_n)\}$, where $E_i$ belongs to a given set of internal energies $\{\tilde{E}_1, \ldots, \tilde{E}_s\}$, such that molecules with different internal energies can have the same velocity, but each couple of velocity and internal energy is unique. A collision obtained with velocity couples from $\mathcal{V}_{\text{pol}}$ is denoted by

$$\{(\xi_i, E_i); (\xi_j, E_j)\} \rightarrow \{(\xi_k, E_k); (\xi_l, E_l)\}. \quad (4.1)$$

\(^1\)To show convergence, the authors discretize the velocity space on a regular grid, and approximate the collision integral by a quadrature formula. Then, with properties such as consistency and stability, one can prove that the numerical method converges.
Since we consider normal models, and still assuming that the symmetry relations (2.11) hold, and since the internal energy enters the energy balance equation (2.7), the collision invariants (cf. (3.3) and (3.4)) will be of the form

$$\phi(\xi_i) = a + b \cdot \xi_i + c(m|\xi_i|^2 + 2E_i), \text{ where } a, c \in \mathbb{R}, b \in \mathbb{R}^d. \quad (4.2)$$

**Geometric interpretation**

We can visualize the DVM, in terms of collisions, geometrically. It follows from the conservation laws given in (2.8) with some algebraic argumentation that an elastic collision \((\xi_i, \xi_j) \leftrightarrow (\xi_k, \xi_l)\) is represented by a (plane) rectangle in \(\mathbb{R}^d\), such that the couple of velocities with indices \((i, j)\) and \((k, l)\) are on diagonal corners, respectively. Similarly, an inelastic collision (4.1), where the internal energy enters in the energy balance equation (2.7), is represented by a (plane) parallelogram in \(\mathbb{R}^d\), see Figure 4.1.

**Conservation laws and normality**

We fix a numbering of all velocities and represent each possible collision \((\Gamma_{ij}^{kl} \neq 0)\) by a collision vector \(\theta\) which is an \(n\)-dimensional vector with \(-1, 0, 1\) as the only coordinates [2]:

$$\theta = [0, \ldots, 0, 1, 0, \ldots, 0, 1, 0, \ldots, 0, -1, 0, \ldots, 0, 0, \ldots, 0] \in \mathbb{Z}^n.$$

If a set of collision vectors is linearly dependent, we say that a collision can be obtained by a combination of the remaining collisions. Otherwise, we say that the collisions are linearly independent. We form a matrix \(\Lambda_{tot}\), which consists of all collision vectors as row vectors, and denote by \(\Lambda\) a matrix consisting of a maximal set of linearly independent collision vectors as row vectors.

We introduce the set of given invariants \(U\) defined such that

$$U = \left\{ \begin{array}{l}
\phi_0 = [1, \ldots, 1] \\
\phi_a = [\xi_1^a, \ldots, \xi_n^a], \quad a = 1, \ldots, d \\
\phi_{d+1} = [m|\xi_1|^2 + 2E_1, \ldots, m|\xi_n|^2 + 2E_n] 
\end{array} \right\}, \quad (4.3)$$
for which $\langle \phi_j, \theta \rangle = 0$ for all $\theta \in \text{Row}(\Lambda)$ and $j \in \{0, \ldots, d+1\}$. The rank of $\Lambda_{\text{tot}}$ cannot, by the construction of the DVM (if the set $U$ is linearly independent and we only have physical collision invariants), exceed $n - (d + 2)$, since for $\xi = [\xi^1, \ldots, \xi^d]$ the functions $\phi_j(\xi)$ in (4.3), then lead to $d + 2$ linearly independent vectors [7, p.5]. In fact, we can introduce the following concepts [8, p.157]:

**Definition 1.** The vector space $\ker(\Lambda)$ is said to be the **vector space of collision invariants** of the discrete velocity model. The number of collision invariants is given by

$$\dim(\ker(\Lambda)) = n - \text{rank}(\Lambda).$$

(4.4)

For the continuous Boltzmann equation the only collision invariants are the physical ones. But in the construction of DVMs for the Boltzmann equation extra collision invariants, so called **spurious collision invariants**, may appear. A DVM without spurious collision invariants is called normal by the following definitions [8, p.158]:

**Definition 2.** A DVM with given invariants $U$ (see (4.3)) is said to be **non-degenerate** if the vectors $\phi_j \in U$, $j \in \{0, \ldots, d+1\}$, are linearly independent. Otherwise, the DVM is called degenerate.

**Definition 3.** A non-degenerate DVM is said to be **normal** if it has exactly $d+2$ linearly independent collision invariants, i.e. if $\dim(\ker(\Lambda)) = d + 2$.

Depending on what we want to study we can be satisfied with different levels of normality. Let $V_j = \{(\xi_i, E_i) | 1 \leq i \leq n, E_i = \tilde{E}_j \} \subseteq V_{\text{pol}}$, $j \in \{1, \ldots, s\}$, and we can distinguish the level of normality, in addition to Definition 4.4, by the following definitions [2, p.747]:

**Definition 4.** A DVM with internal energies $\{\tilde{E}_1, \ldots, \tilde{E}_s\}$ is called **semi-supernormal** if it is normal and the restriction to each set $V_j$, $j \in \{1, \ldots, s\}$, is a normal DVM.

**Definition 5.** A DVM with internal energies $\{\tilde{E}_1, \ldots, \tilde{E}_s\}$ is called **supernormal** if the restriction to each collection

$$\{V_{r_1}, \ldots, V_{r_j}\} \subset \{V_1, \ldots, V_s\}, \quad j \in \{1, \ldots, s\},$$

is a normal DVM.
Chapter 5

A Broadwell Model for Polyatomic Molecules

In this chapter we present a DVM that we consider to be our main new contribution. We wish to describe a gas consisting of a single species of polyatomic molecules in the sense that each molecule has an associated internal energy. We consider a 9-velocity model in $\mathbb{R}^2$ with two levels of internal energy, consisting of two different Broadwell models, as follows

\[
\begin{align*}
\xi_1 &= \{[0,0], E_1\}, & \xi_{2,4} &= \{[\pm1,0], E_1\}, \\
\xi_{3,5} &= \{[0,\pm1], E_1\}, & \xi_{7,8} &= \{[\pm1,1], E_2\}, & \xi_{6,9} &= \{[\pm1,-1], E_2\}.
\end{align*}
\]

Figure 5.1: Linearly independent collisions for the 9-velocity Broadwell model

5.1 Normality of the DVM

In order to comprehend the DVM completely it is suitable to start the discussion with some of the motive behind the particular chosen velocities and then, determine the level of normality. Let us consider the set of velocities $\{\xi_2, \xi_3, \xi_4, \xi_5\}$ – all of them with the same internal energy $E_1$ – which forms a 4-velocity monatomic DVM (also called a
Broadwell model [6]). With these velocities we obtain one linearly independent collision 
\((\xi_2, \xi_4) \leftrightarrow (\xi_3, \xi_5)\). We can represent the collision by the vector \(\theta_1 = [1, -1, 1, -1]\) or, since it is convenient to treat it as a matrix, by the collision matrix

\[
\Lambda_{1 \times 4} = \begin{bmatrix}
1 & -1 & 1 & -1
\end{bmatrix}.
\]

