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МАТЕМАТИЧКО МОДЕЛИРАЊЕ И АНАЛИЗА ВИШЕАТОМСКИХ ГАСОВА И МЕШАВИНА У КОНТЕКСТУ КИНЕТИЧКЕ ТЕОРИЈЕ ГАСОВА И МЕХАНИКЕ ФЛУИДА

– докторска дисертација –

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MATHEMATICAL MODELLING AND ANALYSIS OF POLYATOMIC GASES AND MIXTURES IN THE CONTEXT OF KINETIC THEORY OF GASES AND FLUID MECHANICS

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Paris, 03/06/2014   Milana Pavić

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[1]"The big thank you" — The style of this acknowledgement section reveals a collaborative nature of the thesis, which is itself a Serbian-French cotutelle.

Abstract

This thesis is dedicated to the problems arising in the mathematical modelling of polyatomic gases, and mixtures of monatomic and polyatomic gases, in the context of the kinetic theory of gases and fluid mechanics. The kinetic theory of gases (Boltzmann equation and its variants) is a very active field of applied mathematics. At the same time, continuum theories of physics have quite similar aims and very often treat the same problems as kinetic theory, although from a different point of view. The issues related to their mutual relationships are rather involved and call for the application of mathematical techniques, as well as elaborate physical explanations of modeling problems.

Kinetic theory is a way of modelling a system that consists in a huge number of particles, thanks to the concept of distribution function. The distribution function is defined on the so-called phase space, constituted of typical macroscopic variables, time and position in space, but also of microscopic variables which describe the state of the particles, such as velocity. It aims at describing species (each species when mixtures are concerned) of the gas. The main equation of kinetic theory is the Boltzmann equation. It determines the evolution of the distribution function and introduces the collision operator as a measure of change of the distribution function (due to collisions with other particles). With the help of the distribution function and the corresponding Boltzmann equation, the balance laws for the usual macroscopic observable quantities, such as density, momentum and energy, can be obtained in suitable limits.

For one single monatomic gas, a large literature is available on very different topics of kinetic theory and fluid mechanics. Some aspects are recalled in the introduction part of the thesis. However, in the framework of gaseous mixtures, the models are much more intricate. It is indeed necessary to treat systems of Boltzmann-like equations, rather than one single equation, with multi-species collision kernels (describing the cross interactions between the different distribution functions). The complexity of the models grows dramatically if exchanges of internal energy and chemical reactions are taken into account. The derivation of macroscopic equations from kinetic models remains a very active topic for mixtures, both at the mathematical level and for deducing relevant macroscopic equations based on the modelling of microscopic binary interactions. The aim of this thesis is to establish reliable mathematical models for non-equilibrium processes in polyatomic gases and mixture of monoatomic or polyatomic gases starting from the kinetic theory of gases, that will be compared with models of extended thermodynamics.

Considering polyatomic gases, our aim is to derive a macroscopic model for 14 moments starting from kinetic theory. At the microscopic level, one single parameter is introduced and it becomes an additional argument of the distribution function that enables to recover the proper equation of state at the macroscopic level. We first propose two independent hierarchies of the moment equations for polyatomic gases, which allow to obtain conservation laws for mass density, momentum and total energy of a gas. Such hierarchies are usually truncated at some order. A method which provides an appropriate solution to the closure problem when one performs such a truncation is the maximization of entropy method. We formulate a variational problem for polyatomic gases, and give the solution for any number of moments. We explore in detail the physical case of 14 moments, in which the appropriate approximative distribution function yields the closed system, that is further compared with the model arising from extended thermodynamics. In particular, we compute production terms, and obtain the explicit expressions for relaxation times in terms of two parameters that can be fitted in order to obtain a correct value of the Prandtl number and/or temperature dependence of viscosity.

ABSTRACT

When dealing with mixtures of polyatomic gases, the hydrodynamic approximation in which collisions between molecules of the same component of a mixture are much more frequent than collisions between the molecules of different components is studied. It leads to the so-called maxwellization of a distribution function: the distribution function of each species converges towards a Maxwellian distribution function, each with its own bulk velocity and temperature. With the help of this specified distribution function, balance laws for mass density, momentum and energy can be obtained for each component of the mixture, that can be compared with the multitemperature models for mixtures of Eulerian fluids coming out of extended thermodynamics. In particular, if we restrict the attention to processes which occur in the neighborhood of the average velocity and temperature of the mixture, the phenomenological coefficients of extended thermodynamics can be determined from the source terms provided by the kinetic theory.

Regarding mixtures of monatomic gases, we discuss the diffusion asymptotics of the Boltzmann equations. It amounts to scale the macroscopic arguments of the distribution function - time and space position - with the help of a small parameter interpreted as the mean free path. This asymptotics corresponds to a slow dynamics in space and an even slower one in time. The Hilbert expansion of each distribution function yields two equations. The first equation allows to state that the mixture is close to equilibrium. The second equation is a linear functional equation in the velocity variable. We prove the existence of a solution to this equation. On the one hand, when molecular masses are equal, the techniques introduced by Grad in order to prove the compactness of one part of the kernel can be extended to the multispecies case. On the other hand, we propose a new approach based on a change of variables in velocities for the same issue, which only holds when molecular masses are different.

Résumé

Cette thèse est dédiée aux problèmes de la modélisation mathématique des gaz polyatomiques et des mélanges de gaz monoatomique et polyatomique, dans le contexte de la théorie cinétique des gaz et de la mécanique des fluides. La théorie cinétique des gaz (l'équation de Boltzmann et ses variantes) est un domaine très actif des mathématiques appliquées. En même temps, les théories de la physique des milieux continus ont des objectifs assez similaires et traitent très souvent les mêmes problèmes que la théorie cinétique, bien que d'un point de vue différent. Les questions relatives à leurs relations mutuelles sont complexes et nécessitent l'application de techniques mathématiques, ainsi que des explications heuristiques.

La théorie cinétique permet de modéliser un système constitué d'un grand nombre de particules, grâce à la notion de fonction de distribution. La fonction de distribution est définie sur l'espace des phases, constitué de variables macroscopiques d'une part, comme le temps et la position dans l'espace, mais aussi d'autre part des variables microscopiques qui décrivent l'état des particules, telles que la vitesse. Elle vise à décrire les espèces (chacune des espèces lorsque des mélanges sont concernés) du gaz. Une équation essentielle de la théorie cinétique est l'équation de Boltzmann. Elle détermine l'évolution de la fonction de distribution et fait appel à un opérateur de collision qui mesure la variation de la fonction de distribution (due aux collisions avec d'autres particules). Grâce à l'équation de Boltzmann, les lois pour les quantités macroscopiquement observables habituelles, telles que la densité, le quantité de mouvement et l'énergie, peuvent être obtenus dans des limites appropriées.

Pour un gaz monoatomique, une vaste littérature est disponible sur des sujets reliant la théorie cinétique et la mécanique des fluides. Certains aspects sont rappelés dans la partie introductive de la thèse. Cependant, dans le cadre des mélanges gazeux, les modèles sont beaucoup plus complexes . Il est en effet nécessaire de traiter des systèmes d'équations de Boltzmann, plutôt qu'une seule équation, avec des noyaux de collision multi-espèces (qui décrivent les interactions entre les différentes fonctions de distribution). La complexité des modèles augmente considérablement si l'échange d'énergie et des réactions chimiques sont de plus pris en compte. La dérivation des équations macroscopiques à partir de modèles cinétiques reste un sujet très actif pour les mélanges, tant au niveau mathématique que pour déduire des équations macroscopiques par une modélisation des interactions binaires microscopiques. L'objectif de cette thèse est d'établir des modèles mathématiques pour les processus hors équilibre dans les gaz polyatomiques et les mélanges de gaz monoatomiques ou polyatomiques, à partir de la théorie cinétique des gaz, qui sont comparés ensuite avec les modèles de la thermodynamique étendue.

En ce qui concerne les gaz polyatomiques, notre objectif est d'obtenir un modèle macroscopique de 14 moments à partir de la théorie cinétique. Au niveau microscopique, un seul paramètre est introduit dans la fonction de distribution, qui permet de récupérer l'équation d'état au niveau macroscopique. D'abord, nous proposons deux hiérarchies distinctes formées d'équations de moments pour les gaz polyatomiques, qui permettent d'obtenir des lois de conservation de la densité de masse, de la quantité de mouvement et de l'énergie totale du gaz. Ces hiérarchies sont généralement coupées à un certain ordre. Une méthode qui fournit une solution appropriée au problème de fermeture lorsque l'on effectue une telle troncature est la méthode de la maximisation d'entropie. Nous formulons un problème variationnel pour les gaz polyatomiques, et donnons la solution pour n'importe quel nombre de moments. Nous explorons en détail le cas physique de 14 moments, dans lequel la fonction de distribution approximative fournit le système fermé, qui est ensuite comparé avec les modèles venant de la thermodynamique étendue. En particulier, nous calculons les termes sources, et nous obtenons les expressions explicites pour les temps de relaxation en fonction de deux paramètres qui peuvent être

fixés afin d'obtenir une valeur correcte du nombre de Prandtl et/ou de la dépendance de la viscosité en température.

On étudie un mélange de gaz polyatomiques dans lequel les collisions entre les molécules d'un même composant du mélange sont beaucoup plus fréquentes que les collisions entre les molécules de composants différents. L'asymptotique correspondante conduit à la "maxwellization" des fonctions de distribution: la fonction de distribution de chaque espèce converge vers une Maxwellienne, chacune avec sa propre vitesse moyenne et température. Grâce à la spécification de cette fonction de distribution, les lois pour la densité de masse, de quantité de mouvement et d'énergie peuvent être obtenues pour chaque composant du mélange, qui peut alors être comparé avec les modèles multitempératures pour les mélanges de fluides d'Euler provenant de la thermodynamique étendue. En particulier, si nous restreignons notre attention aux processus pour lesquels les vitesses et températures restent proches de la vitesse moyenne et de la température moyenne du mélange, les coefficients phénoménologiques de la thermodynamique étendue peuvent être déterminés à partir des termes sources fournies par la théorie cinétique.

On présente pour les mélanges de gaz monoatomiques l'asymptotique diffusive des équations de Boltzmann. Elle s'obtient en effectuant un rescaling des arguments de la fonction de distribution – le temps et la position en espace – avec l'aide d'un petit paramètre interprété comme le libre parcours moyen. Cette asymptotique correspond à une dynamique lente dans l'espace et encore plus lente dans le temps. Le développement de Hilbert de chaque fonction de distribution donne deux équations. La première équation permet d'affirmer que le mélange est proche de l'équilibre. La deuxième équation est une équation fonctionnelle linéaire en la variable de vitesse. Nous prouvons l'existence d'une solution de cette équation. D'une part, lorsque les masses moléculaires sont égales, les techniques introduites par Grad afin de prouver la compacité d'une partie du noyau peuvent être étendues au cas de plusieurs espèces. D'autre part, nous proposons une nouvelle approche basée sur un changement de variables des vitesses dans le même but, mais qui est valable lorsque les masses moléculaires sont différentes.

Извод

Ова дисертација је посвећена проблемима математичког моделирања вишеатомских гасова, као и мешавина једноатомских и вишеатомских гасова у оквиру кинетичке теорије гасова и механике флуида. Кинетичка теорија гасова (Болцманова једначина и њене модификације) представља веома активно поље истраживања на пољу примењене математике. У исто време, физичке теорије које материју третирају као непрекидну средину имају сличне циљеве истраживања као кинетичка теорија гасова и врло често анализирају истоветне проблеме, али им приступају на други начин. Питања њиховог међусобног односа су веома дубока и захтевају примену посебних математичких метода, као и детаљно објашњење физичких аспеката моделирања.

Кинетичка теорија је начин моделирања система који се састоји од великог броја честица помоћу концепта функције расподеле. Функција расподеле је дефинисана на такозваном фазном простору који се састоји од уобичајених макроскопских променљивих, времена и простора, али и од микроскопских променљивих које описују микроскопско стање честице, као што је брзина честице. Она има за циљ да опише честице (сваку од компонената када се посматрају мешавине) гаса. Основна једначина кинетичке теорије је Болцманова једначина. Она одређује временску еволуцију функције расподеле и уводи колизиони оператор као меру промене функције расподеле (која се мења због судара честица). Захваљујући функцији расподеле и одговарајућој Болцмановој једначини, могуће је извести једначине баланса уобичајених макроскопских величина, као што су густина, количина кретања и енергија, и то у погодним граничним процесима.

За једнокомпонентни и једноатомски гас је доступна широка литература на врло различите теме кинетичке теорије и механике флуида. Неки аспекти се и наводе у уводном делу дисертације. Међутим, у оквиру гасних мешавина модели су далеко сложенији. Неопходно је узети у обзир систем Болцманових једначина, а не само једну једначину, са вишекомпонентним колизионим операторима (који описују интеракцију између различитих функција расподела). Сложеност модела се драматично повећава уколико се уведу промене унутрашње енергије или хемијске реакције. Извођење макроскопских једначина из кинетичких модела представља веома атрактивну тему у случају мешавина, како на математичком нивоу, тако и за одређивање релевантних макроскопских једначина на основу моделирања микроскопских бинарних интеракција. Циљ ове дисертације јесте да формира поуздане математичке моделе за неравнотежне процесе у случају вишеатомских гасова и мешавина једноатомских и вишеатомских гасова полазећи од кинетичке теорије, који ће бити поређени са моделима проширене термодинамике.

Посматрајући вишеатомске гасове, циљ нам је да формирамо макроскопски модел за 14 момента полазећи од кинетичке теорије гасова. На микроскопском нивоу се уводи један параметар који постаје додатни аргумент функције расподеле и који омогућава добијање једначине стања на макроскопском нивоу. Најпре предлажемо конструисање две независне хијерархије једначина момената за вишеатомске гасове, што омогућава репродуковање закона одржања масе, количине кретања и укупне енергије гаса. Ове хијерархије се обично одсецају на неком реду момената. Једна од метода која пружа адекватно решење за затварање ситема формираног одсецањем хијерархије момената јесте принцип максимума ентропије. Наиме, формулишемо варијациони проблем за вишеатомске гасове и изводимо решење за било који ред момената. Потом проучавамо случај 14 момената у ком се на основу одговарајуће приближне функције расподеле добија затворени систем који се даље пореди са моделом добијеним у оквиру проширене термодинамике. Такође, израчунавамо генеративне чланове, на основу којих добијамо експлицитне изразе за времена релаксације у зависности од два параметра, чија вредност може да се бира тако да се добије

коректна вредност Прантловог броја и/или зависност вискозности од температуре.

Хидродинамичка апроксимација у којој је учестаност судара молекула исте компоненте много већа од учестаности судара молекула различитих компоненти је анализирана за мешавине вишеатомских гасова. Она доводи до тзв. максвелизације функције расподеле: функција расподеле сваке компоненте мешавине формално конвергира ка Максвеловој расподели са различитим брзинама и температурама. Одређивањем функције расподеле једначине баланса густине, количине кретања и енергије се могу извести за сваку компоненту мешавине, а потом упоредити са вишетемпературним моделом за мешавине Ојлеровских флуида проширене термодинамике. Уколико усмеримо нашу пажњу на процесе који се одвијају у околини средње брзине и температуре мешавине можемо одредити феноменолошке коефицијенте проширене термодинамике на основу генеративних чланова кинетичке теорије.

Што се тиче мешавина једноатомских гасова, дискутујемо дифузиону асимптотику Болцманових једначина. Наиме, макроскопски аргументи функције расподеле - време и положај у простору - се скалирају помоћу малог параметра који се интерпретира као дужина слободног пута. Ова асимптотика одговара спорој динамици у простору и још споријој у времену. Хилбертов развој сваке функције расподеле нам даје две једначине. Прва једначина нам омогућава да кажемо да је мешавина у стању блиско равнотежном. Друга једначина је линеарна функционална једначина по брзини. Доказујемо егзистенцију решења ове једначине. Са једне стране, када су масе молекула једнаке, технике, које је увео Град да би доказао компактност оператора у једнокомпонентном случају, могу да се прошире и на вишекомпонентни случај. Са друге стране, предлажемо нови приступ заснован на смени променљивих, који је валидан само када су масе молекула различите.

Contents

Introduction: presentation of models and results

Introduction

The (collisional) kinetic theory is a part of nonequilibrium statistical physics. It was introduced by Boltzmann at the end of the nineteenth century. It provides an alternative to a deterministic, very detailed, approach, in which each molecule i of a gas is considered, together with its position $\mathbf{x}_i$ and velocity $\mathbf{v}_i$, and $t \mapsto (\mathbf{x}_i(t), \mathbf{v}_i(t))_{i=1,\dots,N}$ solves a system of differential equations, essentially Newton's law (we assume that particles obey the laws of classical mechanics - not relativistic, neither quantum). Apart from the impossibility of prescribing initial data $(\mathbf{x}_i(0), \mathbf{v}_i(0))_{i=1,\dots,N}$ for each molecule, such a description would yield an enormous number ($N \sim 10^{26}$ in one cubic meter at normal pressure) of equations. The solution would be so detailed that it would be impossible to grasp all the information. Kinetic theory provides a less complete statistical description of the behavior of the gas.

The objective of kinetic theory is the modelling of a gas through the concept of distribution function. Such a statistical approach makes sense if the number of particles is sufficiently large, so that the gas can be considered as a continuous medium. In short, the state of the gas (in the case of mixture of gases, each of its components) is described by a distribution function f that is a nonnegative function defined on the phase space. This space consists of macroscopic variables (such as time t and position in the physical space $\mathbf{x}$) but also of variables of microscopic nature $\boldsymbol{\xi}$ that describe the particle itself (for example, the velocity of the particle) i.e. $f : (t, \mathbf{x}, \boldsymbol{\xi}) \mapsto f(t, \mathbf{x}, \boldsymbol{\xi}) \geq 0$, where $(t, \mathbf{x}, \boldsymbol{\xi}) \in \mathbb{R}_+ \times \mathbb{R}^N \times \Omega$, and $\Omega \subseteq \mathbb{R}^{\dim(\boldsymbol{\xi})}$. Then $f(t, \mathbf{x}, \boldsymbol{\xi}) \mathrm{d}\mathbf{x} \mathrm{d}\boldsymbol{\xi}$ quantifies the number of particles in the element $\mathrm{d}\mathbf{x}\,\mathrm{d}\boldsymbol{\xi}$ of phase space in the vicinity of the point $(\mathbf{x}, \boldsymbol{\xi})$ at time t.

Once the distribution function is defined as the main object of study of kinetic theory, one wants to understand its evolution. To that purpose, interactions between particles need to be taken into account. In order to do so, several assumptions are considered:

(1) We assume that the ratio of the mean free path of the molecules (distance traversed by a molecule between two collisions) to a typical macroscopic length is of order 1: $\lambda \sim L$, where λ is the mean free path, and L is a typical macroscopic length.

(2) We assume that particles interact via binary collisions. This means that the effect of interactions involving more than two particles can be neglected.

(3) Collisions are assumed localized both in space and time, meaning that they are brief events which occur at a given position and a given time.

(4) We also assume that collisions are microreversible. This means that the microscopic dynamics underlying the collision is time-reversible.

(5) Finally, we introduce a molecular chaos assumption, meaning that collisions involve only uncorrelated particles. In particular, a couple of particles which have already collided are expected not to re-collide in the future.

The previous assumptions can be rigorously proven (on a small interval of time), in the case of one single monatomic gas, under a suitable scaling in which the mean free path of a molecule is of the order of a characteristic length [**46, 24, 32**].

Under the previous assumptions, the appropriate model for the evolution of the distribution function is the Boltzmann equation, precisely described in the sequel of this thesis.

The distribution function is not a directly observable object. It even gives an often unnecessarily detailed description of the gas. Standard experiments enable to obtain only macroscopic quantities, such as density, velocity, energy, or pressure tensor, heat flux of the gas. The distribution function is related to these macroscopic quantities by an averaging over the microscopic state of the molecules $\boldsymbol{\xi}$ against specific functions of $\boldsymbol{\xi}$. As a consequence, macroscopic equations (for example Euler or Navier-Stokes like equations) for a monatomic gas can be derived from the Boltzmann equation at the formal level [**25, 10, 11, 12**], and in some cases rigourously [**51, 43, 35**].

For a monatomic gas, the Euler equations of compressible gases are obtained when a local equilibrium is reached for the distribution function [**25**]. When dissipative effects are taken into account (constitutive equations for the stress tensor and the heat flux as gradients of the velocity and temperature of the gas are introduced), the Navier-Stokes equations of compressible gases are obtained [**25**]. These equations represent a good model when the gas is close to a local equilibrium, but they fail in the description of rapidly changing processes occurring in rarefied gases.

When nonequilibrium phenomena are studied, as in rarefied gas dynamics, the need for a kinetic description arises.

The level of rarefaction of a medium can be expressed in terms of the Knudsen number. The Knudsen number Kn is defined as a ratio of length λ of the mean free path and the macroscopic length L characteristic of the process under consideration, i.e. $\text{Kn} = \lambda/L$. Typically, Navier-Stokes equations are valid as long as $\text{Kn} \ll 1$. This condition fails to hold when the relevant length scale L becomes comparable to the mean free path λ. This can happen either when λ becomes large, or when L becomes small. A typical example of a gas with large mean free path is a high altitude flight in the upper atmosphere. On the other hand, miniaturization produces smaller and smaller devices – for example micro-electro-mechanical systems, where the length L approaches the mean free path λ. More precisely, with help of the Knudsen number, flow regimes can be classified [**57, 44**]:

- $\text{Kn} \lesssim 0.01$ – the hydrodynamic regime, which is very well described by means of macroscopic theory (for example Navier-Stokes equations). When $\text{Kn} \to 0$, which corresponds to the hydrodynamic regime without diffusion, even the Euler equations represent a good model, provided that suitable boundary conditions are introduced.

- $0.01 \lesssim \text{Kn} \lesssim 0.1$ – the slip flow regime, where Navier-Stokes equations or Burnett equations, both supplied with slip boundary conditions, can be taken as models.

- $0.1 \lesssim \text{Kn} \lesssim 10$ – the transition regime where the gas must be described in greater detail by extended macroscopic models. The models that can be used in this regime include the moment methods [**57**].

- $\text{Kn} \gtrsim 10$ – free molecular flow, where the flow is dominated by wall/particle interactions and Boltzmann equation has to be used [**23**].

Even in the hydrodynamic regime, where macroscopic equations are already good models, the kinetic theory plays an important role. Namely, one of its goals is to compute the coefficients that appear in the equations, and that are of phenomenological nature at the macroscopic level. However, the most interesting application of kinetic theory is in the description of processes which occur when the gas is outside of the hydrodynamic regime (with $\text{Kn} \gtrsim 0.01$).

This doctoral dissertation deals with the establishment of reliable mathematical models for nonequilibrium processes in rarefied polyatomic and mixtures of polyatomic gases by the methods of the

kinetic theory of gases. Those models will be compared to the models based on extended thermodynamics.

Part 1 discusses the kinetic models coming out of the existing literature that we use throughout the dissertation.

We first recall the basis of the kinetic modelling in the case of one monatomic gas [23]. In this case, the variable that describes the microscopic state of the particles is the velocity of the particles $\mathbf{v}$ ($\boldsymbol{\xi} = \mathbf{v}$). Moreover, conservation laws of momentum and kinetic energy hold during a collision process of monatomic molecules. As a consequence, the collision transformation can be easily formulated. This makes possible a simple definition of the collision operator and of the corresponding Boltzmann equation. The weak form of the collision operator is presented, enabling the derivation of the conservation laws at the macroscopic level. The equilibrium distribution function is determined by means of the $H-$theorem, which is a manifestation of the second law of thermodynamics.

Then the kinetic model corresponding to a mixture of monatomic gases is briefly presented. In this case, each species $\mathcal{A}_i$, $1 \leq i \leq s$, of a mixture is described by its distribution function $f_i(t, \mathbf{x}, \mathbf{v})$, $i = 1, \ldots, s$. We describe the differences with respect to mono-species gases, that mainly appear because the masses of the different molecules can differ.

Next, we deal with the modelling by kinetic theory of polyatomic gases. The main feature of a polyatomic gas is the presence of additional degrees of freedom (other than the translational ones). This phenomenon can be captured in a variety of ways [33]. We consider the case in which the additional degrees of freedom are modelled by means of one single continuous (that is, non discrete) parameter $I \in \mathbb{R}_+$, the so-called microscopic internal energy of a molecule. This parameter becomes a variable of the distribution function, i.e. $\boldsymbol{\xi} = (\mathbf{v}, I)$. Moreover, it appears in the total energy of the system consisting of two colliding particles. The collision transformation is obtained by following the Borgnakke-Larsen procedure [20], and we formulate it in both $\boldsymbol{\omega}-$ and $\boldsymbol{\sigma}-$ notation [59]. One of the main goals of the modelling of polyatomic gases is to recover the proper equation of state at the macroscopic level. In order to do so, we introduce a weight function $\varphi(I)$ which will follow all integrations with respect to the microscopic state of the particles [22]. We define then the collision operator and its weak forms, together with the Boltzmann equation. The proper choice of the weight function $\varphi(I)$ leads to the derivation at the formal level of the conservation laws for a polyatomic gas [29]. Then, the $H-$theorem is also presented in this case.

Finally, a kinetic model for mixtures of polyatomic gases is formulated: we consider first the collision process at the microscopic level, then we define the collision operator in a weighted framework and its weak forms, which help to write the Boltzmann equation and formulate the macroscopic conservation laws [30]. The equilibrium properties are discussed and the H-theorem is proven. We indicate here that another possibility in the modelling of such gases is to consider the weight as a part of the distribution functions. This approach has been developed in [22] in the context of polyatomic gases. Following this lead, we established a kinetic model for a mixture of polyatomic gases in the conference paper [2]:

Laurent Boudin, Bérénice Grec, Milana Pavić-Čolić, and Francesco Salvarani. A kinetic model for polytropic gases with internal energy. *PAMM*, 13 (1):353–354, 2013.

This model provides a L^2 framework in both variables $\mathbf{v}$ and I, well suited for performing a mathematical study of the diffusion asymptotics, as it was done in [1] for a model without energy exchange. The results of [2] are not presented in this thesis.

Part 2 deals with the presentation of the results which were obtained during the preparation of the PhD thesis.

Chapter 2 deals with the establishment of moment equations for rarefied polyatomic gases and application of the maximum entropy principle for such gases. It is the extended version of the papers [**3**] and [**4**]:

Milana Pavić, Tommaso Ruggeri and Srboljub Simić. Maximum entropy principle for rarefied polyatomic gases. *Phys. A*, 392 (6): 1302–1317, 2013.

Milana Pavić-Čolić and Srboljub Simić. Moment equations for polyatomic gases. *Acta Appl. Math.*, ONline ISSn 1572-9036, DOI 10.1007/s10440-014-9928-6, 2014.

In a monatomic gas, starting from the Boltzmann equation for $f := f(t, \mathbf{x}, \mathbf{v})$, that is

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} = Q(f, f),$$

where Q is a collision kernel, it is possible to construct macroscopic equations of balance type (moment equations) by means of the integration with respect to the velocity variable against monomials of the velocity:

$$
(1) \qquad \partial_t
\begin{pmatrix}
F^{(0)} \\
F_{i_1}^{(1)} \\
F_{i_1 i_2}^{(2)} \\
F_{i_1 i_2 i_3}^{(3)} \\
\vdots \\
F_{i_1 i_2 i_3 \ldots i_n}^{(n)} \\
\vdots
\end{pmatrix}
+ \sum_{j=1}^{3} \partial_{x_j}
\begin{pmatrix}
F_j^{(1)} \\
F_{i_1 j}^{(2)} \\
F_{i_1 i_2 j}^{(3)} \\
F_{i_1 i_2 i_3 j}^{(4)} \\
\vdots \\
F_{i_1 i_2 i_3 \ldots i_n j}^{(n+1)} \\
\vdots
\end{pmatrix}
=
\begin{pmatrix}
P^{(0)} \\
P_{i_1}^{(1)} \\
P_{i_1 i_2}^{(2)} \\
P_{i_1 i_2 i_3}^{(3)} \\
\vdots \\
P_{i_1 i_2 i_3 \ldots i_n}^{(n)} \\
\vdots
\end{pmatrix}, \quad i_k \in \{1, \ldots 3\}, \ \forall k \in \mathbb{N},
$$

where

$$F_{i_1 i_2 \ldots i_n}^{(n)} = \int_{\mathbb{R}^3} v_{i_1} v_{i_2} \ldots v_{i_n} f \, \mathrm{d}\mathbf{v}, \quad P_{i_1 i_2 \ldots i_n}^{(n)} = \int_{\mathbb{R}^3} v_{i_1} v_{i_2} \ldots v_{i_n} Q(f, f) \, \mathrm{d}\mathbf{v}.$$

These equations fit into a hierarchical order: the flux in the moment equation of tensorial order n becomes the density in the moment equation of order $(n+1)$. The first moments are interpreted as usual macroscopic quantities: for example, $F^{(0)}$, $F_{i_1}^{(1)}$ and $F_{i_1 i_2}^{(2)}$ are respectively identified as the macroscopic density, the momentum density and the momentum flux. Moreover, in a monatomic gas, the trace of $F_{i_1 i_2}^{(2)}$ ($\sum_{k=1}^{N} F_{kk}^{(2)}$) is interpreted as the total energy density, because in a monatomic gas there is a link between the internal energy density and the trace of the pressure tensor. The collision invariants (namely, functions $1, \mathbf{v}, \frac{1}{2} |\mathbf{v}|^2$) make the production terms vanish, which enables to recover conservation laws of the mass density, the momentum density and the energy density from $(1)_1$, $(1)_2$ and one half of the trace of $(1)_3$, respectively.

In the case of polyatomic gases, when one wants to build moment equations and to keep their main properties: (i) hierarchical order of the moment equations and (ii) possibility to recover conservation laws; one faces new problems, because of the additional degrees of freedom. Indeed, the collision invariants for a polyatomic gas (functions $1, \mathbf{v}, \frac{m}{2} |\mathbf{v}|^2 + I$) are not well-suited to the construction of a hierarchy analogously to the case of one monatomic gas (that is, with the help of the velocities only). However, moment equations can be generalized to polyatomic gases starting from the Boltzmann equation for $f := f(t, \mathbf{x}, \mathbf{v}, I)$

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} = Q(f, f),$$

where Q is a collision kernel, by constructing two independent hierarchies which we call "momentum" and "energy" hierarchies [**3**]. The "momentum" hierarchy is just a polyatomic version of the usual

hierarchy for monatomic gases:

$$
(2) \quad \partial_t \mathbf{F} + \sum_{j=1}^{3} \partial_{x_j} \mathbf{F}_j = \mathbf{P}, \ \text{with} \ \mathbf{F} = \begin{pmatrix} F^{(0)} \\ F^{(1)}_{i_1} \\ \vdots \\ F^{(n)}_{i_1 i_2 \dots i_n} \\ \vdots \end{pmatrix}, \ F^{(n)}_{i_1 i_2 \dots i_n} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} v_{i_1} v_{i_2} \dots v_{i_n} \, f \, \varphi(I) \mathrm{d}I \, \mathrm{d}\mathbf{v},
$$

while the "energy" hierarchy starts with the energy collisional invariant and proceeds with the usual multiplication by monomials of the velocity:
(3)

$$
\partial_t \mathbf{G} + \sum_{j=1}^{3} \partial_{x_j} \mathbf{G}_j = \mathbf{Q}, \ \text{with} \ \mathbf{G} = \begin{pmatrix} G^{(2)} \\ G^{(3)}_{k_1} \\ \vdots \\ G^{(m+2)}_{k_1 \dots k_m} \\ \vdots \end{pmatrix}, \ G^{(m+2)}_{k_1 \dots k_m} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{m}{2} \, |\mathbf{v}|^2 + I \right) v_{k_1} \dots v_{k_m} f \, \varphi(I) \mathrm{d}I \, \mathrm{d}\mathbf{v}.
$$

Here, $\varphi(I)$ is the weight function which enables to recover the energy law of polyatomic gases. For such hierarchies, the two requirements hold: (i) the hierarchical structure is conserved, albeit separately for the two hierarchies, and (ii) macroscopic equations $(2)_1$, $(2)_2$ respectively correspond to the conservation laws of the mass density and the momentum density, while $(3)_1$ is identified as the conservation law of the energy density.

The two hierarchies are then truncated at some order:

$$
\partial_t \mathbf{F}^{(N)} + \sum_{j=1}^{3} \partial_{x_j} \mathbf{F}^{(N+1)}_j = \mathbf{P}^{(N)}, \quad \partial_t \mathbf{G}^{(M)} + \sum_{j=1}^{3} \partial_{x_j} \mathbf{G}^{(M+1)}_j = \mathbf{Q}^{(M)},
$$

for $N \geq 0$ and $M \geq 2$, where

$$
\mathbf{F}^{(N)} = \begin{pmatrix} F^{(0)} \\ F^{(1)}_{i_1} \\ F^{(2)}_{i_1 i_2} \\ \vdots \\ F^{(n)}_{i_1 i_2 \dots i_N} \end{pmatrix} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \begin{pmatrix} 1 \\ v_{i_1} \\ v_{i_1} v_{i_2} \\ \vdots \\ v_{i_1} v_{i_2} \dots v_{i_N} \end{pmatrix} f \, \varphi(I) \mathrm{d}I \, \mathrm{d}\mathbf{v},
$$

and

$$
\mathbf{G}^{(M)} = \begin{pmatrix} G^{(2)} \\ G^{(3)}_{k_1} \\ \vdots \\ G^{(M)}_{k_1 \dots k_{M-2}} \end{pmatrix} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{m}{2} \, |\mathbf{v}|^2 + I \right) \begin{pmatrix} 1 \\ v_{k_1} \\ \vdots \\ v_{k_1} \dots v_{k_{M-2}} \end{pmatrix} f \, \varphi(I) \mathrm{d}I \, \mathrm{d}\mathbf{v}.
$$

Then, the fluxes $F^{(N+1)}_{i_1 i_2 \dots i_N j}$ and $G^{(M+1)}_{k_1 \dots k_{M-2} j}$, as well as all non-vanishing production terms ($\mathbf{P}^{(N)}$, $N \geq 2$, and $\mathbf{Q}^{(M)}$, $M \geq 3$) remain undetermined, and an unclosed system of equations is obtained.

We detail a computation which provides an appropriate solution to the closure problem, namely the maximization of entropy. The maximum entropy principle used here is inspired by Boltzmann's recognition that entropy counts the number of microscopic states that correspond to a given macroscopic state. This macroscopic state can be described by moments of the distribution function. Then, the maximum entropy principle states that the most likely distribution function (density of microscopic states) is the one which maximizes the physical entropy subject to the constraints that suitable moments are prescribed. In other words, the approximate distribution function comes out as a solution

of the following variational problem:

$$\max_f \quad h$$

$$\text{(4)} \qquad \text{s.t.} \quad \mathbf{F}^{(N)} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \begin{pmatrix} 1 \\ v_{i_1} \\ v_{i_1} v_{i_2} \\ \vdots \\ v_{i_1} v_{i_2} \ldots v_{i_N} \end{pmatrix} f\, \varphi(I) \mathrm{d}I\, \mathrm{d}\mathbf{v},$$

$$\mathbf{G}^{(M)} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\tfrac{m}{2} \left| \mathbf{v} \right|^2 + I \right) \begin{pmatrix} 1 \\ v_{k_1} \\ \vdots \\ v_{k_1} \ldots v_{k_{M-2}} \end{pmatrix} f\, \varphi(I) \mathrm{d}I\, \mathrm{d}\mathbf{v}.$$

Finally, the maximizer $\hat{f}$ enables the computation of the undetermined fluxes and the non-vanishing production terms. Consequently, the system of equations corresponding to the prescribed moments $\mathbf{F}^{(N)}$ and $\mathbf{G}^{(M)}$ is closed.

For $N = 1$ and $M = 2$, the solution to the variational problem (4) is the local equilibrium distribution function, and the corresponding macroscopic equations are the standard Euler equations of compressible polyatomic gases.

Then, we investigate the case when $N = 2$ and $M = 3$. We obtain in this way a non-equilibrium distribution function, called 14 moments approximation. With the help of this distribution function, we compute the fluxes $F^{(3)}_{i_1 i_2 j}$, $G^{(4)}_{k_1 j}$ and the production terms $P^{(2)}_{i_1 i_2}$, $Q^{(3)}_{k_1}$ for the simplest cross section enabling to recover one macroscopic parameter for a simple monoatomic gas, namely the so-called generalized VHS cross section

$$B(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega}) = K\, 2\, R^s\, \left| \mathbf{v} - \mathbf{v}_* \right|^{2s} \left| \boldsymbol{\omega} \cdot \frac{\mathbf{v} - \mathbf{v}_*}{\left| \mathbf{v} - \mathbf{v}_* \right|} \right|,$$

with K being an appropriate dimensional constant and s satisfying the overall assumption $s > -\frac{3}{2}$. The following 14 moments system is obtained after a suitable linearization procedure:

$$\partial_t \rho + \sum_{i=1}^{3} \partial_{x_i} (\rho u_i) = 0,$$

$$\partial_t (\rho u_i) + \sum_{j=1}^{3} \partial_{x_j} (\rho u_i u_j + p_{ij}) = 0,$$

$$\partial_t \left(\rho u_i u_j + p_{ij} \right)$$
$$+ \sum_{k=1}^{3} \partial_{x_k} \left\{ \rho u_i u_j u_k + u_i p_{jk} + u_j p_{ki} + u_k p_{ij} + \left(\alpha + \frac{7}{2} \right)^{-1} (q_i \delta_{jk} + q_j \delta_{ki} + q_k \delta_{ij}) \right\}$$
$$= -K \frac{2^{2s+4} \rho\, (k\, T)^2}{15\, m\, \zeta_0(T)^2} \sqrt{\pi} \left(\frac{k\, T}{m} \right)^s \Gamma \left[s + \frac{3}{2} \right] \left(p_{\langle ij \rangle} + \frac{20}{(2s+5)(2s+7)} \left(\alpha + \frac{5}{2} \right) (\alpha + 1)^{-1} \Pi \delta_{ij} \right)$$

$$\partial_t \left(\tfrac{1}{2} \rho \left| \mathbf{u} \right|^2 + \rho e \right) + \sum_{i=1}^{3} \partial_{x_i} \left\{ \left(\tfrac{1}{2} \rho \left| \mathbf{u} \right|^2 + \rho e \right) u_i + \sum_{j=1}^{3} p_{ij} u_j + q_i \right\} = 0,$$

$$\partial_t \left\{ \left(\tfrac{1}{2} \rho \left| \mathbf{u} \right|^2 + \rho e \right) u_i + \sum_{j=1}^{3} p_{ij} u_j + q_i \right\}$$

$$+ \sum_{j=1}^{3} \partial_{x_j} \left\{ \left(\tfrac{1}{2} \rho \, |\mathbf{u}|^2 + \rho e \right) u_i u_j + \sum_{k=1}^{3} \left(u_i u_k p_{jk} + u_j u_k p_{ik} \right) + \tfrac{1}{2} \rho \, |\mathbf{u}|^2 \, p_{ij} \right.$$

$$+ \left(\alpha + \frac{9}{2} \right) \left(\alpha + \frac{7}{2} \right)^{-1} (q_i u_j + q_j u_i) + \left(\alpha + \frac{7}{2} \right)^{-1} \mathbf{u} \cdot \mathbf{q} \, \delta_{ij} + \left(\alpha + \frac{9}{2} \right) \frac{p}{\rho} \, p_{ij} - \left. \frac{p^2}{\rho} \, \delta_{ij} \right\}$$

$$= - K \sqrt{\pi} \left(\frac{kT}{m} \right)^{s} \Gamma \left[s + \frac{3}{2} \right] \frac{\rho \, (kT)^2}{m \, \zeta_0(T)^2}$$

$$\times \left(\frac{2^{2s+4}}{15} \left(\sum_{k=1}^{3} u_k p_{\langle ik \rangle} + \frac{20}{(2s+5)(2s+7)} \left(\alpha + \frac{5}{2} \right) (\alpha + 1)^{-1} \Pi u_i \right) \right.$$

$$\left. + \left(\frac{7}{2} + \alpha \right)^{-1} \frac{2^{2s+5} \left(s \, (2s+15) + 30 \right)}{9 \, (2s+5) \, (2s+7)} \, q_i \right).$$

The production terms allow to obtain explicit expressions for the transport coefficients (the shear viscosity, the bulk viscosity and the heat conductivity) as functions of the temperature with the coefficients depending on the parameters α and s [4]. Then it is possible to fit the parameter s in order to obtain a correct value of the Prandtl number or an agreement with the transport coefficients dependence upon temperature, according to the experimental data for some specific polyatomic gases. For example, for CO the choice $s = 0.262$ yields a good approximation for both the value of the Prandtl number and temperature dependence of the shear viscosity.

Chapter 3 deals with the establishment of Euler-like equations involving macroscopic velocities and temperatures which are different for each species, when mixtures of polyatomic gases are considered.

Such models are obtained from extended thermodynamics [54] by following Truesdell's principles [58]: (i) all properties of the mixture must be mathematical consequences of properties of the constituents, (ii) to describe the motion of a constituent, we may in imagination isolate it from the rest of the mixture, provided that we properly take into account for the actions of the other constituents upon it, (iii) the motion of the mixture is governed by the same equations as is a single body; and by exploiting the Galilean invariance and the entropy principle.

Our aim is to provide a derivation of those models by kinetic theory. We suppose that each species $\mathcal{A}_i$ of the polyatomic gas mixture, $1 \le i \le s$, is described by a distribution function $f_i := f_i(t, \mathbf{x}, \mathbf{v}, I)$ that satisfies the Boltzmann equation:

$$(5) \qquad \partial_t f_i + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = Q_{ii}(f_i, f_i) + \sum_{\substack{j=1 \\ j \ne i}}^{s} Q_{ij}(f_i, f_j), \quad 1 \le i \le s,$$

where Q_{ii} is a collision operator for molecules of the same species, and Q_{ij} is a collision operator for molecules of different species. In order to obtain at the formal level a multivelocity and multitemperature model, the following asymptotics of the Boltzmann equations (5) is considered: we assume that the Maxwellisation steps for each species are of the same order, but that this scale is much shorter than the equilibration scale between different species. In other words, introducing a small parameter ε, we consider the following system of the Boltzmann equations:

$$\partial_t f_i^{\varepsilon} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i^{\varepsilon} = \frac{1}{\varepsilon} Q_{ii}(f_i^{\varepsilon}, f_i^{\varepsilon}) + \sum_{\substack{j=1 \\ j \ne i}}^{s} Q_{ij}(f_i^{\varepsilon}, f_j^{\varepsilon}), \quad 1 \le i \le s.$$

Note that this scaling has also been proposed and studied in [16] in the case of mixtures of gases with discrete internal energy and in [15] in the case of mixture of reactive monatomic gases. When ε tends to zero, each f_i^{ε} converges at the formal level towards the "mid-equilibrium" distribution function:

$$f_{E_i} = \frac{n_i}{\zeta_{0_i}(T_i)} \left(\frac{m}{2 \, \pi \, k \, T_i} \right)^{N/2} e^{- \frac{1}{k T_i} \left(\frac{m_i}{2} |\mathbf{v} - \mathbf{u}_i|^2 + I \right)},$$

with macroscopic number density $n_i = \rho_i/m_i$, macroscopic velocity $\mathbf{u}_i$ and temperature T_i depending on the species and satisfying the system:

$$\partial_t \rho_i + \nabla_{\mathbf{x}} \cdot (\rho_i \, \mathbf{u}_i) = 0,$$

$$\partial_t \left(\rho_i \, \mathbf{u}_i \right) + \nabla_{\mathbf{x}} \left(\rho_i \, \mathbf{u}_i \otimes \mathbf{u}_i + p_i \, \mathrm{Id} \right) = \mathbf{N}_i,$$

$$\partial_t \left(\tfrac{1}{2} \rho_i \left| \mathbf{u}_i \right|^2 + \rho_i e_i \right) + \nabla_{\mathbf{x}} \cdot \left\{ \left(\tfrac{1}{2} \rho_i \left| \mathbf{u}_i \right|^2 + \rho_i e_i \right) \mathbf{u}_i + p_i \mathbf{u}_i \right\} = E_i, \quad i = 1, ..., s.$$

The formulation of the model consists in the computation of the production terms $\mathbf{T}_i$ and Z_i, which are (according to the second principle of Truesdell) a description of the mutual interactions of the constituents. We perform a computation using the modified VHS model for the cross section, as previously:

$$\mathcal{B}_{ij} \left(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega} \right) = 2^{N-1} K R^{s_{ij}} \left| \mathbf{v} - \mathbf{v}_* \right|^{2s_{ij}} \left| \boldsymbol{\omega} \cdot \frac{\mathbf{v} - \mathbf{v}_*}{\left| \mathbf{v} - \mathbf{v}_* \right|} \right|^{N-2},$$

where the parameter s_{ij} satisfies $s_{ij} = s_{ji}$ and under the restriction $s_{ij} > -\frac{N}{2}$ ($N > 1$ being the dimension of the space). Using the special functions, explicit formulas for the production terms are obtained:

$$\mathbf{N}_i = -\sum_{\substack{j=1 \\ j \neq i}}^{s} \left(\mathbf{u}_i - \mathbf{u}_j \right) K \mu_{ij} \, n_i \, n_j \, \frac{k^2 \, T_i \, T_j}{\zeta_{0_i}(T_i) \zeta_{0_j}(T_j)} \frac{2 \left| S^{N-1} \right| \left| S^{N-2} \right|}{(N + 2s_{ij})(N + 2s_{ij} + 2)}$$

$$\times \left(\frac{2 \, k \, T_i}{m_i} + \frac{2 \, k \, T_j}{m_j} \right)^{s_{ij}} \pi^{\frac{1-N}{2}} e^{-\left(\frac{2 \, k \, T_i}{m_i} + \frac{2 \, k \, T_j}{m_j} \right)^{-1} |\mathbf{u}_i - \mathbf{u}_j|^2} \Gamma \left[\frac{N-1}{2} \right] \Gamma \left[s_{ij} + \frac{N}{2} + 1 \right]$$

$$\times \, {}_1\tilde{F}_1 \left(s_{ij} + \frac{N}{2} + 1; \frac{N}{2} + 1; \left(\frac{2 \, k \, T_i}{m_i} + \frac{2 \, k \, T_j}{m_j} \right)^{-1} |\mathbf{u}_i - \mathbf{u}_j|^2 \right),$$

$$E_i = \left(\frac{m_i}{2 \, k \, T_i} + \frac{m_j}{2 \, k \, T_j} \right)^{-1} \left(\frac{m_i}{2 \, k \, T_i} \mathbf{u}_i + \frac{m_j}{2 \, k \, T_j} \mathbf{u}_j \right) \cdot \mathbf{T}_i$$

$$+ \sum_{\substack{j=1 \\ j \neq i}}^{s} K n_i n_j \frac{k^2 \, T_i \, T_j}{\zeta_{0_i}(T_i) \zeta_{0_j}(T_j)} \frac{2 \left| S^{N-1} \right| \left| S^{N-2} \right|}{(N + 2s_{ij} + 2)}$$

$$\times \left(\frac{2 \, k \, T_i}{m_i} + \frac{2 \, k \, T_j}{m_j} \right)^{s_{ij}} \pi^{\frac{1-N}{2}} e^{-\left(\frac{2 \, k \, T_i}{m_i} + \frac{2 \, k \, T_j}{m_j} \right)^{-1} |\mathbf{u}_i - \mathbf{u}_j|^2} \Gamma \left[\frac{N-1}{2} \right] \Gamma \left[\frac{N + 2s_{ij}}{2} \right]$$

$$\times \left\{ \left(\frac{m_j \, k \, T_i + m_i \, k \, T_j}{m_i + m_j} \right) \left(\mu_{ij} \frac{k \, T_j - k \, T_i}{m_i k T_j + m_j k T_i} + \frac{m_i - m_j}{(m_i + m_j)} \frac{1}{(N + 2s_{ij} + 4)} \right) \right.$$

$$\times \, {}_1\tilde{F}_1 \left(\frac{N + 2s_{ij} + 2}{2}; \frac{N}{2}; \left(\frac{2 \, k \, T_i}{m_i} + \frac{2 \, k \, T_j}{m_j} \right)^{-1} |\mathbf{u}_i - \mathbf{u}_j|^2 \right)$$

$$+ \left(\frac{m_j - m_i}{2 \, (m_i + m_j)} \frac{1}{(N + 2s_{ij} + 4)} \left(k \, T_i + k \, T_j \right) + \frac{1}{2 \, (N + 2s_{ij})} \left(k \, T_j - k \, T_i \right) \right)$$

$$\left. \times \, {}_1\tilde{F}_1 \left(\frac{N + 2s_{ij}}{2}; \frac{N}{2}; \left(\frac{2 \, k \, T_i}{m_i} + \frac{2 \, k \, T_j}{m_j} \right)^{-1} |\mathbf{u}_i - \mathbf{u}_j|^2 \right) \right\}.$$

Chapter 4 is devoted to the study of the diffusion asymptotics of the kinetic model for a mixture of monatomic gases (labeled with $\mathcal{A}_i$, $1 \leq i \leq s$). It is the extended version of the paper [1]:

Laurent Boudin, Bérénice Grec, Milana Pavić, and Francesco Salvarani. Diffusion asymptotics of a kinetic model for gaseous mixtures. *Kinet. Relat. Models* 6 (1): 137–157, 2013.

Each species $\mathcal{A}_i$ of the mixture is described by the distribution function $f_i := f_i(t, \mathbf{x}, \mathbf{v})$. We consider a set of Boltzmann equations:

$$\partial_t f_i + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = \sum_{j=1}^{s} Q_{ij}(f_i, f_j), \quad \forall i = 1, \ldots, s,$$

where Q_{ij} is the collision kernel between species i and j. We perform a scaling of the time t and space position $\mathbf{x}$, with the help of the scaling parameter ε (related to the mean free path), in the following way (this is the traditional scaling of diffusion, [26]):

$$t \mapsto \varepsilon^2 t, \qquad \mathbf{x} \mapsto \varepsilon \mathbf{x}.$$

Then we introduce new distribution functions with scaled arguments:

$$f_i \left(\frac{t^\varepsilon}{\varepsilon^2}, \frac{\mathbf{x}^\varepsilon}{\varepsilon}, \mathbf{v} \right) =: f_i^\varepsilon \left(t^\varepsilon, \mathbf{x}^\varepsilon, \mathbf{v} \right), \quad \forall i = 1, \ldots, s,$$

and we assume

$$\partial_{t^\varepsilon} f_i^\varepsilon = O(1) \quad \text{and} \quad \nabla_{\mathbf{x}^\varepsilon} f_i^\varepsilon = O(1), \quad \text{with} \quad f_i^\varepsilon := f_i^\varepsilon \left(t^\varepsilon, \mathbf{x}^\varepsilon, \mathbf{v} \right), \quad \forall i = 1, \ldots, s.$$

Hence, for any i, each distribution function f_i^ε must solve the following scaled Boltzmann equation, that is

(6) $$\varepsilon \, \partial_t f_i^\varepsilon + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i^\varepsilon = \frac{1}{\varepsilon} \sum_{j=1}^{s} Q_{ij}(f_i^\varepsilon, f_j^\varepsilon), \quad t > 0, \, \mathbf{x} \in \mathbb{R}^3, \, \mathbf{v} \in \mathbb{R}^3.$$

We look for f_i^ε as a formal power series in ε, replace f_i^ε in (6) and identify the coefficients of the same order in ε, as in [21] in the case of one monatomic gas. We only focus on the first two orders.

Thanks to the $H-$theorem, the order -1 of (6) allows to find the zero-th order term of the series, that is the Maxwell functions $n_i(t, \mathbf{x}) \, M_i(\mathbf{v})$, with macroscopic velocity assumed to be equal to 0 (diffusion limit), and temperature scaled to 1, where n_i is the macroscopic density of the species $\mathcal{A}_i$ and $M_i(\mathbf{v})$ is the normalized, centred Maxwell function

$$M_i(\mathbf{v}) = \left(\frac{m_i}{2\pi} \right)^{3/2} e^{-\frac{m_i}{2} |\mathbf{v}|^2}, \quad \forall \mathbf{v} \in \mathbb{R}^3.$$

Therefore, each distribution function f_i^ε, $1 \le i \le s$, can be seen as a perturbation of the equilibrium:

(7) $$f_i^\varepsilon(t, \mathbf{x}, \mathbf{v}) = M_i(\mathbf{v}) \, n_i(t, \mathbf{x}) + \varepsilon \, M_i(\mathbf{v})^{1/2} \, g_i(t, \mathbf{x}, \mathbf{v}) + ..., \quad \forall t \ge 0, \, \forall \mathbf{x}, \mathbf{v} \in \mathbb{R}^3.$$

We choose to put $M_i(\mathbf{v})^{1/2}$ within the first-order term of f_i^ε in (7), since it allows us to work in a plain L^2 framework in the variable $\mathbf{v}$ for g_i.

Focusing on the zero-th order term in ε coming from (6), we obtain a linear functional equation in the velocity variable, holding for any $1 \le i \le s$,

(8) $$M_i^{-1/2} \sum_{j=1}^{s} \left(n_i \, Q_{ij}(M_i, M_j^{1/2} g_j) + n_j \, Q_{ij}(M_i^{1/2} g_i, M_j) \right) = M_i^{1/2} \left(\mathbf{v} \cdot \nabla_{\mathbf{x}} n_i \right),$$

and we wish to show that it can be solved in the natural functional framework. In contrast to the case of one single monatomic gas, studied by Grad [39], where only one functional equation appears, for a mixture of monatomic gases, we have a vector of unknown functions $\mathbf{g} = (g_1, \ldots, g_s)$ satisfying the system (8). For each component g_i of $\mathbf{g}$, we work in L^2 (in the velocity variable), i.e. we investigate the existence of a vector $\mathbf{g}$ satisfying (8) such that $\mathbf{g} \in L^2(\mathbb{R}^3_{\mathbf{v}})^s$. In order to do so, we first rewrite (8) in a more suitable form:

(9) $$(\mathcal{K} - \nu \, \mathrm{Id}) \, \mathbf{g} = \left(M_i^{1/2} \left(\mathbf{v} \cdot \nabla_{\mathbf{x}} n_i \right) \right)_{1 \le i \le s},$$

where we introduce the operator $\mathcal{K}$ with the i-th component of $\mathcal{K}\mathbf{g}$

$$(10) \quad [\mathcal{K}\mathbf{g}]_i(\mathbf{v}) = \sum_{j=1}^{s} \left(\frac{m_j}{2\pi}\right)^{3/4} \iint_{\mathbb{R}^3 \times S^2} \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, e^{-\frac{1}{4}m_i|\mathbf{v}|^2} \, e^{-\frac{1}{2}m_j|\mathbf{v}_*|^2}$$

$$\times \left[n_i \left(\frac{m_i}{2\pi}\right)^{3/4} \left(e^{\frac{1}{4}m_j|\mathbf{v}_*'|^2} g_j(\mathbf{v}_*') - e^{\frac{1}{4}m_j|\mathbf{v}_*|^2} g_j(\mathbf{v}_*) \right) \right.$$

$$\left. + n_j \left(\frac{m_j}{2\pi}\right)^{3/4} e^{\frac{1}{4}m_i|\mathbf{v}'|^2} g_i(\mathbf{v}') \right] \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*,$$

where B_{ij} are the cross section appearing in Q_{ij}, and $\nu_i = \nu_i(\mathbf{v})$ is defined by

$$(11) \quad 0 < \nu_i(\mathbf{v}) = \sum_{j=1}^{s} n_j \left(\frac{m_j}{2\pi}\right)^{3/2} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{2}m_j|\mathbf{v}_*|^2} \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*.$$

The main result of our work is given in the following Theorem.

THEOREM. *Suppose that the cross sections* $(\mathcal{B}_{ij})_{1 \leq i,j \leq s}$ *are positive functions satisfying*

$$\mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{V}) \leq a \, |\sin\theta| \, |\cos\theta| \left(|\mathbf{V}| + \frac{1}{|\mathbf{V}|^{1-\delta}} \right), \quad \forall \, \boldsymbol{\omega} \in S^2, \ \forall \, \mathbf{V} \in \mathbb{R}^3,$$

where $a > 0$, $0 < \delta < 1$ *and* θ *is the angle between* $\boldsymbol{\omega}$ *and* $\mathbf{V} := \mathbf{v} - \mathbf{v}_*$. *If we assume that*

$$(12) \quad \sum_{i=1}^{s} n_i(t, \mathbf{x}) \text{ does not depend on } \mathbf{x},$$

then, for any t, $\mathbf{x}$, *there exists* $\mathbf{g}(t, \mathbf{x}, \cdot) \in L^2(\mathbb{R}_{\mathbf{v}}^3)^s$ *satisfying* (9), *where* $\mathcal{K}$ *and* ν *are given by* (10)–(11).

The proof of this Theorem relies on the application of the Fredholm alternative to the operator $\mathcal{K} - \nu \, \mathrm{Id}$, for which the compactness property in $L^2(\mathbb{R}_{\mathbf{v}}^3)^s$ of the operator $\mathcal{K}$ is required. Indeed, we prove the following Proposition.

PROPOSITION. *The operator* $\mathcal{K}$, *defined by* (10), *is compact from* $L^2(\mathbb{R}_{\mathbf{v}}^3)^s$ *to* $L^2(\mathbb{R}_{\mathbf{v}}^3)^s$.

The compactness of the operator $\mathcal{K}$ is proven by showing a uniform decay at infinity and an equiintegrability property. It is crucial to dissociate the cases when $m_i \neq m_j$ on the one hand, and $m_i = m_j$ on the other hand, because the proofs are quite different. Indeed, for any i, we introduce the set

$$\mathcal{M}_i := \{1 \leq j \leq s \mid m_j = m_i\},$$

which is non empty since $i \in \mathcal{M}_i$, and write $\mathcal{K}$ as the sum of four operators $\mathcal{K}_1, \ldots, \mathcal{K}_4$. For any i, the i-th component of each $\mathcal{K}_\ell \mathbf{g}$, $1 \leq \ell \leq 4$, is given by

$$[\mathcal{K}_1 \mathbf{g}]_i(\mathbf{v}) = -n_i \sum_{j=1}^{s} \left(\frac{m_i m_j}{4\pi^2}\right)^{3/4} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4}m_i|\mathbf{v}|^2} \, e^{-\frac{1}{4}m_j|\mathbf{v}_*|^2} g_j(\mathbf{v}_*)$$

$$\times \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*,$$

$$[\mathcal{K}_2 \mathbf{g}]_i(\mathbf{v}) = n_i \sum_{j \notin \mathcal{M}_i} \left(\frac{m_i m_j}{4\pi^2}\right)^{3/4} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4}m_i|\mathbf{v}|^2} \, e^{-\frac{1}{2}m_j|\mathbf{v}_*|^2} e^{\frac{1}{4}m_j|\mathbf{v}_*'|^2} g_j(\mathbf{v}_*')$$

$$\times \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*,$$

$$[\mathcal{K}_3 \mathbf{g}]_i(\mathbf{v}) = \sum_{j \in \mathcal{M}_i} \left(\frac{m_i}{2\pi}\right)^{3/2} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4}m_i|\mathbf{v}|^2} \, e^{-\frac{1}{2}m_i|\mathbf{v}_*|^2}$$

$$\times \left[n_i \, e^{\frac{1}{4}m_i|\mathbf{v}_*'|^2} g_j(\mathbf{v}_*') + n_j \, e^{\frac{1}{4}m_i|\mathbf{v}'|^2} g_i(\mathbf{v}') \right] \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*,$$

$$[\mathcal{K}_4 \mathbf{g}]_i(\mathbf{v}) = \sum_{j \notin \mathcal{M}_i} n_j \left(\frac{m_j}{2\pi}\right)^{3/2} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4}m_i|\mathbf{v}|^2} \, e^{-\frac{1}{2}m_j|\mathbf{v}_*|^2} e^{\frac{1}{4}m_i|\mathbf{v}'|^2} g_i(\mathbf{v}')$$

$$\times \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*.$$

For the operators $\mathcal{K}_1$, $\mathcal{K}_3$ and $\mathcal{K}_4$, the proof given by Grad in the mono-species case [**39**] can be extended to mixtures. However, the operator $\mathcal{K}_2$ requires a new approach. Grad's geometrical argument on the $\boldsymbol{\omega}$ variable does not hold any longer. Instead of performing a change of variable $\boldsymbol{\omega}$ into another unit vector $\boldsymbol{\omega}^\perp \in S^2$, orthogonal to $\boldsymbol{\omega}$ in the plane $\mathrm{Span}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\omega})$, we change variables in $\mathcal{K}_2$ by transforming $(\mathbf{v}', \mathbf{v}_*)$ into $(\mathbf{v}, \mathbf{v}_*')$. This argument only holds when $m_i \neq m_j$, and its nature is very different from Grad's one.

Notations

- for vectors and tensors, we use boldface letters. For example, vectors of $\mathbb{R}^N$ are denoted by
$$\mathbf{a} = [a_1 \ldots a_N]^T.$$
  Note that the k-th component of the vector $\mathbf{a}$ is denoted by a_k, for some $1 \le k \le N$. When a vector is related to the species $\mathcal{A}_i$, we denote it by $\mathbf{a}_i$. Its k-th component is then $[\mathbf{a}_i]_k$.
- A tensor $\mathbf{T}$ is represented by its components $T_{i_1 i_2 \ldots i_n}$
- round brackets around N indices represent the symmetrization with respect to these indices, that is, the sum over all N! permutations of the indices divided by N!. For example,

$$a_{(i}b_{j)} = \frac{1}{2}\left(a_i b_j + a_j b_i\right)$$

(13)
$$a_{(i}b_j c_{k)} = \frac{1}{3!}\left(a_i\left(b_j c_k + b_k c_j\right) + a_j\left(b_i c_k + b_k c_i\right) + a_k\left(b_j c_k + b_k c_j\right)\right)$$

$$a_{(i}b_{jk)} = \frac{1}{3!}\left(a_i\left(b_{jk} + b_{kj}\right) + a_j\left(b_{ik} + b_{ki}\right) + a_k\left(b_{jk} + b_{kj}\right)\right)$$

Hypergeometric Functions. We are led to introduce the Kummer confluent hypergeometric function, denoted by $M(a, b, z)$ or alternatively by $_1F_1(a; b; z)$, with its integral representation

$$\frac{\Gamma[b-a]\,\Gamma[a]}{\Gamma[b]}\;\,_1F_1(a;b;z) = \int_0^1 e^{zt} t^{a-1}\left(1-t\right)^{b-a-1} \mathrm{d}t, \quad \text{for } b > a > 0,$$

see [5] p. 505, relation 13.2.1. We refer to $_1\tilde{F}_1(a; b; z)$ as its "regularization" given by

$$_1\tilde{F}_1(a;b;z) = \frac{1}{\Gamma[b]}\,_1F_1(a;b;z), \quad \text{where } -b \notin \mathbb{N}.$$

The following property holds:

$$_1\tilde{F}_1(a;b;0) = \frac{1}{\Gamma[b]}.$$

Next, we introduce the following function

$$_0\tilde{F}_1(;b;z) = \frac{1}{\Gamma[b]} e^{-2\sqrt{z}}\,_1F_1\left(b - \frac{1}{2}; 2b - 1; 4\sqrt{z}\right).$$

We recall integral representations of the hypergeometric functions described above that will be useful for us in the sequel [42]:

(14)
$$_1\tilde{F}_1(a;b;z) = \frac{1}{\Gamma[a]} \int_0^\infty e^{-t}\, t^{a-1}\,_0\tilde{F}_1(;b;zt)\mathrm{d}t, \quad \text{for } a > 0,$$

(15)
$$_0\tilde{F}_1(;b;z) = \frac{1}{\sqrt{\pi}\,\Gamma\left[b - \frac{1}{2}\right]} \int_{-1}^1 \left(1 - t^2\right)^{b - \frac{3}{2}} e^{-2t\sqrt{z}}\mathrm{d}t, \quad \text{for } b > \frac{1}{2},$$

(16)
$$_0\tilde{F}_1(;b;z) = \frac{1}{\sqrt{\pi}\,\Gamma\left[b - \frac{1}{2}\right]} \int_0^\pi e^{-2\sqrt{z}\cos t}\left(\sin t\right)^{2b-2}\mathrm{d}t, \quad \text{for } b > \frac{1}{2}.$$

Part 1

Presentation of models

Description of the kinetic models used in this thesis

In this thesis, we will consider three different contexts: mixture of polyatomic gases (Section 2), one single polyatomic gas (Section 3), and mixture of monatomic gases (Section 4). The aim of this Part is to introduce the kinetic models for all three situations. We provide moreover in Section 1 a description of standard mono-species monatomic gas as an introduction.

1. Description of monatomic gases

In this Section, we describe the kinetic modelling of one monatomic gas, such as it is presented in [23] for example.

The variable that describes the microscopic state of a monatomic gas is the velocity, denoted by $\mathbf{v}$ ($\boldsymbol{\xi} = \mathbf{v}$). The state of a monatomic gas is described by a distribution function $f := f(t, \mathbf{x}, \mathbf{v})$, that is a nonnegative function defined on the phase space that consists of time $t \in \mathbb{R}_+$, space position $\mathbf{x} \in \mathbb{R}^N$ and velocity $\mathbf{v} \in \mathbb{R}^N$.

If we consider collisions as the main mechanism of interaction between particles, then the appropriate model for evolution of the distribution function f is the Boltzmann equation. In absence of external forces, the Boltzmann equation reads:

$$(1.1) \qquad \partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = Q(f, f).$$

The right-hand side of the Boltzmann equation (that is $Q(f, f)$) is called the collision integral (operator). It is a quadratic bilinear operator acting only on the velocity $\mathbf{v}$.

The collision integral $Q(f, f)$ corresponds to the effect of the change of velocities of particles due to collisions. Indeed, if we neglect the mutual interactions between particles, i.e. take $Q(f, f) = 0$, then f satisfies the equation of free transport:

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = 0.$$

This means that each particle will travel at constant velocity along characteristics that are straight lines. That is, f will be constant along solutions of

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}, \quad \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = 0.$$

In that case, f at time t can be computed in terms of f at time 0 as follows:

$$f(t, \mathbf{x}, \mathbf{v}) = f(0, \mathbf{x} - t\mathbf{v}, \mathbf{v}).$$

The collision integral can be split into a gain term and a loss term

$$Q(f, f) = Q^+(f, f) - Q^-(f, f).$$

The loss term counts all collisions in which a given particle of velocity $\mathbf{v}$ will encounter another particle, of velocity $\mathbf{v}_*$, and will change its velocity (thus leading to a loss of particles of velocity $\mathbf{v}$). The gain term measures the number of particles of velocity $\mathbf{v}$ which are created due to a collision.

In order to define the collision integral, let us perform an analysis of the collision process between two molecules of a monatomic gas.
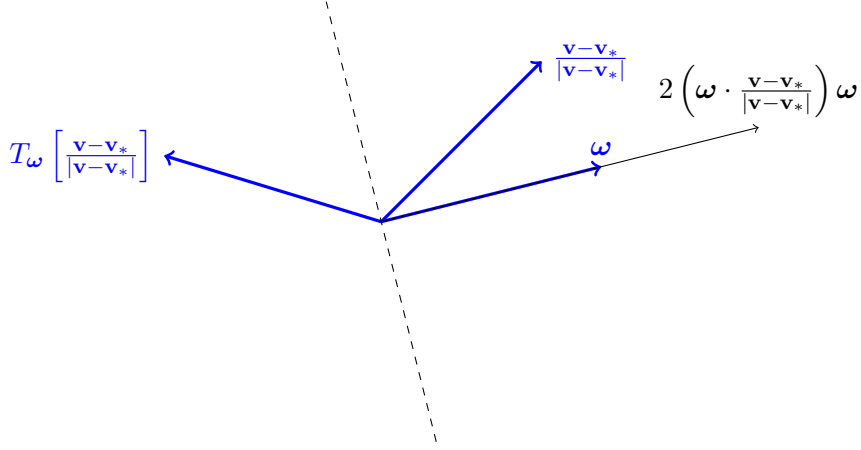
FIGURE 1.1. Transformation (1.4)

Collision transformation. During the collision, the conservation laws of momentum and kinetic energy hold (because since the gas is monatomic, no internal energy is present at the microscopic level). We denote by $\mathbf{v}'$ and $\mathbf{v}'_*$ the pre-collisional velocities of two colliding molecules, that become $\mathbf{v}$ and $\mathbf{v}_*$ after the collision. Then, the microscopic conservation laws take the following form:

$$\begin{aligned} \mathbf{v}' + \mathbf{v}'_* &= \mathbf{v} + \mathbf{v}_*, \\ \left|\mathbf{v}'\right|^2 + \left|\mathbf{v}'_*\right|^2 &= \left|\mathbf{v}\right|^2 + \left|\mathbf{v}_*\right|^2. \end{aligned}$$

(1.2)

Combining these two laws, it follows that the intensity of the relative velocity does not change during a collision:

$$\left|\mathbf{v}' - \mathbf{v}'_*\right| = \left|\mathbf{v} - \mathbf{v}_*\right|.$$

(1.3)

The system of equations (1.2), or equivalently $(1.2)_1$ and (1.3), consists of $(N+1)$ scalar equations for $2N$ scalar variables. We express its solution in terms of $N-1$ parameters: typically, a unit vector of the sphere S^{N-1}. Among all possible ways to do it, of great interest for this work will be two parametrizations: we will call them $\boldsymbol{\omega}-$ and $\boldsymbol{\sigma}-$representation. In the sequel, we explain in detail the $\boldsymbol{\omega}-$representation, while we only define the $\boldsymbol{\sigma}-$representation starting from the $\boldsymbol{\omega}-$one and explain how to pass from one to another.

Model in the $\boldsymbol{\omega}-$notation. Choose a vector $\boldsymbol{\omega} \in S^{N-1}$. Then for a given post-collisional relative velocity $\mathbf{v} - \mathbf{v}_*$, the pre-collisional one $\mathbf{v}' - \mathbf{v}'_*$ will lie in a plane spanned by the vectors $\boldsymbol{\omega}$ and $\frac{\mathbf{v}-\mathbf{v}_*}{|\mathbf{v}-\mathbf{v}_*|}$. Let us define a transformation $T_{\boldsymbol{\omega}}$ as the symmetry with respect to the plane $\{\boldsymbol{\omega}\}^{\perp}$, i.e.

$$T_{\boldsymbol{\omega}}[\mathbf{y}] = \mathbf{y} - 2(\boldsymbol{\omega} \cdot \mathbf{y})\boldsymbol{\omega}, \quad \text{for} \quad \mathbf{y} \in \mathbb{R}^N.$$

(1.4)

To illustrate this transformation, we restrict to the case $N = 3$ and represent a vector $T_{\boldsymbol{\omega}}\left[\frac{\mathbf{v}-\mathbf{v}_*}{|\mathbf{v}-\mathbf{v}_*|}\right]$ in a plane spanned by vectors $\boldsymbol{\omega}$ and $\frac{\mathbf{v}-\mathbf{v}_*}{|\mathbf{v}-\mathbf{v}_*|}$ in Figure 1.1. We parametrize (1.3) with the help of the transformation $T_{\boldsymbol{\omega}}$ as follows:

$$\mathbf{v}' - \mathbf{v}'_* = |\mathbf{v} - \mathbf{v}_*|\, T_{\boldsymbol{\omega}}\left[\frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|}\right] = T_{\boldsymbol{\omega}}[\mathbf{v} - \mathbf{v}_*],$$

(1.5)

Finally, combining (1.5) and $(1.2)_1$, we obtain expressions for the pre-collisional velocities in terms of the post-collisional velocities:

$$\begin{aligned} \mathbf{v}' &= \mathbf{v} - ((\mathbf{v} - \mathbf{v}_*) \cdot \boldsymbol{\omega})\boldsymbol{\omega}, \\ \mathbf{v}'_* &= \mathbf{v}_* + ((\mathbf{v} - \mathbf{v}_*) \cdot \boldsymbol{\omega})\boldsymbol{\omega}, \end{aligned}$$

(1.6)

Collision operator. The collision operator aims at describing the influence of the other particles on the particles of velocity $\mathbf{v}$. Indeed, one observes an elementary velocity volume of size $d\mathbf{v}$, and counts both gains and losses of particles in that volume. The particles that change their velocity into the velocity $\mathbf{v}$ are precisely those that had velocity $\mathbf{v}'$ and that encountered a particle of velocity $\mathbf{v}'_*$. Also, the particle of velocity $\mathbf{v}$ can loose its velocity due to a collision with a particle of velocity $\mathbf{v}_*$. The integration with respect to $\mathbf{v}_*$ and $\boldsymbol{\omega}$ captures all possible particles that may have an influence on gain/loss of particles of velocity $\mathbf{v}$.

Therefore, the collision operator is given by

$$Q(f,f)(t,\mathbf{x},\mathbf{v}) = \iint_{\mathbb{R}^N \times S^{N-1}} \left[f'f'_* - ff_* \right] \check{\mathcal{B}}(\mathbf{v},\mathbf{v}_*,\boldsymbol{\omega}) \, d\boldsymbol{\omega} \, d\mathbf{v}_*,$$

for any $t \in \mathbb{R}_+$ and $\mathbf{x} \in \mathbb{R}^N$, where we have used the standard abbreviations:

$$f' := f(t,\mathbf{x},\mathbf{v}'), \quad f'_* := f(t,\mathbf{x},\mathbf{v}'_*), \quad f_* := f(t,\mathbf{x},\mathbf{v}_*), \quad f := f(t,\mathbf{x},\mathbf{v}).$$

The cross-section $\check{\mathcal{B}}(\mathbf{v},\mathbf{v}_*,\boldsymbol{\omega})$ takes into account the nature of the microscopic interactions. In the case of monatomic gases, $\check{\mathcal{B}}(\mathbf{v},\mathbf{v}_*,\boldsymbol{\omega})$ is a function of $|\mathbf{v} - \mathbf{v}_*|$ and the angle between $\boldsymbol{\omega}$ and $\mathbf{v} - \mathbf{v}_*$ only, thanks to the Galilean invariance, i.e. $\check{\mathcal{B}}(\mathbf{v},\mathbf{v}_*,\boldsymbol{\omega}) = \mathcal{B}\left(|\mathbf{v} - \mathbf{v}_*|, \left| \boldsymbol{\omega} \cdot \frac{\mathbf{v}-\mathbf{v}_*}{|\mathbf{v}-\mathbf{v}_*|} \right| \right) =: \mathcal{B}$.

The structure of the collision integral reflects the general assumptions mentioned in the Introduction. Indeed, the fact that the variables t and $\mathbf{x}$ appear as parameters reflects the assumption that collisions are localized in space and time. The appearance of the products $f'f'_*$ and ff_* is a consequence of the chaos assumption.

The weak form of the collision operator. The formulation of the weak form of the collision operator $Q(f,f)$ allows to recover moment equations at the macroscopic level, especially conservation laws. Indeed, the weak formulation expresses the change in the integral $\int_{\mathbb{R}^N} f\psi(\mathbf{v})d\mathbf{v}$ which is due to the action of collisions.

PROPOSITION 1.1. *Let $\psi : \mathbb{R}^N \to \mathbb{R}$ be an arbitrary function of the velocity $\mathbf{v}$ such that the integral*

$$\int_{\mathbb{R}^N} Q(f,f)(\mathbf{v}) \, \psi(\mathbf{v}) \, d\mathbf{v}$$

makes sense. Then, the following holds

$$(1.7) \quad \int_{\mathbb{R}^N} Q(f,f)(\mathbf{v}) \, \psi(\mathbf{v}) \, d\mathbf{v}$$

$$= -\frac{1}{4} \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \int_{S^{N-1}} \left[f'f'_* - ff_* \right] \times \left[\psi(\mathbf{v}') + \psi(\mathbf{v}'_*) - \psi(\mathbf{v}) - \psi(\mathbf{v}_*) \right] \mathcal{B} \, d\boldsymbol{\omega} \, d\mathbf{v}_* d\mathbf{v}.$$

PROOF. The weak form (1.7) reflects the microscopic reversibility of the collision operator. Namely, the form of the collision operator enables the invariance of the weak form with respect to interchange of pre- and post-collisional velocities $(\mathbf{v},\mathbf{v}_*) \mapsto (\mathbf{v}',\mathbf{v}'_*)$ and of particles themselves $(\mathbf{v},\mathbf{v}_*) \mapsto (\mathbf{v}_*,\mathbf{v})$. Indeed, starting from

$$(1.8) \quad \int_{\mathbb{R}^N} Q(f,f)(\mathbf{v}) \, \psi(\mathbf{v}) \, d\mathbf{v} = \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \int_{S^{N-1}} \left[f'f'_* - ff_* \right] \psi(\mathbf{v}) \mathcal{B} \, d\boldsymbol{\omega} \, d\mathbf{v}_* d\mathbf{v},$$

let us perform the change of the variables $(\mathbf{v},\mathbf{v}_*) \mapsto (\mathbf{v}_*,\mathbf{v})$ with unit Jacobian:

$$(1.9) \quad \int_{\mathbb{R}^N} Q(f,f)(\mathbf{v}) \, \psi(\mathbf{v}) \, d\mathbf{v} = \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \int_{S^{N-1}} \left[f'_*f' - f_*f \right] \psi(\mathbf{v}_*) \mathcal{B} \, d\boldsymbol{\omega} \, d\mathbf{v}_* d\mathbf{v}$$

$$= \int_{\mathbb{R}^N} Q(f,f)(\mathbf{v}) \, \psi(\mathbf{v}_*) \, d\mathbf{v}.$$

Furthermore, let us consider the change of variables $(\mathbf{v}, \mathbf{v}_*) \mapsto (\mathbf{v}', \mathbf{v}'_*)$. The Jacobian of this transformation is 1 because it is based on the symmetry $\mathbf{v} - \mathbf{v}_* \mapsto (\mathbf{v} - \mathbf{v}_*) - 2((\mathbf{v} - \mathbf{v}_*) \cdot \boldsymbol{\omega})\boldsymbol{\omega}$:

$$J_{(\mathbf{v}, \mathbf{v}_*) \mapsto (\mathbf{v}', \mathbf{v}'_*)} = \text{Abs}\left(\begin{vmatrix} I_N - \boldsymbol{\omega}\boldsymbol{\omega}^T & \boldsymbol{\omega}\boldsymbol{\omega}^T \\ -\boldsymbol{\omega}\boldsymbol{\omega}^T & I_N + \boldsymbol{\omega}\boldsymbol{\omega}^T \end{vmatrix}\right) = \text{Abs}\left(\begin{vmatrix} I_N & 0 \\ -\boldsymbol{\omega}\boldsymbol{\omega}^T & I_N \end{vmatrix}\right) = 1.$$

Then, (1.8) becomes

$$(1.10) \qquad \begin{aligned} \int_{\mathbb{R}^N} Q(f,f)(\mathbf{v})\,\psi(\mathbf{v})\,d\mathbf{v} &= \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \int_{S^{N-1}} [ff_* - f'f'_*]\,\psi(\mathbf{v}')\mathcal{B}\,d\boldsymbol{\omega}\,d\mathbf{v}_* d\mathbf{v} \\ &= -\int_{\mathbb{R}^N} Q(f,f)(\mathbf{v})\,\psi(\mathbf{v}')\,d\mathbf{v}. \end{aligned}$$

Moreover, performing the change of variables $(\mathbf{v}, \mathbf{v}_*) \mapsto (\mathbf{v}_*, \mathbf{v})$ in (1.10) with unit Jacobian, we obtain

$$(1.11) \qquad \begin{aligned} \int_{\mathbb{R}^N} Q(f,f)(\mathbf{v})\,\psi(\mathbf{v})\,d\mathbf{v} &= \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \int_{S^{N-1}} [f_*f - f'_*f']\,\psi(\mathbf{v}'_*)\mathcal{B}\,d\boldsymbol{\omega}\,d\mathbf{v}_* d\mathbf{v} \\ &= -\int_{\mathbb{R}^N} Q(f,f)(\mathbf{v})\,\psi(\mathbf{v}'_*)\,d\mathbf{v}. \end{aligned}$$

Finally, summation of equations (1.8), (1.9), (1.10) and (1.11) lead to the required form of the weak formulation (1.7). $\qquad\qquad\square$

Comparing the weak form (1.7) with (1.2), it can be easily seen that the momentum $\psi(\mathbf{v}) = \mathbf{v}$ and kinetic energy $\psi(\mathbf{v}) = \frac{|\mathbf{v}|^2}{2}$ of a molecule make the weak form of the collision operator equal to zero. Such functions are collision invariants, according to the following definition.

We call a function ψ a collision invariant if it satisfies the functional equation:

$$(1.12) \qquad \psi(\mathbf{v}') + \psi(\mathbf{v}'_*) = \psi(\mathbf{v}) + \psi(\mathbf{v}_*), \quad \forall\,(\mathbf{v}, \mathbf{v}_*, \boldsymbol{\omega}) \in \mathbb{R}^{2N} \times S^{N-1}.$$

PROPOSITION 1.2. *The collision invariants (belonging to $L^1_{loc}(\mathbb{R}^N)$) are linear combinations of the following $(N+2)$ functions:*

$$(1.13) \qquad \boldsymbol{\psi}(\mathbf{v}) = \begin{pmatrix} 1 \\ \mathbf{v} \\ |\mathbf{v}|^2 \end{pmatrix}.$$

PROOF. We search for a function $\psi(\mathbf{v})$ such that the equation (1.12) is satisfied. The conservation laws at the microscopic level (1.2) imply that

$$(1.14) \qquad \psi(\mathbf{v}) + \psi(\mathbf{v}_*) = \phi(\mathbf{v} + \mathbf{v}_*, \tfrac{1}{2}|\mathbf{v}|^2 + \tfrac{1}{2}|\mathbf{v}_*|^2).$$

Let us for some function ϕ introduce the operator

$$(1.15) \qquad D_{k\ell} = (v_k - v_{*k})(\partial_{v_\ell} - \partial_{v_{*\ell}}) - (v_\ell - v_{*\ell})(\partial_{v_k} - \partial_{v_{*k}}), \quad \text{for } k \neq \ell.$$

Applying this operator to ϕ, we obtain

$$\begin{aligned} D_{k\ell}\,\phi(\mathbf{v} + \mathbf{v}_*, \tfrac{1}{2}|\mathbf{v}|^2 + \tfrac{1}{2}|\mathbf{v}_*|^2) &= (v_k - v_{*k})(\partial_\ell\phi + v_\ell\,\partial_2\phi - \partial_\ell\phi - v_{*\ell}\,\partial_2\phi) \\ &\quad - (v_\ell - v_{*\ell})(\partial_k\phi + v_k\,\partial_2\phi - \partial_k\phi - v_{*k}\,\partial_2\phi) \\ &= 0. \end{aligned}$$

Thus, in conjunction with (1.14), we obtain

$$D_{k\ell}(\psi(\mathbf{v}) + \psi(\mathbf{v}_*)) = 0.$$

Differentiation with respect to v_k yields

$$\begin{aligned} \partial_{v_k}&(D_{k\ell}(\psi(\mathbf{v}) + \psi(\mathbf{v}_*))) \\ &= \left((v_k - v_{*k})(\partial^2_{v_k v_\ell} - \partial^2_{v_k v_{*\ell}}) + (\partial_{v_\ell} - \partial_{v_{*\ell}}) - (v_\ell - v_{*\ell})(\partial^2_{v_k^2} - \partial^2_{v_k v_{*k}})\right)(\psi(\mathbf{v}) + \psi(\mathbf{v}_*)) \\ (1.16) \quad &= (v_k - v_{*k})\,\partial^2_{k\ell}\psi(\mathbf{v}) + \partial_\ell\psi(\mathbf{v}) - \partial_\ell\psi(\mathbf{v}_*) - (v_\ell - v_{*\ell})\,\partial^2_{k^2}\psi(\mathbf{v}) = 0. \end{aligned}$$

Furthermore, we differentiate (1.16) with respect to $v_{*\ell}$ and obtain

$$(1.17) \qquad\qquad -\partial^2_{\ell^2}\psi(\mathbf{v}_*) + \partial^2_{k^2}\psi(\mathbf{v}) = 0,$$

and we also differentiate (1.16) with respect to v_{*k}, obtaining

$$(1.18) \qquad\qquad -\partial^2_{k\ell}\psi(\mathbf{v}) - \partial^2_{k\ell}\psi(\mathbf{v}_*) = 0.$$

The equality (1.17) would not be possible unless

$$\partial^2_{k^2}\psi(\mathbf{v}) = \text{const}, \qquad \text{for every } k = 1,\dots,N.$$

Also, equality (1.18) implies that the mixed partial derivatives are constant, and because of the "minus" sign, they are equal to zero:

$$\partial^2_{k\ell}\psi(\mathbf{v}) = 0, \qquad 1 \le k,\ell \le N.$$

Note that the proof presented here holds for $\psi \in C^2(\mathbb{R}^N)$ if the derivatives are taken in the classical sense. Using them in the sense of distributions enables to treat $\psi \in L^1_{loc}(\mathbb{R}^N)$. $\qquad\square$

We see that the weak form of the collision integral (1.7) vanishes when the test function $\psi(\mathbf{v})$ is chosen to be a collision invariant (1.13). In other words,

$$\int_{\mathbb{R}^N} Q(f,f)(\mathbf{v}) \begin{pmatrix} 1 \\ \mathbf{v} \\ |\mathbf{v}|^2 \end{pmatrix} \, d\mathbf{v} = 0.$$

This property of the weak form of the collision operator enables to recover the conservation laws of mass, momentum density and total energy density at the macroscopic level. In particular, the fact that (1.13) are the *only* invariants that satisfy the functional equation (1.74) shows that there are no hidden conservation laws in the Boltzmann equation.

Next, we define macroscopic quantities as moments of the distribution function, and link the evolution of these quantities to the solution of the Boltzmann equation.

Macroscopic conservation laws. Even though it only provides a statistical description, the Boltzmann equation is still unnecessary detailed for the majority of problems. In fact, one is most often interested in the moments that can be obtained from the Boltzmann equation by means of integration with respect to the quantities which describe the microscopic state of particles (the velocity $\mathbf{v}$ of the particles in the monatomic case).

To obtain a general macroscopic law, we multiply the Boltzmann equation by some function of the microscopic state of particles, say $\psi(\mathbf{v})$, and integrate over all possible values of microscopic states $\mathbf{v} \in \mathbb{R}^N$ (assuming that f is smooth with respect to $t, \mathbf{x}$, and has good properties of integrability with respect to $\mathbf{v}$):

$$(1.19) \qquad \int_{\mathbb{R}^N} (\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f)\,\psi(\mathbf{v})\, d\mathbf{v} = \int_{\mathbb{R}^N} Q(f,f)(\mathbf{v})\,\psi(\mathbf{v}) d\mathbf{v}.$$

Let us transform the left-hand side of (1.19). By interchanging the order of the integration and differentiation, we obtain

$$\int_{\mathbb{R}^N} (\partial_t f)\,\psi(\mathbf{v})\, d\mathbf{v} = \partial_t \int_{\mathbb{R}^N} f\psi(\mathbf{v})\, d\mathbf{v}.$$

Similarly,

$$\int_{\mathbb{R}^N} (\mathbf{v} \cdot \nabla_{\mathbf{x}} f)\,\psi(\mathbf{v})\, d\mathbf{v} = \nabla_{\mathbf{x}} \cdot \int_{\mathbb{R}^N} f\,\mathbf{v}\,\psi(\mathbf{v})\, d\mathbf{v}.$$

Then (1.19) can be written in the form

$$\partial_t \int_{\mathbb{R}^N} f\psi(\mathbf{v})\, d\mathbf{v} + \nabla_{\mathbf{x}} \cdot \int_{\mathbb{R}^N} f\,\mathbf{v}\,\psi(\mathbf{v})\, d\mathbf{v} = \int_{\mathbb{R}^N} Q(f,f)(\mathbf{v})\,\psi(\mathbf{v}) d\mathbf{v}.$$

This is the general moment equation. Its physical interpretation is obtained by specifying the test function $\psi(\mathbf{v})$. In the sequel we precise the conservation laws when test functions are chosen to be collisional invariants for which the right-hand side of the moment equation becomes zero. But first, let us define macroscopic quantities.

When $\psi(\mathbf{v})$ is chosen to consist of monomials in the velocity variable, i.e. $\psi(\mathbf{v}) = v_{i_1} v_{i_2} \ldots v_{i_n}$, where $i_k \in \{1, 2, 3\}$, for $k = 1, \ldots n$ and $n \in \mathbb{N}$, we obtain monomial moments of the distribution function denoted by $F^{(n)}_{i_1 i_2 \ldots i_n}$:

$$(1.20) \qquad F^{(n)}_{i_1 i_2 \ldots i_n}(t, \mathbf{x}) = \int_{\mathbb{R}^N} m \, v_{i_1} v_{i_2} \ldots v_{i_n} \, f(t, \mathbf{x}, \mathbf{v}) \, \mathrm{d}\mathbf{v}.$$

The moments of order $n \leq 2$ are interpreted as the mass density, the momentum density and the momentum flux:

$$(1.21) \qquad \begin{pmatrix} \rho \\ \rho u_i \\ \rho u_i u_j + p_{ij} \end{pmatrix} = \begin{pmatrix} F^{(0)} \\ F^{(1)}_i \\ F^{(2)}_{ij} \end{pmatrix} = \int_{\mathbb{R}^N} m \begin{pmatrix} 1 \\ v_i \\ v_i v_j \end{pmatrix} f \, \mathrm{d}\mathbf{v},$$

where ρ is the mass density, u_i is i-th component of the macroscopic velocity, while p_{ij} is ij-th element of the pressure tensor. The splitting of the second order moment is obtained by introducing the peculiar[1] velocity of a particle $\mathbf{c} = \mathbf{v} - \mathbf{u}$. Indeed, from the first order moment (using the zero-th order moment) we get:

$$\int_{\mathbb{R}^N} m \, v_i \, f \, \mathrm{d}\mathbf{v} = \int_{\mathbb{R}^N} m \, (u_i + c_i) \, f \, \mathrm{d}\mathbf{v} = \rho u_i + \int_{\mathbb{R}^N} m \, c_i \, f \, \mathrm{d}\mathbf{v},$$

and therefore

$$(1.22) \qquad \int_{\mathbb{R}^N} m \, c_i \, f \, \mathrm{d}\mathbf{v} = 0.$$

Thus, the second order moment becomes

$$\int_{\mathbb{R}^N} m \, v_i v_j \, f \, \mathrm{d}\mathbf{v} = \rho u_i u_j + \int_{\mathbb{R}^N} m \, c_i c_j \, f \, \mathrm{d}\mathbf{v},$$

and

$$(1.23) \qquad p_{ij} = \int_{\mathbb{R}^N} m \, c_i c_j \, f \, \mathrm{d}\mathbf{v}.$$

Moreover, one half of the trace (equalization of indices and summation over them) is interpreted as the energy density:

$$(1.24) \qquad \int_{\mathbb{R}^N} \tfrac{m}{2} \, |\mathbf{v}|^2 \, f \, \mathrm{d}\mathbf{v} = \tfrac{1}{2} \rho \, |\mathbf{u}|^2 + \int_{\mathbb{R}^N} \tfrac{m}{2} \, |\mathbf{c}|^2 \, f \, \mathrm{d}\mathbf{v},$$

using $(1.21)_1$ and (1.22). This definition illustrates the decomposition of the total energy of a gas into the kinetic and internal energy at the macroscopic level. Indeed, using the peculiar velocity $\mathbf{c} = \mathbf{v} - \mathbf{u}$ and property (1.22), starting from kinetic theory we obtain the formula for the internal energy density:

$$(1.25) \qquad \rho e = \int_{\mathbb{R}^N} \tfrac{m}{2} \, |\mathbf{c}|^2 \, f \, \mathrm{d}\mathbf{v}.$$

Comparing the definition of the macroscopic internal energy density (1.25) to the definition of the pressure tensor (1.23), it can be noticed that the macroscopic internal energy density is related to the trace of the pressure tensor. In the case of monatomic gases, the trace of the pressure tensor is linked to the hydrodynamic pressure as follows:

$$(1.26) \qquad p = \tfrac{1}{N} \left(p_{11} + p_{22} + \cdots + p_{NN} \right).$$

Therefore, the caloric equation of state for a monatomic gas is recovered:

$$(1.27) \qquad \rho e = \tfrac{N}{2} p = \tfrac{N}{2} n \, k \, T,$$

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[1] The term "peculiar" is used instead of the term "relative" when one velocity is the macroscopic one, and the other one is a microscopic one: in this case, the velocity $\mathbf{v}$ is the velocity of the particle, so we refer to it as microscopic, while the velocity $\mathbf{u}$ is the macroscopic velocity of a gas.

where n is the macroscopic density $n = \rho/m$, k is the Boltzmann constant and T is the temperature of the gas defined by

$$T = \frac{1}{N} \frac{m}{k} \frac{\int_{\mathbb{R}^N} m \,|\mathbf{c}|^2\, f \,\mathrm{d}\mathbf{v}}{\int_{\mathbb{R}^N} m f \,\mathrm{d}\mathbf{v}}.$$

Finally, the energy flux can be defined and furthermore properly decomposed using the peculiar velocity $\mathbf{c} = \mathbf{v} - \mathbf{u}$ as follows:

$$\int_{\mathbb{R}^N} \tfrac{m}{2} \,|\mathbf{v}|^2\, v_i\, f \,\mathrm{d}\mathbf{v} = \left(\tfrac{1}{2}\rho \,|\mathbf{u}|^2 + \rho e \right) u_i + \sum_{j=1}^N p_{ij} u_j + q_i,$$

where the i-th component of the heat flux $\mathbf{q}$ is defined as

$$q_i = \int_{\mathbb{R}^N} \tfrac{m}{2} \,|\mathbf{c}|^2\, c_i\, f \,\mathrm{d}\mathbf{v}.$$

Once we have the physical interpretation of the low order moments of the distribution function, the corresponding moment equations can be derived from the Boltzmann equation.

PROPOSITION 1.3. *Let f be a solution of the Boltzmann equation (1.1) that is smooth with respect to $t, \mathbf{x}$ and rapidly decaying in $\mathbf{v}$. Then the following local conservation laws hold:*

$$\partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho\, \mathbf{u}) = 0,$$

(1.28)
$$\partial_t \rho u_i + \sum_{j=1}^N \partial_{x_j} (\rho u_i u_j + p_{ij}) = 0, \ \ i = 1, \ldots, N,$$

$$\partial_t \left(\tfrac{1}{2}\, \rho \,|\mathbf{u}|^2 + \rho\, e \right) + \sum_{j=1}^N \partial_{x_j} \left(\left(\tfrac{1}{2}\, \rho \,|\mathbf{u}|^2 + \rho\, e \right) u_j + \sum_{i=1}^N p_{ij} u_i + q_j \right) = 0.$$

They respectively represent the local conservation of mass, momentum and total energy density of a monatomic gas.

$H-$**theorem.** The microscopic mechanics we used until now is time reversible. This means precisely the following. Suppose that at time t_0 two particles of velocities $\mathbf{v}'$ and $\mathbf{v}'_*$ are colliding. After the collision, at time $t_0 + \Delta t$ their velocities are $\mathbf{v}$ and $\mathbf{v}_*$, respectively, thanks to the collisional rules (1.6). Let us now perform a mental experiment. Let change the sign of the velocities at time $t_0 + \Delta t$, that is we consider two particles of velocities $-\mathbf{v}$ and $-\mathbf{v}_*$ at time $t_0 + \Delta t$. Then these particles will collide and at time $t_0 + 2\Delta t$ their velocities can be obtained from the collisional rules (1.6):

$$(-\mathbf{v}) - (((-\mathbf{v}) - (-\mathbf{v}_*)) \cdot \boldsymbol{\omega}) \,\boldsymbol{\omega} = -(\mathbf{v} - ((\mathbf{v} - \mathbf{v}_*) \cdot \boldsymbol{\omega}) \,\boldsymbol{\omega}) = -\mathbf{v}',$$
$$(-\mathbf{v}_*) + (((-\mathbf{v}) - (-\mathbf{v}_*)) \cdot \boldsymbol{\omega}) \,\boldsymbol{\omega} = -(\mathbf{v}_* + ((\mathbf{v} - \mathbf{v}_*) \cdot \boldsymbol{\omega}) \,\boldsymbol{\omega}) = -\mathbf{v}'_*.$$

It can be seen that the velocities are equal to the starting velocities up to a change of sign. Or in other words, the change of sign of velocities at some time makes the system pass through the same sequence of states which it went through in the forward direction. We described a reversible process.