Then, we have

\[
\dim(\ker(\Lambda_{1 \times 4})) = 4 - \text{rank}(\Lambda_{1 \times 4}) = 3,
\]

which, by definition, is a degenerate DVM. For normality, we need \(\dim(\ker(\Lambda_{1 \times 4})) = d + 2 = 4\), and we transform the DVM to be normal by adding one velocity \(\xi_1\) (also with internal energy \(E_1\)) [6]. To see this, let \(\{\xi_1, \xi_2, \xi_3, \xi_4, \xi_5\}\) be the new velocity set (see Figure 5.1(a)). Since \(\xi_1\) do not participate in any collision, \((\xi_2, \xi_4) \leftrightarrow (\xi_3, \xi_5)\) is still the only one, which we now represent by the matrix

\[
\Lambda_{1 \times 5} = \begin{bmatrix}
0 & 1 & -1 & 1 & -1
\end{bmatrix}.
\]

It follows that

\[
\dim(\ker(\Lambda_{1 \times 5})) = 5 - \text{rank}(\Lambda_{1 \times 5}) = 4,
\]

and then, the set \(U\) of given invariants given in (4.3) are linearly independent and spans \(\ker(\Lambda_{1 \times 5})\). Even though the DVM, in some sense, is artificial (since \(\xi_1\) cannot participate in any collision), we have shown that it satisfies the condition of being normal.

**Method of one-extension**

In [6], the authors introduced an inductive method called the *method of one-extension*, in which a model can be extended with an additional velocity. One can easily interpret the method geometrically for a single species collision. By having three corners (velocities) of a rectangle (collision), but not the fourth in the velocity set, one can add the fourth velocity to the velocity set, obtaining a new collision that is linearly independent of the already existing collisions in the DVM. In the inelastic case, of course, the considered collision is represented by a parallelogram.

If we by this method add the velocity \(\xi_6\) with internal energy \(E_2\), we obtain two linearly independent collision vectors that we put as rows in the matrix

\[
\Lambda_{2 \times 6} = \begin{bmatrix}
0 & 1 & -1 & 1 & -1 & 0 \\
1 & 0 & 0 & -1 & 1 & -1
\end{bmatrix}.
\]

It follows that

\[
\dim(\ker(\Lambda_{2 \times 6})) = 6 - \text{rank}(\Lambda_{2 \times 6}) = 4,
\]

which coincides with the number of linearly independent collision invariants and we have a normal DVM. Observe that the model now contains molecules with different levels of
internal energy, and that the collision given by the second row vector in $\Lambda_{2\times6}$ describes an inelastic collision. If we continue with this inductive argument, in fact; "In the inelastic case, one could always construct a new normal model by using the one-extension scheme" [7, p.20], then we complete the model with the remaining velocities given in (5.1), and check below that it is in fact normal.

**Level of normality**

The total number of possible collisions in this model is fourteen (each collision with its inverse collision are counted as one) with the following eight inelastic collisions;

\[
\begin{align*}
(\xi_3, \xi_6) &\leftrightarrow (\xi_1, \xi_2) \leftrightarrow (\xi_5, \xi_7) \\
(\xi_2, \xi_8) &\leftrightarrow (\xi_1, \xi_3) \leftrightarrow (\xi_4, \xi_7) \\
(\xi_3, \xi_9) &\leftrightarrow (\xi_1, \xi_4) \leftrightarrow (\xi_5, \xi_8) \\
(\xi_2, \xi_9) &\leftrightarrow (\xi_1, \xi_5) \leftrightarrow (\xi_4, \xi_6),
\end{align*}
\]

and the following six elastic collisions;

\[
\begin{align*}
(\xi_2, \xi_4) &\leftrightarrow (\xi_3, \xi_5) \\
(\xi_2, \xi_8) &\leftrightarrow (\xi_1, \xi_7) \\
(\xi_3, \xi_6) &\leftrightarrow (\xi_5, \xi_7) \\
(\xi_6, \xi_8) &\leftrightarrow (\xi_7, \xi_9) \\
(\xi_2, \xi_9) &\leftrightarrow (\xi_4, \xi_6) \\
(\xi_3, \xi_9) &\leftrightarrow (\xi_5, \xi_8).
\end{align*}
\]

For brevity, in the collisions above, we only indicate the velocities, since the internal energy is unique for each velocity. Observe that some collisions between particles with different internal energy are classified as elastic collisions. Since we only consider non-trivial collisions, this is the case when we have a perfect transfer of internal energy in the collision. In other words, when we have no contribution of the internal energies to the energy balance equation (2.7).

If we let $\Lambda_{\text{tot}}$ be the matrix with rows given by all possible collision vectors, then $\text{rank}(\Lambda_{\text{tot}}) = 5$. Therefore, every collision in the DVM can be expressed as a linear combination of five linearly independent collision vectors. For instance, we can choose the following linearly independent collisions:

\[
\begin{align*}
(\xi_2, \xi_4) &\leftrightarrow (\xi_3, \xi_5); \quad \theta_1 = [0,1,-1,1,-1,0,0,0,0] \\
(\xi_6, \xi_8) &\leftrightarrow (\xi_7, \xi_9); \quad \theta_2 = [0,0,0,0,0,1,-1,1,-1] \\
(\xi_2, \xi_8) &\leftrightarrow (\xi_4, \xi_7); \quad \theta_3 = [0,1,0,-1,0,0,-1,1,0] \\
(\xi_3, \xi_6) &\leftrightarrow (\xi_5, \xi_7); \quad \theta_4 = [0,0,1,0,-1,1,-1,0,0] \\
(\xi_1, \xi_5) &\leftrightarrow (\xi_4, \xi_6); \quad \theta_5 = [1,0,0,-1,1,-1,0,0,0],
\end{align*}
\]

and then let $\Lambda_{5\times9} = [\theta_1 \theta_2 \theta_3 \theta_4 \theta_5]^T$, with $\text{rank}(\Lambda_{5\times9}) = 5$. The linearly independent collisions are illustrated in Figure 5.1. By (4.4), $\dim(\text{ker}(\Lambda_{5\times9})) = 9 - 5 = 4$. Therefore,
to check that the DVM is normal we only need to make sure that the DVM is non-degenerate. In order to compute the given invariants (4.3) explicitly we determine the relationship between $E_1$ and $E_2$. We consider the inelastic collision $(\xi_1, \xi_3) \leftrightarrow (\xi_4, \xi_7)$ for which the energy balance equation has to be satisfied, i.e.

$$\frac{1}{2} m \gamma^2 |\xi_1|^2 + E_1 + \frac{1}{2} m \gamma^2 |\xi_3|^2 + E_1 = \frac{1}{2} m \gamma^2 |\xi_4|^2 + E_1 + \frac{1}{2} m \gamma^2 |\xi_7|^2 + E_2. \quad (5.3)$$

By (5.3), it follows that

$$E_1 - E_2 = m \gamma^2. \quad (5.4)$$

In (5.4), $\gamma$ is an imagined scale factor for the velocities in (5.1). Because of the symmetry of the DVM, (5.4) is obtained for any inelastic collision, and so is well-defined. We keep the expression in (5.4) as general as possible, since it allows us to make a possible re-scaling of the model. The collision invariants (given invariants) are given by

$$\begin{align*}
\phi_1 &= [1, 1, 1, 1, 1, 1, 1, 1, 1] \\
\phi_2 &= [0, 1, 0, -1, 0, 1, 1, -1, -1] \\
\phi_3 &= [0, 0, 1, 0, -1, -1, 1, 1, -1] \\
\phi_4 &= [0, 1, 1, 1, 0, 0, 0, 0, 0].
\end{align*}$$

Obviously, they are linearly independent and hence, the DVM is non-degenerate by Definition 2. Then, since $\dim(\ker(\Lambda_{5 \times 9})) = 4$, the DVM is normal.

Now, if we consider the DVM consisting of the subset of velocities $\{\xi_6, \xi_7, \xi_8, \xi_9\}$ all with internal energy $E_2$ (see Figure 5.1(b)), then, in correspondence to (5.2), we see that it is formally not normal. Therefore, the original DVM given by (5.1), by Definitions 4 and 5, does not satisfy any level of normality above normal.

### 5.2 Flow axially symmetric around x-axis

We consider the DVM with velocities (5.1) and distribution functions $f_i = f(x, \xi_i, t)$ for $1 \leq i \leq 9$. Then, the complete system of equations for the DVM is given in Appendix A.

**Reduction of system by symmetry**

We assume that our flow is symmetric with respect to the x-axis, or in other words, the distribution functions corresponding to the couples of velocities $(\xi_3, \xi_5)$, $(\xi_6, \xi_7)$, and $(\xi_8, \xi_9)$, respectively, are mutually equal, i.e.

$$f_3 = f_5, \quad f_6 = f_7, \quad f_8 = f_9. \quad (5.5)$$

By the symmetry around the x-axis, we can reduce the system of nine equations to a system of six equations. By reducing the system we mean to apply (5.5), such that, by
adding the equations with equal distribution functions, we get advantageous cancellations. For instance, we add the equations that correspond to \( f_3 \) and \( f_5 \) in the system in Appendix A, and apply (5.5). By the symmetry properties of the model, we can assume that each inelastic collision occur with equal probability. Therefore, it follows that

\[
\frac{\partial f_3}{\partial t} = \Gamma_{23}^{24}(f_2f_4 - f_3f_6) + \Gamma_{31}^{24}(f_2f_8 - f_1f_3) + \Gamma_{31}^{17}(f_4f_7 - f_1f_3) \\
+ \Gamma_{30}^{12}(f_1f_2 - f_3f_6) + \Gamma_{30}^{14}(f_1f_4 - f_3f_6).
\]

With similar argumentation for the remaining equations, and by the symmetry relations (2.11), we reduce the system given in Appendix A. We renumber the indices for the distribution functions \( f_7 \) and \( f_8 \), such that, we denote \( f_7 \) by \( f_5 \), and \( f_8 \) by \( f_6 \). Then, we obtain the following reduced system

\[
\begin{align*}
\frac{1}{2} \frac{\partial f_1}{\partial t} & = \Gamma_{12}^{35}(f_3f_5 - f_1f_2) + \Gamma_{13}^{45}(f_4f_5 - f_1f_3) + \Gamma_{13}^{26}(f_2f_6 - f_1f_3) \\
& + \Gamma_{14}^{36}(f_3f_6 - f_1f_4) \\
\frac{1}{2} \left( \frac{\partial f_2}{\partial t} + \frac{\partial f_2}{\partial x} \right) & = \frac{1}{2} \Gamma_{24}^{32}(f_2f_4 - f_2f_6) + \Gamma_{26}^{45}(f_4f_4 - f_2f_6) + \Gamma_{12}^{35}(f_3f_5 - f_1f_3) \\
& - \Gamma_{13}^{26}(f_2f_6 - f_1f_3) \\
\frac{\partial f_3}{\partial t} & = -\Gamma_{24}^{32}(f_2f_4 - f_2f_6) + \Gamma_{13}^{26}(f_2f_6 - f_1f_3) + \Gamma_{13}^{45}(f_3f_5 - f_1f_3) \\
& - \Gamma_{12}^{35}(f_3f_5 - f_1f_2) - \Gamma_{14}^{36}(f_3f_6 - f_1f_4) \\
\frac{1}{2} \left( \frac{\partial f_4}{\partial t} - \frac{\partial f_4}{\partial x} \right) & = \frac{1}{2} \Gamma_{24}^{35}(f_3f_5 - f_1f_2) - \Gamma_{26}^{45}(f_4f_5 - f_2f_6) - \Gamma_{13}^{45}(f_3f_5 - f_1f_3) \\
& + \Gamma_{14}^{36}(f_3f_6 - f_1f_4) \\
\frac{\partial f_5}{\partial t} + \frac{\partial f_5}{\partial x} & = -\Gamma_{26}^{45}(f_4f_5 - f_2f_6) - \Gamma_{13}^{45}(f_3f_5 - f_1f_2) - \Gamma_{13}^{45}(f_3f_5 - f_1f_3) \\
\frac{\partial f_6}{\partial t} - \frac{\partial f_6}{\partial x} & = \Gamma_{26}^{45}(f_4f_5 - f_2f_6) - \Gamma_{13}^{45}(f_2f_6 - f_1f_3) - \Gamma_{14}^{36}(f_3f_6 - f_1f_4). \quad (5.6)
\end{align*}
\]

Therefore, the original system, containing fourteen possible collisions, is now reduced to contain six possible collisions, i.e. the inelastic collisions;

\[
(\xi_1, \xi_2) \leftrightarrow (\xi_3, \xi_5) \quad (\xi_1, \xi_3) \leftrightarrow (\xi_4, \xi_6) \\
(\xi_1, \xi_3) \leftrightarrow (\xi_2, \xi_6) \quad (\xi_1, \xi_4) \leftrightarrow (\xi_3, \xi_6),
\]

and the elastic collisions;

\[
(\xi_2, \xi_4) \leftrightarrow (\xi_5, \xi_6) \quad (\xi_2, \xi_5) \leftrightarrow (\xi_4, \xi_6).
\]

Observe that the velocities in the collisions given above correspond to the distribution functions \( f_1, ..., f_6 \), and therefore, the numeration differs from the velocities given in (5.1), and can be seen in Figure 5.2.
It is important that in the reduced system, the conservation laws are still satisfied. We rewrite the right-hand side of system (5.6) in the following way

\[
\begin{bmatrix}
1 & 1 & 1 & 1 & 0 & 0 \\
1 & 0 & -1 & 0 & 1/2 & 1 \\
-1 & 1 & 1 & -1 & -1 & 0 \\
0 & -1 & 0 & 1 & 1/2 & -1 \\
-1 & -1 & 0 & 0 & 0 & -1 \\
0 & 0 & -1 & -1 & 0 & 1 \\
\end{bmatrix}
\begin{bmatrix}
\Gamma_{35}^3 (f_3 f_5 - f_1 f_2) \\
\Gamma_{45}^4 (f_4 f_5 - f_1 f_3) \\
\Gamma_{26}^2 (f_2 f_6 - f_1 f_3) \\
\Gamma_{36}^3 (f_3 f_6 - f_2 f_4) \\
\Gamma_{33}^3 (f_3 f_3 - f_2 f_4) \\
\Gamma_{45}^4 (f_4 f_5 - f_2 f_6) \\
\end{bmatrix}.
\]

Then it is easy to see that the collision invariants

\[
\begin{align*}
\phi_1 &= [1, 1, 1, 1, 1, 1] \\
\phi_2 &= [0, 1, 0, -1, 1, -1] \\
\phi_3 &= [0, 1, 1, 0, 0]
\end{align*}
\]

are orthogonal to the column vectors of the $6 \times 6$-matrix given in (5.7).