Disorder, or macroscopic irreversibility, is measured by means of the entropy that is defined starting from the kinetic theory by

(1.29)
$$\eta = \int_{\mathbb{R}^N} f \,\log f \,\mathrm{d}\mathbf{v}.$$

PROPOSITION 1.4 ($H-$theorem)**.** *Assume that the cross section $\mathcal{B}$ is positive almost everywhere, and that $f := f(\mathbf{v}) \geq 0$ is such that all quantities below are well defined. Then*

(a) *The entropy production is non-positive, i.e.*

(1.30)
$$D(f) = \int_{\mathbb{R}^N} Q(f, f)(\mathbf{v}) \,\log f \,\mathrm{d}\mathbf{v} \leq 0.$$

(b) *Moreover, the three following properties are equivalent.*

  i. *For any $\mathbf{v} \in \mathbb{R}^N$*

$$Q(f, f)(\mathbf{v}) = 0.$$

ii.   *The entropy production vanishes, that is*

$$D(f) = \int_{\mathbb{R}^N} Q(f,f)(\mathbf{v}) \log f \, d\mathbf{v} = 0.$$

iii.   *There exist $n > 0$, $T > 0$ and $\mathbf{u} \in \mathbb{R}^N$ such that*

(1.31)
$$f(\mathbf{v}) = n \left(\frac{m}{2\,\pi\,k\,T} \right)^{N/2} e^{-\frac{m}{2kT}|\mathbf{v}-\mathbf{u}|^2}.$$

PROOF. In order to prove the statement (a), we consider the weak form of the collision operator (1.7), choosing the test function $\psi(\mathbf{v}) = \log f(\mathbf{v})$:

$$D(f) = -\frac{1}{4} \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \int_{S^{N-1}} \left[f'f_*' - f f_* \right] \times \left[\log f' + \log f_*' - \log f - \log f_* \right] \mathcal{B} \, d\boldsymbol{\omega} \, d\mathbf{v}_* d\mathbf{v}$$

$$= -\frac{1}{4} \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \int_{S^{N-1}} \left[f'f_*' - f f_* \right] \times \left[\log f' f_*' - \log f f_* \right] \mathcal{B} \, d\boldsymbol{\omega} \, d\mathbf{v}_* d\mathbf{v}.$$

Noticing that the function $(x,y) \mapsto (x-y)(\log x - \log y)$ is nonnegative for $x, y > 0$, the assumptions made on $\mathcal{B}$ and f yield the non-positivity of the entropy production $D(f)$.

Let us show the equivalence of the three statements in the part (b). The following implications are straightforward: (i $\Rightarrow$ ii) and (iii $\Rightarrow$ i). Let us show (ii $\Rightarrow$ iii). Indeed, suppose that ii) holds, i.e.

$$D(f) = -\frac{1}{4} \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \int_{S^{N-1}} \left[f'f_*' - f f_* \right] \times \left[\log f' + \log f_*' - \log f - \log f_* \right] \mathcal{B} \, d\boldsymbol{\omega} \, d\mathbf{v}_* d\mathbf{v} = 0.$$

Thus, $\log f$ is a collisional invariant, and by Proposition 1.2, $\log f$ is a linear combination of $1, \mathbf{v}, |\mathbf{v}|^2$. Therefore, there exist constants $A_0, A_1, \ldots, A_N, A_{N+1}$ such that

$$f = e^{A_0 + A_1 v_1 + \ldots A_N v_N + A_{N+1}|\mathbf{v}|^2}.$$

Finally, the choice

$$A_0 = \ln n \left(\left(\frac{m}{2\,\pi\,k\,T} \right)^{N/2} \right) - \frac{m}{2kT}|\mathbf{u}|^2,$$

$$A_i = \frac{m}{kT} u_i, \quad i = 1, \ldots, N,$$

$$A_{N+1} = -\frac{m}{2kT},$$

for $n \geq 0$, $T > 0$ and $\mathbf{u} \in \mathbb{R}^N$ yields the form of the equilibrium distribution function. $\square$

One of the important implications of the $H-$theorem concerns the additional macroscopic law obtained from the Boltzmann equation. Indeed, for f and $\log f$ rapidly decaying with respect to $\mathbf{v}$ and smooth with respect to $(t, \mathbf{x})$, the integration of the Boltzmann equation over the velocity space against the test function $\log f$, in conjunction with (1.30), yields

(1.32)
$$\partial_t \eta + \sum_{j=1}^{N} \partial_{x_j} \eta_j \leq 0,$$

where η_j is the entropy flux:

$$\eta_j = \int_{\mathbb{R}^N} v_j \, f \, \log f \, d\mathbf{v}.$$

It should be noted that in the physical sense, the entropy (1.29) coincides with the usual entropy from the continuum theories up to a change of sign and multiplication by the Boltzmann constant k. Also, it represents a dynamical entropy in the sense that it is defined for non-equilibrium processes. In particular, the macroscopic law (1.32), obtained from the Boltzmann equation using the $H-$theorem, matches the second law of thermodynamics which says that the physical entropy of an isolated system should not decrease with respect to time. In other words, if a gas does not interact with an external device, its entropy will increase until it has reached the maximum value it can have in accordance with the values of the conserved quantities – mass, momentum and energy density.

The σ−notation. We now present another possible parametrization of equation (1.3). Indeed, we parametrize this equation with a unit vector $\sigma \in S^{N-1}$:

$$(1.33) \qquad \mathbf{v}' - \mathbf{v}'_* = |\mathbf{v} - \mathbf{v}_*|\,\sigma.$$

The last equation in conjunction with $(1.2)_1$ yields formulas for the pre-collisional velocities in terms of the post-collisional velocities and the parameter σ:

$$\mathbf{v}' = \frac{\mathbf{v} + \mathbf{v}_*}{2} + \frac{|\mathbf{v} - \mathbf{v}_*|}{2}\,\sigma,$$

$$\mathbf{v}'_* = \frac{\mathbf{v} + \mathbf{v}_*}{2} - \frac{|\mathbf{v} - \mathbf{v}_*|}{2}\,\sigma.$$

Since this notation will be very useful in further computations, its relation to the ω−notation is discussed in the next paragraph.

Passage from ω− to σ−notation. The relation between parameters ω and σ can be obtained from equations (1.5) and (1.33). Indeed, one can see that

$$(1.34) \qquad \sigma = \mathbf{z} - 2\,(\omega \cdot \mathbf{z})\,\omega, \quad \text{where } \mathbf{z} = \frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|}.$$

We restrict ourselves to space dimension three ($N = 3$). We remind that ω and σ are unit vectors of the sphere S^2. Indeed, the notation ω and σ hides, in fact, two angles. If we introduce angles $\alpha_1, \beta_1 \in [0, \pi]$, $\alpha_2, \beta_2 \in [0, 2\pi]$, then actually the following notation has been used

$$\omega := \begin{pmatrix} \cos\alpha_1 \\ \sin\alpha_1 \cos\alpha_2 \\ \sin\alpha_1 \sin\alpha_2 \end{pmatrix}, \quad \sigma := \begin{pmatrix} \cos\beta_1 \\ \sin\beta_1 \cos\beta_2 \\ \sin\beta_1 \sin\beta_2 \end{pmatrix}.$$

Also, we recall the notation for elements on the sphere S^2:

$$\mathrm{d}\omega := \sin\alpha_1\,\mathrm{d}\alpha_1\,\mathrm{d}\alpha_2, \quad \mathrm{d}\sigma := \sin\beta_1\,\mathrm{d}\beta_1\,\mathrm{d}\beta_2.$$

Therefore, when we say that we pass from ω− to σ−representation, we actually mean that we change variables $(\alpha_1, \alpha_2) \mapsto (\beta_1, \beta_2)$. Thus, it will be useful to compute the Jacobian $J_{(\alpha_1,\alpha_2)\mapsto(\beta_1\beta_2)}$. The relation which holds between the two groups of angles is obtained from (1.34). Indeed, for some $\mathbf{z} = (z_1, z_2, z_3)^{\mathrm{T}}$

$$\cos\beta_1 = \sigma_1 = z_1 - 2\,(z_1 \cos\alpha_1 + z_2 \sin\alpha_1 \, \cos\alpha_2 + z_3 \sin\alpha_1 \sin\alpha_2)\cos\alpha_1,$$
$$(1.35) \qquad \sin\beta_1 \cos\beta_2 = \sigma_2 = z_2 - 2\,(z_1 \cos\alpha_1 + z_2 \sin\alpha_1 \, \cos\alpha_2 + z_3 \sin\alpha_1 \sin\alpha_2)\sin\alpha_1 \, \cos\alpha_2,$$
$$\sin\beta_1 \sin\beta_2 = \sigma_3 = z_3 - 2\,(z_1 \cos\alpha_1 + z_2 \sin\alpha_1 \, \cos\alpha_2 + z_3 \sin\alpha_1 \sin\alpha_2)\sin\alpha_1 \, \sin\alpha_2.$$

Note that $J_{(\alpha_1,\alpha_2)\mapsto(\beta_1\beta_2)}$ can be decomposed as follows

$$J_{(\alpha_1,\alpha_2)\mapsto(\beta_1\beta_2)} = J_{(\alpha_1,\alpha_2)\mapsto(\sigma_1,\sigma_2)}\,J_{(\sigma_1,\sigma_2)\mapsto(\beta_1\beta_2)}.$$

It is an easy task to compute the Jacobian $J_{(\beta_1\beta_2)\mapsto(\sigma_1,\sigma_2)}$ from the first equalities in (1.35):

$$J_{(\beta_1\beta_2)\mapsto(\sigma_1,\sigma_2)} = (\sin\beta_1)^2\,|\sin\beta_2| = |\sigma_3|\sin\beta_1.$$

Therefore

$$J_{(\alpha_1,\alpha_2)\mapsto(\beta_1\beta_2)} = \frac{1}{|\sigma_3|\sin\beta_1}\,J_{(\alpha_1,\alpha_2)\mapsto(\sigma_1,\sigma_2)}.$$

Computation of the Jacobian $J_{(\alpha_1,\alpha_2)\mapsto(\sigma_1,\sigma_2)}$ requires more efforts, and lead to the result

$$J_{(\alpha_1,\alpha_2)\mapsto(\sigma_1,\sigma_2)} = 4\,|\sigma_3|\,|\omega \cdot \mathbf{z}|\sin\alpha_1, \quad \forall\,\mathbf{z} \in \mathbb{R}^3.$$

Summarizing, we obtain

$$\sin\beta_1\mathrm{d}\beta_1\mathrm{d}\beta_2 = 4\,|\omega \cdot \mathbf{z}|\sin\alpha_1\mathrm{d}\alpha_1\mathrm{d}\alpha_2, \quad \forall\,\mathbf{z} \in \mathbb{R}^3.$$

At the end, one should note that when ω moves over the sphere S^2, σ moves twice over the sphere S^2. More precisely, both ω and $-\omega$ give one σ. Since the domain for σ remains S^2, we should add a

factor $1/2$ in the changes of variable between $\boldsymbol{\omega}$ and $\boldsymbol{\sigma}$ in the integrals. This leads to the final result, now expressed in standard notation for kinetic theory:

$$(1.36) \qquad \int_{S^2} F(\boldsymbol{\sigma})\,\mathrm{d}\boldsymbol{\sigma} = \int_{S^2} F(\mathbf{z} - 2\,(\boldsymbol{\omega} \cdot \mathbf{z})\,\boldsymbol{\omega})\,2\,|\boldsymbol{\omega} \cdot \mathbf{z}|\,\mathrm{d}\boldsymbol{\omega}, \quad \forall\,\mathbf{z} \in S^2,$$

for any function F such that the integrals are well defined. For the result in any space dimension, we refer to [59] and give the final result

$$(1.37) \qquad \int_{S^{N-1}} F(\boldsymbol{\sigma})\,\mathrm{d}\boldsymbol{\sigma} = \int_{S^{N-1}} F(\mathbf{z} - 2\,(\boldsymbol{\omega} \cdot \mathbf{z})\,\boldsymbol{\omega})\,2^{N-2}\,|\boldsymbol{\omega} \cdot \mathbf{z}|^{N-2}\,\mathrm{d}\boldsymbol{\omega}, \quad \forall\,\mathbf{z} \in S^{N-1}.$$

2. Description of mixtures of monatomic gases

In Chapter 4 of this thesis, we consider a mixture of monatomic gases. The main problem with respect to the use of a monatomic, mono-species gas is the possibility for molecules to have different masses. Although seeming at first sight easy to overcome, this extension leads to new mathematical problems when, for example, the diffusion asymptoptics of the Boltzmann equation is considered. We write here a brief extension of the preliminaries of the previous Section (under the assumption that the space dimension is $N = 3$) to the case of a mixture of monatomic gases.

Let the gas mixture be constituted of $s \geq 2$ species. Each species $\mathcal{A}_i$ of the mixture, $1 \leq i \leq s$, is described by a microscopic density function f_i. It depends on time $t \in \mathbb{R}_+$, space position $\mathbf{x} \in \mathbb{R}^3$ and molecular velocity $\mathbf{v} \in \mathbb{R}^3$, and is nonnegative. More precisely, $f_i(t, \mathbf{x}, \mathbf{v})\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v}$ allows to quantify the number of molecules of species $\mathcal{A}_i$ at time t in an elementary volume of size $\mathrm{d}\mathbf{x}$, and whose velocities equal $\mathbf{v}$ up to $\mathrm{d}\mathbf{v}$. We can also define at a given point $\mathbf{x}$ and a given time t the macroscopic density n_i of each species $\mathcal{A}_i$ by

$$n_i(t, \mathbf{x}) = \int_{\mathbb{R}^3} f_i(t, \mathbf{x}, \mathbf{v})\,\mathrm{d}\mathbf{v}.$$

The rate of change of distribution functions is measured by means of collision operators Q_{ij} defined below in (1.41). More precisely, each distribution function f_i is supposed to satisfy the Boltzmann equation

$$(1.38) \qquad \partial_t f_i + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = \sum_{j=1}^{s} Q_{ij}(f_i, f_j), \quad \forall\,i = 1, \dots, s.$$

In order to define the collision operators, let us analyze a collision between two molecules.

Collision transformation. We assume that the mixture only involves molecular collisions in which, since the gases are monatomic, kinetic energy is conserved. We consider two colliding molecules of species $\mathcal{A}_i$ and $\mathcal{A}_j$, $1 \leq i, j \leq s$. Their masses are m_i and m_j, and their pre-collisional velocities $\mathbf{v}'$ and $\mathbf{v}'_*$. After a collision, the particles belong to the same species (no chemical reactions), so their masses remain unchanged, and their velocities become $\mathbf{v}$ and $\mathbf{v}_*$. Both momentum and kinetic energy are conserved, i.e.

$$(1.39) \qquad m_i \mathbf{v}' + m_j \mathbf{v}'_* = m_i \mathbf{v} + m_j \mathbf{v}_*, \qquad \tfrac{m_i}{2}\left|\mathbf{v}'\right|^2 + \tfrac{m_j}{2}\left|\mathbf{v}'_*\right|^2 = \tfrac{m_i}{2}\left|\mathbf{v}\right|^2 + \tfrac{m_j}{2}\left|\mathbf{v}_*\right|^2.$$

Consequently, $\mathbf{v}'$ and $\mathbf{v}'_*$ can be written in terms of $\mathbf{v}$ and $\mathbf{v}_*$:

$$(1.40) \qquad \begin{aligned} \mathbf{v}' &= \frac{m_i \mathbf{v} + m_j \mathbf{v}_*}{m_i + m_j} + \frac{m_j}{m_i + m_j}\,T_{\boldsymbol{\omega}}\left[\mathbf{v} - \mathbf{v}_*\right], \\ \mathbf{v}'_* &= \frac{m_i \mathbf{v} + m_j \mathbf{v}_*}{m_i + m_j} - \frac{m_i}{m_i + m_j}\,T_{\boldsymbol{\omega}}\left[\mathbf{v} - \mathbf{v}_*\right], \end{aligned}$$

where $\boldsymbol{\omega} \in S^2$ is arbitrary, and $T_{\boldsymbol{\omega}}$ is the symmetry with respect to the plane $\{\boldsymbol{\omega}\}^{\perp}$, i.e.

$$T_{\boldsymbol{\omega}}\mathbf{z} = \mathbf{z} - 2(\boldsymbol{\omega} \cdot \mathbf{z})\boldsymbol{\omega}, \qquad \forall\,\mathbf{z} \in \mathbb{R}^3.$$

Collision operators. Let $1 \leq i, j \leq s$. The collision operator associated to the species $\mathcal{A}_i$ and $\mathcal{A}_j$ is defined by

$$(1.41) \qquad Q_{ij}(f,g)(\mathbf{v}) = \iint_{\mathbb{R}^3 \times S^2} \left[f(\mathbf{v}') g(\mathbf{v}'_*) - f(\mathbf{v}) g(\mathbf{v}_*) \right] \check{\mathcal{B}}_{ij}(\mathbf{v}, \mathbf{v}_*, \boldsymbol{\omega}) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*,$$

where $\mathbf{v}'$ and $\mathbf{v}'_*$ are defined by (1.40), and f and g are two functions of the velocity variable. The cross-section $\check{\mathcal{B}}_{ij}(\mathbf{v}, \mathbf{v}_*, \boldsymbol{\omega})$ only depends on $\mathbf{v}$, $\mathbf{v}_*$ and $\boldsymbol{\omega}$. In fact, $\check{\mathcal{B}}_{ij}$ is only a function of $|\mathbf{v} - \mathbf{v}_*|$ and the angle θ between $\boldsymbol{\omega}$ and $\mathbf{v} - \mathbf{v}_*$, thanks to Galilean invariance. Let us set

$$(1.42) \qquad \check{\mathcal{B}}_{ij}(\mathbf{v}, \mathbf{v}_*, \boldsymbol{\omega}) = \mathcal{B}_{ij}\left(|\mathbf{v} - \mathbf{v}_*|, \left| \boldsymbol{\omega} \cdot \frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|} \right| \right) =: \mathcal{B}_{ij}, \quad \forall \boldsymbol{\omega} \in S^2, \quad \forall \mathbf{v}, \mathbf{v}_* \in \mathbb{R}^3.$$

The collisions are also supposed microreversible, which ensures that

$$(1.43) \qquad \mathcal{B}_{ij}\left(|\mathbf{v} - \mathbf{v}_*|, \left| \boldsymbol{\omega} \cdot \frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|} \right| \right) = \mathcal{B}_{ji}\left(|\mathbf{v} - \mathbf{v}_*|, \left| \boldsymbol{\omega} \cdot \frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|} \right| \right).$$

The collision operators can also be written under weak forms, obtained from (1.41) using the changes of variables $(\mathbf{v}, \mathbf{v}_*) \mapsto (\mathbf{v}_*, \mathbf{v})$ and $(\mathbf{v}, \mathbf{v}_*) \mapsto (\mathbf{v}', \mathbf{v}'_*)$ for a fixed $\boldsymbol{\omega} \in S^2$:

$$\int_{\mathbb{R}^3} Q_{ij}(f,g)\, \psi_i(\mathbf{v}) \mathrm{d}\mathbf{v} = -\frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{S^2} \left[f(\mathbf{v}') g(\mathbf{v}'_*) - f(\mathbf{v}) g(\mathbf{v}_*) \right] \times \left[\psi_i(\mathbf{v}') - \psi_i(\mathbf{v}) \right] \mathcal{B}_{ij} \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_* \, \mathrm{d}\mathbf{v},$$

$$(1.44) \qquad \int_{\mathbb{R}^3} Q_{ij}(f,g)\, \psi_i(\mathbf{v}) \mathrm{d}\mathbf{v} + \int_{\mathbb{R}^3} Q_{ji}(g,f)\, \psi_j(\mathbf{v}) \mathrm{d}\mathbf{v}$$

$$= -\frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{S^2} \left[f(\mathbf{v}') g(\mathbf{v}'_*) - f(\mathbf{v}) g(\mathbf{v}_*) \right] \times \left[\psi_i(\mathbf{v}') + \psi_j(\mathbf{v}'_*) - \psi_i(\mathbf{v}) - \psi_j(\mathbf{v}_*) \right] \mathcal{B}_{ij} \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_* \, \mathrm{d}\mathbf{v}.$$

We mention that, if we choose suitable test-functions, the weak forms allow to formally write, for any i and j, and any functions f and g for which the following equations make sense:

$$(1.45) \qquad \int_{\mathbb{R}^3} Q_{ij}(f,g)(\mathbf{v}) \, \mathrm{d}\mathbf{v} = 0,$$

$$(1.46) \qquad \int_{\mathbb{R}^3} Q_{ij}(f,g)(\mathbf{v}) \begin{pmatrix} m_i \, \mathbf{v} \\ \frac{m_i}{2} \, |\mathbf{v}|^2 \end{pmatrix} \mathrm{d}\mathbf{v} + \int_{\mathbb{R}^3} Q_{ji}(g,f)(\mathbf{v}) \begin{pmatrix} m_j \, \mathbf{v} \\ \frac{m_j}{2} \, |\mathbf{v}|^2 \end{pmatrix} \mathrm{d}\mathbf{v} = 0.$$

$H-$**theorem.** Let us now write down the $H-$theorem corresponding to the above defined collisional operators and discuss the mechanical equilibrium. The following properties hold.

PROPOSITION 1.5. *Let us assume that the cross sections $(\mathcal{B}_{ij})_{1 \leq i,j \leq s}$ are positive almost everywhere and that all $f_i := f_i(\mathbf{v}) \geq 0$, $1 \leq i \leq s$, are such that both the collisional integrals Q_{ij} and the entropy production D are well defined. Then*

(a) *The entropy production is non-positive, i.e.*

$$D(f_1, \ldots, f_s) := \sum_{i=1}^{s} \sum_{j=1}^{s} \int_{\mathbb{R}^3} Q_{ij}(f_i, f_j)(\mathbf{v}) \log\left(f_i(\mathbf{v}) \right) \mathrm{d}\mathbf{v} \leq 0.$$

(b) *Moreover, the three following properties are equivalent.*
   i. *For any $1 \leq i, j \leq s$ and $\mathbf{v} \in \mathbb{R}^3$*

$$(1.47) \qquad Q_{ij}(f_i, f_j)(\mathbf{v}) = 0.$$

   ii. *The entropy production vanishes, that is*

$$D(f_1, \ldots, f_s) = 0.$$

   iii. *There exist $T > 0$ and $u \in \mathbb{R}^3$ such that, for any i, there exists $n_i \geq 0$ such that*

$$(1.48) \qquad f_i(\mathbf{v}) = n_i \left(\frac{m_i}{2\,\pi\,k\,T} \right)^{3/2} e^{-\frac{m_i}{2kT}|\mathbf{v}-\mathbf{u}|^2}.$$

PROOF. The first part can be proven analogously to the first part of Proposition 1.4, using the weak form (1.44) and some properties of the log function. Let us focus on (ii⇒iii). Considering first the term corresponding to the same species, $Q_{ii} = 0$ implies that f_i has the required form (1.48)

$$f_i(\mathbf{v}) = n_i \left(\frac{m_i}{2\pi k T_i} \right)^{3/2} e^{-\frac{m_i}{2kT_i}|\mathbf{v}-\mathbf{u}_i|^2},$$

but with T_i and $\mathbf{u}_i$ instead of T and $\mathbf{u}$. It remains to prove that T_i and $\mathbf{u}_i$ do not depend on i. Let us consider the terms corresponding to the species $\mathcal{A}_i$ and $\mathcal{A}_j$. Then $Q_{ij} = 0$, $i \neq j$, implies $f_i(\mathbf{v}')f_j(\mathbf{v}'_*) = f_i(\mathbf{v})f_j(\mathbf{v}_*)$, which reduces to

$$\frac{m_i}{2kT_i} \left| \mathbf{v}' - \mathbf{u}_i \right|^2 + \frac{m_j}{2kT_j} \left| \mathbf{v}'_* - \mathbf{u}_j \right|^2 = \frac{m_i}{2kT_i} \left| \mathbf{v} - \mathbf{u}_i \right|^2 + \frac{m_j}{2kT_j} \left| \mathbf{v}_* - \mathbf{u}_i \right|^2.$$

For simplicity, using the $\boldsymbol{\sigma}-$notation, it can be written

$$\frac{m_i}{2kT_i} \left| \frac{m_i\mathbf{v} + m_j\mathbf{v}_*}{m_i + m_j} + \frac{m_j}{m_i + m_j} |\mathbf{v} - \mathbf{v}_*| \boldsymbol{\sigma} - \mathbf{u}_i \right|^2 + \frac{m_j}{2kT_j} \left| \frac{m_i\mathbf{v} + m_j\mathbf{v}_*}{m_i + m_j} - \frac{m_i}{m_i + m_j} |\mathbf{v} - \mathbf{v}_*| \boldsymbol{\sigma} - \mathbf{u}_j \right|^2$$
$$= \frac{m_i}{2kT_i} |\mathbf{v} - \mathbf{u}_i|^2 + \frac{m_j}{2kT_j} |\mathbf{v}_* - \mathbf{u}_i|^2.$$

Equalization of the coefficients in $\boldsymbol{\sigma}$ yields

$$\frac{m_i m_j}{m_i + m_j} |\mathbf{v} - \mathbf{v}_*| \left(\frac{1}{kT_i} \frac{m_i\mathbf{v} + m_j\mathbf{v}_*}{m_i + m_j} - \frac{1}{kT_i}\mathbf{u}_i - \frac{1}{kT_j} \frac{m_i\mathbf{v} + m_j\mathbf{v}_*}{m_i + m_j} + \frac{1}{kT_j}\mathbf{u}_j \right) = 0,$$

for any $\mathbf{v}, \mathbf{v}_* \in \mathbb{R}^3$. Consequently,

$$\frac{m_i\mathbf{v} + m_j\mathbf{v}_*}{m_i + m_j} \left(\frac{1}{kT_i} - \frac{1}{kT_i} \right) - \left(\frac{\mathbf{u}_i}{T_i} - \frac{\mathbf{u}_j}{T_j} \right) = 0,$$

which finally yields $T_i = T_j$ and $\mathbf{u}_i = \mathbf{u}_j$.   □

3. Description of polyatomic gases

It is well known that the macroscopic internal energy of a gas consists of two parts: the part related to the translational degrees of freedom, and the part related to additional (vibrational and rotational) degrees of freedom. At equilibrium, a linear relation links the macroscopic internal energy to the temperature (hydrodynamic pressure) of a (rarefied) gas with a factor of proportionality that is related to the number of degrees of freedom D. In the monatomic case, $D = 3$, which means that molecules can move only in 3 directions in space. The main feature of polyatomic gases is the existence of additional (vibrational and rotational) degrees of freedom (for diatomic $D = 5$, for three-atomic $D = 6$) which reflects the fact that polyatomic gases have more options or liberty for motion during a collision process than monatomic gases have.

From the standpoint of continuum theories, a specificity of polyatomic gases is that the internal energy density is not directly related to the trace of the pressure tensor, as it was in the monatomic case. Indeed, the internal energy is divided into a translational part and a part related to the additional degrees of freedom. Only the translational part is related to the trace of the pressure tensor.

From the kinetic point of view, it is not an easy task to grasp all the peculiarities of polyatomic gases. One approach introduces a discrete set of internal energy levels possibly occupied by molecules. That is, one may think of a polyatomic gas as a mixture of monatomic gases, and attach to each molecule, besides a continuous variable representing its center-of-mass velocity, a discrete variable representing the internal state [40]. The approach that we consider in this thesis is the following: we build a model of collision as simple as possible between two molecules, which enables to recover at the macroscopic level a given correct equation of state for the energy. We refer to [22, 29] for this approach. We introduce one single continuous parameter $I \in \mathbb{R}_+$ for the microscopic internal energy, which becomes an additional argument of the distribution function.

The Boltzmann equation. A polyatomic rarefied gas is described by a distribution function $f \geq 0$, which depends on the usual variables: time $t \in \mathbb{R}_+$, position in the physical space $\mathbf{x} \in \mathbb{R}^N$ (in some parts we will take $N = 3$), velocity of the particle $\mathbf{v} \in \mathbb{R}^N$, but also on a microscopic internal energy $I \in \mathbb{R}_+$. Therefore, the set of variables describing the microscopic state of a particle is extended: $\boldsymbol{\xi} = (\mathbf{v}, I)$. The evolution of the distribution function $f := f(t, \mathbf{x}, \mathbf{v}, I)$ is determined by the Boltzmann equation. It reads

$$(1.49) \qquad \partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = Q(f, f).$$

The right-hand side of the Boltzmann equation, $Q(f, f)$, is a quadratic bilinear operator acting only on the velocity $\mathbf{v}$ and the internal energy I.

We will assume systematically in what follows that f tends to zero sufficiently rapidly with respect to $\mathbf{v}$ and I, and that it is smooth with respect to $t > 0$, $\mathbf{x} \in \mathbb{R}^N$.

As in the case of monatomic gases, the collision operator can be split into a gain term and a loss term

$$Q(f, f) = Q^+(f, f) - Q^-(f, f).$$

The loss term counts all collisions in which a given particle of velocity $\mathbf{v}$ and microscopic internal energy I will encounter another particle, of velocity $\mathbf{v}_*$ and internal energy I_*, and will change its velocity and internal energy, leading thus to a loss of particles of velocity $\mathbf{v}$ and internal energy I. The gain term measures the number of particles of velocity $\mathbf{v}$ and microscopic internal energy I which are created due to a collision. In order to define precisely the collision integral, some preliminary work is needed.

Introduction of a weight. A kinetic model with weight was presented in [**29, 30**] in the context of mixture of polyatomic gases with possible chemical reactions. The introduction of a weight aims at recovering a given energy law. We expose this idea in the framework of one polyatomic gas. Later on, we will extend it for mixtures of polyatomic gases, i.e. we will recall ideas from [**30**] in the context of absence of chemical reactions.

The appropriate energy law at the macroscopic level will be obtained if one defines properly the macroscopic internal energy density. As all the other macroscopic quantities, the macroscopic internal energy density is defined as a moment of the distribution function f, i.e. by means of integration of the distribution function f against some test function with respect to the variables aimed at describing the microscopic state of a gas – in this case, the velocity $\mathbf{v} \in \mathbb{R}^N$ and the microscopic internal energy $I \in \mathbb{R}_+$. Moreover, we consider weighted integrals. We define a weight as a function $\varphi(I)$ of I satisfying the condition of nonnegativity $\varphi(I) \geq 0$.

Let us announce that the weight $\varphi(I)$ will appear in the definitions of all the macroscopic quantities. Therefore when taking averages of the distribution function f, the appropriate space will be $L^1\big(\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}\big)$. In particular, the physical meaning of the distribution function is made clear by defining

$$n = \iint_{\mathbb{R}^N \times \mathbb{R}_+} f\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v},$$

as the macroscopic density n of a gas.

Our goal here is to determine a form of the weight $\varphi(I)$ which will lead to the proper classical caloric equation of state for polyatomic gases in equilibrium, which reads

$$(1.50) \qquad e|_E = \frac{1}{\gamma - 1}\,\frac{k}{m}\,T,$$

where e and T are the respective internal energy and the temperature of a gas, while γ represents the heat capacity ratio, which can be related to the number D of degrees of freedom:

$$\gamma = \frac{D + 2}{D}.$$

The appropriate values for different polyatomic gases and the corresponding form of their equation of state is presented in the Table 1.1.

molecule	value of D	value of γ	equation of state
monatomic	3	$\frac{5}{3}$	$e\vert_E = \frac{3}{2}\frac{k}{m}T$
diatomic	5	$\frac{7}{5}$	$e\vert_E = \frac{5}{2}\frac{k}{m}T$
three-atomic	6	$\frac{4}{3}$	$e\vert_E = 3\frac{k}{m}T$

TABLE 1.1. Values of number of degrees of freedom (D) and heat capacity ratio (γ) for monatomic, diatomic and three-atomic molecules with corresponding equations of state in the case $N = 3$

In order to get a form of the weight $\varphi(I)$, we must connect the equation of state (1.50) with the definition of internal energy density as a moment of the distribution function.

The internal energy density will be properly defined in Proposition 2.2. Here we only anticipate that from the standpoint of kinetic theory, internal energy density in equilibrium in space dimension $N = 3$ reads

$$(1.51) \qquad \rho\, e\vert_E = \frac{3}{2}\, n\, k\, T + n\frac{\zeta_1}{\zeta_0}, \qquad \text{with} \quad \zeta_\beta := \zeta_\beta(T) = \int_{\mathbb{R}_+} I^\beta\, \varphi(I)\, e^{-\frac{1}{kT}I}\, \mathrm{d}I.$$

Comparing to the well-known formula (1.50), we must determine $\varphi(I)$ so that

$$(1.52) \qquad \frac{\zeta_1}{\zeta_0} \propto \lambda\, k\, T,$$

where λ should be some constant. If we introduce the notation $\tau = \frac{1}{kT}$, it can be written

$$\frac{\zeta_1}{\zeta_0} = -\frac{\frac{\mathrm{d}}{\mathrm{d}\tau}\zeta_0}{\zeta_0} = -\frac{\mathrm{d}}{\mathrm{d}\tau}\log\left(\zeta_0\right).$$

Combining the last equation with (1.52), one obtains an ODE

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\log\left(\zeta_0\right) \propto -\lambda\frac{1}{\tau},$$

whose solution yields $\zeta_0 \propto \tau^{-\lambda}$. On the other side, note that ζ_0 is nothing else but the Laplace transform of $\varphi(I)$, i.e. $\zeta_0 = \mathcal{L}\left(\varphi(I)\right)$. Therefore,

$$\varphi(I) \propto \mathcal{L}^{-1}\left(\tau^{-\lambda}\right) = \frac{1}{\Gamma\left[\lambda\right]}\, I^{\lambda-1},$$

where Γ is the Gamma function. In fact, in order to remain coherent with [30], we will rather use the following simplified formula for the weight $\varphi(I)$:

$$(1.53) \qquad \varphi(I) = I^\alpha, \qquad \text{with } \alpha > -1.$$

For this choice of the weight function, one has

$$\zeta_\beta = (kT)^{\beta+1+\alpha}\Gamma\left[\beta + 1 + \alpha\right], \quad \text{and therefore} \quad \frac{\zeta_1}{\zeta_0} = (\alpha + 1)\, k\, T.$$

To conclude, we observe that for the choice $\varphi(I) = I^\alpha$, the last result in conjunction with (1.51) leads to the following form of the internal energy in equilibrium

$$(1.54) \qquad e\vert_E = \left(\alpha + \frac{5}{2}\right)\frac{k}{m}T, \qquad \text{with } \alpha > -1.$$

molecule	value of γ	value of α
diatomic	$\frac{7}{5}$	0
three-atomic	$\frac{4}{3}$	$\frac{1}{2}$

TABLE 1.2. Values of heat capacity ratio (γ) and parameter of the model (α) for some types of molecules

Comparing to the original form of the equation of state (1.50), one obtains the relation between the two coefficients γ and α:

$$\alpha = \frac{-5\,\gamma + 7}{2\,(\gamma - 1)}, \qquad \gamma = \frac{2\,\alpha + 7}{2\,\alpha + 5}.$$

For later purposes, the values for some structure of molecules are presented in the Table 1.2.

Observe that the case of a monatomic gas ($\gamma = 5/3$) cannot be recovered from the one with continuous internal energy, since the value of the parameter α in the monatomic case would violate the overall restriction $\alpha > -1$.

Collision transformation. The goal of this Section is to determine all pre-collisional microscopic quantities as functions of the post-collisional ones.

Let us analyze a collision process between two molecules. Suppose that colliding molecules have velocities $\mathbf{v}'$ and $\mathbf{v}'_*$ and internal energies I' and I'_*, respectively. Those are pre-collisional microscopic quantities. After the collision they are transformed into post-collisional quantities; velocities become $\mathbf{v}$ and $\mathbf{v}_*$, while internal energies transform to I and I_*. The conservation laws of momentum and total energy (kinetic plus internal that captures phenomena related to polyatomic gases) of a system consisting of two molecules are valid during a collision process:

$$m\mathbf{v}' + m\mathbf{v}'_* = m\mathbf{v} + m\mathbf{v}_*,$$

(1.55)

$$\tfrac{m}{2}\left|\mathbf{v}'\right|^2 + \tfrac{m}{2}\left|\mathbf{v}'_*\right|^2 + I' + I'_* = \tfrac{m}{2}\left|\mathbf{v}\right|^2 + \tfrac{m}{2}\left|\mathbf{v}_*\right|^2 + I + I_*.$$

It is convenient to pass to the reference frame of the center of mass. We apply the two body problem, which describes the motion of the particles under mutual interaction only. We introduce the velocity of the center of mass $\mathbf{G}$ and the relative velocity $\mathbf{g}$ via

(1.56)
$$\mathbf{G} = \frac{\mathbf{v} + \mathbf{v}_*}{2} \quad \text{and} \quad \mathbf{g} = \mathbf{v} - \mathbf{v}_*.$$

From the conservation law of momentum, we immediately get that the post- and pre-collisional velocities of the center of mass coincide, i.e.

(1.57)
$$\mathbf{G} = \frac{\mathbf{v}' + \mathbf{v}'_*}{2} =: \mathbf{G}'.$$

The original velocities $\mathbf{v}$ and $\mathbf{v}_*$ can be expressed in terms of the velocities in the center of mass reference frame from (1.56):

(1.58)
$$\mathbf{v} = \mathbf{G} + \tfrac{1}{2}\mathbf{g} \quad \text{and} \quad \mathbf{v}_* = \mathbf{G} - \tfrac{1}{2}\mathbf{g}.$$

Finally, substitution of (1.58) into $(1.55)_2$ yields

$$m\left|\mathbf{G}'\right|^2 + \tfrac{m}{4}\left|\mathbf{g}'\right|^2 + I' + I'_* = m\left|\mathbf{G}\right|^2 + \tfrac{m}{4}\left|\mathbf{g}\right|^2 + I + I_*,$$

where $\mathbf{g}'$ is the relative pre-collisional velocity $\mathbf{g}' := \mathbf{v}' - \mathbf{v}'_*$. Now, relation (1.57) implies that the conservation law of energy $(1.55)_2$ is satisfied if and only if

$$E := \tfrac{m}{4}\left|\mathbf{v}' - \mathbf{v}'_*\right|^2 + I' + I'_* = \tfrac{m}{4}\left|\mathbf{v} - \mathbf{v}_*\right|^2 + I + I_*.$$

To conclude, rewriting system (1.55) in the center of mass reference frame, we obtained an equivalent system

(1.59)
$$m\mathbf{v}' + m\mathbf{v}'_* = m\mathbf{v} + m\mathbf{v}_*,$$
$$E = \frac{m}{4}\left|\mathbf{v}' - \mathbf{v}'_*\right|^2 + I' + I'_* = \frac{m}{4}\left|\mathbf{v} - \mathbf{v}_*\right|^2 + I + I_*,$$

which is easier to handle.

Laws (1.59) represent the connection between post- and pre-collisional microscopic quantities. Thus, they can be seen as a system of $(N+1)$ scalar equations in $(2N+2)$ scalar unknowns. It is natural to expect that the solution of this system will be expressed in terms of $(N+1)$ parameters. To finally express post-collisional quantities in terms of pre-collisional ones, we use the so-called Borgnakke-Larsen procedure [20].

The Borgnakke-Larsen procedure. This method is based on the repartition of the total energy E. At first, the total energy E is divided into kinetic energy and microscopic internal energy. We introduce a parameter $R \in [0,1]$ in order to impose a part RE of the total energy as pre-collisional kinetic energy, and the rest $(1-R)E$ to the microscopic internal energy (of the two colliding molecules):

(1.60)
$$RE = \frac{m}{4}\left|\mathbf{v}' - \mathbf{v}'_*\right|^2,$$
$$(1-R)E = I' + I'_*.$$

Further, with the help of another parameter $r \in [0,1]$, the internal energy itself is distributed between two molecules:

(1.61)
$$I' = r(1-R)E,$$
$$I'_* = (1-r)(1-R)E.$$

For later purposes, let us introduce here the extra parameters $R' \in [0,1]$ and $r' \in [0,1]$ by the following identities

$$\frac{m}{4}\left|\mathbf{v} - \mathbf{v}_*\right|^2 = R'E, \quad I + I_* = (1-R')E, \quad I = r'(1-R')E, \quad I_* = (1-r')(1-R')E,$$

or more precisely,

(1.62)
$$R' = \frac{m}{4E}\left|\mathbf{v} - \mathbf{v}_*\right|^2,$$
$$r' = \frac{I}{I + I_*}.$$

To summarize, we obtained the pre-collisional internal energies as functions of the post-collisional quantities by introducing two parameters R and r, as expressed in equations (1.61). It remains to determine the pre-collisional velocities. This will be done by means of a parametrization of the equation (1.60) with the help of $(N-1)$ parameters. Indeed, in the $\boldsymbol{\omega}-$notation, for some unit vector $\boldsymbol{\omega} \in S^{N-1}$ we parametrize (1.60) as follows:

(1.63)
$$\mathbf{v}' - \mathbf{v}'_* = 2\sqrt{\frac{RE}{m}}\, T_{\boldsymbol{\omega}}\left[\frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|}\right],$$

where $T_{\boldsymbol{\omega}}\left[\mathbf{y}\right] = \mathbf{y} - 2\left(\boldsymbol{\omega} \cdot \mathbf{y}\right)\boldsymbol{\omega}$, for $\mathbf{y} \in \mathbb{R}^N$. Combining (1.63) and (1.55)$_1$, we obtain expressions for the pre-collisional velocities in terms of the post-collisional quantities:

(1.64)
$$\mathbf{v}' = \frac{\mathbf{v} + \mathbf{v}_*}{2} + \sqrt{\frac{RE}{m}}\, T_{\boldsymbol{\omega}}\left[\frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|}\right],$$
$$\mathbf{v}'_* = \frac{\mathbf{v} + \mathbf{v}_*}{2} - \sqrt{\frac{RE}{m}}\, T_{\boldsymbol{\omega}}\left[\frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|}\right].$$

Another possible choice consists in using the $\boldsymbol{\sigma}$- parametrization, leading to

(1.65)
$$\mathbf{v}' - \mathbf{v}'_* = 2\sqrt{\frac{RE}{m}}\,\boldsymbol{\sigma}.$$

The last equation in conjunction with $(1.59)_1$ yields formulas for the pre-collisional velocities in terms of the parameter $\boldsymbol{\sigma}$:

$$\mathbf{v}' = \frac{\mathbf{v} + \mathbf{v}_*}{2} + \sqrt{\frac{R\,E}{m}}\,\boldsymbol{\sigma},$$

$$\mathbf{v}'_* = \frac{\mathbf{v} + \mathbf{v}_*}{2} - \sqrt{\frac{R\,E}{m}}\,\boldsymbol{\sigma}.$$

The passage from one notation to another can be done by means of the change of the variables described by (1.37).

To summarize: we have introduced $(N+1)$ scalar parameters – those are $R, r, \boldsymbol{\omega}$ – with the help of which we managed to express the microscopic pre-collisional quantities in terms of the post-collisional ones. With that tool in hand, we can define the collision operator. But first, it is necessary to analyze more deeply the transformation that is defined by the collisional rules.

Collision transformation. For a fixed $\boldsymbol{\omega} \in S^{N-1}$, we define the collision transformation

$$S_{\boldsymbol{\omega}} : \mathbb{R}^{2N} \times \mathbb{R}_+^2 \times [0,1]^2 \to \mathbb{R}^{2N} \times \mathbb{R}_+^2 \times [0,1]^2$$
$$(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R) \mapsto (\mathbf{v}', \mathbf{v}'_*, I', I'_*, r', R')$$

by the relations (1.64), (1.61) and (1.62). We collect its main properties in Lemma 1.6.

LEMMA 1.6. *For any $\boldsymbol{\omega} \in S^{N-1}$, the transformation $S_{\boldsymbol{\omega}}$ is an involution of the set $\mathbb{R}^{2N} \times \mathbb{R}_+^2 \times [0,1]^2$ and its Jacobian determinant is given by*

(1.66)
$$J_{S_{\boldsymbol{\omega}}} = \frac{(1-R)}{(1-R')} \left(\frac{R}{R'} \right)^{\frac{N}{2}-1} = \frac{(1-R)}{(1-R')} \left(\frac{|\mathbf{v}' - \mathbf{v}'_*|}{|\mathbf{v} - \mathbf{v}_*|} \right)^{N-2}.$$

PROOF. In order to prove the involution property of $S_{\boldsymbol{\omega}}$, we inverse it. This leads to the following relations:

$$E = \frac{m}{4} \left| \mathbf{v}' - \mathbf{v}'_* \right|^2 + I' + I'_*,$$
$$\mathbf{v} = \frac{\mathbf{v}' + \mathbf{v}'_*}{2} + \sqrt{\frac{R'E}{m}} T_{\boldsymbol{\omega}} \left[\frac{\mathbf{v}' - \mathbf{v}'_*}{|\mathbf{v}' - \mathbf{v}'_*|} \right], \qquad \mathbf{v}_* = \frac{\mathbf{v}' + \mathbf{v}'_*}{2} - \sqrt{\frac{R'E}{m}} T_{\boldsymbol{\omega}} \left[\frac{\mathbf{v}' - \mathbf{v}'_*}{|\mathbf{v}' - \mathbf{v}'_*|} \right],$$
$$I = r'(1 - R')E, \qquad I_* = (1 - r')(1 - R')E,$$
$$r = \frac{I'}{I' + I'_*}, \qquad R = \frac{m}{4\,E} \left| \mathbf{v}' - \mathbf{v}'_* \right|^2.$$

As a consequence, the transformation $S_{\boldsymbol{\omega}}$ is an involution.