### 5.3 Linearization

In order to linearize the system, and in particular, to obtain the linearized collision operator, we follow the procedure in (3.9), (3.10), and (3.15). Since we now consider a DVM for polyatomic molecules, the internal energy enters the energy balance equation (2.7). Hence, the Maxwellians will be of the form (cf. (3.5))

\[ M_i = e^{\phi_i} = \exp(a + b \cdot \xi_i + c(m\gamma^2|\xi_i|^2 + 2E_i)), \quad i \in \{1, \ldots, 6\}. \]

We consider the Maxwellians to be non-drifting, i.e. with $b = 0$. Then it follows that

\[ M = \alpha[1, \beta, \beta, \beta, 1, 1], \]

where

\[ \alpha = \exp(a + 2cE_1) \quad \text{and} \quad \beta = \exp(cm\gamma^2). \]
The first equation in the linearized system of (5.6) is, by (3.15), given by

\[
\frac{1}{2} \frac{\partial h_1}{\partial t} = \Gamma_{12}^{35} M_2^{1/2} (M_3^{1/2} h_5 + M_5^{1/2} h_3 - M_1^{1/2} h_2 - M_2^{1/2} h_1)
+ \Gamma_{13}^{45} M_3^{1/2} (M_4^{1/2} h_5 + M_5^{1/2} h_4 - M_1^{1/2} h_3 - M_3^{1/2} h_1)
+ \Gamma_{13}^{26} M_3^{1/2} (M_4^{1/2} h_6 + M_6^{1/2} h_2 - M_1^{1/2} h_3 - M_3^{1/2} h_1)
+ \Gamma_{14}^{36} M_4^{1/2} (M_3^{1/2} h_6 + M_6^{1/2} h_3 - M_1^{1/2} h_4 - M_4^{1/2} h_1).
\]  

(5.10)

We form the linearized collision operator \(L\), given by

\[
L = \begin{bmatrix}
a_{11} & a_{12} & \cdots & a_{16} \\
a_{21} & a_{22} & \cdots & a_{26} \\
\vdots & \vdots & \ddots & \vdots \\
a_{61} & a_{62} & \cdots & a_{66}
\end{bmatrix}
\]

(5.11)

where the entries \(a_{ij}, 1 \leq j \leq 6\), are given by the corresponding coefficients for \(h_j\) that appears in (5.10). With similar argumentation for the remaining equations in (5.6), we complete the matrix. The entries of the matrix (5.11), are given explicitly in Appendix B.

**Transition probabilities**

We continue the investigation of the model by determining the transition probabilities explicitly. By these calculations we expect to reduce the number of terms in some of the entries in matrix (5.11). There are different ways to calculate the transition probabilities suggested in [9, 10].

If we assume, in correspondence with (2.10), that the collision coefficient associated with an elastic collision is calculated by

\[
\Gamma_{ij}^{kl} = S \gamma |\xi_i - \xi_j| a_{ij}^{kl}
\]

where \(i, j, k, l \in \{1, \ldots, n\}\),

\[\Gamma_{45}^{26} = S \gamma |\xi_2 - \xi_6| a_{26}^{45} = \frac{\sqrt{5}}{2} S \gamma\]

and \(\gamma\) is the scale factor of the velocities. Then, the collision \((\xi_2, \xi_6) \leftrightarrow (\xi_4, \xi_5)\) occur with probability

\[
\Gamma_{26}^{45} = S \gamma |\xi_2 - \xi_6| a_{26}^{45} = \frac{\sqrt{5}}{2} S \gamma.
\]

Observe that we only consider non-trivial collisions, i.e. collisions where the molecules just exchange velocities \((\xi_i, \xi_j) \leftrightarrow (\xi_j, \xi_i)\) are of no interest. Therefore, the collision have two possible outcomes which we assume to be equally probable (see a more detailed discussion below), and hence, \(a_{26}^{45} = \frac{1}{2}\).
Cross sectional area and inelastic collisions

Considering the inelastic collisions it is not clear whether the following equation is satisfied or not;

\[ S_\gamma |\xi_i - \xi_j| |\xi_k - \xi_l| a^i_{ij} a^j_{kl} = S_\gamma |\xi_k - \xi_l| |\xi_i - \xi_j| a^k_{ij} a^l_{kl}, \quad i, j, k, l \in \{1, ..., 6\}. \]

For instance, by (2.11) we have \( \Gamma^{26}_{13} = \Gamma^{13}_{26} \), or explicitly given by

\[ S_\gamma |\xi_1 - \xi_3| a^{26}_{13} = S_\gamma |\xi_2 - \xi_6| a^{13}_{26} \iff \frac{1}{2} = \frac{\sqrt{5}}{2}, \quad (5.13) \]

which obviously is a contradiction. In order to obtain equality in (5.13), we can make a distinction such that the cross sectional area \( S \) depends on whether the incoming molecules possess the same internal energy or not. Therefore, we denote by \( S_{11} \) the cross sectional area related to the type of collision

\[ \{ (\xi_i, E_1); (\xi_j, E_1) \} \rightarrow \{ (\xi_k, E_p); (\xi_l, E_q) \}, \]

and by \( S_{12} \), the cross sectional area related to the type of collision

\[ \{ (\xi_i, E_1); (\xi_j, E_2) \} \rightarrow \{ (\xi_k, E_p); (\xi_l, E_q) \}, \]

where \( i, j, k, l \in \{1, ..., 6\} \), and \( p, q \in \{1, 2\} \). Observe that we here assume that the cross sectional area does not depend on the outcome. Then, the symmetry relations (2.11) are satisfied regarding the inelastic collisions if we infer the cross sectional areas \( S_{11} \) and \( S_{12} \), such that, they compensate for the difference in the relative velocity before and after the collision. Then, if we insert \( S_{11} \) and \( S_{12} \) in (5.13), we obtain the relation

\[ S_{11} = \sqrt{5} S_{12}. \quad (5.14) \]

We have now two options to represent the transition probabilities for the inelastic collisions. We want to simplify the expression of matrix (5.11), and therefore, we proceed the discussion with the following simplifying assumption. We assume that the collision between molecules with velocities and internal energies \( (\xi_i, E_1) \), and \( (\xi_j, E_2) \) collide with some probability independently of the outcome. Therefore, by assumption the following collisions

\[ (\xi_2, \xi_6) \leftrightarrow (\xi_4, \xi_5) \quad \text{(elastic collision)} \]
\[ (\xi_2, \xi_6) \leftrightarrow (\xi_1, \xi_3) \quad \text{(inelastic collision)}, \]

are obtained with the same probability. Since the DVM is symmetric around both axis it is natural to assume that all the inelastic collisions are obtained with the same probability.
Hence, the coefficients we need for the reduced system of equations, are given by

\[
\Gamma_{12}^{35} = \Gamma_{13}^{45} = \Gamma_{14}^{26} = \Gamma_{15}^{13} = \Gamma_{16}^{45} = \Gamma_{26}^{13} = \frac{\sqrt{5}}{2} S_{12} \gamma. \tag{5.15}
\]