To compute the Jacobian, we first pass to the reference frame of the center of mass by changing velocities $\mathbf{v}$ and $\mathbf{v}_*$ to the relative velocity $\mathbf{g}$ and the velocity of center of mass $\mathbf{G}$, both defined in (1.56), i.e. we perform the change of variables with unit Jacobian

$$(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R) \mapsto (\mathbf{g}, \mathbf{G}, I, I_*, r, R).$$

Moreover, we pass to the spherical coordinates for the relative velocity $\mathbf{g}$:

$$(\mathbf{g}, \mathbf{G}, I, I_*, r, R) \mapsto \left(|\mathbf{g}|, \frac{\mathbf{g}}{|\mathbf{g}|}, \mathbf{G}, I, I_*, r, R \right).$$

These two transformations result in an easier computation of the Jacobian $J_{S_{\boldsymbol{\omega}}}$, which now takes the form

$$J_{S_{\boldsymbol{\omega}}} = \frac{1}{|\mathbf{g}|^{N-1}} \, J_{\left(|\mathbf{g}|, \frac{\mathbf{g}}{|\mathbf{g}|}, \mathbf{G}, I, I_*, r, R \right) \mapsto \left(|\mathbf{g}'|, \frac{\mathbf{g}'}{|\mathbf{g}'|}, \mathbf{G}', I', I'_*, r', R' \right)} |\mathbf{g}'|^{N-1},$$

the last transformations being defined by

$$\left|\mathbf{g}'\right| = 2\sqrt{\frac{R\,E}{m}}, \quad \frac{\mathbf{g}'}{\left|\mathbf{g}'\right|} = T_{\boldsymbol{\omega}}\left[\frac{\mathbf{g}}{\left|\mathbf{g}\right|}\right], \quad \mathbf{G}' = \mathbf{G},$$

$$I' = r(1-R)E, \quad I'_* = (1-r)(1-R)E, \quad r' = \frac{I}{E - \frac{m}{4}\left|\mathbf{g}\right|^2}, \quad R' = \frac{m}{4E}\left|\mathbf{g}\right|^2,$$

where $E = \frac{m}{4}\left|\mathbf{g}\right|^2 + I + I_*$. Note that the second transformation is just a rotation of the unit vector, and thus has a unit Jacobian. In addition, we can eliminate $\mathbf{G}$ from our consideration. Therefore,

$$J_{S_{\boldsymbol{\omega}}} = \left(\frac{\left|\mathbf{g}'\right|}{\left|\mathbf{g}\right|}\right)^{N-1} J_{(\left|\mathbf{g}\right|,I,I_*,r,R)\mapsto(\left|\mathbf{g}'\right|,I',I'_*,r',R')}.$$

It seems convenient to change variable I_* to E with unit Jacobian, so that

$$J_{S_{\boldsymbol{\omega}}} = \left(\frac{\left|\mathbf{g}'\right|}{\left|\mathbf{g}\right|}\right)^{N-1} J_{(\left|\mathbf{g}\right|,I,E,r,R)\mapsto(\left|\mathbf{g}'\right|,I',I'_*,r',R')}.$$

Now we expand the determinant $J_{S_{\boldsymbol{\omega}}}$ along a column containing the derivatives with respect to I, and since only the expression for r' depends on I, we easily obtain:

$$J_{S_{\boldsymbol{\omega}}} = \left(\frac{\left|\mathbf{g}'\right|}{\left|\mathbf{g}\right|}\right)^{N-1} \frac{1}{E - \frac{m}{4}\left|\mathbf{g}\right|^2} J_{(\left|\mathbf{g}\right|,E,r,R)\mapsto(\left|\mathbf{g}'\right|,I',I'_*,R')}.$$

The same strategy is used for the column containing derivatives with respect to $\left|\mathbf{g}\right|$, and noting that only R' is a function of $\left|\mathbf{g}\right|$ yields

$$J_{S_{\boldsymbol{\omega}}} = \left(\frac{\left|\mathbf{g}'\right|}{\left|\mathbf{g}\right|}\right)^{N-1} \frac{1}{E - \frac{m}{4}\left|\mathbf{g}\right|^2} \frac{m}{2E}\left|\mathbf{g}\right| J_{(E,r,R)\mapsto(\left|\mathbf{g}'\right|,I',I'_*)}.$$

At the end, we simply compute the derivatives

$$J_{S_{\boldsymbol{\omega}}} = \left(\frac{\left|\mathbf{g}'\right|}{\left|\mathbf{g}\right|}\right)^{N-1} \frac{1}{E - \frac{m}{4}\left|\mathbf{g}\right|^2} \frac{m}{2E}\left|\mathbf{g}\right| \text{Abs}\left(\begin{vmatrix} \sqrt{\frac{4R}{mE}} & 0 & \sqrt{\frac{4E}{mR}} \\ r(1-R) & (1-R)E & -rE \\ (1-r)(1-R) & -(1-R)E & -(1-r)E \end{vmatrix}\right)$$

$$= \left(\frac{\left|\mathbf{g}'\right|}{\left|\mathbf{g}\right|}\right)^{N-1} \frac{1}{E - \frac{m}{4}\left|\mathbf{g}\right|^2} \sqrt{\frac{mE}{4R}}\,(1-R)\left|\mathbf{g}\right|$$

$$= \left(\frac{\left|\mathbf{g}'\right|}{\left|\mathbf{g}\right|}\right)^{N-1} \frac{(1-R)\left|\mathbf{g}\right|}{(1-R')\left|\mathbf{g}'\right|}.$$

Then, combining expressions for $\left|\mathbf{g}'\right|$ and R', we notice that

$$\frac{\left|\mathbf{g}'\right|^2}{\left|\mathbf{g}\right|^2} = \frac{R}{R'},$$

which leads to the final expression for the Jacobian $J_{S_{\boldsymbol{\omega}}}$

$$J_{S_{\boldsymbol{\omega}}} = \frac{(1-R)}{(1-R')}\left(\frac{\left|\mathbf{g}'\right|}{\left|\mathbf{g}\right|}\right)^{N-2} = \frac{(1-R)}{(1-R')}\left(\frac{R}{R'}\right)^{\frac{N}{2}-1}.$$

$\square$

After proving this Lemma, all the preliminary work for the construction of the collision integral is done. In the sequel we define the collision operator and present its properties. Before going into details, let us mention the standard abbreviations that we use

$$f' := f\left(t,\mathbf{x},\mathbf{v}',I'\right), \quad f'_* := f\left(t,\mathbf{x},\mathbf{v}'_*,I'_*\right), \quad f_* := f\left(t,\mathbf{x},\mathbf{v}_*,I_*\right), \quad f := f\left(t,\mathbf{x},\mathbf{v},I\right).$$

Collision operator. The collision operator corresponding to the distribution function f is defined for any $t \in \mathbb{R}_+, \mathbf{x} \in \mathbb{R}^N$ by

$$(1.67) \qquad Q(f,f)(\mathbf{v}, I) = \int_\Omega \int_{S^{N-1}} \left[f' f'_* - f f_* \right] \mathcal{B} \left(1 - R \right) R^{\frac{N}{2}-1} \frac{1}{\varphi(I)} \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}r \, \mathrm{d}R \, \mathrm{d}I_* \, \mathrm{d}\mathbf{v}_*,$$

where $\Omega = \mathbb{R}^N \times \mathbb{R}_+ \times [0,1]^2$ and $\mathbf{v}'$, $\mathbf{v}'_*$, I', I'_* are defined in (1.64) and (1.61). The cross section $\mathcal{B} := \mathcal{B}(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega})$ is a nonnegative function that satisfies the microreversibility assumptions:

$$(1.68) \qquad \begin{aligned} \mathcal{B}(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega}) &= \mathcal{B}(\mathbf{v}_*, \mathbf{v}, I_*, I, 1-r, R, \boldsymbol{\omega}), \\ \mathcal{B}(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega}) &= \mathcal{B}(\mathbf{v}', \mathbf{v}'_*, I', I'_*, r', R', \boldsymbol{\omega}). \end{aligned}$$

The cross section $\mathcal{B}$ describes the nature of the microscopic interactions.

As we already mentioned, the collision operator represents the rate of change of the number of particles having velocity $\mathbf{v}$ and internal energy I. Indeed, on one side, with the sign "+" i.e. with the term $f' f'_*$, we count particles that had some other velocity and internal energy before the collision, and after the collision have velocity $\mathbf{v}$ and internal energy I. By the collisional rules, these velocity and internal energy will be created after a collision of particles having precisely velocities $\mathbf{v}'$, $\mathbf{v}'_*$ and internal energies I' and I'_* before the collision. As a byproduct, the other particle will have velocity $\mathbf{v}_*$ and internal energy I_* after the collision. That is why the "prime" quantities are called pre-collisionals. On the other side, the term with the "-" sign, i.e. the term $f f_*$, counts particles that loose velocity $\mathbf{v}$ and internal energy I, which happens when a collision occurs with some other particle of velocity $\mathbf{v}_*$ and internal energy I_*.

Weak form of the collision operator.

PROPOSITION 1.7. *Let $\psi : \mathbb{R}^N \times \mathbb{R}_+ \to \mathbb{R}$ be function of the velocity $\mathbf{v}$ and microscopic internal energy I, such that the integral*

$$\iint_{\mathbb{R}^N \times \mathbb{R}_+} Q(f,f)(\mathbf{v}, I) \, \psi(\mathbf{v}, I) \, \varphi(I) \, \mathrm{d}\mathbf{v} \, \mathrm{d}I$$

makes sense. Then, the following holds

$$(1.69) \qquad \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q(f,f)(\mathbf{v}, I) \, \psi(\mathbf{v}, I) \, \varphi(I) \, \mathrm{d}\mathbf{v} \, \mathrm{d}I$$

$$= -\frac{1}{4} \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_\Omega \int_{S^{N-1}} \left[f' f'_* - f f_* \right] \times \left[\psi(\mathbf{v}', I') + \psi(\mathbf{v}'_*, I'_*) - \psi(\mathbf{v}, I) - \psi(\mathbf{v}_*, I_*) \right]$$

$$\times \mathcal{B}(1-R) R^{\frac{N}{2}-1} \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}r \, \mathrm{d}R \, \mathrm{d}I_* \, \mathrm{d}\mathbf{v}_* \, \mathrm{d}I \, \mathrm{d}\mathbf{v}.$$

PROOF. The proof of this Proposition relies on the application of Lemma 1.6. Indeed, we first write the full expression

$$(1.70) \qquad \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q(f,f)(\mathbf{v}, I) \, \psi(\mathbf{v}, I) \, \varphi(I) \, \mathrm{d}\mathbf{v} \, \mathrm{d}I$$

$$= \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_\Omega \int_{S^{N-1}} \left[f' f'_* - f f_* \right] \psi(\mathbf{v}, I) \, \mathcal{B}(1-R) R^{\frac{N}{2}-1} \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}r \, \mathrm{d}R \, \mathrm{d}I_* \, \mathrm{d}\mathbf{v}_* \, \mathrm{d}I \, \mathrm{d}\mathbf{v}.$$

Then we perform the change of variables (for $\boldsymbol{\omega} \in S^{N-1}$ fixed)

$$(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R) \mapsto (\mathbf{v}', \mathbf{v}'_*, I', I'_*, r', R').$$

Using the invariant properties of the cross section (1.68) and Lemma 1.6, we obtain

$$(1.71) \qquad \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q(f,f)(\mathbf{v}, I) \, \psi(\mathbf{v}, I) \, \varphi(I) \, \mathrm{d}\mathbf{v} \, \mathrm{d}I$$

$$= \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_\Omega \int_{S^{N-1}} \left[f f_* - f' f'_* \right] \psi(\mathbf{v}', I') \, \mathcal{B}(1-R) R^{\frac{N}{2}-1} \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}r \, \mathrm{d}R \, \mathrm{d}I_* \, \mathrm{d}\mathbf{v}_* \, \mathrm{d}I \, \mathrm{d}\mathbf{v}.$$

Further, we mimic the interchange of particles by means of the change of variables

$$(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R) \mapsto (\mathbf{v}_*, \mathbf{v}, I_*, I, 1 - r, R), \quad \text{for } \boldsymbol{\omega} \in S^{N-1} \text{ fixed,}$$

first in the integral (1.70), and then in (1.71). Again, using the invariant properties of the cross section (1.68), we get

$$(1.72) \quad \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q(f, f)(\mathbf{v}, I)\, \psi(\mathbf{v}, I)\, \varphi(I)\, \mathrm{d}\mathbf{v}\, \mathrm{d}I$$

$$= \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_{\Omega} \int_{S^{N-1}} \left[f' f'_* - f f_* \right] \psi(\mathbf{v}_*, I_*)\, \mathcal{B}\,(1 - R)\, R^{\frac{N}{2}-1}\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}r\, \mathrm{d}R\, \mathrm{d}I_*\, \mathrm{d}\mathbf{v}_*\, \mathrm{d}I\, \mathrm{d}\mathbf{v},$$

and

$$(1.73) \quad \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q(f, f)(\mathbf{v}, I)\, \psi(\mathbf{v}, I)\, \varphi(I)\, \mathrm{d}\mathbf{v}\, \mathrm{d}I$$

$$= \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_{\Omega} \int_{S^{N-1}} \left[f f_* - f' f'_* \right] \psi(\mathbf{v}'_*, I'_*)\, \mathcal{B}\,(1 - R)\, R^{\frac{N}{2}-1}\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}r\, \mathrm{d}R\, \mathrm{d}I_*\, \mathrm{d}\mathbf{v}_*\, \mathrm{d}I\, \mathrm{d}\mathbf{v}.$$

Finally, summation of all four expressions (1.70), (1.71), (1.72) and (1.73) yields the result.   □

In the sequel, we investigate when the weak form of the collision operator (1.69) is equal to zero, which amounts to looking for the collision invariants.

Collision invariants. We call a function ψ a *collision invariant* if it satisfies the functional equation

$$(1.74) \quad \forall\, (\mathbf{v}, \mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega}) \in \mathbb{R}^{2N} \times \mathbb{R}_+^2 \times [0,1]^2 \times S^{N-1}, \quad \psi(\mathbf{v}, I) + \psi(\mathbf{v}_*, I_*) = \psi(\mathbf{v}', I') + \psi(\mathbf{v}'_*, I'_*).$$

The following Proposition shows that the collision invariants are precisely quantities invariant during a collision – that is the functions whose invariant property can be seen on the microscopic conservation laws (1.55).

PROPOSITION 1.8. *The collision invariants belonging to L^1_{loc} are linear combinations of the following $(N + 2)$ functions:*

$$(1.75) \qquad\qquad \boldsymbol{\psi}(\mathbf{v}, I) = \begin{pmatrix} 1 \\ m\mathbf{v} \\ \frac{m}{2}\,|\mathbf{v}|^2 + I \end{pmatrix}.$$

PROOF. The proof relies on the proof for collisional invariants in the case of a monatomic gas described in Proposition 1.2. Indeed, we look for a function $\psi(\mathbf{v}, I)$ such that (1.74) holds. The collisional rules (1.55) yield

$$(1.76) \qquad\qquad \psi(\mathbf{v}, I) + \psi(\mathbf{v}_*, I_*) = \phi(\mathbf{v} + \mathbf{v}_*, \tfrac{m}{2}\,|\mathbf{v}|^2 + \tfrac{m}{2}\,|\mathbf{v}_*|^2 + I + I_*),$$

for some function ϕ. We use again the operator $D_{k\ell}$ introduced in (1.15), that is

$$D_{k\ell} = (v_k - v_{*k})\,(\partial_{v_\ell} - \partial_{v_{*\ell}}) - (v_\ell - v_{*\ell})\,(\partial_{v_k} - \partial_{v_{*k}}).$$

Proceeding as in the proof of Proposition 1.2, we obtain

$$\partial_{k^2}^2 \psi(\mathbf{v}, I) = \text{const}, \qquad \partial_{k\ell}^2 \psi(\mathbf{v}, I) = 0,$$

which ensures that ψ is a polynomial of degree 2 with respect to the velocity variable, more precisely

$$(1.77) \qquad\qquad \psi(\mathbf{v}, I) = a(I) + \mathbf{b}(I) \cdot \mathbf{v} + c(I)\tfrac{m}{2}\,|\mathbf{v}|^2.$$

In order to make clear the dependence of $\psi(\mathbf{v}, I)$ with respect to I, we apply the operator $\partial_I - \partial_{I_*}$ on identity (1.76), and get

$$\partial_I \psi(\mathbf{v}, I) - \partial_{I_*} \psi(\mathbf{v}_*, I_*) = 0.$$

Now, using the form (1.77), we obtain

$$a'(I) + \mathbf{b}'(I) \cdot \mathbf{v} + c'(I)\tfrac{m}{2}\,|\mathbf{v}|^2 = a'(I_*) + \mathbf{b}'(I_*) \cdot \mathbf{v}_* + c'(I_*)\tfrac{m}{2}\,|\mathbf{v}_*|^2.$$

This identity can hold only if

$$a'(I) = \text{const}, \quad \mathbf{b}'(I) = 0 \quad \text{and} \quad c'(I) = 0,$$

which implies that a is an affine function of I and $\mathbf{b}$, c are pure constants. Inserting this function into (1.77), the required form of the collision invariants is obtained:

$$\psi(\mathbf{v}, I) = \mathbf{c} \cdot \boldsymbol{\psi}(\mathbf{v}, I),$$

for some constant vector $\mathbf{c} \in \mathbb{R}^{N+2}$.

As in the monoatomic case, the differential operators are taken in the sense of distributions in the computation above. $\qquad \square$

According to Proposition 1.7, for any f such that the integrals converge, the following holds

$$(1.78) \qquad \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q(f, f)(\mathbf{v}, I) \begin{pmatrix} 1 \\ m\mathbf{v} \\ \frac{m}{2}|\mathbf{v}|^2 + I \end{pmatrix} \varphi(I)\, dI\, d\mathbf{v} = 0.$$

$H-$**theorem.** The microscopic model described by the collision transformation $S_{\boldsymbol{\omega}}$ is time reversible. Indeed, suppose that there are two particles of velocities $\mathbf{v}'$, $\mathbf{v}'_*$ and internal energies I', I'_* at some time t_0, that are going to collide. After the collision, at some time $t_0 + \Delta t$, their state is precisely $S_{\boldsymbol{\omega}}(\mathbf{v}', \mathbf{v}'_*, I', I'_*, r', R') = (\mathbf{v}, \mathbf{v}_*, I, I_*, r, R)$. If we change the sign of the velocities, i.e. if we consider particles of velocities $-\mathbf{v}$, $-\mathbf{v}_*$ and internal energies I, I_* at the time $t_0 + \Delta t$, then they will collide, and at the time $t_0 + 2\Delta t$, their state will be $S_{\boldsymbol{\omega}}(-\mathbf{v}, -\mathbf{v}_*, I, I_*, r, R) = (-\mathbf{v}', -\mathbf{v}'_*, I', I'_*, r', R'_*)$. Therefore, if the sign of the velocities of the particles is changed, the system passes in the reverse direction through the same sequence of states which it went through in the forward direction (there will be a change only in the sign of the velocities).

We now introduce the entropy production functional, whose explicit form is given by

$$D(f) := \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q(f, f)(\mathbf{v}, I)\, (\log f(\mathbf{v}, I))\, \varphi(I)\, dI\, d\mathbf{v}.$$

It is well defined when f is nonnegative and satisfies some suitable assumptions of regularity, lower bound, and decay at infinity. The following properties hold.

PROPOSITION 1.9. *Assume that the cross section $\mathcal{B}$ is positive almost everywhere and that $f \geq 0$ is such that both the collisional integral Q and the entropy production D are well defined. Then*

(a) *The entropy production is non-positive, i.e.*

$$D(f) \leq 0.$$

(b) *Moreover, the three following properties are equivalent.*
    i. *For any $\mathbf{v} \in \mathbb{R}^N$, $I \in \mathbb{R}_+$*

$$Q(f, f)(\mathbf{v}, I) = 0.$$

    ii. *The entropy production vanishes, that is*

$$D(f) = 0.$$

    iii. *There exist $n > 0$, $T > 0$ and $\mathbf{u} \in \mathbb{R}^N$ such that*

$$f(\mathbf{v}, I) = \frac{n}{\zeta_0(T)} \left(\frac{m}{2\pi k T}\right)^{N/2} e^{-\frac{1}{kT}\left(\frac{m}{2}|\mathbf{v} - \mathbf{u}|^2 + I\right)},$$

where $\zeta_0(T)$ is given by (1.51):

$$\zeta_0(T) = \int_{\mathbb{R}_+} \varphi(I)\, e^{-\frac{1}{kT}I}\, dI.$$

PROOF. To prove statement (a), let us consider a weak form of the collisional operator for the choice $\log f$ for test function. Then (1.69) implies

$$(1.79) \quad D(f) = -\frac{1}{4} \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_{\Omega} \int_{S^{N-1}} \left[f' f'_* - f f_*\right] \times \left[\log\left(f' f'_*\right) - \log\left(f f_*\right)\right]$$

$$\times \mathcal{B}\, (1 - R)\, R^{\frac{N}{2} - 1}\, d\boldsymbol{\omega}\, dr\, dR\, dI_*\, d\mathbf{v}_*\, dI\, d\mathbf{v}.$$

Note that for $x, y \in \mathbb{R}_+$ the function $(x, y) \mapsto (x - y)(\log x - \log y)$ is nonnegative. Since all other functions under the integral are nonnegative on theirs domains, the non-positivity of the entropy production $D(f)$ follows.

As regards the second part of the theorem, note that the following implications are straightforward: (i $\Rightarrow$ ii) and (iii $\Rightarrow$ i). Let us now show (ii $\Rightarrow$ iii). Suppose that ii) holds, i.e. $D(f) = 0$. From the full expression for $D(f)$, already written in (1.79), $\log f$ is a collisional invariant. Then, Proposition 1.8 implies that $\log f$ is a linear combination of $1, mv_k, \frac{m}{2}|\mathbf{v}|^2 + I$, for $k = 1, \ldots, N$, i.e. there exists $A_0, A_1, \ldots, A_N, A_{N+1}$, all constants, such that

$$f = e^{A_0 + mA_1 v_1 + \cdots + mA_N v_N + A_{N+1}\left(\frac{m}{2}|\mathbf{v}|^2 + I\right)}.$$

For the choice

$$A_0 = \ln\left(\frac{n}{\zeta_0(T)}\left(\frac{m}{2\pi k T}\right)^{N/2}\right) - \frac{m}{2kT}|\mathbf{u}|^2,$$

$$A_i = \frac{1}{kT}u_i, \quad 1 \leq i \leq N,$$

$$A_{N+1} = -\frac{1}{kT},$$

where n and T are chosen to be positive, and $\mathbf{u} \in \mathbb{R}^N$, the required form of the equilibrium distribution function is obtained. $\qquad\square$

Let us point out an important detail. The necessary condition for $Q(f, f) = 0$ to hold is that f is the local Maxwellian distribution function, i.e. that f takes the following shape

$$(1.80) \qquad f_E(t, \mathbf{x}, \mathbf{v}, I) = \frac{n(t, \mathbf{x})}{\zeta_0(T(t, \mathbf{x}))}\left(\frac{m}{2\pi k T(t, \mathbf{x})}\right)^{N/2} e^{-\frac{1}{k T(t, \mathbf{x})}\left(\frac{m}{2}|\mathbf{v} - \mathbf{u}(t, \mathbf{x})|^2 + I\right)},$$

where the quantities $n, T, \mathbf{u}$ are allowed to depend on time t and space position $\mathbf{x}$. For this distribution function, the gas is in equilibrium with respect to the velocity and microscopic internal energy, but not with respect to the time and position variables.

Although the local Maxwellian (1.80) makes the entropy vanish regardless the form of $n(t, \mathbf{x})$, $T(t, \mathbf{x})$, $\mathbf{u}(t, \mathbf{x})$, it does not in general provide a solution to the Boltzmann equation. Indeed, the left-hand side of the Boltzmann equation imposes conditions on the change of the hydrodynamic quantities with respect to t and $\mathbf{x}$.

Macroscopic conservation laws. We multiply the Boltzmann equation by some function of the microscopic state of particles, say $\psi(\mathbf{v}, I)$, and integrate (with the weight $\varphi(I)$!) over all possible values of the microscopic states ($\mathbf{v} \in \mathbb{R}^N, I \in \mathbb{R}_+$). Similarly to the monatomic case, interchange of the order of the integration and differentiation leads to the general moment equation:

$$(1.81) \quad \partial_t \iint_{\mathbb{R}^N \times \mathbb{R}_+} f\psi(\mathbf{v}, I)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v} + \nabla_\mathbf{x} \cdot \iint_{\mathbb{R}^N \times \mathbb{R}_+} f\,\mathbf{v}\,\psi(\mathbf{v}, I)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}$$

$$= \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q(f, f)(\mathbf{v}, I)\,\psi(\mathbf{v}, I)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}.$$

In order to identify this general equation with some well-known physical laws, let us define the macroscopic quantities appearing in the theory of polyatomic gases.

Definition of macroscopic quantities. We recall the definition of the macroscopic density

$$n = \iint_{\mathbb{R}^N \times \mathbb{R}_+} f\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v},$$

or mass density

$$(1.82) \qquad \rho = \iint_{\mathbb{R}^N \times \mathbb{R}_+} m\,f\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v} = m\,n.$$

The momentum density of a gas is obtained by means of integration against velocity $\mathbf{v}$

$$\rho\,\mathbf{u} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} m\,\mathbf{v}\,f\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v},$$

where $\mathbf{u}$ represents the macroscopic velocity of the gas.

The total energy density is defined as the integral against the energy collision invariant $\frac{m}{2}\,|\mathbf{v}|^2 + I$:

$$(1.83) \qquad \text{total energy density} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} \left(\tfrac{m}{2}\,|\mathbf{v}|^2 + I\right) f\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}.$$

Classically, the total energy density is split into the kinetic and internal energy density. In the case of polyatomic gases, the internal energy density $\rho\,e$ is further divided into the translational part $\rho\,e_T$ and the part related to the internal degrees of freedom $\rho\,e_I$. This splitting is followed by the decomposition of the energy collision invariant. Indeed, if we introduce the peculiar velocity $\mathbf{c}$ with respect to the macroscopic velocity $\mathbf{u}$ by the relation $\mathbf{c} = \mathbf{v} - \mathbf{u}$, then we can rewrite the energy collision invariant as follows

$$\tfrac{m}{2}\,|\mathbf{v}|^2 + I = \tfrac{m}{2}\,|\mathbf{u}|^2 + m\,\mathbf{u}\cdot\mathbf{c} + \tfrac{m}{2}\,|\mathbf{c}|^2 + I.$$

Substitution of this decomposition into (1.83) in conjunction with (1.82) yields the decomposition of the total macroscopic energy density itself:

$$\text{total energy density} = \tfrac{1}{2}\,\rho\,|\mathbf{u}|^2 + \rho e,$$

where $\frac{1}{2}\rho\,|\mathbf{u}|^2$ is the kinetic energy of the gas and ρe is the macroscopic internal energy density that is additionally decomposed:

$$(1.84) \qquad \rho e = \iint_{\mathbb{R}^N \times \mathbb{R}_+} \left(\tfrac{m}{2}\,|\mathbf{c}|^2 + I\right) f\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v} = \rho\,e_T + \rho\,e_I.$$

The translational part of the macroscopic internal energy density is defined as the polyatomic version (in the sense that we just have additional integration with respect to I) of the internal energy density in the monatomic case:

$$(1.85) \qquad \rho\,e_T = \iint_{\mathbb{R}^N \times \mathbb{R}_+} \tfrac{m}{2}\,|\mathbf{c}|^2 f\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v},$$

while the part related to the internal degrees of freedom defined as

$$(1.86) \qquad \rho\,e_I = \iint_{\mathbb{R}^N \times \mathbb{R}_+} I f\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}$$

captures the specific properties of polyatomic gases.

One can then decompose the momentum flux:

$$\text{momentum flux} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} v_i\,v_j\,f\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v} = \rho\,u_i\,u_j + p_{ij},$$

where p_{ij} is $ij-$th element of pressure tensor defined by

$$(1.87) \qquad p_{ij} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} m\,c_i\,c_j\,f\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}.$$

Comparing (1.85) and (1.87), the following difference with respect to the monatomic gases can be immediately noticed: the internal energy density of a gas ρe is not anymore equal to one half of the trace of the pressure tensor p_{ij}. Namely, in the case of polyatomic gases, only the translational part of the internal energy density ρe_T given by (1.85) is related to the trace of the pressure tensor:

$$\rho e_T = \frac{1}{2}\left(p_{11} + p_{22} + \cdots + p_{NN}\right).$$

Furthermore, the pressure tensor can be divided into the equilibrium and non-equilibrium part with the help of the local equilibrium distribution function (1.80):

$$(1.88) \qquad p_{ij} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} m\,c_i\,c_j\,f_E\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v} + \iint_{\mathbb{R}^N \times \mathbb{R}_+} m\,c_i\,c_j\,(f - f_E)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}.$$

Defining the hydrodynamic pressure p and the non-equilibrium part σ_{ij} of the pressure tensor by

$$(1.89) \qquad p = \tfrac{1}{N} \iint_{\mathbb{R}^N \times \mathbb{R}_+} m \, |\mathbf{c}|^2 \, f_E \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}, \quad \sigma_{ij} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} m \, c_i \, c_j \, (f - f_E) \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v},$$

the splitting of the pressure tensor (1.88) can be rewritten:

$$(1.90) \qquad\qquad\qquad\qquad\qquad p_{ij} = p \, \delta_{ij} + \sigma_{ij},$$

where δ_{ij} is Kronecker symbol. Moreover, we can write σ_{ij} in the following form

$$\sigma_{ij} = \Pi \, \delta_{ij} + p_{\langle ij \rangle},$$

where $p_{\langle ij \rangle}$ is a traceless part of the pressure tensor and Π is the so-called dynamic pressure defined by

$$(1.91) \qquad\qquad\qquad\qquad \Pi = \tfrac{1}{N} \iint_{\mathbb{R}^N \times \mathbb{R}_+} m \, |\mathbf{c}|^2 \, (f - f_E) \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}.$$

Finally, the pressure tensor is structured as follows

$$(1.92) \qquad\qquad\qquad\qquad\qquad p_{ij} = (p + \Pi) \, \delta_{ij} + p_{\langle ij \rangle}.$$

Comparing definitions (1.85) and $(1.89)_1$, one more difference between polyatomic and monatomic gases can be noticed: in the case of a polyatomic gas, only a part of the internal energy density (namely, the translational part) is related to the the hydrodynamic pressure

$$(1.93) \qquad\qquad\qquad\qquad\qquad \rho \, e_T|_E = \tfrac{N}{2} p,$$

and this only happens in equilibrium. Moreover, defining temperature with

$$T = \frac{1}{N} \frac{1}{k} \frac{\iint_{\mathbb{R}^N \times \mathbb{R}_+} m \, |\mathbf{c}|^2 \, f_E \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}}{\iint_{\mathbb{R}^N \times \mathbb{R}_+} f \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}},$$

the equation of state can be recovered:

$$(1.94) \qquad\qquad\qquad\qquad\qquad p = n \, k \, T.$$

Finally, the energy flux is decomposed as

$$(1.95) \quad \text{energy flux} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} \left(\tfrac{m}{2} \, |\mathbf{v}|^2 + I \right) v_j \, f \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v} = \left(\tfrac{1}{2} \rho \, |\mathbf{u}|^2 + \rho \, e \right) u_j + \sum_{i=1}^{N} p_{ij} u_i + q_j,$$

where the heat flux $\mathbf{q}$ is defined by

$$q_j = \iint_{\mathbb{R}^N \times \mathbb{R}_+} \left(\tfrac{m}{2} \, |\mathbf{c}|^2 + I \right) c_j \, f \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}, \qquad j = 1, \dots, N.$$

Having in mind all these definitions, the next question which arises is the determination of the identities that the quantities defined above satisfy.

Local macroscopic conservation laws. Using the definitions of the macroscopic quantities given above, (1.81) and (1.78), we can derive macroscopic identities for these quantities that will be valid for any solution of the Boltzmann equation.

PROPOSITION 1.10. *Let f be a solution of the Boltzmann equation (1.49) that is rapidly decaying with respect to $(\mathbf{v}, I)$, and smooth with respect to $(t, \mathbf{x})$. Then the following local conservation laws hold:*

$$\partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho \, \mathbf{u}) = 0,$$

$$\partial_t \rho u_i + \sum_{j=1}^{N} \partial_{x_j} (\rho u_i u_j + p_{ij}) = 0, \; i = 1, \dots, N,$$

(1.96)

$$\partial_t \left(\tfrac{1}{2} \, \rho \, |\mathbf{u}|^2 + \rho \, e \right) + \sum_{j=1}^{N} \partial_{x_j} \left(\left(\tfrac{1}{2} \, \rho \, |\mathbf{u}|^2 + \rho \, e \right) u_j + \sum_{i=1}^{N} p_{ij} u_i + q_j \right) = 0.$$

Those are respectively the local conservation of mass, momentum and total energy density of a polyatomic gas.

The entropy law. One of the consequences of the $H-$theorem is the entropy law. Let us define the entropy and the entropy flux by

$$(1.97) \qquad \eta = \iint_{\mathbb{R}^N \times \mathbb{R}_+} f \log f \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}, \qquad \eta_j = \iint_{\mathbb{R}^N \times \mathbb{R}_+} v_j \, f \log f \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}, \ 1 \leq j \leq N.$$

Then, the integration of the Boltzmann equation against the test function $\log f$ in conjunction with Proposition 1.9 (a) yields the entropy law (valid when f and $\log f$ are rapidly decaying with respect to $(\mathbf{v}, I)$ and smooth with respect to $(t, \mathbf{x})$)

$$\partial_t \eta + \sum_{j=1}^N \partial_{x_j} \eta_j \leq 0.$$

4. Description of mixtures of polyatomic gases

Mixture of polyatomic gases are considered in this thesis in Chapter 3. We wish to describe a mixture of s species – namely species $\mathcal{A}_i$, $1 \leq i \leq s$ – thanks to the introduction of s different distribution functions, in such a way that each distribution function f_i describes the species $\mathcal{A}_i$, $1 \leq i \leq s$.

The constitution of a kinetic model for such a mixture requires ideas from the previous Section. Indeed, we capture additional degrees of freedom with one continuous parameter, that is the microscopic internal energy $I \in \mathbb{R}_+$. The derivation of the correct equation of state for each species can be achieved through the introduction of a suitable weight $\varphi_i(I)$ (which can be different for each species) appearing in the integration with respect to the microscopic state of the particles.

The distribution function f_i describes the species $\mathcal{A}_i$, $1 \leq i \leq s$. It is supposed to be a non-negative function that depends on the usual variables, time $t > 0$ and space position $\mathbf{x} \in \mathbb{R}^N$, the velocity $\mathbf{v} \in \mathbb{R}^N$ of a particle, together with its microscopic internal energy $I \in \mathbb{R}_+$. Any change in the $i-$th distribution function along the trajectory of a particle in phase space is due to collisions both with molecules of the same kind, and with molecules of the other species. Therefore, the collision integral in (1.49) should be replaced by a sum of similar integrals, each of which takes into account the collisions of the molecules of the species $\mathcal{A}_i$ with molecules of the species $\mathcal{A}_j$ (including $i = j$):

$$(1.98) \qquad \partial_t f_i + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = \sum_{j=1}^s Q_{ij}(f_i, f_j)(\mathbf{v}, I), \quad 1 \leq i \leq s.$$

Thus, the change of state of an $s-$component mixture is described by a system of s equations for the s distribution functions f_i, $1 \leq i \leq s$.

In order to provide formulas for the collisional operator Q_{ij}, we perform an analysis at the level of two colliding particles.

The microscopic model. Let us consider two colliding molecules of the species $\mathcal{A}_i$ and $\mathcal{A}_j$, $1 \leq i, j \leq s$, with masses m_i and m_j. Suppose that their pre-collisional velocities are $\mathbf{v}'$ and $\mathbf{v}'_*$ and internal energies I' and I'_*, respectively. Since we exclude chemical reactions, after collision, molecules belong to the same species, and their masses are unchanged. Velocities become $\mathbf{v}$ and $\mathbf{v}_*$, while internal energies transform to I and I_*. During that collision process, conservation laws of momentum and total energy – that consists of kinetic plus microscopic internal energy of particles – remain valid:

$$(1.99) \qquad m_i \mathbf{v} + m_j \mathbf{v}_* = m_i \mathbf{v}' + m_j \mathbf{v}'_*,$$
$$\frac{m_i}{2} |\mathbf{v}|^2 + \frac{m_j}{2} |\mathbf{v}_*|^2 + I + I_* = \frac{m_i}{2} |\mathbf{v}'|^2 + \frac{m_j}{2} |\mathbf{v}'_*|^2 + I' + I'_*.$$

We pass to the reference frame of the center of mass by means of introducing the velocity of the center of mass $\mathbf{G}$ and the relative velocity $\mathbf{g}$:

$$\mathbf{G} = \frac{m_i \mathbf{v} + m_j \mathbf{v}_*}{m_i + m_j} \quad \text{and} \quad \mathbf{g} = \mathbf{v} - \mathbf{v}_*.$$

Then system (1.99) is equivalent to the system

$$m_i \mathbf{v} + m_j \mathbf{v}_* = m_i \mathbf{v}' + m_j \mathbf{v}'_*,$$

(1.100)

$$E := \frac{\mu_{ij}}{2} |\mathbf{v} - \mathbf{v}_*|^2 + I + I_* = \frac{\mu_{ij}}{2} |\mathbf{v}' - \mathbf{v}'_*|^2 + I' + I'_*.$$

This system consists of $(N+1)$ scalar equations in $(2N+2)$ scalar unknowns $(\mathbf{v}', \mathbf{v}'_*, I', I'_*)$, and its solution will be expressed in terms of $N+1$ scalar parameters – those will be $R, r \in [0,1]$ and a unit vector of the sphere S^{N-1}. More precisely, we use again the Borgnakke-Larsen procedure in order to express the pre-collisional quantities in terms of the post-collisional ones. In $\boldsymbol{\omega}$−notation, it yields

$$\mathbf{v}' = \frac{m_i \mathbf{v} + m_j \mathbf{v}_*}{m_i + m_j} + \frac{m_j}{m_i + m_j} \sqrt{\frac{2\,RE}{\mu_{ij}}} \, T_{\boldsymbol{\omega}} \left[\frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|} \right],$$

$$\mathbf{v}'_* = \frac{m_i \mathbf{v} + m_j \mathbf{v}_*}{m_i + m_j} - \frac{m_i}{m_i + m_j} \sqrt{\frac{2\,RE}{\mu_{ij}}} \, T_{\boldsymbol{\omega}} \left[\frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|} \right],$$

(1.101)

$$I' = r(1-R)E,$$

$$I'_* = (1-r)(1-R)E,$$

$$R' = \frac{\mu_{ij}}{2E} |\mathbf{v} - \mathbf{v}_*|^2,$$

$$r' = \frac{I}{I + I_*},$$

where $T_{\boldsymbol{\omega}} \mathbf{z} = \mathbf{z} - 2\,(\boldsymbol{\omega} \cdot \mathbf{z})\,\boldsymbol{\omega}, \, \forall \mathbf{z} \in \mathbb{R}^N$. Alternatively, $\mathbf{v}'$ and $\mathbf{v}'_*$ could be expressed in terms of a vector $\boldsymbol{\sigma} \in S^{N-1}$ in the following manner

$$\mathbf{v}' = \frac{m_i \mathbf{v} + m_j \mathbf{v}_*}{m_i + m_j} + \frac{m_j}{m_i + m_j} \sqrt{\frac{2\,RE}{\mu_{ij}}} \, \boldsymbol{\sigma}, \qquad \mathbf{v}'_* = \frac{m_i \mathbf{v} + m_j \mathbf{v}_*}{m_i + m_j} - \frac{m_i}{m_i + m_j} \sqrt{\frac{2\,RE}{\mu_{ij}}} \, \boldsymbol{\sigma}.$$

It is easy to pass from one notation to the other one by means of the change of variables $\boldsymbol{\sigma} = T_{\boldsymbol{\omega}} \mathbf{z}, \, \forall \mathbf{z} \in \mathbb{R}^N$, as described by (1.34).

Lemma 1.11 collects properties of the collision transformation in $\boldsymbol{\omega}$−notation.

LEMMA 1.11. *For any* $\boldsymbol{\omega} \in S^{N-1}$, *the transformation* $(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R) \mapsto (\mathbf{v}', \mathbf{v}'_*, I', I'_*, r', R')$ *given by the relation* (1.101) *is an involution of the set* $\mathbb{R}^{2N} \times \mathbb{R}_+^2 \times [0,1]^2$ *and its Jacobian determinant is*

(1.102) $$J_{(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R) \mapsto (\mathbf{v}', \mathbf{v}'_*, I', I'_*, r', R')} = \frac{(1-R)}{(1-R')} \left(\frac{R}{R'} \right)^{\frac{N}{2}-1} = \frac{(1-R)}{(1-R')} \left(\frac{|\mathbf{v}' - \mathbf{v}'_*|}{|\mathbf{v} - \mathbf{v}_*|} \right)^{N-2}.$$

The proof of this Lemma will be omitted, since it is completely analogous to the proof of Lemma 1.6. It can be found in [**30**].

Collision operators and their weak forms. Let $1 \leq i, j \leq s$. The collision operator associated to species $\mathcal{A}_i$ and $\mathcal{A}_j$ is defined for any $t \in \mathbb{R}_+, \mathbf{x} \in \mathbb{R}^N$ by

(1.103) $$Q_{ij}(f,g)(\mathbf{v}, I) = \int_\Omega \int_{S^{N-1}} \left[f' g'_* - f g_* \right] \mathcal{B}_{ij}\,(1-R)\,R^{\frac{N}{2}-1} \frac{1}{\varphi_i(I)} \, \mathrm{d}\omega\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{v}_*,$$

where $\mathbf{v}'$, $\mathbf{v}'_*$, I' and I'_* are defined by (1.101), $\Omega = \mathbb{R} \times \mathbb{R}_+ \times [0,1]^2$, and $f, g : \mathbb{R}^N \times \mathbb{R}_+ \to \mathbb{R}$ are two functions. The cross section $\mathcal{B}_{ij} := \mathcal{B}_{ij}(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega})$ is supposed to satisfy the microreversibility assumptions:

(1.104)

$$\mathcal{B}_{ij}(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega}) = \mathcal{B}_{ji}(\mathbf{v}_*, \mathbf{v}, I_*, I, 1-r, R, \boldsymbol{\omega}),$$

$$\mathcal{B}_{ij}(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega}) = \mathcal{B}_{ij}(\mathbf{v}', \mathbf{v}'_*, I', I'_*, r', R', \boldsymbol{\omega}).$$

In the sequel we describe the weak forms of collision integrals. Because of the presence of different species, two different weak formulations are presented.

PROPOSITION 1.12. *Let* $\psi_i : \mathbb{R}^N \times \mathbb{R}_+ \to \mathbb{R}$ *be functions such that the integrals*

$$\iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ij}\left(f,g\right)\left(\mathbf{v},I\right)\psi_i\left(\mathbf{v},I\right)\varphi_i\left(I\right)\mathrm{d}\mathbf{v}\,\mathrm{d}I \ and \ \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ji}\left(g,f\right)\left(\mathbf{v},I\right)\psi_j\left(\mathbf{v},I\right)\varphi_j\left(I\right)\mathrm{d}\mathbf{v}\,\mathrm{d}I$$

make sense. Then, the following holds

$$(1.105) \quad \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ij}\left(f,g\right)\left(\mathbf{v},I\right)\psi_i\left(\mathbf{v},I\right)\varphi_i\left(I\right)\mathrm{d}\mathbf{v}\,\mathrm{d}I$$

$$= -\frac{1}{2}\iint_{\mathbb{R}^N \times \mathbb{R}_+}\int_\Omega\int_{S^2}\left[f'g'_* - fg_*\right]\times\left[\psi_i\left(\mathbf{v}',I'\right) - \psi_i\left(\mathbf{v},I\right)\right]\mathcal{B}_{ij}\left(1-R\right)R^{\frac{N}{2}-1}\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{v}_*\,\mathrm{d}I\,\mathrm{d}\mathbf{v},$$

and

$$(1.106)$$
$$\iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ij}\left(f,g\right)\left(\mathbf{v},I\right)\psi_i\left(\mathbf{v},I\right)\varphi_i\left(I\right)\mathrm{d}\mathbf{v}\,\mathrm{d}I + \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ji}\left(g,f\right)\left(\mathbf{v},I\right)\psi_j\left(\mathbf{v},I\right)\varphi_j\left(I\right)\mathrm{d}\mathbf{v}\,\mathrm{d}I$$

$$= -\frac{1}{2}\iint_{\mathbb{R}^N \times \mathbb{R}_+}\int_\Omega\int_{S^2}\left[f'g'_* - fg_*\right]\times\left[\psi_i\left(\mathbf{v}',I'\right) + \psi_j\left(\mathbf{v}'_*,I'_*\right) - \psi_i\left(\mathbf{v},I\right) - \psi_j\left(\mathbf{v}_*,I_*\right)\right]$$

$$\times\mathcal{B}_{ij}\left(1-R\right)R^{\frac{N}{2}-1}\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{v}_*\,\mathrm{d}I\,\mathrm{d}\mathbf{v}.$$

PROOF. Let us write the full expression

$$(1.107) \quad \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ij}\left(f,g\right)\left(\mathbf{v},I\right)\psi_i\left(\mathbf{v},I\right)\varphi_i\left(I\right)\mathrm{d}\mathbf{v}\,\mathrm{d}I$$

$$= \iint_{\mathbb{R}^N \times \mathbb{R}_+}\int_\Omega\int_{S^2}\left[f'g'_* - fg_*\right]\psi_i\left(\mathbf{v},I\right)\mathcal{B}_{ij}\left(1-R\right)R^{\frac{N}{2}-1}\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{v}_*\,\mathrm{d}I\,\mathrm{d}\mathbf{v}.$$

In order to get formula (1.105) it is enough to perform the change of variables

$$(1.108) \qquad\qquad \left(\mathbf{v},\mathbf{v}_*,I,I_*,r,R\right)\mapsto\left(\mathbf{v}',\mathbf{v}'_*,I',I'_*,r',R'\right) \quad \text{for } \boldsymbol{\omega}\in S^{N-1} \text{ fixed,}$$

with Jacobian (1.102). Using property $(1.104)_2$ we obtain

$$(1.109) \quad \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ij}\left(f,g\right)\left(\mathbf{v},I\right)\psi_i\left(\mathbf{v},I\right)\varphi_i\left(I\right)\mathrm{d}\mathbf{v}\,\mathrm{d}I$$

$$= \iint_{\mathbb{R}^N \times \mathbb{R}_+}\int_\Omega\int_{S^2}\left[fg_* - f'g'_*\right]\psi_i\left(\mathbf{v}',I'\right)\mathcal{B}_{ij}\left(1-R\right)R^{\frac{N}{2}-1}\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{v}_*\,\mathrm{d}I\,\mathrm{d}\mathbf{v}.$$

Summing equations (1.107) and (1.109), we obtain the formula (1.105).

The second part of the proof uses the same strategy. We write the second integral appearing in the left-hand side of (1.106):

$$\iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ji}\left(g,f\right)\left(\mathbf{v},I\right)\psi_j\left(\mathbf{v},I\right)\varphi_j\left(I\right)\mathrm{d}\mathbf{v}\,\mathrm{d}I$$

$$= \iint_{\mathbb{R}^N \times \mathbb{R}_+}\int_\Omega\int_{S^2}\left[g\left(\frac{m_j\mathbf{v}+m_i\mathbf{v}_*}{m_i+m_j} + \frac{m_i}{m_i+m_j}\sqrt{\frac{2\,RE}{\mu_{ij}}}T_{\boldsymbol{\omega}}\left[\frac{\mathbf{v}-\mathbf{v}_*}{|\mathbf{v}-\mathbf{v}_*|}\right],r\left(1-R\right)E\right)\right.$$

$$\times f\left(\frac{m_j\mathbf{v}+m_i\mathbf{v}_*}{m_i+m_j} - \frac{m_j}{m_i+m_j}\sqrt{\frac{2\,RE}{\mu_{ij}}}T_{\boldsymbol{\omega}}\left[\frac{\mathbf{v}-\mathbf{v}_*}{|\mathbf{v}-\mathbf{v}_*|}\right],\left(1-r\right)\left(1-R\right)E\right) - g\left(\mathbf{v},I\right)f\left(\mathbf{v}_*,I_*\right)\right]$$

$$\times\psi_j\left(\mathbf{v},I\right)\mathcal{B}_{ij}\left(1-R\right)R^{\frac{N}{2}-1}\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{v}_*\,\mathrm{d}I\,\mathrm{d}\mathbf{v}.$$

We mimic the interchange of particles in the last integral by changing variables

$$\left(\mathbf{v},\mathbf{v}_*,I,I_*,r,R\right)\mapsto\left(\mathbf{v}_*,\mathbf{v},I_*,I,1-r,R\right), \quad \text{for } \boldsymbol{\omega}\in S^{N-1} \text{ fixed,}$$

so that we obtain

$$\iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ji}(g,f)(\mathbf{v},I)\, \psi_j(\mathbf{v},I)\, \varphi_j(I)\, \mathrm{d}\mathbf{v}\, \mathrm{d}I$$

$$= \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_\Omega \int_{S^2} [g_*' f' - g_* f]\, \psi_j(\mathbf{v}_*, I_*)\, \mathcal{B}_{ij}\, (1-R)\, R^{\frac{N}{2}-1}\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}r\, \mathrm{d}R\, \mathrm{d}I_*\, \mathrm{d}\mathbf{v}_*\, \mathrm{d}I\, \mathrm{d}\mathbf{v}.$$

Next, we perform the change (1.108) and get

$$\iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ji}(g,f)(\mathbf{v},I)\, \psi_j(\mathbf{v},I)\, \varphi_j(I)\, \mathrm{d}\mathbf{v}\, \mathrm{d}I$$

$$= \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_\Omega \int_{S^2} [g_* f - g_*' f']\, \psi_j(\mathbf{v}_*', I_*')\, \mathcal{B}_{ij}\, (1-R)\, R^{\frac{N}{2}-1}\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}r\, \mathrm{d}R\, \mathrm{d}I_*\, \mathrm{d}\mathbf{v}_*\, \mathrm{d}I\, \mathrm{d}\mathbf{v}.$$

Finally, summing the last two formulas together with the form (1.105) of the first integral appearing in the left-hand side of (1.106), we obtain the expression (1.106). $\qquad\square$

In the case of mixtures, collision invariants are linked to each species of the mixture. Namely, a set of functions ψ_i, $i=1,\ldots,s$ is called collision invariant if the functional equation

(1.110) $$\forall i,j = 1,\ldots,s, \qquad \psi_i(\mathbf{v},I) + \psi_j(\mathbf{v}_*, I_*) = \psi_i(\mathbf{v}',I') + \psi_j(\mathbf{v}_*', I_*').$$

is satisfied for every $(\mathbf{v},\mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega}) \in \mathbb{R}^{2N} \times \mathbb{R}_+^2 \times [0,1]^2 \times S^{N-1}$.