Regarding the remaining elastic collision \(\Gamma_{23}^{35}\) (or in the original notation \(\Gamma_{21}^{35}\)), we have two colliding molecules with internal energy \(E_1\). We want to express all the transition probabilities with the same cross sectional area \(S_{12}\), therefore, in accordance to (5.12), and with respect to the relation (5.14), we obtain

\[
\Gamma_{23}^{35} = \Gamma_{24}^{35} = S_{11} \gamma | \xi_2 - \xi_4 | a_{21}^{35} = 2 S_{11} \gamma = 2 \sqrt{5} S_{12} \gamma. \tag{5.16}
\]

The linearized collision operator

Now, if we insert (5.15) and (5.16) in the entries given in Appendix B, we can reduce the linearized collision operator \(L\) such that it is given by

\[
L = \sqrt{5} \alpha S \gamma \begin{bmatrix}
2\beta & 0 & 0 & 0 & -\beta & -\beta \\
0 & \frac{3}{2} + \beta & -1 - 2\beta & \beta - \frac{1}{2} & -\sqrt{3} & \sqrt{3} \\
0 & -1 - 2\beta & 2 + 4\beta & -1 - 2\beta & 0 & 0 \\
0 & \beta - \frac{1}{2} & -1 - 2\beta & \frac{3}{2} + \beta & \sqrt{3} & -\sqrt{3} \\
-\beta & -\sqrt{3} & 0 & \sqrt{3} & 3/2\beta & -1/2\beta \\
-\beta & \sqrt{3} & 0 & -\sqrt{3} & -1/2\beta & 3/2\beta
\end{bmatrix}, \tag{5.17}
\]

where we removed the indices of the cross sectional area \(S = S_{12}\), and \(\alpha\) and \(\beta\) are given in (5.9). As a basis for the kernel of the linearized operator \(L\) we can choose

\[
\begin{align*}
\phi_1 &= [0, 1, 1, 1, 0, 0] \\
\phi_2 &= [1, 0, 0, 0, 1, 1] \\
\phi_3 &= [0, \sqrt{3}, 0, -\sqrt{3}, 1, -1].
\end{align*} \tag{5.18}
\]

5.4 The spatially homogeneous Boltzmann equation

Statement of the problem

We consider the Cauchy problem for the spatially homogeneous system of equations

\[
\begin{align*}
\frac{df}{dt} &= Q(f, f), \quad t \in \mathbb{R}_+, \\
f(0) &= f_0,
\end{align*} \tag{5.19}
\]

where \(f = [f_1, ..., f_9]\), and \(f_i(t) = f(\xi_i, t) \in C^1(\mathbb{R}_+)\) with velocities \(\xi_i, 1 \leq i \leq 9\), given in (5.1), and details of \(Q(f, f)\) can be found in Appendix A. Stabilization of the solution
as $t \to \infty$ is assumed, that is
\[ f \to M \text{ as } t \to \infty, \quad (5.20) \]

where $M$ is a Maxwellian. In fact, as a consequence of the $H$-theorem \[13, p.139\], and with similar methods as in \[4, p.829\], one can prove that (5.20) holds. We reduce the system by the assumption of a symmetric flow around the $x$-axis as in (5.6), and by the expansion
\[ f = M + M^{1/2}h, \quad (5.21) \]
we obtain (if neglecting the non-linear term $S(h)$) the reduced linearized Cauchy problem
\[
\begin{align*}
  C \frac{dh}{dt} &= -Lh, \quad t \in \mathbb{R}_+, \\
  h(0) &= h_0,
\end{align*}
\quad (5.22)
\]
where $h = [h_1, ..., h_6]$, and $h_i(t) = h(\xi_i, t) \in C^1(\mathbb{R}_+)$ with velocities $\xi_i$, $1 \leq i \leq 6$, given in Figure 5.2. The linearized collision operator $L$ is given by (5.17), and $C = \text{diag}(2, 2, 1, 2, 1, 1)^{-1}$. Observe that we consider the system to be close to equilibrium, why the quadratic part $S(h)$ can be considered to be small.

We rewrite the system of equations given in (5.22) in the following way
\[
\frac{\partial h}{\partial t} = -C^{-1/2}LC^{-1/2}h, \quad (5.23)
\]
then multiplying both sides with $C^{1/2}$, we obtain
\[
\frac{\partial}{\partial t} C^{1/2}h = -C^{-1/2}LC^{-1/2}C^{1/2}h.
\]
We observe that since $L$ is symmetric, it follows that $C^{-1/2}LC^{-1/2}$ is also symmetric, and hence, diagonalizable. We have
\[
C^{-1/2}LC^{-1/2} = PD{P}^{-1}, \quad (5.24)
\]
for a diagonal matrix $D$ with the eigenvalues of $C^{-1/2}LC^{-1/2}$ on its diagonal, and an invertible matrix $P$ with the corresponding eigenvectors as column vectors. If we insert (5.24) in (5.23), it follows that
\[
\frac{\partial h}{\partial t} = -C^{-1}Lh
\]
\[
= -C^{-1/2}PD{P}^{-1}C^{1/2}h
\]
\[
= \Big(C^{-1/2}P\Big)D\Big(C^{-1/2}P\Big)^{-1}h.
\]
It is clear that we obtain the eigenvalues with the corresponding eigenvectors by solving
the equation
\[ C^{-1}Lx = \lambda x, \tag{5.25} \]
where \( \lambda \geq 0 \), since \( L \) is semi-positive and \( C \) is positive.

**Eigenvectors of \( C^{-1}L \)**

We observe that \( \phi_1, \phi_2, \) and \( \phi_3 \), given in (5.18), are all solutions to (5.25), and hence, we have obtained three eigenvectors, all with eigenvalue \( \lambda = 0 \).

To solve (5.25) for the remaining eigenvectors, we first make the following observation. Multiplying the right-hand side of (5.25) with \( C\phi \), where \( \phi \in \ker(L) = \text{span}\{\phi_1, \phi_2, \phi_3\} \), we obtain by (3.17) and (5.25) that
\[
\lambda \langle x, C\phi \rangle = \langle C^{-1}Lx, C\phi \rangle = \langle Lx, \phi \rangle = \langle x, L\phi \rangle = 0.
\]
Therefore, the problem of finding the remaining eigenvectors to \( C^{-1}L \) is reduced to find three linearly independent vectors in the vector space \( C \ker(L) \perp \), that satisfy (5.25) (for some \( \lambda > 0 \)). The vector space \( C \ker(L) \) is given explicitly by
\[
C \ker(L) = \text{span}\left\{ \begin{array}{c} C\phi_1 = [0, \frac{1}{2}, 1, \frac{1}{2}, 0, 0], \\
C\phi_2 = [\frac{1}{2}, 0, 0, 0, 1, 1], \\
C\phi_3 = [0, \frac{1}{2} \sqrt{3}, 0, -\frac{1}{2} \sqrt{3}, 1, -1] \end{array} \right\}. \tag{5.26}
\]

**Remark.** If we consider two distinct eigenvalues \( \lambda_1 \) and \( \lambda_2 \) with corresponding eigenvectors \( x \) and \( y \), respectively, then by (3.17) and (5.25)
\[
\lambda_1 \langle x, C\phi \rangle = \langle C^{-1}Lx, C\phi \rangle = \langle Lx, y \rangle = \langle x, Ly \rangle = \langle Cx, C^{-1}Ly \rangle = \lambda_2 \langle Cx, y \rangle = \lambda_2 \langle x, Cy \rangle.
\]
It follows that \( (\lambda_1 - \lambda_2) \langle x, Cy \rangle = 0 \), but since \( \lambda_1 \neq \lambda_2 \), we must have
\[
\langle x, Cy \rangle = 0. \tag{5.27}
\]

Now, we assume that a first basis vector of \( (C \ker(L)) \perp \) take the form \( \psi_1 = [a, 0, 0, 0, b, c] \), \( a, b, c \in \mathbb{R} \), since then, we have \( \langle \psi_1, C\phi_1 \rangle = 0 \). In order for \( \psi_1 \) to also be orthogonal to \( C\phi_2 \) and \( C\phi_3 \), we obtain that \( \psi_1 = [-4b, 0, 0, 0, b, b] \). If we let \( b = 1 \), and insert in (5.25), we see that \( \psi_1 \) is in fact an eigenvector. Solving the equation (5.25) for \( \lambda \), we obtain
\[
\psi_1 = [-4, 0, 0, 0, 1, 1] \quad \text{and} \quad \lambda_1 = 5\sqrt{5}\alpha\beta\gamma S. \tag{5.28}
\]
Regarding a second basis vector of \( (C \ker(L)) \perp \), we assume \( \psi_2 \) to take a form such that \( \langle \psi_2, C\phi_2 \rangle = 0 \), and therefore, we have \( \psi_2 = [0, a, b, c, 0, 0] \), \( a, b, c \in \mathbb{R} \). With similar argumentation as above, i.e. such that the orthogonality conditions are satisfied, we obtain that \( \psi_2 = [0, a, -a, a, 0, 0] \). We let \( a = 1 \) and observe that \( \psi_2 \) is an eigenvector,
and it follows by (5.25) that
\[\psi_2 = [0, 1, -1, 1, 0, 0] \text{ and } \lambda_2 = 4\sqrt{5}\alpha\gamma S(1 + 2\beta). \quad (5.29)\]

Moreover, \(\langle \psi_1, \psi_2 \rangle = 0\), and \(\psi_1\) and \(\psi_2\) both satisfy the condition (5.27) for any other eigenvector with distinct eigenvalue. Hence, we have an orthogonal basis \(\{C\phi_1, C\phi_2, C\phi_3, \psi_1, \psi_2\}\) of a subspace in \(\mathbb{R}^6\). Regarding the last eigenvector \(\psi_3\): if we can find \(\psi_3 \in (\text{ker}(L))^\perp\) such that (5.27) is satisfied for any other eigenvector, then we are done. Now, if we complete the basis for \(\mathbb{R}^6\) by choosing \(B = [0, 1, 0, 0, 0, 0]\), and apply the Gram-Schmidt orthogonalization procedure, we obtain \(\tilde{\psi}_3 = 1/(\beta + 4)[0, 2, 0, -2, -\sqrt{\beta}, \sqrt{\beta}]\). Then, this basis vector is indeed the last eigenvector. If we multiply \(\tilde{\psi}_3\) with \(\beta + 4\), and insert in (5.25) solving for \(\lambda\), we obtain
\[\psi_3 = [0, 2, 0, -2, -\sqrt{\beta}, \sqrt{\beta}] \text{ and } \lambda_3 = 2\sqrt{5}\alpha\gamma S(2 + \beta). \quad (5.30)\]

**Solution of the reduced linearized problem**

Let us return to the problem (5.22). We have
\[
\frac{dh}{dt} = -C^{-1}Lh = -PDP^{-1}h, \quad (5.31)
\]
where \(P = [\psi_1 \psi_2 \psi_3 \phi_1 \phi_2 \phi_3]\), or explicitly
\[
P = \begin{bmatrix}
-4 & 0 & 0 & 1 & 0 \\
0 & 1 & 2 & 1 & 0 & \sqrt{\beta} \\
0 & -1 & 1 & 0 & 0 \\
0 & 1 & -2 & 1 & 0 & -\sqrt{\beta} \\
1 & 0 & -\sqrt{\beta} & 0 & 1 & 1 \\
1 & 0 & \sqrt{\beta} & 0 & 1 & -1
\end{bmatrix}, \quad (5.32)
\]
and \(D = \text{diag}(\lambda_1, \lambda_2, \lambda_3, 0, 0, 0)\). Observe that \(P\) in (5.32) should not be confused with \(P\) in (5.24). We multiply both sides of the system (5.31) with \(P^{-1}\) and obtain
\[
\frac{d}{dt}P^{-1}h = -DP^{-1}h.
\]
If we substitute \(w = P^{-1}h\) in the above equation, it follows that
\[
\frac{dw}{dt} = -Dw.
\]
By the fundamental theorem for linear systems [18, p.17], we obtain the solution \( w = e^{-Dt}C_0 = \text{diag}(c_1, \ldots, c_6) \), or explicitly

\[
\begin{align*}
    w_1 &= c_1 e^{-\lambda_1 t}, \\
    w_2 &= c_2 e^{-\lambda_2 t}, \\
    w_3 &= c_3 e^{-\lambda_3 t}, \\
    w_4 &= c_4, \\
    w_5 &= c_5, \\
    w_6 &= c_6,
\end{align*}
\]

where \( c_i = w_i(0) \in \mathbb{R} \) for \( i \in \{1, \ldots, 6\} \), and \( \lambda_1, \lambda_2, \) and \( \lambda_3 \) are given in (5.28), (5.29), and (5.30), respectively.