PROPOSITION 1.13. *The collision invariants corresponding to the species $\mathcal{A}_i$, that belongs to L_{loc}^1, are the following $(N+2)$ functions:*

$$\boldsymbol{\psi}_i(\mathbf{v},I) = \begin{pmatrix} 1 \\ m_i \mathbf{v} \\ \frac{m_i}{2}\, |\mathbf{v}|^2 + I \end{pmatrix}.$$

PROOF. The proof uses ideas of the proof for the corresponding Lemma 1.8 for one polyatomic gas. We search for a function ψ_i such that it satisfies equation (1.110), for $1 \leq i,j \leq s$. Collisional rules $(1.101)_{1-4}$ imply that functions of the pre-collisional quantities, i.e. the right-hand side of (1.110), can be expressed with the help of a function ϕ as follows:

(1.111) $$\psi_i(\mathbf{v},I) + \psi_j(\mathbf{v}_*, I_*) = \phi(m_i \mathbf{v} + m_j \mathbf{v}_*, \tfrac{m_i}{2}\, |\mathbf{v}|^2 + \tfrac{m_j}{2}\, |\mathbf{v}_*|^2 + I + I_*).$$

Let us introduce the operator $D_{k\ell}^{ij}$ corresponding to the species $\mathcal{A}_i$ and $\mathcal{A}_j$, $1 \leq i,j \leq s$, for $k,\ell = 1,\ldots,N$ and $k \neq \ell$:

$$D_{k\ell}^{ij} = (v_k - v_{*k}) \left(\tfrac{1}{m_i} \partial_{v_\ell} - \tfrac{1}{m_j} \partial_{v_{*\ell}} \right) - (v_\ell - v_{*\ell}) \left(\tfrac{1}{m_i} \partial_{v_k} - \tfrac{1}{m_j} \partial_{v_{*k}} \right).$$

Applying the operator $D_{k\ell}^{ij}$ to the function ϕ, similarly as in the proof of Proposition 1.8, we obtain

$$D_{k\ell}^{ij} \phi(m_i \mathbf{v} + m_j \mathbf{v}_*, \tfrac{m_i}{2}\, |\mathbf{v}|^2 + \tfrac{m_j}{2}\, |\mathbf{v}_*|^2 + I + I_*) = 0,$$

which yields

$$D_{k\ell}^{ij} (\psi_i(\mathbf{v},I) + \psi_j(\mathbf{v}_*, I_*)) = 0.$$

Differentiating with respect to v_k, we obtain

(1.112) $$\tfrac{1}{m_i} \partial_\ell\, \psi_i(\mathbf{v},I) - \tfrac{1}{m_j} \partial_\ell\, \psi_j(\mathbf{v}_*, I_*) + \tfrac{1}{m_i}(v_k - v_{*k}) \partial_{\ell k}^2 \psi_i(\mathbf{v},I) - \tfrac{1}{m_i}(v_\ell - v_{*\ell}) \partial_{k^2}^2 \psi_i(\mathbf{v},I) = 0.$$

Furthermore, we differentiate (1.112) with respect to $v_{*\ell}$, obtaining

$$-\tfrac{1}{m_j} \partial_{\ell^2}^2 \psi_j(\mathbf{v}_*, I_*) + \tfrac{1}{m_i} \partial_{k^2}^2 \psi_i(\mathbf{v},I) = 0,$$

while differentiation of (1.112) with respect to $v_{*\ell}$ yields

$$-\tfrac{1}{m_j} \partial_{\ell k}^2 \psi_j(\mathbf{v}_*, I_*) - \tfrac{1}{m_i} \partial_{\ell k}^2 \psi_i(\mathbf{v},I) = 0.$$

The last two equalities imply

$$\partial_{k^2}^2 \psi_i(\mathbf{v},I) = m_i \, \text{const}, \qquad \partial_{k\ell}^2 \psi_i(\mathbf{v},I) = 0,$$

which ensures that ψ is a polynomial of order 2 with respect to the velocity variable with coefficients depending on the species and I, more precisely

$$(1.113) \qquad \psi_i(\mathbf{v}, I) = a_i(I) + \mathbf{b}_i(I) \cdot \mathbf{v} + c(I)\tfrac{m_i}{2} |\mathbf{v}|^2 .$$

In order to make clear the dependence of $\psi(\mathbf{v}, I)$ with respect to I, we apply the operator $\partial_I - \partial_{I_*}$ on identity (1.111), and get

$$\partial_I \psi(\mathbf{v}, I) - \partial_{I_*} \psi(\mathbf{v}_*, I_*) = 0.$$

Now, using the form (1.113) we obtain

$$a_i'(I) + \mathbf{b}_i'(I) \cdot \mathbf{v} + c'(I)\tfrac{m_i}{2} |\mathbf{v}|^2 = a_j'(I_*) + \mathbf{b}_j'(I_*) \cdot \mathbf{v}_* + c'(I_*)\tfrac{m_j}{2} |\mathbf{v}_*|^2 ,$$

which imposes conditions on coefficients:

$$a_i'(I) = \text{const}, \quad \mathbf{b}_i'(I) = 0 \quad \text{and} \quad c'(I) = 0.$$

Thus, a_i takes the form $a_i(I) = aI + a_i$, while $\mathbf{b}_i$ is a constant that depends on the species, and c is a pure constant. Finally, (1.113) becomes

$$\psi_i(\mathbf{v}, I) = a_i + \mathbf{b}_i \cdot \mathbf{v} + c(\tfrac{m_i}{2} |\mathbf{v}|^2 + I).$$

$\square$

Let us point out an important difference between mixtures and single-component gases. In order to define the collision invariant for the species $\mathcal{A}_i$, it is necessary to consider simultaneously two species $\mathcal{A}_i$ and $\mathcal{A}_j$, since the collision process itself is formed by two (possible) different species. Moreover, the weak form (1.106) is defined for species $\mathcal{A}_i$ and $\mathcal{A}_j$ simultaneously. Therefore, considering the species $\mathcal{A}_i$ and taking the weak form of the corresponding collision operator $\sum_{j=1}^s Q_{ij}$, in order to get the right-hand side of (1.106), one needs to add Q_{ji}'s for all $j = 1, \ldots, s$. Consequently, the cancelation of the weak form can be obtained only for mixture as a whole, when ψ_i from (1.106) is chosen to be a collision invariant. An exception is the weak form (1.105), since it vanishes for the first collision invariant when only one species, e.g. $\mathcal{A}_i$ is considered.

Macroscopic conservation laws for mixtures. In order to formulate macroscopic conservation laws for mixtures, we define macroscopic quantities. Mass density, momentum density and total energy density of the species $\mathcal{A}_i$ are defined as the following moments of the distribution function:

$$(1.114) \qquad \begin{pmatrix} \rho_i \\ \rho_i \mathbf{u}_i \\ \frac{1}{2} \rho_i |\mathbf{u}_i|^2 + \rho_i e_i \end{pmatrix} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} \begin{pmatrix} m_i \\ m_i \mathbf{v} \\ \frac{m_i}{2} |\mathbf{v}|^2 + I \end{pmatrix} f_i \, \varphi_i(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}.$$

If we introduce the peculiar velocity that corresponds to the specie $\mathcal{A}_i$ with $\mathbf{c}_i = \mathbf{v} - \mathbf{u}_i$, then pressure tensor and heat flux corresponding to the species $\mathcal{A}_i$ are defined as follows

$$(1.115) \qquad \begin{pmatrix} [\mathbf{p}_i]_{k\ell} \\ \mathbf{q}_i \end{pmatrix} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} \begin{pmatrix} m_i \, [\mathbf{c}_i]_k \, [\mathbf{c}_i]_\ell \\ \left(\frac{m_i}{2} |\mathbf{c}_i|^2 + I \right) \mathbf{c} \end{pmatrix} f_i \, \varphi_i(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}.$$

The conservation laws are specified in the following Proposition.

PROPOSITION 1.14. *Let f_i be a solution of the Boltzmann equation (1.98) which is rapidly decaying with respect to $\mathbf{v}$ and smooth with respect to $t, \mathbf{x}$. Then the conservation law of mass density for a species $\mathcal{A}_i$ and conservation laws of momentum and total energy density for the mixture hold:*

$$(1.116) \qquad \partial_t \rho_i + \nabla_{\mathbf{x}} \cdot \rho_i \mathbf{u}_i = 0, \; i = 1, \ldots, s$$

$$(1.117) \qquad \sum_{i=1}^s \left(\partial_t \rho_i \mathbf{u}_i + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i + \mathbf{p}_i) \right) = 0,$$

$$(1.118) \qquad \sum_{i=1}^s \left(\partial_t \left(\tfrac{1}{2} \rho_i |\mathbf{u}_i|^2 + \rho_i e_i \right) + \nabla_{\mathbf{x}} \cdot \left(\left(\tfrac{1}{2} \rho_i |\mathbf{u}_i|^2 + \rho_i e_i \right) \mathbf{u}_i + \mathbf{p}_i \mathbf{u}_i + \mathbf{q}_i \right) \right) = 0.$$

PROOF. The conservation law of mass density for the species $\mathcal{A}_i$ (1.116) is obtained by means of the integration of the Boltzmann equation (1.98) with respect to $\mathbf{v}$ and I, using the definitions (1.114)$_{1,2}$ and the property (1.105) of the weak form which ensures that the right-hand side of (1.116) vanishes. Starting from the Boltzmann equation (1.98), the integration against $m_i \mathbf{v}$ yields

$$\partial_t \rho_i \mathbf{u}_i + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i + \mathbf{p}_i) = \sum_{j=1}^{s} \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ij}(f_i, f_j)(\mathbf{v}, I)\, m_i\, \mathbf{v}\, \varphi_i(I)\, \mathrm{d}\mathbf{v}\, \mathrm{d}I,$$

using definitions (1.114)$_2$ and (1.115)$_1$. If we sum the last equality over i, then the property (1.106) makes the right-hand side equal to zero, and therefore the conservation law of momentum (1.117) is obtained. Finally, integrating the Boltzmann equation (1.98) against $\frac{m_i}{2}|\mathbf{v}|^2 + I$, the same procedure yields the conservation law of energy (1.118). $\qquad\square$

$H-$*theorem.* We conclude this Section by writing down the $H-$theorem corresponding to the collisional operators we defined and by determining the mechanical equilibrium.

PROPOSITION 1.15. *Assume that the cross sections $\mathcal{B}_{ij}$, $1 \leq i, j \leq s$, are positive almost everywhere and that all $f_i \geq 0$, $1 \leq i \leq s$, are such that the collisional integrals Q_{ij} and the entropy productions $D(f_1, \ldots, f_s)$ are well defined. Then*

(a) *The entropy production is non-positive, i.e.*

$$D(f_1, \ldots, f_s) := \sum_{i=1}^{s} \sum_{j=1}^{s} \iint_{\mathbb{R}^N \times \mathbb{R}_+} Q_{ij}(f_i, f_j)(\mathbf{v}, I) \log(f_i(\mathbf{v}, I))\, \varphi_i(I)\, \mathrm{d}I\, \mathrm{d}\mathbf{v} \leq 0.$$

(b) *Moreover, the three following properties are equivalent.*
  i. *For any $1 \leq i, j \leq s$ and $\mathbf{v} \in \mathbb{R}^N$, $I \in \mathbb{R}_+$*

  $$Q_{ij}(f_i, f_j)(\mathbf{v}, I) = 0.$$

  ii. *The entropy production vanishes, that is*

  $$D(f_1, \ldots, f_s) = 0.$$

  iii. *There exist $T > 0$, $\mathbf{u} \in \mathbb{R}^N$ and for any $i = 1, \ldots, s$ there exists $n_i \geq 0$ such that*

  $$f_i(\mathbf{v}, I) = \frac{n_i}{\zeta_{0_i}(T)} \left(\frac{m_i}{2\pi k T}\right)^{N/2} e^{-\frac{1}{kT}\left(\frac{m_i}{2}|\mathbf{v}-\mathbf{u}|^2 + I\right)}.$$

PROOF. The proof follows the same strategy as in [**30**]. The part (a) can be proven, using the properties of the weak form (1.106) for $\psi_i(\mathbf{v}, I) = \log f_i(\mathbf{v}, I)$ and nonnegativity of the function $(x, y) \mapsto (x - y)(\log x - \log y)$. Concerning the part (b), the implications (i$\Rightarrow$ ii) and (ii$\Rightarrow$ i) are straightforward. Let us suppose that ii) holds and let us prove iii). Then, the collision integral corresponding to the same species Q_{ii} is equal to zero, which implies that there exists $n_i \geq 0$, $\mathbf{u}_i \in \mathbb{R}^N$ and $T_i \geq 0$ such that

$$(1.119) \qquad f_i(\mathbf{v}, I) = \frac{n_i}{\zeta_{0_i}(T_i)} \left(\frac{m_i}{2\pi k T_i}\right)^{N/2} e^{-\frac{1}{kT_i}\left(\frac{m_i}{2}|\mathbf{v}-\mathbf{u}_i|^2 + I\right)}.$$

Then, it remains to show that $\mathbf{u}_i = \mathbf{u}_j$ and $T_i = T_j$ for every $i \neq j$. Using the terms corresponding to the collisions between particles of the species $\mathcal{A}_i$ and $\mathcal{A}_j$, we can write $f_i(\mathbf{v}', I')f_j(\mathbf{v}'_*, I'_*) = f_i(\mathbf{v}, I)f_j(\mathbf{v}_*, I_*)$, which simplifies into

$$\frac{1}{kT_i}\left(\frac{m_i}{2}\left|\frac{m_i\mathbf{v} + m_j\mathbf{v}_*}{m_i + m_j} + \frac{m_j}{m_i + m_j}\sqrt{\frac{2RE}{\mu_{ij}}}\,T_{\boldsymbol{\omega}}\left[\frac{\mathbf{v}-\mathbf{v}_*}{|\mathbf{v}-\mathbf{v}_*|}\right] - \mathbf{u}_i\right|^2 + r(1-R)E\right)$$

$$+ \frac{1}{kT_j}\left(\frac{m_j}{2}\left|\frac{m_i\mathbf{v} + m_j\mathbf{v}_*}{m_i + m_j} - \frac{m_i}{m_i + m_j}\sqrt{\frac{2RE}{\mu_{ij}}}\,T_{\boldsymbol{\omega}}\left[\frac{\mathbf{v}-\mathbf{v}_*}{|\mathbf{v}-\mathbf{v}_*|}\right] - \mathbf{u}_j\right|^2 + (1-r)(1-R)E\right)$$

$$= \frac{1}{kT_i}\left(\frac{m_i}{2}|\mathbf{v}-\mathbf{u}_i|^2 + I\right) + \frac{1}{kT_j}\left(\frac{m_j}{2}|\mathbf{v}_*-\mathbf{u}_j|^2 + I_*\right)$$

Considering the coefficients of the degree 1 in r, we get

$$\frac{1}{T_i} - \frac{1}{T_j} = 0,$$

which implies $T_i = T_j$. Moreover, the coefficients of degree $1/2$ in R yield $\mathbf{u}_i = \mathbf{u}_j$. $\qquad\square$

The entropy law. Let us define for each species $\mathcal{A}_i$, $i = 1, \ldots, s$, the entropy and the entropy flux by

$$\eta_i = \iint_{\mathbb{R}^N \times \mathbb{R}_+} f_i \, \log f_i \, \varphi_i(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}, \qquad \eta_{i_j} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} v_j \, f_i \, \log f_i \, \varphi_i(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}, \ 1 \le j \le N,$$

under the assumption that each f_i and $\log f_i$ are rapidly decaying with respect to $(\mathbf{v}, I)$ and smooth with respect to $(t, \mathbf{x})$, for every $i = 1, \ldots, s$. Then Proposition 1.15 (b) implies the entropy law:

$$\sum_{i=1}^{s} \left(\partial_t \eta_i + \sum_{j=1}^{N} \partial_{x_j} \eta_{i_j} \right) \le 0.$$

Part 2

Presentation of the results of the thesis

CHAPTER 2

Maximum entropy principle for polyatomic gases

Extended thermodynamics is closely related to the mathematical theory of hyperbolic systems [**50**]. Indeed, the basic equations of extended thermodynamics that aim at describing a monatomic gas are the balance laws:

$$(2.1) \qquad \partial_t \mathbf{F} + \sum_{j=1}^{3} \partial_{x_j} \mathbf{F}_j = \mathbf{P},$$

where $\mathbf{F}$, $\mathbf{F}_j$ are densities and fluxes of macroscopic quantities (fields) and $\mathbf{P}$ are production densities.

Ordinary thermodynamics already uses such field equations, but it restricts the vector $\mathbf{F}$ to have five components – the densities of mass, momentum and energy, which define the state of a fluid [**27, 48**]. In that case (and in absence of chemical reactions), the production terms $\mathbf{P}$ vanish, so that the field equations are in fact conservation laws. The closure of the system is achieved by relating the fluxes $\mathbf{F}_j$ to the densities $\mathbf{F}$ through constitutive relations.

The simplest constitutive relation is the thermal equation of state, which relates the pressure at one point and time to the densities of mass and energy at that point and time. By neglecting viscosity and heat conduction, one obtains the Euler hyperbolic system for compressible fluids.

The other well-known constitutive equations are those of Navier-Stokes and Fourier for viscous stress and heat flux. These laws rely on the assumption that the fluxes $\mathbf{F}_j$ at some position depend on $\mathbf{F}$ as well as on the gradients of $\mathbf{F}$. This enables to write down Navier-Stokes-Fourier equations, which include derivatives of second order with respect to $\mathbf{x}$ in the momentum and energy equations.

Extended thermodynamics *extends* the state $\mathbf{F}$ in order to include further densities, typically the densities of the fluxes of momentum and energy. In such a way, extended thermodynamics can describe processes with steep gradients and rapid changes. Whatever the additional variables are, all the basic equations have the structure of balance equations, although not all of them are conservation laws [**50**]. The closure is achieved by constitutive equations for the fluxes $\mathbf{F}_j$ and the production terms $\mathbf{P}$, that are local and instantaneous so that $\mathbf{F}_j$ and $\mathbf{P}$ at one point and time depend only on the state at that point and time (and not of the gradients). Moreover, the constitutive equations are restricted to satisfy two universal principles: the objectivity or relativity principle (stating that the field equations (2.1) have the same form in all Galilean frames) and the entropy principle (requiring that the entropy inequality holds for all solutions of the field equations (2.1) and that the entropy density is a convex function). The two principles together ensure that system (2.1) is symmetric hyperbolic [**17, 55, 50**].

Extended thermodynamics is connected to the kinetic theory of gases. Indeed, moments of the distribution function – solution to the Boltzmann equation – can be identified with field variables. Then, moment equations can be obtained from the Boltzmann equation by integrating with respect to the variables that describe microscopic states of the gas against some test functions. It is worth mentioning that kinetic theory of monatomic gases forces the moment equations to have a hierarchical structure: the flux in one equation becomes the density in the next equation, so that the fluxes in the moment equations are in fact also densities. This is not the case in general for fluxes in field equations arising from extended thermodynamics. Namely, when moments of distribution function are interpreted as macroscopic fields, we refer to extended thermodynamics at a *kinetic level*, contrary to extended thermodynamics at a *macroscopic level* in general [**19**]. An important aspect that enables hierarchical arrangement in the case of monatomic gases is the the simple relation that holds between

the internal energy density and the hydrodynamic pressure, that is the trace of the pressure tensor.

The moment method builds an infinite number of moments starting from the Boltzmann equation. Apart from the intractability of an infinite number of equations, the description that it suggests is too much detailed. On the other side, it is common in extended thermodynamics that an approximation of a thermodynamical process under consideration is obtained by means of a finite number of field equations. As a consequence, moment equations are usually truncated at some order. Then, an important aspect of the contact between extended thermodynamics and kinetic theory becomes the closure problem.

For a monatomic gas, the most popular system that describes its behavior (beyond the usual Euler and Navier-Stokes equations) is the system of equations for 13 moments – precisely:

mass density	1	
momentum density	3	
pressure tensor	5 =	9(full matrix)
		− 3(symmetry of pressure tensor)
		− 1(relation of the trace of pressure tensor and energy)
energy density	1	
heat flux	3,	

whose closure is at the heart of the following three procedures: (i) Grad's moment method, (ii) extended thermodynamics of viscous, heat-conducting gases and (iii) maximization of entropy. It was shown [50] that in the case of 13 fields these three procedures yield the same macroscopic equations.

The Grad's moment method is focused on finding an approximate non-equilibrium velocity distribution function $f(t, \mathbf{x}, \mathbf{v})$ which closes the system of balance laws for the 13 moments. The celebrated solution, given by Grad [37], is based upon the expansion of the distribution function in terms of tensorial Hermite polynomials. It enables to compute fluxes and production terms and in such a way closes the system.

The extended thermodynamics [50] yields the same set of equations by imposing universal principles of relativity and entropy inequality (with a convex entropy).

Motivated by the similarity of extended thermodynamics and moment equations derived from the Boltzmann equation on one hand, and the observation that Grad's distribution function maximizes the entropy [44] on the other hand, a maximum entropy principle was established [31, 47]. In [50] this procedure was extended for any number of moments of a monatomic gas.

The moment method and procedures for solving the closure problem when moment equations are truncated at some order described above were established only within the theory of monatomic gases. Aiming to go beyond this framework – one wishes to consider rarefied polyatomic gases or real (dense) gases, one immediately faces a new problem. The simple relationship between the trace of the pressure tensor and the internal energy density does not exist any more, which disturbs the nice hierarchical structure of the moment equations.

In the macroscopic framework, an extended thermodynamics theory for real (dense) gases [9] was only very recently developed. It involves 14 fields:

mass density	1	
momentum density	3	
pressure tensor	6 =	9(full matrix)
		− 3(symmetry of pressure tensor)
energy density	1	
heat flux	3.	

The presence of one more parameter in the pressure tensor (dynamical pressure) is also a feature of rarefied polyatomic gases, and its consideration leads to the same problems as in dense gases. This

Chapter deals first with the construction of moment equations for rarefied polyatomic gases. Another aim of this Chapter is to establish the maximum entropy principle for rarefied polyatomic gases. To that end, a variational problem is formulated and solved thanks to the following result [7]: When $F, G \in C^2$ with respect to all variables, if a function $x = x(t)$, $t \in [a, b]$ is a critical point of the integral $J(x) = \int_a^b F(t, x, x')\,\mathrm{d}t$ that satisfies the conditions

$$K(x) = \int_a^b G(t, x, x')\mathrm{d}t = L, \quad x(a) = A, \quad x(b) = B,$$

then there exists a constant $\alpha \in \mathbb{R}$ such that the function $x = x(t)$ is an extremum of the extended functional $\mathcal{L} = \int_a^b (F - \alpha G)\,\mathrm{d}t$, i.e. the Euler-Lagrange equation holds for the extended functional $\mathcal{L}$:

$$(2.2) \qquad \frac{\partial \mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial x'} = 0.$$

The moment method and the maximum entropy principle for monatomic gases is recalled, in order to point out the main problems that appear when polyatomic gases are considered. Then, some ideas – that were originally developed within the extended thermodynamics theory of dense gases [9] – about how to overcome these problems will be presented. Finally, the kinetic theory for polyatomic gases contributed to the justification of these ideas and the establishment of moment equations for polyatomic gases. Afterwards, the maximum entropy principle is applied in order to close the system for 14 moments.

1. The state of the art for monatomic gases

In a monatomic gas, the macroscopic quantities are averages of the distribution function $f(t, \mathbf{x}, \mathbf{v})$ over the velocity space against monomials in $\mathbf{v}$. Therefore, one naturally obtains evolution equation for the macroscopic quantities by taking moments of the evolution equation for the distribution function (that is the Boltzmann equation) – integrating with respect to $\mathbf{v}$ after multiplication by some monomials of $\mathbf{v}$. Moments are therefore governed by the moment equations of balance type:

$$(2.3) \quad \partial_t \int_{\mathbb{R}^3} m \begin{pmatrix} 1 \\ v_{i_1} \\ v_{i_1} v_{i_2} \\ \vdots \\ v_{i_1} \cdots v_{i_n} \\ \vdots \end{pmatrix} f(t, \mathbf{x}, \mathbf{v})\,\mathrm{d}\mathbf{v} + \sum_{j=1}^3 \partial_{x_j} \int_{\mathbb{R}^3} m\, v_j \begin{pmatrix} 1 \\ v_{i_1} \\ v_{i_1} v_{i_2} \\ \vdots \\ v_{i_1} \cdots v_{i_n} \\ \vdots \end{pmatrix} f(t, \mathbf{x}, \mathbf{v})\,\mathrm{d}\mathbf{v}$$

$$= \int_{\mathbb{R}^3} m \begin{pmatrix} 1 \\ v_{i_1} \\ v_{i_1} v_{i_2} \\ \vdots \\ v_{i_1} \cdots v_{i_n} \\ \vdots \end{pmatrix} Q(f, f)(\mathbf{v})\,\mathrm{d}\mathbf{v}, \quad i_k \in \{1, 2, 3\}, \ \forall k \in \mathbb{N}.$$

The main characteristic of this infinite sequence of equations is that the flux (the term after the derivative with respect to $\mathbf{x}$) in the moment equation of tensorial order n becomes the density (the term after the derivative with respect to t) in the moment equation of order $n+1$. Fluxes and densities essentially coincide – the flux in one equation becomes the density in the next equation.

We remind (1.13) that the collision invariants for monatomic gases are $1, \mathbf{v}, |\mathbf{v}|^2$. Consequently, the first two equations are the conservation laws of the mass density and the i_1-th component of momentum density. In addition, one half of the trace (equalization of indices and summation over them) of the third equation is interpreted as the conservation law of the total (kinetic + internal) energy density.

Let us devote more attention to the last property. The total energy density (1.24) is defined as the moment of the distribution function against the energy collisional invariant and it can be decomposed into macroscopic kinetic and internal energy. The macroscopic internal energy density is related to the

hydrodynamic pressure (which is, according to (1.26), one third of the trace of the pressure tensor) via the caloric equation of state for ideal gases (1.27):

$$(2.4) \qquad\qquad \rho\, e = \tfrac{1}{2}\left(p_{11} + p_{22} + p_{33}\right) = \tfrac{3}{2}\,p.$$

where k is the Boltzmann constant $k = 1.38 \cdot 10^{-23} J/K$.

The description by an infinite number of moment equations is equivalent to the description by the distribution function. Its presentation is perhaps more physically intuitive, since one is usually interested in the evolution of macroscopic observable quantities, but an infinite number of moment equations is untractable, and also too much detailed. Therefore, the hierarchy of macroscopic equations (2.3) is usually truncated at some order of moments, say N.

A method which provides an appropriate solution to the closure problem when one performs such a truncation is the maximization of entropy method [44]. It is well known that each solution f of the Boltzmann equation of monatomic gases satisfies the extra entropy balance law:

$$(2.5) \qquad\qquad \partial_t h + \sum_{j=1}^{3} \partial_{x_j} h_j = \Sigma \geq 0,$$

where

$$(2.6) \qquad h = -k \int_{\mathbb{R}^3} f \log f \, d\mathbf{v}, \quad h_j = -k \int_{\mathbb{R}^3} v_j f \log f \, d\mathbf{v}, \quad \Sigma = -k \int_{\mathbb{R}^3} Q(f) \log f \, d\mathbf{v},$$

k being the Boltzmann constant (this result with factor $-k$ dropped is known as $H-$theorem, see Proposition 1.4 in Introduction, equality being satisfied when f is the Maxwellian distribution (1.31)). In other words, the entropy inequality (2.5) automatically holds for the infinite hierarchy. But, when the hierarchy is truncated at some order, the entropy inequality (2.5) needs not be satisfied anymore. In fact, it becomes a strong restriction for the choice of the distribution function that satisfies the truncated moment equations. At the same time, it is known that the local Maxwellian distribution (with hydrodynamic variables which depend on t and $\mathbf{x}$), as well as Grad's distribution, maximizes the physical entropy h.

These results motivated the formulation of the maximum entropy principle. It states that one can use in the closure problem the distribution function f which maximizes the physical entropy under the constraints that its moments are prescribed:

$$\max_f \quad h$$
$$(2.7) \qquad\qquad \text{s.t.} \quad \mathbf{F}^{(N)}(t,\mathbf{x}) = \int_{\mathbb{R}^3} m\,\mathbf{\Psi}^{(N)}(\mathbf{v})\, f(t,\mathbf{x},\mathbf{v})\, d\mathbf{v},$$

where $\mathbf{F}^{(N)} := \mathbf{F}^{(N)}(t,\mathbf{x})$ is the truncated vector of moments up to tensorial order N[1], and $\mathbf{\Psi}^{(N)}$ is the vector $\mathbf{\Psi}$ given in (2.11) truncated at order N:

$$\mathbf{\Psi}^{(N)}(\mathbf{v}) = \begin{pmatrix} 1 \\ v_{i_1} \\ v_{i_1} v_{i_2} \\ \vdots \\ v_{i_1} \cdots v_{i_N} \end{pmatrix}.$$

Thus, the distribution function used in the closure problem comes out as solution of a variational problem with constraints.

The problem can be put on physical ground in the following way: the maximization of entropy is the search for the most probable distribution function. On the other hand, the only information we get about the system is its macroscopic state, described by the moments (2.7) of the distribution function. Therefore, we look for a distribution function f within the set of functions compatible with a given macroscopic state which maximizes the entropy. To be more precise we should write $f^{(N)}$ instead of f,

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[1]Let us remark an abuse of notation: in some Sections N denotes a dimension of space. However, in this Section, the dimension of space is 3, and N denotes an order of truncation of moment (equations).

but to avoid a cumbersome notation we omit the index N. Nevertheless, it is important to note that $f^{(N)}$ is not solution of the Boltzmann equation (1.49) and it is an open problem to prove that $f^{(N)}$ converge to the solution f of the Boltzmann equation when $N \to \infty$.

The variational problem with the constraints (2.7) is solved by introducing the vector of multipliers

$$\boldsymbol{\lambda}^{(N)} = \left(\lambda^{(0)} \quad \lambda_{i_1}^{(1)} \quad \lambda_{i_1 i_2}^{(2)} \quad \cdots \quad \lambda_{i_1 i_2 \ldots i_N}^{(N)} \right)^T$$

and yields the following solution $\hat{f} := \hat{f}(t, \mathbf{x}, \mathbf{v})^2$:

(2.8)
$$\hat{f} = F(\chi) = e^{\left(-1 - \frac{m}{k}\chi\right)},$$

where

$$\chi = \boldsymbol{\lambda}^{(N)} \cdot \boldsymbol{\Psi}^{(N)} = \lambda^{(0)} + \sum_{i_1=1}^{3} \lambda_{i_1}^{(1)} v_{i_1} + \sum_{i_1,i_2=1}^{3} \lambda_{i_1 i_2}^{(2)} v_{i_1} v_{i_2} + \cdots + \sum_{i_1,\ldots,i_n=1}^{3} \lambda_{i_1 \ldots i_n}^{(n)} v_{i_1} \ldots v_{i_n}.$$

Finally, plugging the solution (2.8) into constraints of the problem (2.7), we obtain algebraic equations for the multipliers $\boldsymbol{\lambda}^{(N)}$:

$$\hat{\mathbf{F}}^{(N)} = \int_{\mathbb{R}^3} m \, \boldsymbol{\Psi}^{(N)} e^{\left(-1 - \frac{m}{k} \boldsymbol{\lambda}^{(N)} \cdot \boldsymbol{\Psi}^{(N)}\right)} \, d\mathbf{v},$$

where we have denoted by $\hat{\mathbf{F}}^{(N)}$ the densities evaluated at the maximizer $\hat{f}$. Note that the multipliers, and consequently the distribution function, depend on t and $\mathbf{x}$ through the moments, $\boldsymbol{\lambda}^{(N)} := \boldsymbol{\lambda}^{(N)}(\mathbf{F}^{(N)}(t, \mathbf{x}))$.

Once the maximizer $\hat{f}$ is determined, one can compute all macroscopic quantities and in such a way obtain a closed system of macroscopic equations that determines their time rate of change. Indeed, truncating the hierarchy (2.3) at the order N and choosing $\hat{f}$ for the distribution function, we obtain the following set of macroscopic equations

(2.9)
$$\partial_t \hat{\mathbf{F}}^{(N)} + \sum_{j=1}^{3} \partial_{x_j} \hat{\mathbf{F}}_j^{(N+1)} = \hat{\mathbf{P}}^{(N)},$$

where $\hat{\mathbf{F}}_j^{(N+1)}$ and $\hat{\mathbf{P}}^{(N)}$ are respectively the fluxes and the production terms evaluated at the maximizer $\hat{f}$:

$$\hat{\mathbf{F}}_j^{(N+1)} = \int_{\mathbb{R}^3} m \, v_j \boldsymbol{\Psi}^{(N)}(\mathbf{v}) \, \hat{f} \, d\mathbf{v}, \quad \hat{\mathbf{P}}^{(N)} = \int_{\mathbb{R}^3} m \, \boldsymbol{\Psi}^{(N)}(\mathbf{v}) \, Q(\hat{f}, \hat{f}) \, d\mathbf{v}.$$

Let us explain the notation we use. The moment of *of order n*, for $n \geq 0$, is represented by $F_{i_1 i_1 \ldots i_n}^{(n)}$, as pointed out in (1.20). The moments *up to the order n* are denoted by $\mathbf{F}^{(n)}$. The notation $\mathbf{F}_j^{(n+1)}$ means that we consider moments up to the order $(n+1)$ (starting from the first order moment, since $n \geq 0$) with indices containing index j. More precisely,

$$\mathbf{F}^{(n)} = \begin{pmatrix} F^{(0)} \\ F_{i_1}^{(1)} \\ \ldots \\ F_{i_1 i_2 \ldots i_n}^{(n)} \end{pmatrix}, \quad \mathbf{F}_j^{(n+1)} = \begin{pmatrix} F_j^{(1)} \\ F_{i_1 j}^{(2)} \\ \ldots \\ F_{i_1 i_2 \ldots i_n j}^{(n+1)} \end{pmatrix}.$$

Note that, by definition, the moments are symmetric with respect to change of indices, for example $F_{i_1 i_2}^{(2)} = F_{i_2 i_1}^{(2)}$.

However, the solution of the variational problem (2.7) does not provide, in general, an integrable function (in particular, when N is odd).

One way to overcome this problem is to approximate the solution $\hat{f}$ by assuming that processes are not far from local equilibrium. In order to do so, let us first characterize the equilibrium state from the standpoint of maximum entropy principle.

---

[2]With $\hat{f} := \hat{f}(t, \mathbf{x}, \mathbf{v})$ we denote a solution of the variational problem under consideration.

If the densities of mass, momentum and energy (densities of Euler system of equations) are taken as constraints:

$$\mathbf{F}^{(2)} = \begin{pmatrix} \rho \\ \rho u_i \\ \frac{1}{2}\rho\,|\mathbf{u}|^2 + \rho e \end{pmatrix} = \int_{\mathbb{R}^3} m \begin{pmatrix} 1 \\ v_i \\ \frac{1}{2}\,|\mathbf{v}|^2 \end{pmatrix} f\,d\mathbf{v}, \qquad i = 1, 2, 3,$$

the maximum entropy principle yields an equilibrium distribution function (that is, a local Maxwellian function) as a maximizer, i.e. determines $\boldsymbol{\lambda}_E^{(N)}$:

$$\boldsymbol{\lambda}_E^{(N)} := \left(-\tfrac{k}{m}\log\left(n\left(\tfrac{m}{2\pi kT}\right)^{3/2}\right) \quad -\tfrac{1}{T}u_i \quad \tfrac{1}{2T}\delta_{ij} \quad 0 \quad \cdots \quad 0 \right)^T,$$

for $i, j = 1, 2, 3$ and δ_{ij} representing the Kronecker delta. In such a way, we obtain χ at local equilibrium state ($\chi_E = \boldsymbol{\lambda}_E^{(N)} \cdot \boldsymbol{\Psi}^{(N)}$), and consequently the solution of the variational problem is

$$\hat{f} = F(\chi_E) = f_E,$$

where f_E is the local equilibrium distribution function of the form (1.31) with coefficients that depend on $(t, \mathbf{x})$.

Aiming to expand the maximizer (2.8) in the neighborhood of the local equilibrium [44], we assume that $\chi \approx \chi_E$ or $\boldsymbol{\lambda}^{(N)} \approx \boldsymbol{\lambda}_E^{(N)}$, for a given N, which yields that the exact solution $\hat{f}$ of the variational problem (2.7) is approximated as:

$$\hat{f} \approx F(\chi_E)\left(1 - \tfrac{m}{k}\left(\chi - \chi_E\right)\right).$$

Since $F(\chi_E) = f_E$, the approximate distribution function reads

(2.10) $$\hat{f} \approx f_E\left(1 - \tfrac{m}{k}\tilde{\boldsymbol{\lambda}}^{(N)} \cdot \boldsymbol{\Psi}^{(N)}\right), \quad \tilde{\boldsymbol{\lambda}}^{(N)} = \boldsymbol{\lambda}^{(N)} - \boldsymbol{\lambda}_E^{(N)}.$$

Plugging this approximate distribution function into constraints (2.7) we obtain a linear system of equations for the coefficients $\tilde{\boldsymbol{\lambda}}^{(N)}$, and consequently the distribution function expressed in terms of the known densities $\mathbf{F}^{(N)}$. Finally, the substitution of such distribution function into the moment equations (2.9) closes this system.

Let us consider an example of (2.10). Taking the following moments as constraints

$$\mathbf{F}^{(3)} = \begin{pmatrix} \rho \\ \rho u_i \\ \rho u_i u_j + p_{ij} \\ \left(\frac{1}{2}\rho\,|\mathbf{u}|^2 + \rho e\right)u_i + \sum_{j=1}^3 p_{ij}u_j + q_i \end{pmatrix} = \int_{\mathbb{R}^3} m \begin{pmatrix} 1 \\ v_i \\ v_i v_j \\ \frac{1}{2}\,|\mathbf{v}|^2 v_i \end{pmatrix} f\,d\mathbf{v}, \qquad i = 1, 2, 3,$$

and considering the solution (2.10) for $N = 3$, we obtain the Lagrange multipliers

$$\tilde{\boldsymbol{\lambda}}^{(3)} = \begin{pmatrix} \tilde{\lambda}^{(0)} \\ \tilde{\lambda}_i^{(1)} \\ \tilde{\lambda}_{ij}^{(2)} \\ \tilde{\lambda}_{ijk}^{(3)} \end{pmatrix} = \begin{pmatrix} 1 + \frac{\rho}{2p^2}\sum_{i,j=1}^3 p_{\langle ij\rangle}u_i u_j - \frac{\rho^2}{5p^3}\mathbf{q}\cdot\mathbf{u}\,|\mathbf{u}|^2 + \frac{\rho}{p^2}\mathbf{q}\cdot\mathbf{u} \\ -\frac{\rho}{p^2}\sum_{j=1}^3 p_{\langle ij\rangle}u_j + \frac{\rho^2}{5p^3}|\mathbf{u}|^2 q_i + \frac{2}{5}\frac{\rho^2}{p^3}\mathbf{q}\cdot\mathbf{u}\,q_i - \frac{\rho}{p^2}q_i \\ \frac{\rho}{2p^2}p_{\langle ij\rangle} - \frac{2}{5}\frac{\rho^2}{p^3}q_i u_j - \frac{\rho^2}{5p^3}\mathbf{q}\cdot\mathbf{u}\,\delta_{ij} \\ \frac{\rho^2}{5p^3}\delta_{jk} \end{pmatrix}.$$

Then the approximate distribution function (2.10) for $N = 3$ for this choice of $\tilde{\boldsymbol{\lambda}}^{(3)}$ coincides with Grad's 13 moments distribution function:

$$f_G = n\left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{m}{2kT}|\mathbf{c}|^2}\left(1 - \frac{\rho}{p^2}\mathbf{q}\cdot\mathbf{c} + \frac{\rho}{2p^2}\sum_{i,j=1}^3 p_{\langle ij\rangle}c_i c_j + \frac{1}{5}\frac{\rho^2}{p^3}\mathbf{q}\cdot|\mathbf{c}|^2\mathbf{c}\right), \quad \text{with } \mathbf{c} = \mathbf{v} - \mathbf{u},$$

based upon expansion of distribution function in terms of Hermite polynomials [37]. Consequently, the two approaches yield the same set of balance equations for 13 moments. At the same time, at the macroscopic level the same set of balance laws is obtained by the maximum entropy principle on one side, and extended thermodynamics on the other side [19].

Let us present another possibility about how to overcome the convergence problem. Grad's distribution can be regarded as finite-dimensional approximation of a non-equilibrium distribution function. At the same time, it provides a solution to the closure problem for the truncated set of moment equations. A brief comment may be given about the closure procedure provided by Levermore [47] and the one given here. Namely, the aim of [47] was to give a nonperturbative closure for the moment hierarchy, thus imposing integrability condition to the exact solution of the variational problem (2.7) (typically, it amounts to take into account only some even powers of the velocity variable in $\mathbf{F}^{(N)}$). This condition is rather stringent and eventually rules out the exact solution at Grad's level as inadmissible, since it is not integrable. However, its approximation in the neighborhood of Maxwellian is integrable. To put the derivation of Grad's distribution, or any higher order one, to a firm mathematical ground, one has to make a compromise and drop the condition of integrability of the exact solution. The way out is to search for a solution of the variational problem (2.7) among the set of admissible functions of the form:

$$ f = f_E \left(1 + \boldsymbol{\alpha}^{(N)} \cdot \boldsymbol{\Psi}^{(N)} \right), $$

for a properly defined equilibrium distribution f_E, where $\boldsymbol{\alpha}^{(N)}$ is the vector of functions which has to be determined from the variational problem. Two additional requirements are needed:

(1) the equilibrium distribution f_E has to be taken exact solution of the variational problem with constaints $\mathbf{F}^{(2)}$;
(2) a smallness assumption has to be imposed on $\boldsymbol{\alpha}^{(N)} \cdot \boldsymbol{\Psi}^{(N)}$.

The first condition ensures that f_E is Maxwellian, while the second one implies that admissible functions are small perturbations of the equilibrium distribution. Under these assumptions, it can be shown that $\boldsymbol{\alpha}^{(N)} = -(m/k)\boldsymbol{\lambda}^{(N)}$ is the solution of the constrained variational problem.

In this Chapter, we will build a moment hierarchy for polyatomic gases. A problem that arises in such a construction is that there is no simple relation between the internal energy density and the trace of the pressure tensor, such as (2.4). Indeed, the evolution equation of energy cannot be recovered from any moment equation hierarchically structured as (2.3). This happens for polyatomic rarefied gases in which we are interested, but also for dense gases. Considering dense gases [9], the system of field equations was adapted to a different hierarchy than (2.3). We will validate this idea from the standpoint of kinetic theory in the context of rarefied polyatomic gases [3].

Afterwards, the maximum entropy principle in the case of polyatomic rarefied gases will be presented. In particular, for the 14 moments case, the obtained model can be compared with the model arising from the extended thermodynamics [9], as it was done in the 13 moments case for monatomic gases.

2. Heuristic viewpoint of the model for dense gases

Let us briefly survey the development of ideas for building two independent hierarchies in the case of dense gases [9].

The Navier-Stokes-Fourier theory can be seen as a limiting case of extended thermodynamics obtained by carrying out the Maxwellian iteration (see [9] and references therein), i.e. as an approximation of extended thermodynamics when the relaxation times of dissipative fluxes (viscous stress and heat flux) are neglected.

The Navier-Stokes-Fourier system consists of the usual conservation laws

$$ \partial_t \rho + \sum_{j=1}^{3} \partial_{x_j} \left(\rho \, u_j \right) = 0, $$

$$ \partial_t \rho u_i + \sum_{j=1}^{3} \partial_{x_j} \left(\rho u_i u_j + p_{ij} \right) = 0, \ i = 1, 2, 3, $$

$$ \partial_t \left(\tfrac{1}{2} \rho \left| \mathbf{u} \right|^2 + \rho \, e \right) + \sum_{j=1}^{3} \partial_{x_j} \left(\left(\tfrac{1}{2} \rho \left| \mathbf{u} \right|^2 + \rho \, e \right) u_j + \sum_{i=1}^{3} p_{ij} u_i + q_j \right) = 0, $$

and recalling the structure of the pressure tensor (1.92): $p_{ij} = (p + \Pi)\delta_{ij} + p_{\langle ij \rangle}$, the constitutive equations for the traceless part of the pressure tensor, dynamic pressure and heat flux write

$$p_{\langle ij \rangle} = 2\,\mu\,\frac{\partial u_{\langle i}}{\partial x_{j\rangle}}, \quad \Pi = -\nu\,\nabla_{\mathbf{x}} \cdot \mathbf{u}, \quad \mathbf{q} = -\kappa\,\nabla_{\mathbf{x}} T,$$

where μ is the shear viscosity, ν the bulk viscosity and κ the heat conductivity. This system can be rewritten as follows:

$$\partial_t \rho \qquad\qquad + \sum_{j=1}^{3} \partial_{x_j}\left(\rho\,u_j\right) \qquad\qquad = 0,$$

$$\partial_t\left(\rho\,u_i\right) \qquad\qquad + \sum_{j=1}^{3} \partial_{x_j}\left(\rho\,u_i\,u_j + p_{ij}\right) \qquad\qquad = 0,$$

$$\partial_t\left(\tfrac{1}{2}\,\rho\,|\mathbf{u}|^2 + \rho\,e\right) + \sum_{j=1}^{3}\partial_{x_j}\left(\left(\tfrac{1}{2}\,\rho\,|\mathbf{u}|^2 + \rho\,e\right)u_j + \sum_{i=1}^{3}p_{ij}\,u_i + q_j\right) = 0,$$

$$\sum_{k=1}^{3}\partial_{x_k}\left(u_i\,\delta_{jk} + u_j\,\delta_{ik} - \tfrac{2}{3}\,u_k\,\delta_{ij}\right) \qquad\qquad = \frac{S_{\langle ij\rangle}}{\mu},$$

$$\sum_{j=1}^{3}\partial_{x_j}u_j \qquad\qquad = -\frac{\Pi}{\nu},$$

$$\partial_{x_i}T \qquad\qquad = -\frac{q_i}{\kappa}.$$

Then, it can be seen as a degenerate (some derivatives with respect to time are missing) balance-type system of 14 equations for the 14 unknown variables: ρ, u_i, e, q_i, $p_{\langle ij\rangle}$, Π, for $i,j = 1,2,3$. It seems natural to build a hyperbolic system, i.e. to include missing terms with time derivatives, and then to see the above system as a partly steady case of the new hyperbolic system. Indeed, the following structure of balance laws is assumed in extended thermodynamics of dense gases [9]:

$$\partial_t F + \sum_{j=1}^{3}\partial_{x_j}F_j = 0,$$

$$\partial_t F_{i_1} + \sum_{j=1}^{3}\partial_{x_j}F_{i_1 j} = 0,$$

$$\partial_t F_{i_1 i_2} + \sum_{j=1}^{3}\partial_{x_j}F_{i_1 i_2 j} = P_{i_1 i_2}, \qquad\qquad \partial_t G + \sum_{j=1}^{3}\partial_{x_j}G_j = 0,$$

$$\partial_t G_{k_1} + \sum_{j=1}^{3}\partial_{x_j}G_{k_1 j} = Q_{k_1},$$

where F is the mass density, F_{i_1} is the momentum density, $F_{i_1 i_2}$ is the momentum flux, G is the total energy density and G_{k_1} is the total energy flux. Then $F_{i_1 i_2 j}$ and $G_{k_1 j}$ are fluxes of $F_{i_1 i_2}$, G_{k_1}, respectively, and $P_{i_1 i_2}$, Q_{k_1} are productions with respect to $F_{i_1 i_2}$, G_{k_1} respectively. This structure makes sense when $\sum_{i=1}^{3} F_{ii}$ is not simply related to G.

We describe in Section 3 how it is possible to obtain the same (and in fact an even more general) set of moment equations in the context of kinetic theory of polyatomic gases.

3. Moment equations for polyatomic gases

From the kinetic point of view, it can be easily noticed from the structure of the energy collision invariant $(\frac{m}{2}\,|\mathbf{v}|^2 + I)$ that the energy equation will never fit into any of the moment equations built as (2.3), i.e. with the help of velocities only. Indeed, the moment corresponding to the energy collision invariant is not equal to one half of the trace of the second order moment anymore, because of the

presence of an additional parameter I. Thus, the kinetic theory confirms that the hierarchy of moments equations cannot be constructed in the same fashion as in the monatomic case.

Motivated by the idea stated in [9] within the framework of dense gases, we build moment equations for rarefied polyatomic gases [3] by constructing two independent hierarchies starting from the kinetic theory of polyatomic gases. One of them called "momentum" hierarchy, or $F-$hierarchy, will be similar to the classical hierarchy of monatomic gases; the other one, called "energy" hierarchy, or $G-$hierarchy, begins with the moment related to the energy collision invariant and proceeds with standard increase of the order through multiplication by velocities.

Starting from the kinetic model of polyatomic gases, we define moments of the $F-$hierarchy in the usual way:

$$\mathbf{F}(t, \mathbf{x}) = \iint_{\mathbb{R}^N \times \mathbb{R}_+} m \, \boldsymbol{\Psi}(\mathbf{v}) \, f(t, \mathbf{x}, \mathbf{v}, I) \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v},$$

where $\boldsymbol{\Psi}(\mathbf{v})$ is the vector of monomials:

$$(2.11) \qquad \boldsymbol{\Psi}(\mathbf{v}) = \begin{pmatrix} 1 \\ v_{i_1} \\ v_{i_1} v_{i_2} \\ \vdots \\ v_{i_1} \cdots v_{i_n} \\ \vdots \end{pmatrix}.$$

Then, the integration of the Bolzmann equation (1.49) leads to the balance laws for the $F-$hierarchy:

$$(2.12) \qquad \partial_t \mathbf{F} + \sum_{j=1}^{3} \partial_{x_j} \mathbf{F}_j = \mathbf{P},$$

where fluxes and productions of the $F-$hierarchy are defined as:

$$(2.13) \qquad \begin{aligned} \mathbf{F}_j(t, \mathbf{x}) &= \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \, v_j \, \boldsymbol{\Psi}(\mathbf{v}) \, f(t, \mathbf{x}, \mathbf{v}, I) \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}, \\ \mathbf{P}(t, \mathbf{x}) &= \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \, \boldsymbol{\Psi}(\mathbf{v}) \, Q(f, f)(t, \mathbf{x}, \mathbf{v}, I) \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}. \end{aligned}$$

Since the second hierarchy aims at recovering equations for the energy density (1.83) and energy flux (1.95), the first two densities of this hierarchy have to be defined by means of integration of the distribution function against $\left(\frac{m}{2} |\mathbf{v}|^2 + I\right)$ and $\left(\frac{m}{2} |\mathbf{v}|^2 + I\right) v_j$, for some $1 \le j \le 3$. Therefore, it seems natural to define moments of the $G-$hierarchy by keeping energy collision invariant and proceeding as before – multiplying by monomial of velocity:

$$\mathbf{G}(t, \mathbf{x}) = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \boldsymbol{\Theta}(\mathbf{v}, I) \, f(t, \mathbf{x}, \mathbf{v}, I) \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v},$$

where

$$\boldsymbol{\Theta}(\mathbf{v}, I) = \begin{pmatrix} \frac{m}{2} |\mathbf{v}|^2 + I \\ \left(\frac{m}{2} |\mathbf{v}|^2 + I\right) v_{k_1} \\ \left(\frac{m}{2} |\mathbf{v}|^2 + I\right) v_{k_1} v_{k_2} \\ \vdots \\ \left(\frac{m}{2} |\mathbf{v}|^2 + I\right) v_{k_1} \cdots v_{k_m} \\ \vdots \end{pmatrix} = \left(\frac{m}{2} |\mathbf{v}|^2 + I\right) \boldsymbol{\Psi}(\mathbf{v}).$$

The corresponding fluxes and production terms are defined in the usual way:

(2.14)
$$\mathbf{G}_j(t, \mathbf{x}) = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} v_j \, \Theta(\mathbf{v}, I) \, f(t, \mathbf{x}, \mathbf{v}, I) \, \varphi(I) \, dI \, d\mathbf{v},$$

$$\mathbf{Q}(t, \mathbf{x}) = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \Theta(\mathbf{v}, I) \, Q(f, f)(t, \mathbf{x}, \mathbf{v}, I) \, \varphi(I) \, dI \, d\mathbf{v}.$$

Then, the balance laws for the $G-$hierarchy obtained from the Boltzmann equation (1.49) read:

(2.15)
$$\partial_t \mathbf{G} + \sum_{j=1}^{3} \partial_{x_j} \mathbf{G}_j = \mathbf{Q}.$$

Note that the minimal order of the moment in the $F-$hierarchy is 0, while the minimal order in the $G-$hierarchy is 2. Then, the property that the flux in the moment equation of order n becomes the density in the moment equation of order $n+1$ holds, albeit separately for the $F-$ and for the $G-$hierarchy.

Let us introduce some notations. We represent the moment of the $F-$ ($G-$) hierarchy of the order, say n, componentwise with $F_{i_1 i_2 \ldots i_n}^{(n)}$ ($G_{i_1 i_2 \ldots i_{n-2}}^{(n)}$) for any integer $n \geq 0$ ($n \geq 2$) and $i_k = \{1, 2, 3\}$ for every $k = 1, \ldots, n$. When we deal with moments of the $F-$ ($G-$) hierarchy up to some order, say n, then we write them in vector form $\mathbf{F}^{(n)}$ ($\mathbf{G}^{(n)}$).

Then $F^{(0)}$ is the mass density, $F_{i_1}^{(1)}$ is the i_1-th component of the momentum density, while $F_{i_1 i_2}^{(2)}$ is the $i_1 i_2$-th element of the momentum flux:

(2.16)
$$F^{(0)} = \rho, \quad F_{i_1}^{(1)} = \rho \, u_{i_1}, \quad F_{i_1 i_2}^{(2)} = \rho \, u_{i_1} \, u_{i_2} + p_{i_1 i_2}.$$

As desired, $G^{(2)}$ is the energy density and $G_{k_1}^{(3)}$ is the k_1-component of the energy flux:

(2.17)
$$G^{(2)} = \tfrac{1}{2} \rho \, |\mathbf{u}|^2 + \rho e, \quad G_{k_1}^{(3)} = \left(\tfrac{1}{2} \rho \, |\mathbf{u}|^2 + \rho e \right) u_{k_1} + \sum_{i=1}^{3} p_{i k_1} u_i + q_{k_1}.$$

Furthermore, the first two moment equations from the $F-$hierarchy have physical meaning of the conservation laws for the mass and momentum, while the first moment equation from the $G-$hierarchy physically is interpreted as the conservation law of the total energy.

Central moments for polyatomic gases. In practice, "full" moments are too heavy to work with. Even more, any physical problem we deal with should not depend upon the (value) of the macroscopic velocity $\mathbf{u}$. Therefore, it will be very useful to define the central moments – moments centered around the macroscopic velocity $\mathbf{u}$.

Central moments are defined with help of the velocity $\mathbf{c} = \mathbf{v} - \mathbf{u}$. For the $F-$ and $G-$ hierarchy, they read

$$\mathcal{F} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} m \, \boldsymbol{\Psi}(\mathbf{c}) \, f \, \varphi(I) \, dI \, d\mathbf{v}, \quad \mathcal{G} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} \Theta(\mathbf{c}, I) \, f \, \varphi(I) \, dI \, d\mathbf{v}.$$

We recall the physical interpretation of the first few central moments:

(2.18)
$$\mathcal{F}^{(0)} = \rho, \quad \mathcal{F}_{i_1}^{(1)} = 0_{i_1}, \quad \mathcal{F}_{i_1 i_2}^{(2)} = p_{i_1 i_2}, \quad \mathcal{G}^{(0)} = \rho e, \quad \mathcal{G}_{i_1}^{(1)} = q_{i_1}.$$

It is useful to express "full" moments in terms of the central ones. Indeed, the $N-$th order moment for the $F-$hierarchy $F_{i_1 \ldots i_N}^{(N)}$ can be written with the help of the central moments of order N and lower than N as follows

$$F_{i_1 \ldots i_N}^{(N)} = \mathcal{F}_{i_1 \ldots i_N}^{(N)} + \sum_{k=1}^{N} \binom{N}{k} \mathcal{F}_{(i_1 \ldots i_{N-k}}^{(N-k)} u_{i_{N-k+1}} \ldots u_{i_N)},$$

where we have used the notation (13). In particular,

$$F^{(0)} = \mathcal{F}^{(0)}, \quad F_{i_1}^{(1)} = \mathcal{F}^{(0)} u_{i_1}, \quad F_{i_1 i_2}^{(2)} = \mathcal{F}_{i_1 i_2}^{(2)} + \mathcal{F}^{(0)} u_{i_1} u_{i_2}.$$

Furthermore, we rewrite the $(M+2)$-th order moment for the $G-$hierarchy $G^{(M+2)}_{i_1...i_M}$ in terms of the central moments for the $G-$hierarchy of the order $(M+2)$ and lower than $(M+2)$, as well as the moments for the $F-$hierarchy of orders $(M-1)$ and $(M+1)$:

$$(2.19) \qquad G^{(M+2)}_{i_1...i_M} = \mathcal{G}^{(M+2)}_{i_1...i_M} + \sum_{k=1}^{M} \binom{M}{k} \mathcal{G}^{(M+2-k)}_{(i_1...i_{M-k}} u_{i_{M-k+1}}...u_{i_M)} + \sum_{k=1}^{3} u_k F^{(M+1)}_{k\,i_1...i_M} - \frac{1}{2}|\mathbf{u}|^2 F^{(M)}_{i_1...i_M}.$$

The first two moments are therefore:

$$G^{(2)} = \mathcal{G}^{(0)} + \sum_{k=1}^{3} u_k F^{(1)}_k - \tfrac{1}{2}|\mathbf{u}|^2 F^{(0)},$$

$$G^{(3)}_{i_1} = \mathcal{G}^{(3)}_{i_1} + \mathcal{G}^{(2)} u_{i_1} + \sum_{k=1}^{3} u_k F^{(2)}_{k\,i_1} - \tfrac{1}{2}|\mathbf{u}|^2 F^{(1)}_{i_1}.$$

The dependence of the moment for the $G-$hierarchy upon moments of the $F-$hierarchy observed in (2.19) is crucial for the determination of the relation between the orders of truncation N and M. Namely, it is clear that the $F-$hierarchy should contain at least moments necessary for expressing the $(M+2)$-th moment (2.19) for the $G-$hierarchy. Since the highest order of the $F-$hierarchy appearing in (2.19) is $(M+1)$, we obtain the following restriction: $N \geq M+1$ [8].

4. Maximum entropy principle for polyatomic gases

Like in monatomic gases, infinite sequences of moment equations for polyatomic gases may be truncated to form a finite set of balance laws:

$$(2.20) \qquad \partial_t \mathbf{F}^{(N)} + \sum_{j=1}^{3} \partial_{x_j} \mathbf{F}^{(N+1)}_j = \mathbf{P}^{(N)}, \quad \partial_t \mathbf{G}^{(M)} + \sum_{j=1}^{3} \partial_{x_j} \mathbf{G}^{(M+1)}_j = \mathbf{Q}^{(M)}.$$

for $N \geq 0$ and $M \geq 2$. On the other hand, truncation calls for the solution of the closure problem. We present one method that aims at solving the closure problem, namely the maximum entropy principle, in the context of polyatomic gases.

In the case of polyatomic gases, entropy is defined by the following relation:

$$(2.21) \qquad h = -k \iint_{\mathbb{R}^3 \times \mathbb{R}_+} f \log f \varphi(I)\, \mathrm{d}I\, \mathrm{d}\mathbf{v} = -k\eta,$$

where η is given in $(1.97)_1$. The maximum entropy principle amounts to stating the following variational problem:

$$\max_f \quad h$$

$$(2.22) \qquad \text{s.t.} \quad \mathbf{F}^{(N)} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m\, \mathbf{\Psi}^{(N)}(\mathbf{v})\, f\, \varphi(I)\mathrm{d}I\, \mathrm{d}\mathbf{v},$$

$$\mathbf{G}^{(M)} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \mathbf{\Theta}^{(M)}(\mathbf{v}, I)\, f\, \varphi(I)\mathrm{d}I\, \mathrm{d}\mathbf{v},$$

with

$$\mathbf{\Psi}^{(N)}(\mathbf{v}) = \begin{pmatrix} 1 \\ v_{i_1} \\ v_{i_1} v_{i_2} \\ \vdots \\ v_{i_1} v_{i_2} \ldots v_{i_N} \end{pmatrix} \quad \text{and} \quad \mathbf{\Theta}^{(M)}(\mathbf{v}, I) = \left(\frac{m}{2}|\mathbf{v}|^2 + I \right) \mathbf{\Psi}^{(M)}(\mathbf{v}).$$

This variational problem is solved by introducing the vector of multipliers

$$\boldsymbol{\lambda}^{(N)} = \begin{pmatrix} \lambda^{(0)} \\ \lambda^{(1)}_{i_1} \\ \vdots \\ \lambda^{(N)}_{i_1...i_N} \end{pmatrix}, \quad \boldsymbol{\mu}^{(M)} = \begin{pmatrix} \mu^{(2)} \\ \mu^{(3)}_{k_1} \\ \vdots \\ \mu^{(M)}_{k_1...k_M} \end{pmatrix}.$$

Then, the appropriate extended functional $\mathcal{L}$ reads

$$\mathcal{L} = h - \boldsymbol{\lambda}^{(N)} \cdot \left(\iint_{\mathbb{R}^3 \times \mathbb{R}_+} m\, \boldsymbol{\Psi}^{(N)}(\mathbf{v})\, f\, \varphi(I)\, \mathrm{d}I\, \mathrm{d}\mathbf{c} \right) - \boldsymbol{\mu}^{(M)} \cdot \left(\iint_{\mathbb{R}^3 \times \mathbb{R}_+} \boldsymbol{\Theta}^{(M)}(\mathbf{v}, I)\, \varphi(I)\, \mathrm{d}I\, \mathrm{d}\mathbf{c} \right).$$

The Euler-Lagrange equation (2.2) reduces to $\delta \mathcal{L}/\delta f = 0$, which is satisfied if and only if

$$-k\,(\log f + 1) - m\boldsymbol{\lambda}^{(N)} \cdot \boldsymbol{\Psi}^{(N)} - \boldsymbol{\mu}^{(M)} \cdot \boldsymbol{\Theta}^{(M)} = 0.$$

Therefore, the solution $\hat{f} := \hat{f}(t, \mathbf{x}, \mathbf{v}, I)$ to the variational problem (2.22) is

(2.23) $$\hat{f} = e^{-1 - \frac{m}{k} \boldsymbol{\lambda}^{(N)} \cdot \boldsymbol{\Psi}^{(N)} - \frac{1}{k} \boldsymbol{\mu}^{(M)} \cdot \boldsymbol{\Theta}^{(M)}}.$$

Plugging the solution $\hat{f}$ into densities, fluxes and production terms from (2.20), a closed system of equations is obtained:

(2.24) $$\partial_t \hat{\mathbf{F}}^{(N)} + \sum_{j=1}^{3} \partial_{x_j} \hat{\mathbf{F}}_j^{(N+1)} = \hat{\mathbf{P}}^{(N)}, \quad \partial_t \hat{\mathbf{G}}^{(M)} + \sum_{j=1}^{3} \partial_{x_j} \hat{\mathbf{G}}_j^{(M+1)} = \hat{\mathbf{Q}}^{(M)},$$

where $\hat{\mathbf{F}}^{(N)}$, $\hat{\mathbf{F}}_j^{(N+1)}$, $\hat{\mathbf{P}}^{(N)}$, $\hat{\mathbf{G}}^{(M)}$, $\hat{\mathbf{G}}_j^{(M+1)}$, $\hat{\mathbf{Q}}^{(M)}$ respectively denotes quantities $\mathbf{F}^{(N)}$, $\mathbf{F}_j^{(N+1)}$, $\mathbf{P}^{(N)}$, $\mathbf{G}^{(M)}$, $\mathbf{G}_j^{(M+1)}$, $\mathbf{Q}^{(M)}$ evaluated at the maximizer $\hat{f}$.

As in the case of monatomic gases, our attention is focused on the convergence problem. Namely, not every variational problem yields an integrable function $\hat{f}$. To ensure the convergence of the quantities appearing in (2.24), we are led to approximate the exact solution $\hat{f}$ to the variational problem (2.22) around an equilibrium state. We anticipate that this assumption amounts to suppose:

$$\boldsymbol{\lambda}^{(N)} \approx \boldsymbol{\lambda}_E^{(N)} := \begin{pmatrix} -\frac{k}{m}\left(\log\left(\frac{\rho}{m\zeta_0(T)} \left(\frac{m}{2\pi kT}\right)^{3/2}\right) + 1\right) + \frac{1}{2T}|\mathbf{u}|^2 \\ -\frac{1}{T}\mathbf{u} \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \qquad \boldsymbol{\mu}^{(M)} \approx \boldsymbol{\mu}_E^{(M)} := \begin{pmatrix} \frac{1}{T} \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

The multipliers $\boldsymbol{\lambda}_E^{(N)}$ and $\boldsymbol{\mu}_E^{(M)}$ will be derived in Proposition 2.1. In particular, the equilibrium distribution function f_E will be obtained. It will be shown that

(2.25) $$f_E = e^{-1 - \frac{m}{k} \boldsymbol{\lambda}_E^{(N)} \cdot \boldsymbol{\Psi}^{(N)} - \frac{1}{k} \boldsymbol{\mu}_E^{(M)} \cdot \boldsymbol{\Theta}^{(M)}}.$$

In order to expand $\hat{f}$ in the neighborhood of local equilibrium state, let us denote

$$\chi = m\boldsymbol{\lambda}^{(N)} \cdot \boldsymbol{\Psi}^{(N)} + \boldsymbol{\mu}^{(M)} \cdot \boldsymbol{\Theta}^{(M)},$$

and

$$\chi_E = m\boldsymbol{\lambda}_E^{(N)} \cdot \boldsymbol{\Psi}^{(N)} + \boldsymbol{\mu}_E^{(M)} \cdot \boldsymbol{\Theta}^{(M)}.$$

Then, introducing the function F, (2.23) can be rewritten as follows

$$\hat{f} = F(\chi) = e^{-1 - \frac{1}{k}\chi}.$$

Assuming that $\chi \approx \chi_E$, a Taylor expansion yields

$$F(\chi) \approx F(\chi_E)\left(1 - \frac{1}{k}(\chi - \chi_E)\right).$$

Taking into account (2.25), the exact solution (2.23) to the variational problem (2.22) can be approximated around a local equilibrium state as follows

$$\hat{f} \approx f_E \left(1 - \frac{1}{k}\left(m\tilde{\boldsymbol{\lambda}}^{(N)} \cdot \boldsymbol{\Psi}^{(N)} + \tilde{\boldsymbol{\mu}}_E^{(M)} \cdot \boldsymbol{\Theta}^{(M)}\right)\right),$$

for $\tilde{\boldsymbol{\lambda}}^{(N)} := \boldsymbol{\lambda}^{(N)} - \boldsymbol{\lambda}_E^{(N)}$ and $\tilde{\boldsymbol{\mu}}^{(M)} := \boldsymbol{\mu}^{(M)} - \boldsymbol{\mu}_E^{(M)}$.

In the sequel, we describe the Euler approximation obtained for the choice $N = 1$ and $M = 2$, and the 14 moments approximation obtained by choosing $N = 2$ and $M = 3$.

5. Euler approximation for polyatomic gases obtained by means of the maximum entropy principle

Our first aim is to recover the equilibrium distribution function and appropriate field equations for hydrodynamic variables (i.e. transfer equations for moments) via the maximum entropy principle.

5.1. Equilibrium distribution function for polyatomic gases.
The maximum entropy principle is expressed in terms of the following variational problem: determine the distribution function $f := f(t, \mathbf{x}, \mathbf{v}, I)$ such that

$$\max_f \quad h$$

(2.26)
$$\text{s.t.} \quad \mathbf{F}^{(1)} = \begin{pmatrix} \rho \\ \rho \, u_i \end{pmatrix} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \begin{pmatrix} 1 \\ v_i \end{pmatrix} f \, \varphi(I) \, dI \, d\mathbf{v},$$

$$\mathbf{G}^{(2)} = \tfrac{1}{2} \rho \, |\mathbf{u}|^2 + \rho \, e = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\tfrac{m}{2} \, |\mathbf{v}|^2 + I \right) f \, \varphi(I) \, dI \, d\mathbf{v}.$$

Due to Galilean invariance, the problem can be reformulated using the velocity $\mathbf{c} = \mathbf{v} - \mathbf{u}$ in such a way that it does not depend upon the macroscopic velocity $\mathbf{u}$:

$$\max_f \quad h$$

(2.27)
$$\text{s.t.} \quad \mathcal{F}^{(1)} = \begin{pmatrix} \rho \\ 0_i \end{pmatrix} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \begin{pmatrix} 1 \\ c_i \end{pmatrix} f \, \varphi(I) \, dI \, d\mathbf{c},$$

$$\mathcal{G}^{(2)} = \rho \, e = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\tfrac{m}{2} \, |\mathbf{c}|^2 + I \right) f \, \varphi(I) \, dI \, d\mathbf{c},$$

bearing in mind that the velocity argument of the distribution function is translated i.e. $f = f(t, \mathbf{x}, \mathbf{c} + \mathbf{u}, I)$. The solution is given as follows.

PROPOSITION 2.1. *The distribution function which comes out as a solution to the variational problem* (2.27) *has the form:*

(2.28)
$$\hat{f} = f_E = \frac{\rho}{m \, \zeta_0(T)} \left(\frac{m}{2\pi kT} \right)^{3/2} e^{-\frac{1}{kT} \left(\frac{m}{2} |\mathbf{v} - \mathbf{u}|^2 + I \right)},$$

where

(2.29)
$$\zeta_0(T) = \int_{\mathbb{R}_+} e^{-\frac{1}{kT} I} \varphi(I) \, dI.$$

PROOF. In order to prove the statement, we introduce the vector of multipliers $\boldsymbol{\lambda}^{(1)} := \left(\lambda^{(0)} \quad \lambda_i^{(1)} \right)^T$, for $i = 1, 2, 3$, and the multiplier $\boldsymbol{\mu}^{(2)} := \mu^{(2)}$. Superscripts indicates the tensorial order of the moment to which the multiplier is related. The appropriate extended functional is defined as follows:

(2.30)
$$\mathcal{L} = h - \lambda^{(0)} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \, f \varphi(I) \, dI \, d\mathbf{v} - \sum_{i=1}^{3} \lambda_i^{(1)} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \, v_i \, f \varphi(I) \, dI \, d\mathbf{v}$$
$$- \mu^{(2)} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\tfrac{m}{2} \, |\mathbf{v}|^2 + I \right) f \varphi(I) \, dI \, d\mathbf{v}.$$

Since $\mathcal{L}$ is a scalar, it must retain the same value also for zero hydrodynamic velocity $\mathbf{u} = \mathbf{0}$, due to the Galilean invariance. So, in order to work with the reformulated problem (2.27), we introduce $\check{\boldsymbol{\lambda}}^{(1)} := \left(\check{\lambda}^{(0)} \quad \check{\lambda}_i^{(1)} \right)^T$, $i = 1, 2, 3$, and $\check{\boldsymbol{\mu}}^{(2)} := \check{\mu}^{(2)}$, via

(2.31)
$$\lambda^{(0)} = \check{\lambda}^{(0)} - \sum_{k=1}^{3} \check{\lambda}_k^{(1)} u_k + \tfrac{1}{2} \check{\mu}^{(2)} |\mathbf{u}|^2 ; \quad \lambda_i^{(1)} = \check{\lambda}_i^{(1)} - \check{\mu}^{(2)} u_i, \text{ for any } i = 1, 2, 3; \quad \mu^{(2)} = \check{\mu}^{(2)}.$$

Then using relations that hold between full and central moments (2.16), (2.17), (2.18), the following extended functional is obtained:

$$(2.32) \quad \mathcal{L} = -k \int_{\mathbb{R}^3} \int_0^\infty f \log f \varphi(I) \, dI \, d\mathbf{c} - \check{\lambda}^{(0)} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \, f \varphi(I) \, dI \, d\mathbf{c}$$

$$- \sum_{i=1}^3 \check{\lambda}_i^{(1)} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \, c_i \, f \varphi(I) \, dI \, d\mathbf{c} - \check{\mu}^{(2)} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{m}{2} \, |\mathbf{c}|^2 + I \right) f \varphi(I) \, dI \, d\mathbf{c}.$$

The Euler-Lagrange equation $\delta \mathcal{L} / \delta f = 0$ is satisfied if and only if

$$f = e^{-1 - \frac{1}{k} \left[m \, \check{\lambda}^{(0)} + m \sum_{i=1}^3 \left(\check{\lambda}_i^{(1)} c_i \right) + \check{\mu}^{(2)} \left(\frac{m}{2} |\mathbf{c}|^2 + I \right) \right]}.$$

Plugging the solution into the constraints of the problem (2.27), we precisely obtain the following system:

$$\rho = m e^{-1 - \frac{m}{k} \check{\lambda}^{(0)}} \left(\frac{2\pi k}{m \check{\mu}^{(2)}} \right)^{\frac{3}{2}} \zeta_0 \left(\frac{1}{\check{\mu}^{(2)}} \right) e^{\frac{m}{2k\check{\mu}^{(2)}} \sum_{k=1}^3 \left(\check{\lambda}_k^{(1)} \right)^2},$$

$$0_i = -m e^{-1 - \frac{m}{k} \check{\lambda}^{(0)}} \left(\frac{2\pi k}{m \check{\mu}^{(2)}} \right)^{\frac{3}{2}} \zeta_0 \left(\frac{1}{\check{\mu}^{(2)}} \right) \frac{1}{\check{\mu}^{(2)}} \check{\lambda}_i^{(1)},$$

$$e = \frac{1}{2 \left(\check{\mu}^{(2)} \right)^2} \left(\sum_{k=1}^3 \left(\check{\lambda}_k^{(1)} \right)^2 + 3 \frac{k}{m} \check{\mu}^{(2)} \right) + \frac{1}{m} \frac{\zeta_1 \left(\frac{1}{\check{\mu}^{(2)}} \right)}{\zeta_0 \left(\frac{1}{\check{\mu}^{(2)}} \right)},$$

where

$$\zeta_\beta(x) = \int_{\mathbb{R}_+} I^\beta \, e^{-\frac{1}{kx} I} \varphi(I) \, dI.$$

Then, we immediately obtain:

$$\check{\lambda}_i^{(1)} = 0, \qquad i = 1, 2, 3,$$

$$e = \frac{3}{2} \frac{k}{m} \frac{1}{\check{\mu}^{(2)}} + \frac{1}{m} \frac{\zeta_1 \left(\frac{1}{\check{\mu}^{(2)}} \right)}{\zeta_0 \left(\frac{1}{\check{\mu}^{(2)}} \right)},$$

$$\rho = m \, e^{-1 - \frac{m}{k} \check{\lambda}^{(0)}} \left(\frac{2\pi k}{m \check{\mu}^{(2)}} \right)^{\frac{3}{2}} \zeta_0 \left(\frac{1}{\check{\mu}^{(2)}} \right).$$

The first term of the internal energy is its translational part and comparison to (1.93) yields final formulas for the zero velocity multipliers in terms of the hydrodynamic variables:

$$(2.33) \qquad e^{-1 - \frac{m}{k} \check{\lambda}^{(0)}} = \frac{\rho}{m \, \zeta_0(T)} \left(\frac{m}{2\pi k T} \right)^{3/2}, \qquad \check{\lambda}_i^{(1)} = 0, \quad i = 1, 2, 3, \qquad \check{\mu}^{(2)} = \frac{1}{T},$$

with $\zeta_0(T)$ defined by (2.29), which completes the proof. $\qquad \square$

The distribution (2.28) is the generalization of the classical Maxwellian equilibrium distribution in the case of polyatomic gases. It was derived in **[30, 22]** by means of the H−theorem. The model chosen to describe the polyatomic structure, i.e. the measure $\varphi(I) dI$, determines (2.28) through $\zeta_0(T)$.

5.2. Euler equations for polyatomic gases. Once the equilibrium distribution function (2.28) is determined, it enables to derive a closed system of macroscopic variables which corresponds to truncated moments that were constraints in the problem (2.26). As a matter of fact, for the proper choice of the weight function $\varphi(I)$, we obtain Euler equations for polyatomic gases.

PROPOSITION 2.2. *In equilibrium, the internal part of internal energy e_I has the following form:*

$$(2.34) \qquad e_I|_E = \frac{\rho}{m} \frac{\zeta_1(T)}{\zeta_0(T)}, \quad \zeta_1(T) = \int_{\mathbb{R}_+} I \varphi(I) e^{-\frac{1}{kT} I} \, dI.$$

Moreover, if the weight function is chosen to be $\varphi(I) = I^\alpha$, the internal energy of a polyatomic gas in equilibrium reads:

$$(2.35) \qquad e|_E = \left(\frac{5}{2} + \alpha\right)\frac{k}{m}T, \quad \alpha > -1.$$

PROOF. We recall the definition (1.86) of the internal part of the internal energy density:

$$\rho\, e_I = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} I f\, \varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}$$

To prove (2.34), one only has to put the equilibrium distribution (2.28) into (1.86). Furthermore, choosing $\varphi(I) = I^\alpha$, and taking into account the identity:

$$\zeta_\beta(T) = \int_{\mathbb{R}_+} I^\beta \varphi(I) e^{-\frac{1}{kT}I}\,\mathrm{d}I = (kT)^{\beta+1+\alpha}\Gamma(\beta+1+\alpha),$$

for $\beta \geq 0$, auxiliary functions can be expressed in terms of the Gamma function:

$$(2.36) \qquad \zeta_0(T) = (kT)^{1+\alpha}\Gamma(1+\alpha), \quad \zeta_1(T) = (kT)^{2+\alpha}\Gamma(2+\alpha),$$

with overall restriction $\alpha > -1$. With the help of the relation $\Gamma(z+1) = z\Gamma(z)$, one obtains $\zeta_1(T)/\zeta_0(T) = (1+\alpha)kT$, which in turn leads to (2.35) by combining with translational energy (1.85). $\qquad\square$

If the hydrodynamic variables ρ, $\mathbf{u}$ and T in (2.28) are constants, the distribution function identically satisfies the Boltzmann equation. If they are functions of $(t, \mathbf{x})$, we have so-called local Maxwellian distribution, that is not in general solution to the Boltzmann equation, but at least the hydrodynamic variables – moments of distribution function – cannot be arbitrary: they have to satisfy the transfer equations for moments. As a matter of fact, these equations are the Euler gas dynamics equations for polyatomic perfect gases.

PROPOSITION 2.3. *If (2.28) is a local equilibrium distribution, then the hydrodynamic variables $\rho := \rho(t, \mathbf{x})$, $\mathbf{u} := \mathbf{u}(t, \mathbf{x})$ and $T := T(t, \mathbf{x})$ satisfy the following systems of equations (Euler system):*

$$\partial_t \rho + \sum_{j=1}^3 \partial_{x_j}(\rho u_j) = 0,$$

$$(2.37) \qquad \partial_t(\rho u_i) + \sum_{j=1}^3 \partial_{x_j}\left(\rho\, u_i\, u_j + p\,\delta_{ij}\right) = 0, \qquad i = 1, 2, 3,$$

$$\partial_t\left(\tfrac{1}{2}\rho\,|\mathbf{u}|^2 + \rho\, e\right) + \sum_{j=1}^3 \partial_{x_j}\left\{\left(\tfrac{1}{2}\rho\,|\mathbf{u}|^2 + \rho\, e + p\right)u_j\right\} = 0,$$

(where δ_{ij} is Kronecker delta) and

$$p = \frac{k}{m}\rho\, T \quad \text{and} \quad e = \left(\frac{5}{2} + \alpha\right)\frac{k}{m}T, \quad \alpha > -1.$$

PROOF. Equations (2.37) are obtained as moment equations (2.20) for $N = 1$ and $M = 2$, i.e. moment equations that correspond to moments appearing as constraints in (2.26), evaluated for the distribution function (2.28). In fact, in Euler approximation, fluxes and production terms can be explicitly computed using

$$\mathbf{F}_j^{(2)} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \begin{pmatrix} 1 \\ v_i \end{pmatrix} v_j\, f_E\, I^\alpha\,\mathrm{d}I\,\mathrm{d}\mathbf{v}, \qquad \mathbf{G}_j^{(3)} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{m}{2}\,|\mathbf{v}|^2 + I\right) v_j\, f_E\, I^\alpha\,\mathrm{d}I\,\mathrm{d}\mathbf{v},$$

$$\mathbf{P}^{(1)} = \mathbf{0}, \qquad\qquad\qquad\qquad \mathbf{Q}^{(2)} = \mathbf{0}.$$

In particular, when the pressure tensor p_{ij} and heat flux q_i are evaluated as fluxes of local Maxwellian (2.28), one obtains:

$$p_{ij} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \, c_i \, c_j \, f_E \, I^\alpha \, \mathrm{d}I \, \mathrm{d}\mathbf{c} = \frac{k}{m} \, \rho \, T \, \delta_{ij} = p \, \delta_{ij},$$

$$q_j = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{m}{2} \, |\mathbf{c}|^2 + I \right) c_j \, f_E \, I^\alpha \, \mathrm{d}I \, \mathrm{d}\mathbf{c} = 0,$$

which completes the proof. $\qquad \square$

Note that equations (2.37) have the same form in the case of monatomic gases, except for the fact that the internal energy in the monatomic case is strictly $e = \frac{3}{2} \frac{k}{m} T$.

6. The 14 moments approximation for polyatomic gases obtained by means of the maximum entropy principle

It is shown that the local equilibrium case (equations (2.37) from previous Section) is recovered for $N = 1$ and $M = 2$, with closure achieved through the equilibrium distribution (2.28). For higher order approximations, the closure problem remains open. In this Section, we shall study the most interesting physical case of non-equilibrium, involving 14 moments.

6.1. The 14 moments distribution function.
In this Section, we apply the maximum entropy principle in order to close the following system of moment equations for 14 moments:

$$(2.38) \qquad \partial_t \mathbf{F}^{(2)} + \partial_{x_j} \mathbf{F}_j^{(3)} = \mathbf{P}^{(2)}, \quad \partial_t \mathbf{G}^{(3)} + \partial_{x_j} \mathbf{G}_j^{(4)} = \mathbf{Q}^{(3)}.$$

For the entropy defined by (2.21), the following variational problem can be formulated, expressing the maximum entropy principle: determine the distribution function $f := f(t, \mathbf{x}, \mathbf{v}, I)$ such that

$$\max_f \quad h$$

(2.39)

$$\text{s.t.} \quad \mathbf{F}^{(2)} = \begin{pmatrix} \rho \\ \rho \, u_i \\ \rho \, u_i \, u_j + p_{ij} \end{pmatrix} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \begin{pmatrix} 1 \\ v_i \\ v_i \, v_j \end{pmatrix} f \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v},$$

$$\mathbf{G}^{(3)} = \begin{pmatrix} \frac{1}{2} \rho \, |\mathbf{u}|^2 + \rho e \\ \left(\frac{1}{2} \rho \, |\mathbf{u}|^2 + \rho e \right) u_i + \sum_{j=1}^{3} p_{ij} u_j + q_i \end{pmatrix} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{m}{2} \, |\mathbf{v}|^2 + I \right) \begin{pmatrix} 1 \\ v_i \end{pmatrix} f \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v}.$$

Note that (2.39) determines 14 constraints for 14 scalar moments of the distribution function, in contrast to 13 moments in the case of monatomic gases. The number of constrained moments is increased since $\sum_{i=1}^{3} F_{ii}^{(2)} \neq G^{(2)}$ in polyatomic gases.

As in the previous Section, the full moments can be replaced by central moments, due to Galilean invariance. Indeed, the problem (2.39) can be reformulated as:

$$\max_f \quad h$$

$$(2.40) \qquad \text{s.t.} \quad \mathcal{F}^{(2)} = \begin{pmatrix} \rho \\ 0 \\ p_{ij} \end{pmatrix} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \begin{pmatrix} 1 \\ c_i \\ c_i \, c_j \end{pmatrix} f \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{c},$$

$$\mathcal{G}^{(3)} = \begin{pmatrix} \rho e \\ q_i \end{pmatrix} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{m}{2} \, |\mathbf{c}|^2 + I \right) \begin{pmatrix} 1 \\ c_i \end{pmatrix} f \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{c}.$$

The solution of the problem for the choice $\varphi(I) = I^\alpha$ is as follows.

PROPOSITION 2.4. *The linearized distribution function which maximizes the entropy (2.21) subject to constraints (2.40) for the choice of the weighting function $\varphi(I) = I^\alpha$, has the form:*

$$(2.41) \quad \hat{f}(t, \mathbf{x}, \mathbf{c} + \mathbf{u}, I) \approx f_{14}(t, \mathbf{x}, \mathbf{c} + \mathbf{u}, I) = f_E(t, \mathbf{x}, \mathbf{c} + \mathbf{u}, I) \left\{ 1 - \frac{\rho}{p^2} \mathbf{q} \cdot \mathbf{c} \right.$$

$$+ \frac{\rho}{2p^2} \sum_{i,j=1}^{3} \left[p_{\langle ij \rangle} + \left(\frac{5}{2} + \alpha \right)(1 + \alpha)^{-1} \Pi \delta_{ij} \right] c_i c_j$$

$$\left. - \frac{3}{2(1+\alpha)} \frac{\rho}{mp^2} \Pi \left(\frac{m}{2} |\mathbf{c}|^2 + I \right) + \left(\frac{7}{2} + \alpha \right)^{-1} \frac{\rho^2}{mp^3} \mathbf{q} \cdot \left(\frac{m}{2} |\mathbf{c}|^2 + I \right) \mathbf{c} \right\},$$

where f_E is the equilibrium distribution (2.28) and $\zeta_0(T)$ is the auxiliary function (2.29).

PROOF. To solve the problem we shall introduce the following vectors of multipliers:

$$\check{\boldsymbol{\lambda}}^{(2)} := \left(\check{\lambda}^{(0)} \quad \check{\lambda}_i^{(1)} \quad \check{\lambda}_{ij}^{(2)} \right)^T, \quad \check{\boldsymbol{\mu}}^{(3)} := \left(\check{\mu}^{(2)} \quad \check{\mu}_i^{(3)} \right)^T, \qquad i, j = 1, 2, 3,$$

where $\check{\boldsymbol{\lambda}}^{(2)}$ corresponds to constraints $\mathcal{F}^{(2)}$ and $\check{\boldsymbol{\mu}}^{(3)}$ corresponds to constraints $\mathcal{G}^{(3)}$.

The extended functional for the constrained variational problem reads:

$$(2.42) \qquad \mathcal{L} = h - \check{\boldsymbol{\lambda}}^{(2)} \cdot \left(\iint_{\mathbb{R}^3 \times \mathbb{R}_+} m \, \boldsymbol{\Psi}^{(2)}(\mathbf{c}) \, f \, I^\alpha \, dI \, d\mathbf{c} \right) - \check{\boldsymbol{\mu}}^{(3)} \cdot \left(\iint_{\mathbb{R}^3 \times \mathbb{R}_+} \boldsymbol{\Theta}^{(3)}(\mathbf{c}, I) \, I^\alpha \, dI \, d\mathbf{c} \right).$$

The solution of the Euler-Lagrange equation $\delta \mathcal{L}/\delta f = 0$ is given by:

$$\hat{f} = e^{-1 - \frac{1}{k} \chi}, \qquad \chi = m \, \check{\boldsymbol{\lambda}}^{(2)} \cdot \boldsymbol{\Psi}^{(2)}(\mathbf{c}) + \check{\boldsymbol{\mu}}^{(3)} \cdot \boldsymbol{\Theta}^{(3)}(\mathbf{c}, I).$$

To ensure the convergence of moments of the distribution function, we shall replace the exact form of the maximizer by its expansion in the neighborhood of the local equilibrium:

$$(2.43) \qquad \hat{f} \approx f_E \left(1 - \frac{1}{k} \left(m \, \tilde{\boldsymbol{\lambda}}^{(2)} \cdot \boldsymbol{\Psi}^{(2)}(\mathbf{c}) + \tilde{\boldsymbol{\mu}}^{(3)} \cdot \boldsymbol{\Theta}^{(3)}(\mathbf{c}, I) \right) \right),$$

where f_E is the equilibrium distribution (2.28) and $\tilde{\boldsymbol{\lambda}}^{(2)} = \check{\boldsymbol{\lambda}}^{(2)} - \check{\boldsymbol{\lambda}}_E^{(2)}$, $\tilde{\boldsymbol{\mu}}^{(3)} = \check{\boldsymbol{\mu}}^{(3)} - \check{\boldsymbol{\mu}}_E^{(3)}$, where subscript E indicates the values of the multipliers at the local equilibrium state:

$$\check{\boldsymbol{\lambda}}_E^{(2)} = \begin{pmatrix} -\frac{k}{m} \left(\log \left(\frac{\rho}{m\zeta_0(T)} \left(\frac{m}{2\pi k T} \right)^{3/2} \right) + 1 \right) \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \qquad \check{\boldsymbol{\mu}}^{(3)} = \begin{pmatrix} \frac{1}{T} \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

Insertion of (2.43) into the constraints (2.40) yields the appropriate equations for multipliers. Indeed, the following system of algebraic equations emerges for $i, j = 1, 2, 3$:

$$0 = m\tilde{\lambda}^{(0)} + kT \left(\sum_{k=1}^{3} \tilde{\lambda}_{kk}^{(2)} \right) + kT \left(\alpha + \frac{5}{2} \right) \tilde{\mu}^{(2)},$$

$$0 = \tilde{\lambda}_i^{(1)} + \left(\alpha + \frac{7}{2} \right) \frac{kT}{m} \tilde{\mu}_i^{(3)},$$

$$(2.44) \qquad p_{ij} = -2 \frac{kT^2}{m} \rho \, \tilde{\lambda}_{ij}^{(2)} + \delta_{ij} \frac{kT}{m} \rho \left(1 - T\tilde{\mu}^{(2)} \right),$$

$$\rho e = \frac{kT}{m} \rho \left(\alpha + \frac{5}{2} \right) - \rho \frac{kT^2}{m} \left(\left(\sum_{k=1}^{3} \tilde{\lambda}_{kk}^{(2)} \right) + \left(\alpha + \frac{5}{2} \right) \tilde{\mu}^{(2)} \right),$$

$$q_i = -\frac{kT^2}{m} \rho \left(\alpha + \frac{7}{2} \right) \left(\tilde{\lambda}_i^{(1)} + \frac{kT}{m} \left(\alpha + \frac{9}{2} \right) \tilde{\mu}_i^{(3)} \right).$$

The equations $(2.44)_{1-3}$ come out from the constraints (2.40) concerning the $\mathcal{F}$ hierarchy, while $(2.44)_{4-5}$ come out from the $\mathcal{G}$ hierarchy. Equations $(2.44)_{2,5}$ in conjunction with (1.94) yield the following solution

$$\tilde{\mu}_i^{(3)} = -\frac{k}{m}\left(\frac{7}{2}+\alpha\right)^{-1}\frac{\rho^2}{p^3}\,q_i,$$

$$\tilde{\lambda}_i^{(1)} = \frac{k}{m}\frac{\rho}{p^2}\,q_i.$$

Using (2.35) and taking the trace of $(2.44)_3$ with the help of (1.92) and (1.94), equations $(2.44)_{3,4}$ yield the following system

$$\sum_{k=1}^3 p_{kk} = -2\frac{kT^2}{m}\rho\left(\sum_{k=1}^3 \tilde{\lambda}_{kk}^{(2)}\right) + 3\frac{kT}{m}\rho\left(1 - T\tilde{\mu}^{(2)}\right),$$

$$0 = \left(\sum_{k=1}^3 \tilde{\lambda}_{kk}^{(2)}\right) + \left(\alpha + \frac{5}{2}\right)\tilde{\mu}^{(2)},$$

whose solution is

(2.45)

$$\tilde{\mu}^{(2)} = \frac{k}{m}\frac{3}{2(\alpha+1)}\frac{\rho}{p^2}\Pi,$$

$$\tilde{\lambda}_{ii}^{(2)} = -\frac{k}{m}\frac{1}{2(\alpha+1)}\left(\alpha + \frac{5}{2}\right)\frac{\rho}{p^2}\Pi,$$

which implies $\tilde{\lambda}^{(0)} = 0$ by $(2.44)_1$. Combining $(2.44)_3$, (1.90) and $(2.45)_1$ we obtain

$$\tilde{\lambda}_{ij}^{(2)} = -\frac{k}{m}\frac{\rho}{2p^2}\left\{p_{\langle ij\rangle} + \left(\frac{5}{2}+\alpha\right)(1+\alpha)^{-1}\Pi\delta_{ij}\right\},$$

and thus the non-equilibrium velocity distribution (2.41) is obtained. $\square$

A remarkable property of real gases, anticipated at the beginning of the Section, is the existence of the dynamic pressure, which does not appear in monatomic gases. Namely, in the monatomic case, i.e. classical Grad's distribution, constraint $(2.40)_3$, or equivalently the trace of $(2.44)_3$ yields $\tilde{\lambda}_{ii}^{(2)} = 0$, and consequently $\Pi = 0$. The additional term $\tilde{\mu}^{(2)}$ is due to the presence of the internal energy parameter I in the equilibrium distribution (2.28).

An interesting feature of the non-equilibrium distribution (2.41) is its compatibility with other distributions obtained in the context of polyatomic gases. Firstly, it reduces to the velocity distribution obtained by Mallinger [49] for diatomic molecules $(\alpha = 0)$. Furthermore, a comparison could be made with the semi-classical model [60], which assumes that molecules can occupy discrete states of internal energy. It may be observed (see [45], Section 5.2) that the auxiliary function $\zeta_0(T)$ plays the role of the partition function $\mathcal{Z} = \sum_\alpha \exp(-e_\alpha/kT)$. The complete compatibility with the corresponding non-equilibrium function can be observed when I is substituted by e_α and macroscopic quantities are defined by summation over α instead of integration over I.