In order to determine the complete solution of problem (5.22) we take into account the initial conditions \( h(0) = h_0 \), and the fact that the solution tends to zero at infinity, i.e.

\[ h(t) \to 0 \text{ as } t \to \infty. \]

The boundary condition at infinity is a direct consequence from the fact that the original function \( f \), before the expansion (5.21), tends to the Maxwellian distribution as \( t \to \infty \). Therefore, in order to satisfy (5.34), we see that \( c_4, c_5, \) and \( c_6 \), must be equal to zero. Then, we get \( h = h(t) \) by

\[

h(t) = Pw = \begin{bmatrix}
-4c_1 e^{-\lambda_1 t} \\
2c_2 e^{-\lambda_2 t} + 2c_3 e^{-\lambda_3 t} \\
-c_2 e^{-\lambda_2 t} \\
c_2 e^{-\lambda_2 t} - 2c_3 e^{-\lambda_3 t} \\
c_1 e^{-\lambda_1 t} - \sqrt{\beta}c_3 e^{-\lambda_3 t} \\
c_1 e^{-\lambda_1 t} + \sqrt{\beta}c_3 e^{-\lambda_3 t}
\end{bmatrix}.
\]

We apply the initial condition at \( t = 0 \) in (5.35), from where it follows that

\[
\begin{align*}
    c_1 &= -\frac{1}{4} h_{01}, \\
    c_2 &= -h_{03}, \\
    c_3 &= \frac{h_{02} + h_{03}}{2}.
\end{align*}
\]

The initial condition \( h_0 = [h_{01}, \ldots, h_{06}] \), must be of the form

\[ h_0 = -\frac{1}{4} h_{01} \psi_1 - h_{03} \psi_2 + \frac{h_{02} + h_{03}}{2} \psi_3 \]

in order to obtain a solution \( h \). Then by inserting (5.36) in (5.35), the solution is given
by

\[ h = \frac{1}{4} h_0_1 e^{-\lambda_1 t} \psi_1 - h_0_2 e^{-\lambda_2 t} \psi_2 + \frac{h_0_2 + h_0_3}{2} e^{-\lambda_3 t} \psi_3. \]

**Remark.** To obtain the solution \( h \), it is necessary and sufficient that \( h_0 \in (C \ker(L))^\perp \).

In fact, \( h \in (C \ker(L))^\perp \) for every \( t \geq 0 \). This follows from the fact that \( \langle \psi_j, C \phi_i \rangle = 0 \) for every \( i, j \in \{1, 2, 3\} \), and since

\[ h = w_1 \psi_1 + w_2 \psi_2 + w_3 \psi_3, \]

we have \( \langle h, C \phi_i \rangle = 0 \) for \( i \in \{1, 2, 3\} \), with the coefficients \( w_1, w_2, \) and \( w_3 \) given in (5.33), and \( C \phi_i \) given in (5.26).

**Solution of the original Cauchy problem**

In order to represent the solution in terms of \( f = [f_1, ..., f_6] \), we first observe that by relation (5.21), we have

\[ h_0_j = M_j^{-1/2} (f_0_j - M_j), \quad j \in \{1, 2, 3\}, \]

and solutions exist, if and only if

\[ f_0 \in M + M^{1/2} (C \ker(L))^\perp. \]

Accordingly, if the initial condition is on the form \( f_0 = M + M^{1/2} h_0 \), with \( h_0 \) from (5.37), then the approximate solution of the non-linear reduced problem (problem (5.19) reduced by assumption of a symmetric flow as in (5.6)), close to equilibrium, is given by

\[ f = M + M^{1/2} \left( -\frac{1}{4} M_1^{-1/2} (f_0_1 - M_1) e^{-\lambda_1 t} \psi_1 - M_3^{-1/2} (f_0_3 - M_3) e^{-\lambda_3 t} \psi_3 + \frac{M_2^{-1/2} (f_0_2 - M_2) + M_3^{-1/2} (f_0_3 - M_3)}{2} e^{-\lambda_3 t} \psi_3 \right), \quad (5.38) \]

where the Maxwellian \( M \) is given in (5.8), and the eigenvectors \( \psi_j \) with corresponding eigenvalues \( \lambda_j \) for \( j \in \{1, 2, 3\} \), are all given in (5.28), (5.29), and (5.30), respectively. The initial data \( f_0 = [f_0_1, ..., f_0_6] \) is given in (5.19).
By the insertion of the Maxwellian and the eigenvectors in (5.38), we obtain the explicit, and more illustrating solution

\[
\begin{align*}
  f_1 &= \alpha + e^{-\lambda_1 t}(f_0 - \alpha) \\
  f_2 &= \alpha \beta - e^{-\lambda_2 t}(f_0 - \alpha \beta) + e^{-\lambda_3 t}(f_0 + f_0 - 2\alpha \beta) \\
  f_3 &= \alpha \beta + e^{-\lambda_2 t}(f_0 - \alpha \beta) \\
  f_4 &= \alpha \beta - e^{-\lambda_2 t}(f_0 - \alpha \beta) - e^{-\lambda_3 t}(f_0 + f_0 - 2\alpha \beta) \\
  f_5 &= \alpha - \frac{1}{4} e^{-\lambda_1 t}(f_0 - \alpha) - \frac{1}{2} e^{-\lambda_3 t}(f_0 + f_0 - 2\alpha \beta) \\
  f_6 &= \alpha - \frac{1}{4} e^{-\lambda_1 t}(f_0 - \alpha) + \frac{1}{2} e^{-\lambda_3 t}(f_0 + f_0 - 2\alpha \beta),
\end{align*}
\]

where \(\alpha\) and \(\beta\) are given in (5.9). By studying the right-hand side of (5.39), one can verify that the approximate solution close to equilibrium (i.e. as \(t \to \infty\)) have small deviation from the Maxwellian \(M\) given in (5.8), and of course, the deviation depends on the initial distribution \(f_0\). Accordingly, the approximate solution \(f = [f_1, ..., f_6]\) to the original problem (5.19), under the assumption of symmetric flow around the \(x\)-axis, is equal to

\[
f = [f_1, f_2, f_3, f_4, f_5, f_6, f_6],
\]

where \(f_i\), for \(i \in \{1, ..., 6\}\), are given in system (5.39).
Chapter 6

Conclusion

In this work we have studied the Boltzmann equation (BE) and discrete velocity models (DVMs). We introduced and derived the evolution equation for the continuous BE, and then, we made a transition to a more detailed discussion regarding the discrete BE.

It was a challenge to present a descriptive connection between colliding molecules in the continuous case (discussed in Section 2.3), and the collision operator with a discretized velocity variable (discussed in Section 2.4). However, it was helpful to clarify the discussion with ideas borrowed from the derivation of the continuous collision operator in [12, p.3].

To further clarify the theory presented, we have with explicit calculations examined a 9-velocity Broadwell model for polyatomic molecules. Another challenge, due to the inelastic collisions of the model, was to specify the linearized collision operator. We presented an idea, based on symmetries and a dependence between colliding particles and the cross sectional area (discussed in Section 5.3), to calculate the transition probabilities for collisions of polyatomic molecules, which in the extension was helpful to obtain the linearized collision operator.

To conclude this work, and to make use of the explicit calculations of the model, we solved a Cauchy problem for the spatially homogeneous BE for a gas with a symmetric flow.

In addition to the solution of the spatially homogeneous system, we can extend the discussion to cover the planar stationary systems, and the shock wave systems. They can all be written in the unified form

\[ D \frac{\partial f}{\partial t} = Q(f, f), \quad \text{with } t \in \mathbb{R} \text{ and } D = \text{diag}(d_1, ..., d_n), \]

where in the former case \( d_i = \xi^1_i \), and in the latter case, \( d_i = \xi^1_i - c^1_i \), for \( i \in \{1, ..., n\} \). See [3, p.11] for a more detailed description. However, by the linearization procedure (discussed in Section 3.2), the system transforms into

\[ D \frac{\partial f}{\partial t} + Lh = S(h), \]

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where $L$ is the linearized collision operator, and $S(h)$ is the quadratic part.