6.2. The 14 moments system. The non-equilibrium distribution function (2.41) can be regarded as an approximation of the exact solution of the Boltzmann equation expressed in terms of moments. It is a way by which closure of the transfer equations for moments is achieved. As already noticed, fluxes in transfer equations of order n become densities in equations of order $n+1$. This leaves the fluxes in equations of order $n+1$ undetermined, as well as all the production terms.

Closure of the fluxes. Once the distribution function is obtained via maximization of entropy subject to constraints (2.39), it enables to compute the fluxes:

$$\mathbf{F}_j^{(3)} = \begin{pmatrix} F_i^{(1)} \\ F_{ij}^{(2)} \\ F_{ijk}^{(3)} \end{pmatrix}, \quad \mathbf{G}_j^{(4)} = \begin{pmatrix} G_i^{(3)} \\ G_{ij}^{(4)} \end{pmatrix}.$$

Taking into account the Galilean invariance, the fluxes above can be expressed in terms of non-convective fluxes as follows

$$F_{ijk}^{(3)} = \rho u_i u_j u_k + u_i p_{jk} + u_j p_{ki} + u_k p_{ij} + p_{ijk},$$

$$G_{ij}^{(4)} = \left(\tfrac{1}{2}\rho\,|\mathbf{u}|^2 + \rho e\right) u_i u_j + \sum_{k=1}^{3} u_i u_k p_{jk} + \sum_{k=1}^{3} u_j u_k p_{ik} + \tfrac{1}{2}\,|\mathbf{u}|^2\, p_{ij} + \sum_{k=1}^{3} u_k p_{ijk} + q_i u_j + q_j u_i + q_{ij}.$$

Starting from kinetic theory, the non-convective fluxes are defined as:

$$p_{ijk} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} m c_i c_j c_k f(t, \mathbf{x}, \mathbf{c} + \mathbf{u}, I)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{c},$$

$$q_{ij} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} \left(\tfrac{m}{2}\,|\mathbf{c}|^2 + I\right) c_i c_j f(t, \mathbf{x}, \mathbf{c} + \mathbf{u}, I)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{c}.$$

PROPOSITION 2.5. *The non-convective fluxes p_{ijk} and q_{ij} in the 14 moments approximation and for the choice $\varphi(I) = I^\alpha$, $\alpha > -1$, have the following form:*

$$(2.46) \qquad\qquad p_{ijk} = \left(\alpha + \frac{7}{2}\right)^{-1} \left(q_i \delta_{jk} + q_j \delta_{ki} + q_k \delta_{ij}\right),$$

$$(2.47) \qquad\qquad q_{ij} = \left(\alpha + \frac{9}{2}\right) \frac{p}{\rho}\, p_{ij} - \frac{p^2}{\rho}\, \delta_{ij}.$$

PROOF. Expressions (2.46) and (2.47) for non-convective fluxes are derived in a straightforward way by plugging (2.41) in the above given definitions. □

It must be emphasized that the structure of non-convective fluxes (2.46) and (2.47) implies a genuine coupling of two hierarchies – the heat flux q_i appears in the $F-$hierarchy, whereas the pressure tensor p_{ij} appears in the $G-$hierarchy. It also resembles the structure of the non-convective fluxes in Grad's approximation for monatomic gases and can be regarded as its generalization. However, it is not only the parameter α which brings the flavor of polyatomic gases, but also the pressure tensor whose trace contains a dynamic pressure (apart from the ideal gas one).

The 14 moments equations. At this step, the explicit form of the 14 moments equations is given, up to production terms. The equations of the $F-$hierarchy have the form (for any $i, j = 1, 2, 3$):

$$\partial_t \rho + \sum_{i=1}^{3} \partial_{x_i}(\rho u_i) = 0,$$

$$(2.48) \quad \partial_t(\rho u_i) + \sum_{j=1}^{3} \partial_{x_j}(\rho u_i u_j + p_{ij}) = 0,$$

$$\partial_t\left(\rho u_i u_j + p_{ij}\right)$$
$$+ \sum_{k=1}^{3} \partial_{x_k}\left\{\rho u_i u_j u_k + u_i p_{jk} + u_j p_{ki} + u_k p_{ij} + \left(\alpha + \frac{7}{2}\right)^{-1}\left(q_i \delta_{jk} + q_j \delta_{ki} + q_k \delta_{ij}\right)\right\} = P_{ij}^{14},$$

while the equations of the $G-$hierarchy read:

$$\partial_t \left(\tfrac{1}{2}\rho \left| \mathbf{u} \right|^2 + \rho e \right) + \sum_{i=1}^{3} \partial_{x_i} \left\{ \left(\tfrac{1}{2}\rho \left| \mathbf{u} \right|^2 + \rho e \right) u_i + \sum_{j=1}^{3} p_{ij} u_j + q_i \right\} = 0,$$

(2.49)

$$\partial_t \left\{ \left(\tfrac{1}{2}\rho \left| \mathbf{u} \right|^2 + \rho e \right) u_i + \sum_{j=1}^{3} p_{ij} u_j + q_i \right\}$$

$$+ \sum_{j=1}^{3} \partial_{x_j} \left\{ \left(\tfrac{1}{2}\rho \left| \mathbf{u} \right|^2 + \rho e \right) u_i u_j + \sum_{k=1}^{3} (u_i u_k p_{jk} + u_j u_k p_{ik}) + \tfrac{1}{2}\rho \left| \mathbf{u} \right|^2 p_{ij} \right.$$

$$\left. + \left(\alpha + \tfrac{9}{2} \right) \left(\alpha + \tfrac{7}{2} \right)^{-1} (q_i u_j + q_j u_i) + \left(\alpha + \tfrac{7}{2} \right)^{-1} \mathbf{u} \cdot \mathbf{q}\, \delta_{ij} + \left(\alpha + \tfrac{9}{2} \right) \frac{p}{\rho}\, p_{ij} - \frac{p^2}{\rho}\, \delta_{ij} \right\} = Q_i^{14},$$

where the production terms are given by:

$$(2.50) \qquad\qquad P_{ij}^{14} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} m v_i v_j\, Q(f_{14}, f_{14})(\mathbf{v}, I)\, \varphi(I)\, \mathrm{d}I\, \mathrm{d}\mathbf{v},$$

$$(2.51) \qquad\qquad Q_i^{14} = \iint_{\mathbb{R}^N \times \mathbb{R}_+} \left(\tfrac{m}{2} \left| \mathbf{v} \right|^2 + I \right) v_i\, Q(f_{14}, f_{14})(\mathbf{v}, I)\, \varphi(I)\, \mathrm{d}I\, \mathrm{d}\mathbf{v}.$$

The internal energy e is determined by (2.35) and $\zeta_0(T)$ by (2.36). We also exploited expressions for non-convective fluxes (2.46)-(2.47).

The system (2.48)-(2.49) coincides with the equations of extended thermodynamics. To obtain this result, one must take into account (1.92), use the material derivative $(\;)^{\cdot} = \partial_t(\;) + \sum_{j=1}^{3} u_j \partial_j(\;)$, and exploit the relation between α and the number D of degrees of freedom $\alpha = (D-5)/2$. In such a way, the system (2.48)-(2.49) is transformed into Eq. (67) given in [9], which represents the 14 moments system of extended thermodynamics for dense gases in the rarefied gas limit. In this way the same set of equations arises from maximum entropy principle and extended thermodynamics, as it was the case for monatomic gases [31, 19].

Production terms. All the analysis performed thus far is independent of the collision cross section. Therefore, it is valid for any model of interaction of the molecules. However, the closure of the moments system (2.38) needs an explicit computation of the production terms P_{ij}, Q_i given by (2.50) and (2.51). Zero entries which appear in the right hand sides of moments equations are due to collision invariants. A typical obstacle in the computation of the production terms is the complicated structure of the collision integral $Q(f, f)$. And so, even for an approximate form of the distribution function like f_{14}, the explicit computation of production terms is tedious. It is therefore common practice to make further approximations and determine production terms as a linear form of the non-convective macroscopic fluxes. In this Section, the appropriate approximations for source terms that correspond to the distribution function (2.41) will be determined using one simple model of collision cross section.

We recall the structure of the collision integral (1.67) in the case $N = 3$:

$$Q(f, f)(\mathbf{v}, I) = \int_{\Omega_3} \int_{S^2} \left[f' f'_* - f f_* \right] \mathcal{B}\, (1 - R)\, R^{\frac{1}{2}} \frac{1}{\varphi(I)}\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}r\, \mathrm{d}R\, \mathrm{d}I_*\, \mathrm{d}\mathbf{v}_*,$$

where $\Omega_3 = \mathbb{R}^3 \times \mathbb{R}_+ \times [0,1] \times [0,1]$. As in the classical case, the model of interaction between molecules is reflected on the collision cross section $\mathcal{B}$, and its choice is of the utmost importance in the study of macroscopic transport processes. The more realistic the model of interaction is, the more complicated are the computations of collision integral and production terms. We shall use the following form of the cross section:

$$(2.52) \qquad\qquad B(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega}) = K\, 2\, R^s\, \left| \mathbf{v} - \mathbf{v}_* \right|^{2s} \left| \boldsymbol{\omega} \cdot \frac{\mathbf{v} - \mathbf{v}_*}{\left| \mathbf{v} - \mathbf{v}_* \right|} \right|,$$

where K is an appropriate dimensional constant and the parameter s satisfies the overall assumption $s > -\frac{3}{2}$. This cross section resembles the variable hard spheres model and enables the derivation of the production terms in closed form.

As usual, computations are facilitated when one deals with the velocity

$$\text{(2.53)} \qquad\qquad \mathbf{c} = \mathbf{v} - \mathbf{u}.$$

Indeed, let us rewrite the collision transformations from Section 3. As one expects, they take the same form as for the velocity $\mathbf{v}$, since in general the problem should not depend upon the macroscopic velocity $\mathbf{u}$. The conservation laws at a microscopic level (1.55) in terms of $\mathbf{c}$ read:

$$m\,\mathbf{c}' + m\,\mathbf{c}'_* = m\,\mathbf{c} + m\,\mathbf{c}_*,$$

$$\text{(2.54)}$$

$$\tfrac{m}{2}\left|\mathbf{c}'\right|^2 + \tfrac{m}{2}\left|\mathbf{c}'_*\right|^2 + I' + I'_* = \tfrac{m}{2}\left|\mathbf{c}\right|^2 + \tfrac{m}{2}\left|\mathbf{c}_*\right|^2 + I + I_*.$$

They allow to write the pre-collisional velocities in $\boldsymbol{\omega}-$notation as follows

$$\mathbf{c}' = \frac{\mathbf{c} + \mathbf{c}_*}{2} + \sqrt{\frac{R\,E}{m}}\,T_{\boldsymbol{\omega}}\left[\frac{\mathbf{c} - \mathbf{c}_*}{|\mathbf{c} - \mathbf{c}_*|}\right],$$

$$\text{(2.55)}$$

$$\mathbf{c}'_* = \frac{\mathbf{c} + \mathbf{c}_*}{2} - \sqrt{\frac{R\,E}{m}}\,T_{\boldsymbol{\omega}}\left[\frac{\mathbf{c} - \mathbf{c}_*}{|\mathbf{c} - \mathbf{c}_*|}\right],$$

where

$$\text{(2.56)} \qquad E = \tfrac{m}{4}\left|\mathbf{c}' - \mathbf{c}'_*\right|^2 + I' + I'_* = \tfrac{m}{4}\left|\mathbf{c} - \mathbf{c}_*\right|^2 + I + I_*,$$

and $T_{\boldsymbol{\omega}}\left[\mathbf{y}\right] = \mathbf{y} - 2\left(\boldsymbol{\omega}\cdot\mathbf{y}\right)\boldsymbol{\omega}$ (for any $\mathbf{y}\in\mathbb{R}^3$). We recall the invariant properties of the collision operator (1.78):

$$\text{(2.57)} \qquad \iint_{\mathbb{R}^3\times\mathbb{R}_+}\begin{pmatrix}1\\v_i\\\tfrac{m}{2}\left|\mathbf{v}\right|^2 + I\end{pmatrix} Q(f,f)\,(\mathbf{v},I)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v} = 0, \qquad \text{for any}\quad i = 1,2,3.$$

Combination of the first two properties yields

$$\text{(2.58)} \qquad \iint_{\mathbb{R}^3\times\mathbb{R}_+} c_i\,Q(f,f)\,(\mathbf{v},I)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v} = 0, \qquad \text{for any}\quad i = 1,2,3.$$

The decomposition of velocity $\mathbf{v} = \mathbf{u} + \mathbf{c}$ in conjunction with properties (2.57) and (2.58) leads to the following form of the production terms:

$$P_{ij}^{(2)} = \iint_{\mathbb{R}^3\times\mathbb{R}_+} m\,(u_i\,u_j + c_i\,u_j + c_j\,u_i + c_i\,c_j)\,Q(f,f)\,(\mathbf{v},I)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}$$

$$\text{(2.59)}$$

$$= \iint_{\mathbb{R}^3\times\mathbb{R}_+} m\,c_i\,c_j\,Q(f,f)\,(\mathbf{v},I)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}$$

and

$$Q_i^{(3)} = \iint_{\mathbb{R}^3\times\mathbb{R}_+}\left(\left(\tfrac{m}{2}\left|\mathbf{v}\right|^2 + I\right)u_i + \left(\tfrac{m}{2}\left|\mathbf{u}\right|^2 + m\,\mathbf{u}\cdot\mathbf{c} + \tfrac{m}{2}\left|\mathbf{c}\right|^2 + I\right)c_i\right) Q(f,f)\,(\mathbf{v},I)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}$$

$$\text{(2.60)}$$

$$= \sum_{k=1}^{3} u_k\,P_{ki}^{(2)} + \iint_{\mathbb{R}^3\times\mathbb{R}_+}\left(\tfrac{m}{2}\left|\mathbf{c}\right|^2 + I\right)c_i\,Q(f,f)\,(\mathbf{v},I)\,\varphi(I)\,\mathrm{d}I\,\mathrm{d}\mathbf{v}.$$

Furthermore, the cross section (2.52) takes the following form

$$\mathcal{B}(\mathbf{v},\mathbf{v}_*,I,I_*,r,R,\boldsymbol{\omega}) = K\,2\,R^s\,|\mathbf{v} - \mathbf{v}_*|^{2s}\left|\boldsymbol{\omega}\cdot\frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|}\right|$$

$$\text{(2.61)}$$

$$= K\,2\,R^s\,|\mathbf{c} - \mathbf{c}_*|^{2s}\left|\boldsymbol{\omega}\cdot\frac{\mathbf{c} - \mathbf{c}_*}{|\mathbf{c} - \mathbf{c}_*|}\right| = \mathcal{B}(\mathbf{c},\mathbf{c}_*,I,I_*,r,R,\boldsymbol{\omega}).$$

For this choice of cross section, we aim to compute the production terms in the 14 moments approximation obtained by plugging (2.41) into (2.59) and (2.60):

$$P_{ij}^{14} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} m\, c_i\, c_j\, Q\left(f_{14}, f_{14}\right)(\mathbf{v}, I)\, \varphi(I)\, \mathrm{d}I\, \mathrm{d}\mathbf{v},$$

$$= \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \int_{\Omega_3} \int_{S^2} m\, c_i\, c_j\, \left(f_{14}' f_{14*}' - f_{14} f_{14*}\right)$$

$$\text{(2.62)} \hspace{5cm} \times \mathcal{B}\left(1 - R\right) R^{\frac{1}{2}}\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}r\, \mathrm{d}R\, \mathrm{d}I_*\, \mathrm{d}\mathbf{v}_*\, \mathrm{d}I\, \mathrm{d}\mathbf{v},$$

$$Q_i^{14} = \sum_{k=1}^{3} u_k P_{ki}^{14} + \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{m}{2} |\mathbf{c}|^2 + I\right) c_i\, Q\left(f_{14}, f_{14}\right)(\mathbf{v}, I)\, \varphi(I)\, \mathrm{d}I\, \mathrm{d}\mathbf{v}$$

$$= \sum_{k=1}^{3} u_k P_{ki}^{14} + \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \int_{\Omega_3} \int_{S^2} \left(\frac{m}{2} |\mathbf{c}|^2 + I\right) c_i\, \left(f_{14}' f_{14*}' - f_{14} f_{14*}\right)$$

$$\text{(2.63)} \hspace{5cm} \times \mathcal{B}\left(1 - R\right) R^{\frac{1}{2}}\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}r\, \mathrm{d}R\, \mathrm{d}I_*\, \mathrm{d}\mathbf{v}_*\, \mathrm{d}I\, \mathrm{d}\mathbf{v}.$$

Moreover, we shall assume that the state of the gas during the processes is not far from local equilibrium. Therefore, the products of non-equilibrium distribution functions which appear in the collision integral will be linearized with respect to the moments of the distribution functions, i.e. the stress tensor p_{ij} and heat flux q_i.

PROPOSITION 2.6. *The linearized production terms in the 14 moments approximation for the choice (2.52) read:*

$$\text{(2.64)} \hspace{2cm} \overline{P}_{ij}^{14} = -\frac{2^{2s+4} \rho\, (k\,T)^2}{15\, m\, \zeta_0(T)^2} \sqrt{\pi} \left(\frac{k\,T}{m}\right)^s \Gamma\left[s + \frac{3}{2}\right] \times$$

$$\times K\left(p_{\langle ij \rangle} + \frac{20}{(2s+5)(2s+7)} \left(\alpha + \frac{5}{2}\right)(\alpha + 1)^{-1} \Pi \delta_{ij}\right),$$

$$\text{(2.65)} \hspace{2cm} \overline{Q}_i^{14} = \sum_{k=1}^{3} \left(u_k \overline{P}_{ik}^{14}\right) - \left(\frac{7}{2} + \alpha\right)^{-1} \times$$

$$\times K \frac{2^{2s+5}\left(s\,(2s+15)+30\right)}{9\,(2s+5)\,(2s+7)} \frac{\rho\,(k\,T)^2}{m\, \zeta_0(T)^2} \sqrt{\pi} \left(\frac{k\,T}{m}\right)^s \Gamma\left[s + \frac{3}{2}\right] q_i.$$

PROOF. As non-equilibrium effects are supposed small, we linearize products of the distribution functions appearing in the collision integral with respect to the non-equilibrium quantities manifested in our setting – the traceless part of the pressure tensor $p_{\langle k\ell \rangle}$, the dynamic pressure Π and the heat flux q_n. Using the microscopic conservation laws (2.54), we are led to

(2.66)

$$f_{14}' f_{14*}' - f_{14} f_{14*} \approx f_E f_{E*} \left(\sum_{k,\ell=1}^{3} \frac{\rho}{2p^2} \left[p_{\langle k\ell \rangle} + \left(\frac{5}{2} + \alpha\right)(1+\alpha)^{-1} \Pi \delta_{k\ell}\right] \left(c_k' c_\ell' + c_{*k}' c_{*\ell}' - c_k c_\ell - c_{*k} c_{*\ell}\right)\right.$$

$$+ \sum_{n=1}^{3} \left(\frac{7}{2} + \alpha\right)^{-1} \frac{\rho^2}{mp^3} q_n \left(\left(\frac{m}{2}\left|\mathbf{c}'\right|^2 + I'\right) c_n' + \left(\frac{m}{2}\left|\mathbf{c}_*'\right|^2 + I_*'\right) c_{*n}'\right.$$

$$\left.\left. - \left(\frac{m}{2}|\mathbf{c}|^2 + I\right) c_n - \left(\frac{m}{2}|\mathbf{c}_*|^2 + I_*\right) c_{*n}\right)\right).$$

The insertion of (2.66) into (2.62) and (2.63) leads to a suitable approximation for the source term P_{ij}^{14}, denoted by $\overline{P}_{ij}^{14}$, and for the source term Q_i^{14}, denoted by $\overline{Q}_i^{14}$.

Let us start the computation of the production terms with an analysis of parity of their ingredients. From (2.55), we can see that both $\mathbf{c}'$ and $\mathbf{c}_*'$ are odd functions of $(\mathbf{c}, \mathbf{c}_*)$ for $\boldsymbol{\omega}$ fixed i.e. $\mathbf{c}'(-\mathbf{c}, -\mathbf{c}_*, \boldsymbol{\omega}) = -\mathbf{c}'(\mathbf{c}, \mathbf{c}_*, \boldsymbol{\omega})$ and $\mathbf{c}_*'(-\mathbf{c}, -\mathbf{c}_*, \boldsymbol{\omega}) = -\mathbf{c}_*'(\mathbf{c}, \mathbf{c}_*, \boldsymbol{\omega})$. Consequently, (2.66) consists of two parts: one part

that is even and the other one that is odd with respect to $(\mathbf{c}, \mathbf{c}_*)$. Likewise, the cross section is an even function of $(\mathbf{c}, \mathbf{c}_*)$. This consideration leads to the conclusion that only the even part of (2.66) is of importance for the computation of the production term $\overline{P}_{ij}^{14}$, whereas only the odd part of (2.66) contributes to the production term $\overline{Q}_i^{14}$. Therefore, if we introduce the following notation:

$$
\mathcal{P}_{ijk\ell} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \int_{\Omega_3} \int_{S^2} m\, c_i\, c_j\, f_E\left(t, \mathbf{x}, \mathbf{c} + \mathbf{u}, I\right) f_E\left(t, \mathbf{x}, \mathbf{c}_* + \mathbf{u}, I_*\right)
$$
$$
\times \left(c'_k c'_\ell + c'_{*k} c'_{*\ell} - c_k c_\ell - c_{*k} c_{*\ell}\right)
$$
$$
\times K\, 2\left(1 - R\right) R^{s + \frac{1}{2}} \left|\mathbf{c} - \mathbf{c}_*\right|^{2s} \left|\boldsymbol{\omega} \cdot \frac{\mathbf{c} - \mathbf{c}_*}{|\mathbf{c} - \mathbf{c}_*|}\right|\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}r\, \mathrm{d}R\, \mathrm{d}I_*\, \mathrm{d}\mathbf{c}_*\, \mathrm{d}I\, \mathrm{d}\mathbf{c},
$$

$$
\mathcal{Q}_{in} = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \int_{\Omega_3} \int_{S^2} \left(\frac{m}{2}\left|\mathbf{c}\right|^2 + I\right) c_i f_E\left(t, \mathbf{x}, \mathbf{c} + \mathbf{u}, I\right) f_E\left(t, \mathbf{x}, \mathbf{c}_* + \mathbf{u}, I_*\right)
$$
$$
\times \left(\left(\frac{m}{2}\left|\mathbf{c}'\right|^2 + I'\right) c'_n + \left(\frac{m}{2}\left|\mathbf{c}'_*\right|^2 + I'_*\right) c'_{*n}\right.
$$
$$
\left. - \left(\frac{m}{2}\left|\mathbf{c}\right|^2 + I\right) c_n - \left(\frac{m}{2}\left|\mathbf{c}_*\right|^2 + I_*\right) c_{*n}\right)
$$
$$
\times K\, 2\left(1 - R\right) R^{s + \frac{1}{2}} \left|\mathbf{c} - \mathbf{c}_*\right|^{2s} \left|\boldsymbol{\omega} \cdot \frac{\mathbf{c} - \mathbf{c}_*}{|\mathbf{c} - \mathbf{c}_*|}\right|\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}r\, \mathrm{d}R\, \mathrm{d}I_*\, \mathrm{d}\mathbf{c}_*\, \mathrm{d}I\, \mathrm{d}\mathbf{c},
$$

it can be written:

(2.67)
$$
\overline{P}_{ij}^{14} = \frac{\rho}{2p^2}\left[p_{\langle k\ell\rangle} + \left(\frac{5}{2} + \alpha\right)(1+\alpha)^{-1}\Pi\delta_{k\ell}\right]\mathcal{P}_{ijk\ell},
$$
$$
\overline{Q}_i^{14} = \sum_{k=1}^{3} u_k \overline{P}_{ki}^{14} + \sum_{n=1}^{3}\left(\frac{7}{2} + \alpha\right)^{-1}\frac{\rho^2}{m\,p^3}\, q_n \mathcal{Q}_{in}.
$$

Note that $\mathcal{P}_{ijkl}$ vanishes unless indices are equal by pairs – the integral is non-zero when $i = j$ and $k = \ell$ or $i = k$ and $j = \ell$ or $i = \ell$ and $j = k$. By symmetry, the last two terms lead to the same result and thus $\mathcal{P}_{ijkl}$ may be represented in the form:

(2.68)
$$
\mathcal{P}_{ijk\ell} = \mathcal{P}_1 \delta_{ij}\delta_{k\ell} + \mathcal{P}_2\left(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}\right).
$$

Combining (2.67) and (2.68) in conjunction with (1.90) and the symmetry of the pressure tensor, we can extract some more information

$$
\overline{P}_{ij}^{14} = \frac{\rho}{2p^2}\left(2p_{\langle ij\rangle}\mathcal{P}_2 + \sum_{t=1}^{3}\left(\frac{5}{2} + \alpha\right)(1+\alpha)^{-1}\Pi\,\mathcal{P}_{ijtt}\right)
$$
(2.69)
$$
= \frac{\rho}{2p^2}\left(2p_{\langle ij\rangle}\mathcal{P}_2 + \frac{1}{3}\delta_{ij}\left(\frac{5}{2} + \alpha\right)(1+\alpha)^{-1}\Pi\sum_{r,t=1}^{3}\mathcal{P}_{rrtt}\right).
$$

The term $\mathcal{P}_2$ can be determined from the system of equations obtained from the representation (2.68):

$$
\sum_{r,t=1}^{3}\mathcal{P}_{rrtt} = 9\,\mathcal{P}_1 + 6\,\mathcal{P}_2, \qquad \sum_{r,t=1}^{3}\mathcal{P}_{rtrt} = 3\,\mathcal{P}_1 + 12\,\mathcal{P}_2,
$$

whose solution is

$$
\mathcal{P}_1 = \frac{\sum_{r,t=1}^{3} 2\,\mathcal{P}_{rrtt} - \mathcal{P}_{rtrt}}{15}, \qquad \mathcal{P}_2 = \frac{\sum_{r,t=1}^{3} 3\,\mathcal{P}_{rtrt} - \mathcal{P}_{rrtt}}{30}.
$$

Therefore, (2.69) reduces to

(2.70)
$$
\overline{P}_{ij}^{14} = \frac{\rho}{2p^2}\left(p_{\langle ij\rangle}\frac{\sum_{r,t=1}^{3}\left(3\,\mathcal{P}_{rtrt} - \mathcal{P}_{rrtt}\right)}{15} + \frac{1}{3}\delta_{ij}\left(\frac{5}{2} + \alpha\right)(1+\alpha)^{-1}\Pi\sum_{r,t=1}^{3}\mathcal{P}_{rrtt}\right).
$$

On the other hand, one can see that $\mathcal{Q}_{in}$ vanishes unless $i = n$. Therefore, it can be written

$$(2.71) \qquad \overline{Q}_i^{14} = \sum_{k=1}^{3} u_k \overline{P}_{ki}^{14} + \left(\frac{7}{2} + \alpha\right)^{-1} \frac{\rho^2}{m\,p^3}\, q_i\, \frac{1}{3} \sum_{r=1}^{3} \mathcal{Q}_{rr}.$$

The rest of the computation is straightforward.

In order to compute $\overline{P}_{ij}^{14}$, we have to compute only the contractions $\sum_{r,t=1}^{3} \mathcal{P}_{rrtt}$ and $\sum_{r,t=1}^{3} \mathcal{P}_{rtrt}$. Let us begin with the computation of $\sum_{r,t=1}^{3} \mathcal{P}_{rrtt}$. Its full expression reads

$$\sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = K\, 2 \frac{\rho^2}{m\,\zeta_0(T)^2} \left(\frac{m}{2\pi kT}\right)^3 \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \int_{\Omega_3} \int_{S^2} e^{-\frac{m}{2kT}\left(|\mathbf{c}|^2 + |\mathbf{c}_*|^2\right) - \frac{1}{kT}(I + I_*)}$$

$$\times |\mathbf{c}|^2 \left(|\mathbf{c}'|^2 + |\mathbf{c}_*'|^2 - |\mathbf{c}|^2 - |\mathbf{c}_*|^2\right)$$

$$\times (1 - R)\, R^{s+\frac{1}{2}} |\mathbf{c} - \mathbf{c}_*|^{2s} \left|\boldsymbol{\omega} \cdot \frac{\mathbf{c} - \mathbf{c}_*}{|\mathbf{c} - \mathbf{c}_*|}\right| d\boldsymbol{\omega}\, dr\, dR\, dI_*\, d\mathbf{c}_*\, dI\, d\mathbf{c}.$$

We perform the following change of variables with unit Jacobian

$$(2.72) \qquad (\mathbf{c}, \mathbf{c}_*) \mapsto \left(\mathbf{g} = \mathbf{c} - \mathbf{c}_*, \mathbf{G} = \frac{\mathbf{c} + \mathbf{c}_*}{2}\right),$$

which allows to express

$$\mathbf{c} = \mathbf{G} + \frac{1}{2}\mathbf{g}, \qquad \mathbf{c}_* = \mathbf{G} - \frac{1}{2}\mathbf{g}.$$

By microscopic conservation law of momentum (2.54), it holds $\frac{\mathbf{c}' + \mathbf{c}_*'}{2} =: \mathbf{G}' = \mathbf{G}$. Also, using (2.55), we can see that

$$(2.73) \qquad \mathbf{g}' := \mathbf{c}' - \mathbf{c}_*' = 2\sqrt{\frac{R\,E}{m}} T_{\boldsymbol{\omega}}\left[\frac{\mathbf{c} - \mathbf{c}_*}{|\mathbf{c} - \mathbf{c}_*|}\right],$$

and therefore

$$\mathbf{c}' = \mathbf{G} + \frac{1}{2}\mathbf{g}', \qquad \mathbf{c}_*' = \mathbf{G} - \frac{1}{2}\mathbf{g}'.$$

We are led to rewrite the terms under the integration sign using new variables

$$|\mathbf{c}'|^2 + |\mathbf{c}_*'|^2 - |\mathbf{c}|^2 - |\mathbf{c}_*|^2 = \left|\mathbf{G} + \frac{1}{2}\mathbf{g}'\right|^2 - \left|\mathbf{G} + \frac{1}{2}\mathbf{g}\right|^2 + \left|\mathbf{G} - \frac{1}{2}\mathbf{g}'\right|^2 - \left|\mathbf{G} - \frac{1}{2}\mathbf{g}\right|^2$$

$$= \left(\mathbf{G} + \frac{1}{4}(\mathbf{g}' + \mathbf{g})\right) \cdot (\mathbf{g}' - \mathbf{g}) + \left(\mathbf{G} - \frac{1}{4}(\mathbf{g}' + \mathbf{g})\right) \cdot (-(\mathbf{g}' - \mathbf{g}))$$

$$= \frac{1}{2}\left(|\mathbf{g}'|^2 - |\mathbf{g}|^2\right)$$

$$= \frac{1}{2}(R - 1)|\mathbf{g}|^2 + \frac{2R}{m}(I + I_*).$$

The terms appearing in the power of the exponential read:

$$|\mathbf{c}|^2 + |\mathbf{c}_*|^2 = \left|\mathbf{G} + \frac{1}{2}\mathbf{g}\right|^2 + \left|\mathbf{G} - \frac{1}{2}\mathbf{g}\right|^2$$

$$(2.74) \qquad = 2|\mathbf{G}|^2 + \frac{1}{2}|\mathbf{g}|^2.$$

Passage to velocities **g** and **G** and insertion of the formulas above yield

$$\sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = K\, 2\frac{\rho^2}{m\,\zeta_0(T)^2}\left(\frac{m}{2\pi kT}\right)^3 \iint_{\mathbb{R}^3\times\mathbb{R}_+}\int_{\Omega_3}\int_{S^2} e^{-\frac{m}{kT}|\mathbf{G}|^2}e^{-\frac{m}{4kT}|\mathbf{g}|^2}e^{-\frac{1}{kT}I}e^{-\frac{1}{kT}I_*}$$

$$\times\left(|\mathbf{G}|^2 + \mathbf{G}\cdot\mathbf{g} + \frac{1}{4}|\mathbf{g}|^2\right)\left(\frac{1}{2}(R-1)|\mathbf{g}|^2 + \frac{2R}{m}(I+I_*)\right)$$

$$\times(1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\left|\boldsymbol{\omega}\cdot\frac{\mathbf{g}}{|\mathbf{g}|}\right|\,\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I\,\mathrm{d}\mathbf{G}.$$

Next, we pass to the $\boldsymbol{\sigma}-$ notation and recalling (1.36) we obtain the following expression

$$\sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = K\frac{\rho^2}{m\,\zeta_0(T)^2}\left(\frac{m}{2\pi kT}\right)^3 \iint_{\mathbb{R}^3\times\mathbb{R}_+}\int_{\Omega_3}\int_{S^2} e^{-\frac{m}{kT}|\mathbf{G}|^2}e^{-\frac{m}{4kT}|\mathbf{g}|^2}e^{-\frac{1}{kT}I}e^{-\frac{1}{kT}I_*}$$

$$\times\left(|\mathbf{G}|^2 + \mathbf{G}\cdot\mathbf{g} + \frac{1}{4}|\mathbf{g}|^2\right)\left(\frac{1}{2}(R-1)|\mathbf{g}|^2 + \frac{2R}{m}(I+I_*)\right)$$

$$\times(1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\,\mathrm{d}\boldsymbol{\sigma}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I\,\mathrm{d}\mathbf{G},$$

which is easy to compute. We proceed step by step. First, let us integrate with respect to $\boldsymbol{\sigma}$ and **G**

$$\sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = K\frac{\rho^2}{m\,\zeta_0(T)^2}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}4\pi\int_{\mathbb{R}_+}\int_{\Omega_3} e^{-\frac{m}{4kT}|\mathbf{g}|^2}e^{-\frac{1}{kT}I}e^{-\frac{1}{kT}I_*}$$

$$\times\left(\frac{3}{4\sqrt{2}}\frac{kT}{m} + \frac{1}{8\sqrt{2}}|\mathbf{g}|^2\right)\left(\frac{1}{2}(R-1)|\mathbf{g}|^2 + \frac{2R}{m}(I+I_*)\right)$$

$$\times(1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I.$$

Next, we integrate with respect to I and I_*

$$\sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = K\frac{\rho^2}{m\,\zeta_0(T)^2}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\frac{\pi}{\sqrt{2}}(kT)^2\int_{\mathbb{R}^3}\int_{[0,1]}\int_{[0,1]}|\mathbf{g}|^{2s}\,e^{-\frac{m}{4kT}|\mathbf{g}|^2}$$

$$\times\left(3\frac{kT}{m} + \frac{1}{2}|\mathbf{g}|^2\right)\left(\frac{1}{2}(R-1)|\mathbf{g}|^2 + \frac{4kT}{m}R\right)(1-R)\,R^{s+\frac{1}{2}}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}\mathbf{g}.$$

Now, we proceed with the integration with respect to r and R

$$\sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = K\frac{\rho^2}{m\,\zeta_0(T)^2}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\frac{\pi}{\sqrt{2}}(kT)^2\frac{4}{(2s+5)(2s+7)}$$

$$\times\int_{\mathbb{R}^3}|\mathbf{g}|^{2s}\,e^{-\frac{m}{4kT}|\mathbf{g}|^2}\left(3\frac{kT}{m} + \frac{1}{2}|\mathbf{g}|^2\right)\left(-\frac{2}{(2s+3)}|\mathbf{g}|^2 + 4\frac{kT}{m}\right)\mathrm{d}\mathbf{g}.$$

Passage to spherical coordinates yields

$$\sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = K\frac{\rho^2}{m\,\zeta_0(T)^2}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\frac{\pi^2}{\sqrt{2}}(kT)^2\frac{16}{(2s+5)(2s+7)}$$

$$\times\int_{\mathbb{R}_+} e^{-\frac{m}{4kT}|\mathbf{g}|^2}\left(-\frac{1}{2s+3}|\mathbf{g}|^{2s+6} + \frac{4s}{2s+3}\left(\frac{kT}{m}\right)|\mathbf{g}|^{2s+4} + 12\left(\frac{kT}{m}\right)^2|\mathbf{g}|^{2s+2}\right)\mathrm{d}|\mathbf{g}|.$$

We perform the following change of variables

$$(2.75)\qquad\qquad \frac{m}{4\,k\,T}|\mathbf{g}|^2 \mapsto x,\qquad \text{with}\quad \mathrm{d}|\mathbf{g}| = \frac{1}{2}\left(\frac{m}{4\,k\,T}\right)^{-\frac{1}{2}}x^{-\frac{1}{2}}\mathrm{d}x,$$

so that the integral above becomes

$$\sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = K \frac{\rho^2}{m\,\zeta_0(T)^2} \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \frac{\pi^2}{\sqrt{2}} \,(kT)^2 \frac{16}{(2s+5)\,(2s+7)}$$

$$\times \frac{1}{2} \int_{\mathbb{R}_+} e^{-x} \left(-\frac{1}{2s+3} \left(\frac{m}{4\,kT}\right)^{-s-\frac{7}{2}} x^{s+\frac{5}{2}} + \frac{4s}{2s+3} \left(\frac{kT}{m}\right) \left(\frac{m}{4\,kT}\right)^{-s-\frac{5}{2}} x^{s+\frac{3}{2}} \right.$$

$$\left. +12 \left(\frac{kT}{m}\right)^2 \left(\frac{m}{4\,kT}\right)^{-s-\frac{3}{2}} x^{s+\frac{1}{2}} \right) \, \mathrm{d}x.$$

Factorizing, we obtain the following integral

$$\sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = K \frac{\rho^2}{m\,\zeta_0(T)^2} \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \frac{\pi^2}{\sqrt{2}} \,(kT)^2 \frac{16}{(2s+5)\,(2s+7)}$$

$$\times 2^{2s+6} \left(\frac{kT}{m}\right)^{s+\frac{7}{2}} \int_{\mathbb{R}_+} e^{-x} \left(-\frac{1}{2s+3} x^{s+\frac{7}{2}-1} + \frac{s}{2s+3} x^{s+\frac{5}{2}-1} + \frac{3}{4} x^{s+\frac{3}{2}-1} \right) \, \mathrm{d}x.$$

Comparing this identity to the definition of the gamma function, we conclude that

$$\sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = K \frac{\rho^2}{m^3\,\zeta_0(T)^2} \,(kT)^4 \,\sqrt{\pi} \left(\frac{kT}{m}\right)^s \frac{2^{2s+8}}{(2s+5)\,(2s+7)}$$

$$\left(-\frac{1}{2s+3} \Gamma\left[s+\frac{7}{2}\right] + \frac{s}{2s+3} \Gamma\left[s+\frac{5}{2}\right] + \frac{3}{4} \Gamma\left[s+\frac{3}{2}\right] \right).$$

Now, using the property of the gamma function $\Gamma\,(z+1) = z\Gamma\,(z)$, we obtain the following result

$$\sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = K \frac{\rho^2}{m^3\,\zeta_0(T)^2} \,(kT)^4 \,\sqrt{\pi} \left(\frac{kT}{m}\right)^s \frac{2^{2s+8}}{(2s+5)\,(2s+7)} \Gamma\left[s+\frac{3}{2}\right] \left(-\frac{\left(s+\frac{5}{2}\right)}{2} + \frac{s}{2} + \frac{3}{4} \right),$$

which leads to the final result using (1.94)

$$(2.76) \qquad \sum_{r,t=1}^{3} \mathcal{P}_{rrtt} = -K \frac{2^{2s+7}}{(2s+5)(2s+7)} \frac{m\,p^4}{\rho^2\zeta_0(T)^2} \sqrt{\pi} \left(\frac{kT}{m}\right)^s \Gamma\left[s+\frac{3}{2}\right].$$

Let us compute the integral $\sum_{r,t=1}^{3} \mathcal{P}_{rtrt}$ given by

$$\sum_{r,t=1}^{3} \mathcal{P}_{rtrt} = K\,2 \frac{\rho^2}{m\,\zeta_0(T)^2} \left(\frac{m}{2\pi kT}\right)^3 \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \int_{\Omega_3} \int_{S^2} e^{-\frac{m}{2kT}\left(|\mathbf{c}|^2 + |\mathbf{c}_*|^2\right) - \frac{1}{kT}(I+I_*)}$$

$$\times \left((\mathbf{c}\cdot\mathbf{c}')^2 + (\mathbf{c}\cdot\mathbf{c}_*')^2 - (\mathbf{c}\cdot\mathbf{c})^2 - (\mathbf{c}\cdot\mathbf{c}_*)^2 \right)$$

$$\times (1-R)\,R^{s+\frac{1}{2}} \,|\mathbf{c}-\mathbf{c}_*|^{2s} \left|\boldsymbol{\omega}\cdot\frac{\mathbf{c}-\mathbf{c}_*}{|\mathbf{c}-\mathbf{c}_*|}\right| \, \mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{c}_*\,\mathrm{d}I\,\mathrm{d}\mathbf{c}.$$

As in the previous case, we first pass to the new variables (2.72). We are therefore led to express

$$\left(\mathbf{c}\cdot\mathbf{c}'\right)^2 + \left(\mathbf{c}\cdot\mathbf{c}'_*\right)^2 - \left(\mathbf{c}\cdot\mathbf{c}\right)^2 - \left(\mathbf{c}\cdot\mathbf{c}_*\right)^2$$

$$= \left(\mathbf{c}\cdot\left(\mathbf{c}'+\mathbf{c}\right)\right)\left(\mathbf{c}\cdot\left(\mathbf{c}'-\mathbf{c}\right)\right) + \left(\mathbf{c}\cdot\left(\mathbf{c}'_*+\mathbf{c}_*\right)\right)\left(\mathbf{c}\cdot\left(\mathbf{c}'_*-\mathbf{c}_*\right)\right)$$

$$= \frac{1}{2}\left\{\left(\mathbf{c}\cdot\left(2\,\mathbf{G}+\frac{1}{2}\left(\mathbf{g}'+\mathbf{g}\right)\right)\right)\left(\mathbf{c}\cdot\left(\mathbf{g}'-\mathbf{g}\right)\right) - \left(\mathbf{c}\cdot\left(2\mathbf{G}-\frac{1}{2}\left(\mathbf{g}'+\mathbf{g}\right)\right)\right)\left(\mathbf{c}\cdot\left(\mathbf{g}'-\mathbf{g}\right)\right)\right\}$$

$$= \frac{1}{2}\left(\mathbf{c}\cdot\left(\mathbf{g}'-\mathbf{g}\right)\right)\left(\mathbf{c}\cdot\left(\mathbf{g}'+\mathbf{g}\right)\right)$$

$$= \frac{1}{2}\left(\left(\mathbf{c}\cdot\mathbf{g}'\right)^2 - \left(\mathbf{c}\cdot\mathbf{g}\right)^2\right)$$

$$= \frac{1}{2}\left(\mathbf{G}\cdot\mathbf{g}'\right)^2 + \frac{1}{2}\left(\mathbf{G}\cdot\mathbf{g}'\right)\left(\mathbf{g}\cdot\mathbf{g}'\right) + \frac{1}{8}\left(\mathbf{g}\cdot\mathbf{g}'\right)^2 - \frac{1}{2}\left(\mathbf{G}\cdot\mathbf{g}\right)^2 - \frac{1}{2}\left(\mathbf{G}\cdot\mathbf{g}\right)\left|\mathbf{g}\right|^2 - \frac{1}{8}\left|\mathbf{g}\right|^4,$$

so that it can be written

$$\sum_{r,t=1}^{3}\mathcal{P}_{rtrt} = K\,2\frac{\rho^2}{m\,\zeta_0(T)^2}\left(\frac{m}{2\pi kT}\right)^3 \iint_{\mathbb{R}^3\times\mathbb{R}_+}\int_{\Omega_3}\int_{S^2} e^{-\frac{m}{kT}|\mathbf{G}|^2}e^{-\frac{m}{4kT}|\mathbf{g}|^2}e^{-\frac{1}{kT}I}e^{-\frac{1}{kT}I_*}$$

$$\times\left(\frac{1}{2}\left(\mathbf{G}\cdot\mathbf{g}'\right)^2 - \frac{1}{2}\left(\mathbf{G}\cdot\mathbf{g}\right)^2 + \frac{1}{2}\left(\mathbf{g}\cdot\mathbf{g}'\right)\left(\mathbf{G}\cdot\mathbf{g}'\right) - \frac{1}{2}\left|\mathbf{g}\right|^2\left(\mathbf{G}\cdot\mathbf{g}\right) + \frac{1}{8}\left(\mathbf{g}\cdot\mathbf{g}'\right)^2 - \frac{1}{8}\left|\mathbf{g}\right|^4\right)$$

$$\times\left(1-R\right)R^{s+\frac{1}{2}}\left|\mathbf{g}\right|^{2s}\left|\boldsymbol{\omega}\cdot\frac{\mathbf{g}}{\left|\mathbf{g}\right|}\right|\,\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I\,\mathrm{d}\mathbf{G}.$$

Integration with respect to $\mathbf{G}$ simplifies the integral which now takes the following form

$$\sum_{r,t=1}^{3}\mathcal{P}_{rtrt} = K\,2\frac{\rho^2}{m\,\zeta_0(T)^2}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}2^{-\frac{7}{2}}\int_{\mathbb{R}_+}\int_{\Omega_3}\int_{S^2} e^{-\frac{m}{4kT}|\mathbf{g}|^2}e^{-\frac{1}{kT}I}e^{-\frac{1}{kT}I_*}$$

$$\times\left(\frac{kT}{m}\left(\left|\mathbf{g}'\right|^2 - \left|\mathbf{g}\right|^2\right) + \frac{1}{2}\left(\left(\mathbf{g}\cdot\mathbf{g}'\right)^2 - \left|\mathbf{g}\right|^4\right)\right)$$

$$\times\left(1-R\right)R^{s+\frac{1}{2}}\left|\mathbf{g}\right|^{2s}\left|\boldsymbol{\omega}\cdot\frac{\mathbf{g}}{\left|\mathbf{g}\right|}\right|\,\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I.$$

Next, we pass to the $\boldsymbol{\sigma}$−notation and using (2.56), we are led to express

$$\left|\mathbf{g}'\right|^2 = \frac{4RE}{m} = R\left|\mathbf{g}\right|^2 + \frac{4R}{m}\left(I+I_*\right),$$

$$\left(\mathbf{g}\cdot\mathbf{g}'\right)^2 = \frac{4RE}{m}\left(\mathbf{g}\cdot\boldsymbol{\sigma}\right)^2 = \left(R\left|\mathbf{g}\right|^2 + \frac{4R}{m}\left(I+I_*\right)\right)\left(\mathbf{g}\cdot\boldsymbol{\sigma}\right)^2,$$

so that we can write

$$\sum_{r,t=1}^{3}\mathcal{P}_{rtrt} = K\frac{\rho^2}{m\,\zeta_0(T)^2}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}2^{-\frac{7}{2}}\int_{\mathbb{R}_+}\int_{\Omega_3}\int_{S^2} e^{-\frac{m}{4kT}|\mathbf{g}|^2}e^{-\frac{1}{kT}I}e^{-\frac{1}{kT}I_*}$$

$$\times\left\{\frac{kT}{m}\left(\left(R-1\right)\left|\mathbf{g}\right|^2 + \frac{4R}{m}\left(I+I_*\right)\right) + \frac{1}{2}\left(\left(R\left|\mathbf{g}\right|^2 + \frac{4R}{m}\left(I+I_*\right)\right)\left(\mathbf{g}\cdot\boldsymbol{\sigma}\right)^2 - \left|\mathbf{g}\right|^4\right)\right\}$$

$$\times\left(1-R\right)R^{s+\frac{1}{2}}\left|\mathbf{g}\right|^{2s}\,\mathrm{d}\boldsymbol{\sigma}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I.$$