To further examine the DVM (introduced in Section 5.1), one could apply the model on these problems and investigate properties of the solutions, such as, existence, uniqueness, if the problem is well-posed etc. Even though there are some similarities to obtaining the solution for the spatially homogeneous system (discussed in Section 5.4), the computations will be more challenging for these problems, since they are more complex and also (at least for the shock wave problem) require handling the non-linear parts of the system.
Appendix A

The DVM with velocities given in (5.1) and with distribution functions \( f_i = f(x, \xi_i, t) \) for \( 1 \leq i \leq 9 \) is given explicitly by

\[
\begin{align*}
\frac{\partial f_1}{\partial t} &= \Gamma_{12}^2(f_3 f_6 - f_1 f_2) + \Gamma_{12}^5(f_5 f_7 - f_1 f_2) + \Gamma_{13}^7(f_4 f_7 - f_1 f_3) + \Gamma_{13}^8(f_2 f_8 - f_1 f_3) + \Gamma_{14}^9(f_5 f_8 - f_1 f_4) + \Gamma_{14}^{10}(f_3 f_9 - f_1 f_4) \\
\frac{\partial f_2}{\partial t} + \frac{\partial f_2}{\partial x} &= \Gamma_{24}^7(f_3 f_5 - f_2 f_4) + \Gamma_{28}^7(f_4 f_7 - f_2 f_8) + \Gamma_{29}^6(f_2 f_9 - f_1 f_5) + \Gamma_{15}^6(f_4 f_6 - f_1 f_5) \\
\frac{\partial f_3}{\partial t} + \frac{\partial f_3}{\partial y} &= \Gamma_{35}^2(f_3 f_5 - f_3 f_6) + \Gamma_{37}^5(f_5 f_7 - f_3 f_6) + \Gamma_{38}^5(f_5 f_8 - f_3 f_6) + \Gamma_{39}^5(f_3 f_9 - f_3 f_6) \\
\frac{\partial f_4}{\partial t} - \frac{\partial f_4}{\partial x} &= \Gamma_{44}^2(f_3 f_5 - f_2 f_4) + \Gamma_{48}^2(f_2 f_9 - f_3 f_6) + \Gamma_{47}^2(f_2 f_8 - f_4 f_7) + \Gamma_{41}^1(f_3 f_9 - f_1 f_4) + \Gamma_{45}^1(f_5 f_8 - f_1 f_4) + \Gamma_{46}^1(f_1 f_5 - f_4 f_6) \\
\frac{\partial f_5}{\partial t} - \frac{\partial f_5}{\partial y} &= \Gamma_{57}^2(f_3 f_5 - f_3 f_6) + \Gamma_{55}^5(f_5 f_7 - f_5 f_7) + \Gamma_{56}^5(f_5 f_8 - f_5 f_7) + \Gamma_{58}^5(f_3 f_9 - f_5 f_8) + \Gamma_{59}^5(f_3 f_9 - f_1 f_4) + \Gamma_{51}^1(f_3 f_9 - f_1 f_4) + \Gamma_{52}^1(f_3 f_9 - f_1 f_4) + \Gamma_{53}^1(f_3 f_9 - f_1 f_4) + \Gamma_{54}^1(f_3 f_9 - f_1 f_4) + \Gamma_{55}^1(f_3 f_9 - f_1 f_4) + \Gamma_{56}^1(f_3 f_9 - f_1 f_4) + \Gamma_{57}^1(f_3 f_9 - f_1 f_4)
\end{align*}
\]
Appendix B

The entries of the linearized collision operator $L$ (6 × 6-matrix) in (5.11) are given by:

\[
\begin{align*}
\alpha_{11} &= \alpha \beta \langle \Gamma_{12}^{35}, \Gamma_{13}^{14}, \Gamma_{13}^{26}, \Gamma_{13}^{14}, [1, 1, 1, 1] \rangle \\
\alpha_{12} &= \alpha_{21} = \alpha \beta^{1/2} \langle \Gamma_{12}^{35}, \Gamma_{13}^{26}, [1, -1] \rangle \\
\alpha_{13} &= \alpha_{31} = \alpha \beta^{1/2} \langle \Gamma_{12}^{35}, \Gamma_{13}^{26}, \Gamma_{13}^{14}, \Gamma_{13}^{36}, [-1, 1, 1, -1] \rangle \\
\alpha_{14} &= \alpha_{41} = \alpha \beta^{1/2} \langle \Gamma_{13}^{14}, \Gamma_{13}^{26}, [-1, 1] \rangle \\
\alpha_{15} &= \alpha_{51} = -\alpha \beta \langle \Gamma_{12}^{35}, \Gamma_{13}^{26}, [1, 1] \rangle \\
\alpha_{16} &= \alpha_{61} = -\alpha \beta \langle \Gamma_{13}^{26}, \Gamma_{13}^{14}, [1, 1] \rangle
\end{align*}
\]

\[
\begin{align*}
\alpha_{22} &= \alpha \langle \Gamma_{12}^{35}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, [1, 1, \beta/2, 1] \rangle \\
\alpha_{23} &= \alpha_{32} = -\alpha \langle \Gamma_{12}^{35}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, [1, 1, \beta] \rangle \\
\alpha_{24} &= \alpha_{42} = \alpha \langle \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \beta/2, -1 \rangle \\
\alpha_{25} &= \alpha_{52} = -\alpha \beta^{1/2} \langle \Gamma_{12}^{35}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, [1, 1] \rangle \\
\alpha_{26} &= \alpha_{62} = \alpha \beta^{1/2} \langle \Gamma_{13}^{26}, \Gamma_{13}^{26}, [1, 1] \rangle
\end{align*}
\]

\[
\begin{align*}
\alpha_{33} &= \alpha \langle \Gamma_{12}^{35}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, [1, 1, 1, 1, 1, 2\beta] \rangle \\
\alpha_{34} &= \alpha_{43} = -\alpha \langle \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, [1, 1, \beta] \rangle \\
\alpha_{35} &= \alpha_{53} = \alpha \beta^{1/2} \langle \Gamma_{12}^{35}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, [-1, 1] \rangle \\
\alpha_{36} &= \alpha_{63} = \alpha \beta^{1/2} \langle \Gamma_{13}^{26}, \Gamma_{13}^{26}, [-1, 1] \rangle
\end{align*}
\]

\[
\begin{align*}
\alpha_{44} &= \alpha \langle \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, [1, 1, \beta/2, 1] \rangle \\
\alpha_{45} &= \alpha_{54} = \alpha \beta^{1/2} \langle \Gamma_{13}^{26}, \Gamma_{13}^{26}, [1, 1] \rangle \\
\alpha_{46} &= \alpha_{64} = -\alpha \beta^{1/2} \langle \Gamma_{13}^{26}, \Gamma_{13}^{26}, [1, 1] \rangle
\end{align*}
\]

\[
\begin{align*}
\alpha_{55} &= \alpha \beta \langle \Gamma_{12}^{35}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, [1, 1, 1] \rangle \\
\alpha_{56} &= \alpha_{65} = -\alpha \beta \Gamma_{13}^{26}
\end{align*}
\]

\[
\begin{align*}
\alpha_{66} &= \alpha \beta \langle \Gamma_{13}^{26}, \Gamma_{13}^{26}, \Gamma_{13}^{26}, [1, 1, 1] \rangle
\end{align*}
\]
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