The integration with respect to $\boldsymbol{\sigma}$ gives

$$\sum_{r,t=1}^{3}\mathcal{P}_{rtrt} = K\frac{\rho^2}{m\,\zeta_0(T)^2}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}2^{-\frac{3}{2}}\pi\int_{\mathbb{R}_+}\int_{\Omega_3} e^{-\frac{m}{4kT}|\mathbf{g}|^2}e^{-\frac{1}{kT}I}e^{-\frac{1}{kT}I_*}$$

$$\times\left\{\frac{kT}{m}\left(\left(R-1\right)\left|\mathbf{g}\right|^2 + \frac{4R}{m}\left(I+I_*\right)\right) + \frac{1}{2}\left(\left(\frac{R}{3}-1\right)\left|\mathbf{g}\right|^4 + \frac{4R}{3\,m}\left(I+I_*\right)\left|\mathbf{g}\right|^2\right)\right\}$$

$$\times\left(1-R\right)R^{s+\frac{1}{2}}\left|\mathbf{g}\right|^{2s}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I.$$

Now, we integrate with respect to I and I_*

$$\sum_{r,t=1}^{3} \mathcal{P}_{rtrt} = K \frac{\rho^2}{m\,\zeta_0(T)^2} \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} 2^{-\frac{3}{2}} \pi\,(k\,T)^2 \int_{\mathbb{R}^3} \int_{[0,1]} \int_{[0,1]} e^{-\frac{m}{4kT}|\mathbf{g}|^2}$$
$$\times \left\{ \frac{kT}{m} \left((R-1)\,|\mathbf{g}|^2 + \frac{8\,k\,T}{m} R \right) + \frac{1}{2} \left(\left(\frac{R}{3} - 1\right) |\mathbf{g}|^4 + \frac{8\,k\,T}{3\,m} R\,|\mathbf{g}|^2 \right) \right\}$$
$$\times (1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}\mathbf{g}.$$

Integration with respect to r and R gives

$$\sum_{r,t=1}^{3} \mathcal{P}_{rtrt} = K \frac{\rho^2}{m\,\zeta_0(T)^2} \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \sqrt{2}\,\pi\,(k\,T)^2 \frac{1}{(2s+5)\,(2s+7)} \int_{\mathbb{R}^3} |\mathbf{g}|^{2s}\,e^{-\frac{m}{4kT}|\mathbf{g}|^2}$$
$$\times \left\{ \frac{kT}{m} \left(\left(-\frac{4}{(2s+3)}\right) |\mathbf{g}|^2 + \frac{8\,k\,T}{m} \right) - \frac{(2s+9)}{3\,(2s+3)} |\mathbf{g}|^4 + \frac{4\,k\,T}{3\,m} |\mathbf{g}|^2 \right\}\,\mathrm{d}\mathbf{g}.$$

Passage to spherical coordinate yields

$$\sum_{r,t=1}^{3} \mathcal{P}_{rtrt} = K \frac{\rho^2}{m\,\zeta_0(T)^2} \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \sqrt{2}\,\pi^2\,(k\,T)^2 \frac{4}{(2s+5)\,(2s+7)}$$
$$\times \int_{\mathbb{R}_+} e^{-\frac{m}{4kT}|\mathbf{g}|^2} \left(-\frac{(2s+9)}{3\,(2s+3)} |\mathbf{g}|^{2s+6} + \frac{8s}{3\,(2s+3)} \left(\frac{kT}{m}\right) |\mathbf{g}|^{2s+4} + 8 \left(\frac{kT}{m}\right)^2 |\mathbf{g}|^{2s+2} \right)\,\mathrm{d}\,|\mathbf{g}|.$$

Applying the change of variable (2.75) we obtain the following result

$$\sum_{r,t=1}^{3} \mathcal{P}_{rtrt} = K \frac{\rho^2}{m\,\zeta_0(T)^2} \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \sqrt{2}\,\pi^2\,(k\,T)^2 \frac{4}{(2s+5)\,(2s+7)}$$
$$\times \frac{1}{2} \int_{\mathbb{R}_+} e^{-x} \left(-\frac{(2s+9)}{3\,(2s+3)} \left(\frac{m}{4\,k\,T}\right)^{-s-\frac{7}{2}} x^{s+\frac{5}{2}} + \frac{8s}{3\,(2s+3)} \left(\frac{kT}{m}\right) \left(\frac{m}{4\,k\,T}\right)^{-s-\frac{5}{2}} x^{s+\frac{3}{2}} \right.$$
$$\left. +8 \left(\frac{kT}{m}\right)^2 \left(\frac{m}{4\,k\,T}\right)^{-s-\frac{3}{2}} x^{s+\frac{1}{2}} \right)\,\mathrm{d}x.$$

Now, the factorization leads to

$$\sum_{r,t=1}^{3} \mathcal{P}_{rtrt} = K \frac{\rho^2}{m\,\zeta_0(T)^2} \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \sqrt{2}\,\pi^2\,(k\,T)^2 \frac{4}{(2s+5)\,(2s+7)}$$
$$\times 2^{2s+6} \left(\frac{k\,T}{m}\right)^{s+\frac{7}{2}} \int_{\mathbb{R}_+} e^{-x} \left(-\frac{(2s+9)}{3\,(2s+3)} x^{s+\frac{7}{2}-1} + \frac{2s}{3\,(2s+3)} x^{s+\frac{5}{2}-1} + \frac{1}{2} x^{s+\frac{3}{2}-1} \right)\,\mathrm{d}x.$$

Comparing the last integrals with the definition of the gamma function, we obtain

$$\sum_{r,t=1}^{3} \mathcal{P}_{rtrt} = K \frac{\rho^2}{m^3\,\zeta_0(T)^2} (k\,T)^4 \sqrt{\pi} \left(\frac{k\,T}{m}\right)^s \frac{2^{2s+7}}{(2s+5)\,(2s+7)}$$
$$\times \left(-\frac{(2s+9)}{3\,(2s+3)} \Gamma\left[s+\frac{7}{2}\right] + \frac{2s}{3\,(2s+3)} \Gamma\left[s+\frac{5}{2}\right] + \frac{1}{2} \Gamma\left[s+\frac{3}{2}\right] \right).$$

Using the property of the gamma function $\Gamma\,(z+1) = z\Gamma\,(z)$ we get the following result

$$\sum_{r,t=1}^{3} \mathcal{P}_{rtrt} = K \frac{\rho^2}{m^3\,\zeta_0(T)^2} (k\,T)^4 \sqrt{\pi} \left(\frac{k\,T}{m}\right)^s \frac{2^{2s+7}}{(2s+5)\,(2s+7)} \Gamma\left[s+\frac{3}{2}\right] \left(-\frac{(2s+9)\,(2s+5)}{12} + \frac{s}{3} + \frac{1}{2} \right),$$

which leads to the final expression

$$(2.77) \qquad \sum_{r,t=1}^{3} \mathcal{P}_{rtrt} = -K \frac{2^{2s+5}(39 + 4s(s+6))}{3(2s+5)(2s+7)} \frac{m\,p^4}{\rho^2 \zeta_0(T)^2} \sqrt{\pi} \left(\frac{kT}{m}\right)^s \Gamma\left[s + \frac{3}{2}\right].$$

Injection of the computed integrals (2.76) and (2.77) into (2.70) allows us to write the final expression for the linearized production term which corresponds to the equation for the flux of momentum:
(2.78)
$$\overline{P}_{ij}^{14} = -K \frac{2^{2s+4}\rho\,(kT)^2}{15\,m\,\zeta_0(T)^2} \sqrt{\pi} \left(\frac{kT}{m}\right)^s \Gamma\left[s + \frac{3}{2}\right] \left(p_{\langle ij \rangle} + \frac{20}{(2s+5)(2s+7)}\left(\alpha + \frac{5}{2}\right)(\alpha+1)^{-1}\Pi\delta_{ij}\right),$$

which completes the first part of the proof.

In order to compute production term $\overline{Q}_i^{14}$, the following integral has to be computed:

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K\,2\frac{\rho^2}{m^2\,\zeta_0(T)^2}\left(\frac{m}{2\,\pi\,kT}\right)^3 \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \int_{\Omega_3} \int_{S^2} \left(\frac{m}{2}\,|\mathbf{c}|^2 + I\right) e^{-\frac{m}{2kT}\left(|\mathbf{c}|^2 + |\mathbf{c}_*|^2\right) - \frac{1}{kT}(I + I_*)}$$
$$\times \left(\left(\frac{m}{2}\,|\mathbf{c}'|^2 + I'\right)\mathbf{c}' \cdot \mathbf{c} + \left(\frac{m}{2}\,|\mathbf{c}_*'|^2 + I_*'\right)\mathbf{c}_*' \cdot \mathbf{c} - \left(\frac{m}{2}\,|\mathbf{c}|^2 + I\right)\mathbf{c} \cdot \mathbf{c} - \left(\frac{m}{2}\,|\mathbf{c}_*|^2 + I_*\right)\mathbf{c}_* \cdot \mathbf{c}\right)$$
$$\times (1 - R)\,R^{s + \frac{1}{2}}\,|\mathbf{c} - \mathbf{c}_*|^{2s}\left|\boldsymbol{\omega} \cdot \frac{\mathbf{c} - \mathbf{c}_*}{|\mathbf{c} - \mathbf{c}_*|}\right|\,d\boldsymbol{\omega}dr\,dR\,dI_*\,d\mathbf{c}_*\,dI\,d\mathbf{c}.$$

We are led to pass to the variables (2.72). Indeed, let us express terms appearing in the integral above:

$$\mathbf{c} \cdot \left(\frac{m}{2}\left(|\mathbf{c}'|^2\,\mathbf{c}' + |\mathbf{c}_*'|^2\,\mathbf{c}_*' - |\mathbf{c}|^2\,\mathbf{c} - |\mathbf{c}_*|^2\,\mathbf{c}_*\right) + \left(I'\mathbf{c}' + I_*'\mathbf{c}_*' - I\mathbf{c} - I_*\mathbf{c}_*\right)\right)$$
$$= \mathbf{c} \cdot \left(\frac{m}{2}\left(|\mathbf{c}'|^2\left(\mathbf{G} + \frac{1}{2}\mathbf{g}'\right) + |\mathbf{c}_*'|^2\left(\mathbf{G} - \frac{1}{2}\mathbf{g}'\right) - |\mathbf{c}|^2\left(\mathbf{G} + \frac{1}{2}\mathbf{g}\right) - |\mathbf{c}_*|^2\left(\mathbf{G} - \frac{1}{2}\mathbf{g}\right)\right)\right.$$
$$\left. + \left(I'\left(\mathbf{G} + \frac{1}{2}\mathbf{g}'\right) + I_*'\left(\mathbf{G} - \frac{1}{2}\mathbf{g}'\right) - I\left(\mathbf{G} + \frac{1}{2}\mathbf{g}\right) - I_*\left(\mathbf{G} - \frac{1}{2}\mathbf{g}\right)\right)\right)$$
$$= \mathbf{c} \cdot \left(\mathbf{G}\left(\frac{m}{2}\left(|\mathbf{c}'|^2 + |\mathbf{c}_*'|^2 - |\mathbf{c}|^2 - |\mathbf{c}_*|^2\right) + I' + I_*' - I - I_*\right)\right.$$
$$\left. + \frac{m}{4}\left(\mathbf{g}'\left(|\mathbf{c}'|^2 - |\mathbf{c}_*'|^2\right) - \mathbf{g}\left(|\mathbf{c}|^2 - |\mathbf{c}_*|^2\right)\right) + \frac{1}{2}\mathbf{g}'\left(I' - I_*'\right) - \frac{1}{2}\mathbf{g}\left(I - I_*\right)\right)$$
$$= \mathbf{c} \cdot \left(\frac{m}{4}\left(\mathbf{g}'\left((\mathbf{c}' - \mathbf{c}_*') \cdot (\mathbf{c}' + \mathbf{c}_*')\right) - \mathbf{g}\left((\mathbf{c} - \mathbf{c}_*) \cdot (\mathbf{c} + \mathbf{c}_*)\right)\right) + \frac{1}{2}\mathbf{g}'\left(I' - I_*'\right) - \frac{1}{2}\mathbf{g}\left(I - I_*\right)\right)$$
$$= \left(\mathbf{G} + \frac{1}{2}\mathbf{g}\right) \cdot \left(\frac{m}{4}\left(\mathbf{g}'\left(\mathbf{g}' \cdot 2\mathbf{G}\right) - \mathbf{g}\left(\mathbf{g} \cdot 2\mathbf{G}\right)\right) + \frac{1}{2}\mathbf{g}'\left(I' - I_*'\right) - \frac{1}{2}\mathbf{g}\left(I - I_*\right)\right)$$
$$= \frac{m}{2}\left(\mathbf{g}' \cdot \mathbf{G}\right)^2 - \frac{m}{2}\left(\mathbf{g} \cdot \mathbf{G}\right)^2 + \frac{m}{4}\left(\mathbf{g} \cdot \mathbf{g}'\right)\left(\mathbf{g}' \cdot \mathbf{G}\right) - \frac{m}{4}\,|\mathbf{g}|^2\left(\mathbf{g} \cdot \mathbf{G}\right)$$
$$+ \frac{1}{2}\left(I' - I_*'\right)\left(\mathbf{g}' \cdot \mathbf{G} + \frac{1}{2}\mathbf{g} \cdot \mathbf{g}'\right) - \frac{1}{2}\left(I - I_*\right)\left(\mathbf{g} \cdot \mathbf{G} + \frac{1}{2}\,|\mathbf{g}|^2\right),$$

which in conjunction with (2.74), yields

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K \, 2 \frac{\rho^2}{m^2 \, \zeta_0(T)^2} \left(\frac{m}{2\,\pi\,kT}\right)^3 \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \int_{\Omega_3} \int_{S^2} e^{-\frac{m}{kT}|\mathbf{G}|^2} e^{-\frac{m}{4kT}|\mathbf{g}|^2} e^{-\frac{1}{kT}I} e^{-\frac{1}{kT}I_*}$$

$$\left(\frac{m}{2}\,\mathbf{g}\cdot\mathbf{G} + \frac{m}{2}\,|\mathbf{G}|^2 + \frac{m}{8}\,|\mathbf{g}|^2 + I\right)$$

$$\times \left\{ \frac{m}{2}\left(\mathbf{g}'\cdot\mathbf{G}\right)^2 - \frac{m}{2}\left(\mathbf{g}\cdot\mathbf{G}\right)^2 + \frac{m}{4}\left(\mathbf{g}\cdot\mathbf{g}'\right)\left(\mathbf{g}'\cdot\mathbf{G}\right) - \frac{m}{4}\,|\mathbf{g}|^2\left(\mathbf{g}\cdot\mathbf{G}\right)\right.$$

$$\left. + \frac{1}{2}\left(I' - I_*'\right)\left(\mathbf{g}'\cdot\mathbf{G} + \frac{1}{2}\mathbf{g}\cdot\mathbf{g}'\right) - \frac{1}{2}\left(I - I_*\right)\left(\mathbf{g}\cdot\mathbf{G} + \frac{1}{2}\,|\mathbf{g}|^2\right)\right\}$$

$$\times (1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\left|\boldsymbol{\omega}\cdot\frac{\mathbf{g}}{|\mathbf{g}|}\right|\,\mathrm{d}\boldsymbol{\omega}\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I\,\mathrm{d}\mathbf{G}.$$

Considering integral with respect to $\mathbf{G}$, we first discard all vanishing terms due to parity

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K \, 2 \frac{\rho^2}{m^2 \, \zeta_0(T)^2} \left(\frac{m}{2\,\pi\,kT}\right)^3 \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \int_{\Omega_3} \int_{S^2} e^{-\frac{m}{kT}|\mathbf{G}|^2} e^{-\frac{m}{4kT}|\mathbf{g}|^2} e^{-\frac{1}{kT}I} e^{-\frac{1}{kT}I_*}$$

$$\left(\frac{m}{2}\,\mathbf{g}\cdot\mathbf{G}\left\{\frac{m}{4}\left(\mathbf{g}\cdot\mathbf{g}'\right)\left(\mathbf{g}'\cdot\mathbf{G}\right) - \frac{m}{4}\,|\mathbf{g}|^2\left(\mathbf{g}\cdot\mathbf{G}\right) + \frac{1}{2}\left(I'-I_*'\right)\mathbf{g}'\cdot\mathbf{G} - \frac{1}{2}\left(I-I_*\right)\mathbf{g}\cdot\mathbf{G}\right\}\right.$$

$$+ \frac{m}{2}\,|\mathbf{G}|^2\left\{\frac{m}{2}\left(\mathbf{g}'\cdot\mathbf{G}\right)^2 - \frac{m}{2}\left(\mathbf{g}\cdot\mathbf{G}\right)^2 + \frac{1}{4}\left(I'-I_*'\right)\mathbf{g}\cdot\mathbf{g}' - \frac{1}{4}\left(I-I_*\right)|\mathbf{g}|^2\right\}$$

$$+ \left(\frac{m}{8}\,|\mathbf{g}|^2 + I\right)\left\{\frac{m}{2}\left(\mathbf{g}'\cdot\mathbf{G}\right)^2 - \frac{m}{2}\left(\mathbf{g}\cdot\mathbf{G}\right)^2 + \frac{1}{4}\left(I'-I_*'\right)\mathbf{g}\cdot\mathbf{g}' - \frac{1}{4}\left(I-I_*\right)|\mathbf{g}|^2\right\}\right)$$

$$\times (1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\left|\boldsymbol{\omega}\cdot\frac{\mathbf{g}}{|\mathbf{g}|}\right|\,\mathrm{d}\boldsymbol{\omega}\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I\,\mathrm{d}\mathbf{G},$$

and then

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K \, 2 \frac{\rho^2}{m^2 \, \zeta_0(T)^2} \left(\frac{m}{2\,\pi\,kT}\right)^3 \int_{\mathbb{R}_+} \int_{\Omega_3} \int_{S^2} e^{-\frac{m}{4kT}|\mathbf{g}|^2} e^{-\frac{1}{kT}I} e^{-\frac{1}{kT}I_*}$$

$$\left(\frac{m}{4}\,\pi^{\frac{3}{2}}\left(\frac{kT}{m}\right)^{\frac{5}{2}}\left\{\frac{m}{4}\left(\left(\mathbf{g}\cdot\mathbf{g}'\right)^2 - |\mathbf{g}|^4\right) + \frac{1}{2}\left(I'-I_*'\right)\mathbf{g}\cdot\mathbf{g}' - \frac{1}{2}\left(I-I_*\right)|\mathbf{g}|^2\right\}\right.$$

$$+ \frac{m}{8}\pi^{\frac{3}{2}}\left(\frac{kT}{m}\right)^{\frac{5}{2}}\left\{\frac{5}{2}kT\left(|\mathbf{g}'|^2 - |\mathbf{g}|^2\right) + \frac{3}{2}\left(\left(I'-I_*'\right)\mathbf{g}\cdot\mathbf{g}' - \left(I-I_*\right)|\mathbf{g}|^2\right)\right\}$$

$$+ \left(\frac{m}{8}\,|\mathbf{g}|^2 + I\right)\pi^{\frac{3}{2}}\left(\frac{kT}{m}\right)^{\frac{3}{2}}\left\{\frac{kT}{4}\left(|\mathbf{g}'|^2 - |\mathbf{g}|^2\right) + \frac{1}{4}\left(I'-I_*'\right)\mathbf{g}\cdot\mathbf{g}' - \frac{1}{4}\left(I-I_*\right)|\mathbf{g}|^2\right\}\right)$$

$$\times (1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\left|\boldsymbol{\omega}\cdot\frac{\mathbf{g}}{|\mathbf{g}|}\right|\,\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I.$$

A rearrangement yields the following integral

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K\, 2\frac{\rho^2}{m^2\, \zeta_0(T)^2}\frac{1}{8}\left(\frac{m}{\pi\, k\, T}\right)^{\frac{3}{2}}\int_{\mathbb{R}_+}\int_{\Omega_3}\int_{S^2}e^{-\frac{m}{4kT}|\mathbf{g}|^2}e^{-\frac{1}{kT}I}e^{-\frac{1}{kT}I_*}$$

$$\left(\frac{1}{4}\left(\frac{5}{4}k\,T + \frac{m}{8}\,|\mathbf{g}|^2 + I\right)\left((I'-I'_*)\,\mathbf{g}\cdot\mathbf{g}' - (I-I_*)\,|\mathbf{g}|^2\right)\right.$$

$$+\frac{m\,k\,T}{32}\left(|\mathbf{g}|^2\left(|\mathbf{g}'|^2 - 3\,|\mathbf{g}|^2\right) + 2\left(\mathbf{g}\cdot\mathbf{g}'\right)^2\right)$$

$$\left.+\left(\frac{1}{4}I + \frac{5}{16}k\,T\right)k\,T\left(|\mathbf{g}'|^2 - |\mathbf{g}|^2\right)\right)$$

$$\times\, (1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\left|\boldsymbol{\omega}\cdot\frac{\mathbf{g}}{|\mathbf{g}|}\right|\,\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I.$$

Next, we pass to the $\boldsymbol{\sigma}$−representation with Jacobian (1.36). Recalling (2.73) and (2.56), we express

$$\left|\mathbf{g}'\right|^2 = R\,|\mathbf{g}|^2 + \frac{4\,R}{m}\,(I+I_*),$$

$$\mathbf{g}\cdot\mathbf{g}' = 2\sqrt{\frac{R\,E}{m}}\mathbf{g}\cdot\boldsymbol{\sigma},$$

$$\left(\mathbf{g}\cdot\mathbf{g}'\right)^2 = \left(R\,|\mathbf{g}|^2 + \frac{4\,R}{m}\,(I+I_*)\right)(\mathbf{g}\cdot\boldsymbol{\sigma})^2.$$

and consequently consider the following integral

$$\sum_{r=1}^{3}\mathcal{Q}_{rr} = K\frac{\rho^2}{m^2\,\zeta_0(T)^2}\frac{1}{8}\left(\frac{m}{\pi\,k\,T}\right)^{\frac{3}{2}}\int_{\mathbb{R}_+}\int_{\Omega_3}\int_{S^2}e^{-\frac{m}{4kT}|\mathbf{g}|^2}e^{-\frac{1}{kT}I}e^{-\frac{1}{kT}I_*}$$

$$\left(-\frac{1}{4}\left(\frac{5}{4}k\,T + \frac{m}{8}\,|\mathbf{g}|^2 + I\right)(I-I_*)\,|\mathbf{g}|^2\right.$$

$$+\frac{m\,k\,T}{32}\left(|\mathbf{g}|^2\left((R-3)\,|\mathbf{g}|^2 + \frac{4\,R}{m}\,(I+I_*)\right) + 2\left(R\,|\mathbf{g}|^2 + \frac{4\,R}{m}\,(I+I_*)\right)(\mathbf{g}\cdot\boldsymbol{\sigma})^2\right)$$

$$\left.+\left(\frac{1}{4}I + \frac{5}{16}k\,T\right)k\,T\left((R-1)\,|\mathbf{g}|^2 + \frac{4\,R}{m}\,(I+I_*)\right)\right)$$

$$\times\,(1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\,\mathrm{d}\boldsymbol{\sigma}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I.$$

Integration with respect to $\boldsymbol{\sigma}$ is easy and we are led to proceed in that direction:

$$\sum_{r=1}^{3}\mathcal{Q}_{rr} = K\frac{\rho^2}{m^2\,\zeta_0(T)^2}\frac{\pi}{2}\left(\frac{m}{\pi\,k\,T}\right)^{\frac{3}{2}}\int_{\mathbb{R}_+}\int_{\Omega_3}e^{-\frac{m}{4kT}|\mathbf{g}|^2}e^{-\frac{1}{kT}I}e^{-\frac{1}{kT}I_*}$$

$$\left\{-\frac{1}{4}\left(\frac{5}{4}k\,T + \frac{m}{8}\,|\mathbf{g}|^2 + I\right)(I-I_*)\,|\mathbf{g}|^2 + \frac{m\,k\,T}{32}\,|\mathbf{g}|^2\left(\left(\frac{5}{3}R - 3\right)|\mathbf{g}|^2 + \frac{20\,R}{3\,m}\,(I+I_*)\right)\right.$$

$$\left.+\left(\frac{1}{4}I + \frac{5}{16}k\,T\right)k\,T\left((R-1)\,|\mathbf{g}|^2 + \frac{4\,R}{m}\,(I+I_*)\right)\right\}\times\,(1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I.$$

Next, integration with respect to I and I_* yields

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K \frac{\rho^2}{m^2\,\zeta_0(T)^2} \frac{\pi}{2} \left(\frac{m}{\pi\,k\,T}\right)^{\frac{3}{2}} \int_{\mathbb{R}^3} \int_{[0,1]} \int_{[0,1]} e^{-\frac{m}{4kT}|\mathbf{g}|^2}$$

$$\left\{ -\frac{1}{4}\,(k\,T)^4\,|\mathbf{g}|^2 + \frac{m\,k\,T}{32}\,|\mathbf{g}|^2 \left(\left(\frac{5}{3}R - 3\right)(k\,T)^2\,|\mathbf{g}|^2 + \frac{40\,R}{3\,m}\,(k\,T)^3 \right) \right.$$

$$+ \left(\frac{1}{4}k\,T \left((R-1)\,(k\,T)^3\,|\mathbf{g}|^2 + \frac{12\,R}{m}\,(k\,T)^4 \right) \right.$$

$$\left. + \frac{5}{16}\,(k\,T)^2 \left((R-1)\,(k\,T)^2\,|\mathbf{g}|^2 + \frac{8\,R}{m}\,(k\,T)^3 \right) \right) \right\} \times (1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}\mathbf{g}.$$

A rearrangement leads to

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K \frac{\rho^2}{m^2\,\zeta_0(T)^2} \frac{\pi}{2} \left(\frac{m}{\pi\,k\,T}\right)^{\frac{3}{2}} (k\,T)^3 \int_{\mathbb{R}^3} \int_{[0,1]} \int_{[0,1]} e^{-\frac{m}{4kT}|\mathbf{g}|^2}$$

$$\left(\frac{m}{32}\left(\frac{5}{3}R - 3\right)|\mathbf{g}|^4 + k\,T\left(\frac{47}{48}R - \frac{13}{16}\right)|\mathbf{g}|^2 + \frac{11}{2}\,(k\,T)^2\,\frac{R}{m} \right)(1-R)\,R^{s+\frac{1}{2}}\,|\mathbf{g}|^{2s}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}\mathbf{g}.$$

Integration with respect to r and R gives the following result

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K \frac{\rho^2}{m^2\,\zeta_0(T)^2} \pi \left(\frac{m}{\pi\,k\,T}\right)^{\frac{3}{2}} (k\,T)^3 \frac{2}{(2s+5)} \int_{\mathbb{R}^3} |\mathbf{g}|^{2s}\,e^{-\frac{m}{4kT}|\mathbf{g}|^2}$$

$$\left(\frac{m}{32}\left(\frac{5}{3\,(2s+7)} - \frac{3}{(2s+3)}\right)|\mathbf{g}|^4 + k\,T\left(\frac{47}{48\,(2s+7)} - \frac{13}{16\,(2s+3)}\right)|\mathbf{g}|^2 + \frac{(k\,T)^2}{m}\frac{11}{2\,(2s+7)} \right)\mathrm{d}\mathbf{g}.$$

A rearrangement and a passage to the spherical coordinates lead to

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K \frac{\rho^2}{m^2\,\zeta_0(T)^2} \pi^2 \left(\frac{m}{\pi\,k\,T}\right)^{\frac{3}{2}} (k\,T)^3 \frac{8}{(2s+5)} \int_{\mathbb{R}_+} e^{-\frac{m}{4kT}|\mathbf{g}|^2}$$

$$\left(-m\frac{(s+6)}{12\,(2s+3)\,(2s+7)}\,|\mathbf{g}|^{2s+6} + k\,T\frac{(4s-33)}{12\,(2s+3)\,(2s+7)}\,|\mathbf{g}|^{2s+4} + \frac{(k\,T)^2}{m}\frac{11}{2\,(2s+7)}\,|\mathbf{g}|^{2s+2} \right)\mathrm{d}|\mathbf{g}|.$$

Now, we perform the change of variable (2.75)

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K \frac{\rho^2}{m^2\,\zeta_0(T)^2} \pi^2 \left(\frac{m}{\pi\,k\,T}\right)^{\frac{3}{2}} (k\,T)^3 \frac{8}{(2s+5)\,(2s+7)}$$

$$\times \frac{1}{2} \int_{\mathbb{R}_+} e^{-x} \left(-m\frac{(s+6)}{12\,(2s+3)} \left(\frac{m}{4\,k\,T}\right)^{-s-\frac{7}{2}} x^{s+\frac{5}{2}} + \left(k\,T\frac{(4s-33)}{12\,(2s+3)} \right)\left(\frac{m}{4\,k\,T}\right)^{-s-\frac{5}{2}} x^{s+\frac{3}{2}} \right.$$

$$\left. + \frac{(k\,T)^2}{m}\frac{11}{2}\left(\frac{m}{4\,k\,T}\right)^{-s-\frac{3}{2}} x^{s+\frac{1}{2}} \right)\mathrm{d}x.$$

A factorization yields the following integral

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K \frac{\rho^2}{m^2\,\zeta_0(T)^2} \pi^2 \left(\frac{m}{\pi\,k\,T}\right)^{\frac{3}{2}} (k\,T)^3 \frac{8}{(2s+5)\,(2s+7)}$$

$$\times m\,2^{2s+6} \left(\frac{k\,T}{m}\right)^{s+\frac{7}{2}} \int_{\mathbb{R}_+} e^{-x} \left(-\frac{(s+6)}{12\,(2s+3)} x^{s+\frac{7}{2}-1} + \frac{(4s-33)}{48\,(2s+3)} x^{s+\frac{5}{2}-1} + \frac{11}{32} x^{s+\frac{3}{2}-1} \right)\mathrm{d}x.$$

Comparing to the definition of gamma function, we obtain

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K \frac{\rho^2}{m^3 \zeta_0(T)^2} (kT)^5 \sqrt{\pi} \left(\frac{kT}{m}\right)^s \frac{2^{2s+9}}{(2s+5)(2s+7)}$$
$$\times \left(-\frac{(s+6)}{12(2s+3)} \Gamma\left[s+\frac{7}{2}\right] + \frac{(4s-33)}{48(2s+3)} \Gamma\left[s+\frac{5}{2}\right] + \frac{11}{32} \Gamma\left[s+\frac{3}{2}\right]\right),$$

and then using the property of the gamma function $\Gamma[x+1] = x\Gamma[x]$ yields

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = K \frac{\rho^2}{m^3 \zeta_0(T)^2} (kT)^5 \sqrt{\pi} \left(\frac{kT}{m}\right)^s \frac{2^{2s+9}}{(2s+5)(2s+7)}$$
$$\times \Gamma\left[s+\frac{3}{2}\right] \left(-\frac{(s+6)(2s+5)}{48} + \frac{(4s-33)}{96} + \frac{11}{32}\right).$$

Using (1.94) we can rearrange once more

$$\sum_{r=1}^{3} \mathcal{Q}_{rr} = -K \frac{(kT)^2}{\zeta_0(T)^2} \frac{p^3}{\rho} \sqrt{\pi} \left(\frac{kT}{m}\right)^s \frac{2^{2s+5}(s(2s+15)+30)}{3(2s+5)(2s+7)} \Gamma\left[s+\frac{3}{2}\right].$$

Finally, insertion of this result into (2.71) together with (2.78) lead to the expression for the linearized source term corresponding to the equation for the heat flux in the 14-moments approximation:

$$\overline{Q}_i^{14} = \sum_{k=1}^{3} u_k \overline{P}_{ik}^{14} - K \left(\frac{7}{2} + \alpha\right)^{-1} \frac{2^{2s+5}(s(2s+15)+30)}{9(2s+5)(2s+7)} \frac{\rho(kT)^2}{m\zeta_0(T)^2} \sqrt{\pi} \left(\frac{kT}{m}\right)^s \Gamma\left[s+\frac{3}{2}\right] q_i.$$

This completes the proof. □

Transport coefficients. The results obtained here are a consequence of the model of interaction between the molecules. The production terms thus represent the macroscopic dissipative effects. However, their structure reflects the mesoscopic mechanism of interaction without any prior recourse to phenomenological relations.

Since the maximization of entropy and extended thermodynamics obtain the same set of moment equations, it enables explicit computation of the relaxation times of the extended thermodynamics model, τ_S for viscous stress, τ_Π for dynamic pressure and τ_q for heat flux, from our production terms. Indeed, It is in the spirit of extended thermodynamics, as well as the theory of hyperbolic systems of balance laws, to recast the production terms in the following form:

$$P_{ij}^{14} = \frac{1}{\tau_s} p_{\langle ij \rangle} + \frac{1}{\tau_\Pi} \Pi \delta_{ij}, \quad Q_i^{14} = u_k P_{ik}^{14} - \frac{1}{\tau_q} q_i,$$

where τ_s, τ_Π and τ_q are appropriate relaxation times. They estimate the rate of decay of non-equilibrium quantities. It is easy to recognize from (2.64)-(2.65) that:

$$\frac{1}{\tau_s} = K \frac{2^{2s+4}}{15} \frac{\rho(kT)^2}{m\zeta_0(T)^2} \sqrt{\pi} \left(\frac{kT}{m}\right)^s \Gamma\left[s+\frac{3}{2}\right],$$

$$\frac{1}{\tau_\Pi} = K \left(\alpha + \frac{5}{2}\right)(\alpha+1)^{-1} \frac{2^{2s+6}}{3(2s+5)(2s+7)} \frac{\rho(kT)^2}{m\zeta_0(T)^2} \sqrt{\pi} \left(\frac{kT}{m}\right)^s \Gamma\left[s+\frac{3}{2}\right],$$

$$\frac{1}{\tau_q} = K \left(\frac{7}{2} + \alpha\right)^{-1} \frac{2^{2s+5}(s(2s+15)+30)}{9(2s+5)(2s+7)} \frac{\rho(kT)^2}{m\zeta_0(T)^2} \sqrt{\pi} \left(\frac{kT}{m}\right)^s \Gamma\left[s+\frac{3}{2}\right].$$

On the other hand, it was shown [9] that the relaxation times can be related to the transport coefficients – shear viscosity μ, bulk viscosity ν, and heat conductivity κ:

$$\mu = p\tau_S, \quad \nu = \frac{4(1+\alpha)}{3(5+2\alpha)} p\tau_\Pi, \quad \kappa = \left(\alpha + \frac{7}{2}\right) \frac{p^2}{\rho T} \tau_q,$$

so that one obtains:

$$\mu = \frac{15}{2^{2s+4}} \frac{m^s}{\sqrt{\pi} K \Gamma\left[s + \frac{3}{2}\right]} (kT)^{-s-1} q(T)^2,$$

$$(2.79) \qquad \nu = \frac{(\alpha+1)^2}{(2\alpha+5)^2} \frac{(2s+5)(2s+7)}{2^{2s+3}} \frac{m^s}{\sqrt{\pi} K \Gamma\left[s + \frac{3}{2}\right]} (kT)^{-s-1} q(T)^2,$$

$$\kappa = \left(\alpha + \frac{7}{2}\right)^2 \frac{9(2s+5)(2s+7)}{2^{2s+5}(s(2s+15)+30)} \frac{k}{m} \frac{m^s}{\sqrt{\pi} K \Gamma\left[s + \frac{3}{2}\right]} (kT)^{-s-1} q(T).$$

Although we arrived at (2.79) by an *ad-hoc* procedure, in contrast to the standard asymptotic methods like Chapman-Enskog one, it gives some hint impression about the dependence of transport coefficients with respect to the collision model.

In [3] results similar to (2.79) were obtained in the special case $s = 0$. Generalized form of the transport coefficients, obtained in [4], leaves the possibility to adapt the collision cross section and match certain macroscopic quantities. For example, we can choose s to obtain the appropriate value of Prandtl number, $\mathrm{Pr} = c_p \mu / \kappa$. A theoretically obtained value for Prandtl number for polyatomic gases is given by Eucken's relation, $\mathrm{Pr} = 4\gamma/(9\gamma - 5)$, while from (2.79) one obtains:

$$\mathrm{Pr} = \left(\alpha + \frac{7}{2}\right)^{-1} \frac{10(s(2s+15)+30)}{3(2s+5)(2s+7)}.$$

Matching these two relations, with the aid of the restriction $s > -3/2$, the following values of parameter s are obtained:

TABLE 2.1. Prandtl number and values of the parameter s

Gas	γ	α	Pr	s
diatomic	7/5	0	28/38	0.678
three-atomic	4/3	1/2	16/21	−0.311

Since we only have one free parameter in the model, we can adapt it to match only one macroscopic quantity, while for the others we may expect just better or worse matching. One of these important properties is the dependence of the viscosity with respect to the temperature, for which it is easy to determine from $(2.79)_1$ that $\mu \propto T^{2\alpha+s-1}$. For the values from Table 2.1 one can determine that one obtains $\mu \propto T^{0.322}$ for diatomic gases, and $\mu \propto T^{2.311}$ for three-atomic gases, both results being unsatisfactory when compared with experiment.

However, a different strategy can be applied: first to adapt s to match the temperature dependence, and then to compute the corresponding Prandtl number. According to [25], for CO one has $\mu \propto T^{0.734}$, which gives $s = 0.262$ and yields $\mathrm{Pr} = 0.781$, which is in satisfactory agreement with the theoretical value for diatomic gases ($\mathrm{Pr} = 0.737$ from Table 2.1). For three-atomic gases the results are a bit worse.

Entropy density and entropy flux. Another important feature which we need to discuss is the structure of entropy density and entropy flux for non-equilibrium distribution (2.41). Macroscopic entropy is defined by (2.21):

$$(2.80) \qquad h = \rho s = -k \int_{\mathbb{R}^3} \int_0^\infty f \log f \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v},$$

while entropy flux has the form:

$$(2.81) \qquad h_j = \rho s u_j + \tilde{h}_j, \quad \tilde{h}_j = -k \int_{\mathbb{R}^3} \int_0^\infty c_j f \log f \, \varphi(I) \, \mathrm{d}I \, \mathrm{d}\mathbf{v},$$

where $\tilde{h}_j$ is a non-convective entropy flux. As a first step, we shall derive them for the equilibrium distribution (2.28).

PROPOSITION 2.7. *The entropy density and the non-convective entropy flux for polyatomic gases in local equilibrium state have the following form:*

$$(2.82) \qquad \rho s|_E = -k \frac{\rho}{m} \left\{ \log \left(\frac{\rho}{m \zeta_0(T)} \left(\frac{m}{2\pi k T} \right)^{3/2} \right) - \left(\frac{5}{2} + \alpha \right) \right\}, \quad \tilde{h}_j|_E = 0.$$

Moreover, Gibbs relation holds in equilibrium:

$$(2.83) \qquad ds|_E = \frac{1}{T} \left\{ de|_E - \frac{p}{\rho^2} d\rho \right\},$$

where $e|_E$ is the internal energy density of polyatomic gas (2.35).

For both relations (2.82) and (2.83) the proof is straightforward. They are derived by direct insertion of the equilibrium distribution (2.28) into (2.80) and (2.81). Gibbs relation comes out after differentiation of $(2.82)_1$.

We can conclude from the last Proposition that the equilibrium entropy density is a generalization of the one for monatomic gases, and that the form of Gibbs relation is also preserved. The form of the non-equilibrium entropy density and entropy flux is dictated by the form of the non-equilibrium distribution function, and thus can be expressed in terms of 14 scalar fields.

PROPOSITION 2.8. *The non-equilibrium entropy density and entropy flux for polyatomic gases in the 14 moments approximation have the following form:*

$$\rho s = \rho s|_E - \frac{1}{4} \frac{k}{m} \frac{\rho}{p^2} \sum_{i,j=1}^{3} \left(p_{\langle ij \rangle} p_{\langle ij \rangle} \right) - \frac{1}{2} \left(\frac{7}{2} + \alpha \right)^{-1} \frac{k}{m} \frac{\rho^2}{p^3} \mathbf{q} \cdot \mathbf{q}$$

$$(2.84) \qquad - \frac{3}{4} \left(\frac{5}{2} + \alpha \right) (1 + \alpha)^{-1} \frac{k}{m} \frac{\rho}{p^2} \Pi^2,$$

$$(2.85) \qquad \tilde{h}_i = \frac{q_i}{T} - \frac{k}{m} \frac{\rho}{p^2} \left(\frac{7}{2} + \alpha \right)^{-1} \sum_{j=1}^{3} p_{\langle ij \rangle} q_j - \frac{k}{m} \frac{\rho}{p^2} \left(\frac{7}{2} + \alpha \right)^{-1} \Pi q_i, \qquad i = 1, 2, 3.$$

PROOF. To prove these results, it is sufficient to follow the procedure used in the derivation of the entropy density and the entropy flux in the case of Grad's distribution function [37]. First, one has to put the non-equilibrium distribution function (2.41) into (2.80) and (2.81). Since we shall restrict our study to second order terms with respect to non-equilibrium densities – pressure tensor p_{ij}, heat flux q_i and dynamic pressure Π – we shall exploit the approximation $\log(1+x) \approx x - x^2/2$, valid for $|x| \ll 1$. Under these assumptions, the relations (2.84)-(2.85) are obtained after tedious, but straightforward integration of (2.80) and (2.81). □

The non-equilibrium entropy density (2.84) comprises the equilibrium one ρs_E and non-linear, quadratic terms related to pressure tensor, heat flux and dynamic pressure. It is a generalization of Grad's entropy density since it contains the polyatomic parameter α and term Π^2 which do not exist in the monatomic case. Moreover, it fulfills the convexity conditions provided $\alpha > -1$ (or equivalently $D > 3$), ensuring that the 14 moments system (2.48)-(2.49) can be put into symmetric hyperbolic form [18].

The entropy flux (2.85) shares the same properties as the entropy density. It contains the linear term, q_i/T, typical for linear theory, but comprises non-linear terms $p_{\langle ij \rangle} q_j$, present also in the monatomic case, and Πq_i which is the non-linear contribution specific of polyatomic gases. The coefficients contain the parameter of the model α, as well. The results presented above are in perfect agreement with the ones of extended thermodynamics [9].

Multivelocity and multitemperature models of Eulerian polyatomic gases

Mixtures of Eulerian (inviscid) gases are usually described by monovelocity and monotemperature models, where the state of the mixture of s species is determined by the mass densities of each constituent ρ_i, $i = 1, \ldots, s$, the mixture velocity $\mathbf{u}$ and the common temperature T or the internal energy density e. They stay in the framework of ordinary thermodynamics, and the corresponding equations write, as long as chemical reactions are not taken into account [50],

$$\partial_t \rho_i + \nabla_{\mathbf{x}} \cdot (\rho_i \, \mathbf{u}) = 0, \quad \text{for any} \ \ i = 1, \ldots, s,$$
$$\partial_t \left(\rho \, \mathbf{u} \right) + \nabla_{\mathbf{x}} \left(\rho \, \mathbf{u} \otimes \mathbf{u} + p \, \text{Id} \right) = \mathbf{0},$$
$$\partial_t \left(\tfrac{1}{2} \rho \, |\mathbf{u}|^2 + \rho e \right) + \nabla_{\mathbf{x}} \cdot \left\{ \left(\tfrac{1}{2} \rho \, |\mathbf{u}|^2 + \rho e \right) \mathbf{u} + p \, \mathbf{u} \right\} = 0,$$

where $\rho = \sum_{i=1}^{s} \rho_i$. They become complete once state laws are written for the pressure p and the energy e in terms of the mass densities ρ_i and the common temperature T.

Models involving one velocity and one temperature/internal energy per species (resp. called $\mathbf{u}_i$ and T_i/e_i) have lately been developed in the context of extended thermodynamics. Let us recall that the first rational model of homogeneous mixtures was proposed by Truesdell in the context of rational thermodynamics [58]. It is based on three principles that we briefly comment:

(1) All properties of the mixture must be mathematical consequences of properties of the constituents.
(2) In order to describe the motion of a constituent, we may in imagination isolate it from the rest of the mixture, if the actions of the other constituents upon it are properly described.
(3) The motion of the mixture is governed by the same equations as in a single body.

Roughly speaking, the first principle asserts that the whole is just a sum of its parts and the third that a body, in its motion as a whole, behaves in the same way whether it is a mixture or not. The second principle implies that each component of the mixture obeys balance laws of mass, momentum and energy. We mention that these laws are not conservative, because of the mutual interaction of the constituents. Indeed, if the mixture is constituted of s species: $\mathcal{A}_1, \ldots \mathcal{A}_s$, and if chemical reactions are excluded from our consideration, then the species $\mathcal{A}_i$ satisfy the following system of equations

(3.1)
$$\partial_t \rho_i + \nabla_{\mathbf{x}} \cdot (\rho_i \, \mathbf{u}_i) = 0,$$
$$\partial_t \left(\rho_i \, \mathbf{u}_i \right) + \nabla_{\mathbf{x}} \left(\rho_i \, \mathbf{u}_i \otimes \mathbf{u}_i + \mathbf{p}_i \right) = \mathbf{N}_i,$$
$$\partial_t \left(\tfrac{1}{2} \rho_i \, |\mathbf{u}_i|^2 + \rho_i e_i \right) + \nabla_{\mathbf{x}} \cdot \left\{ \left(\tfrac{1}{2} \rho_i \, |\mathbf{u}_i|^2 + \rho_i e_i \right) \mathbf{u}_i + \mathbf{p}_i \mathbf{u}_i + \mathbf{q}_i \right\} = E_i, \quad \text{for any} \ \ i = 1, \ldots, s,$$

ρ_i being the density, $\mathbf{u}_i$ the velocity, e_i the internal energy, $\mathbf{p}_i$ the pressure tensor and $\mathbf{q}_i$ the heat flux of the species $\mathcal{A}_i$. In order to recover conservation laws of mass, momentum and energy for the mixture as a whole, the production terms must satisfy the following relations:

(3.2)
$$\sum_{i=1}^{s} \mathbf{N}_i = \mathbf{0}, \qquad \sum_{i=1}^{s} E_i = 0.$$

In fact, the third principle implies that the mixture obeys conservation laws identical to those of a single fluid:

$$\partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho\,\mathbf{u}) = 0,$$

(3.3)
$$\partial_t (\rho\,\mathbf{u}) + \nabla_{\mathbf{x}} (\rho\,\mathbf{u} \otimes \mathbf{u} + \mathbf{p}) = \mathbf{0},$$

$$\partial_t \left(\tfrac{1}{2} \rho\,|\mathbf{u}|^2 + \rho e \right) + \nabla_{\mathbf{x}} \cdot \left\{ \left(\tfrac{1}{2}\rho\,|\mathbf{u}|^2 + \rho e \right)\mathbf{u} + \mathbf{p}\mathbf{u} + \mathbf{q} \right\} = 0,$$

where ρ is the density, $\mathbf{u}$ the velocity, e the internal energy, $\mathbf{p}$ the pressure tensor and $\mathbf{q}$ the heat flux of the mixture. At the same time, these field variables have to be deduced from the ones of the components of the mixture, by the first principle. They are defined with the following relations:

$$\rho = \sum_{i=1}^{s} \rho_i \qquad\qquad \text{mass density of mixture,}$$

$$\mathbf{u} = \frac{1}{\rho} \sum_{i=1}^{s} \rho_i \mathbf{u}_i \qquad\qquad \text{mixture velocity,}$$

$$\mathbf{U}_i = \mathbf{u}_i - \mathbf{u}, \quad \text{with } \sum_{i=1}^{s} \rho_i \mathbf{U}_i = 0 \qquad\qquad \text{diffusion velocity,}$$

$$\mathbf{p} = \sum_{i=1}^{s} (\mathbf{p}_i + \rho_i \mathbf{U}_i \otimes \mathbf{U}_i) \qquad\qquad \text{pressure tensor,}$$

$$e = \frac{1}{\rho} \sum_{i=1}^{s} \rho_i \left(e_i + \tfrac{1}{2}\,|\mathbf{U}_i|^2 \right) \qquad\qquad \text{internal energy,}$$

$$\mathbf{q} = \sum_{i=1}^{s} \left(\mathbf{q}_i + \rho_i \left(e_i + \tfrac{1}{2}\,|\mathbf{U}_i|^2 \right) + \mathbf{p}_i \mathbf{U}_i \right) \qquad \text{flux of internal energy.}$$

Then it is easy to recover the conservation laws for mixture (3.3) by summation of balance laws for constituents (3.1), having in mind (3.2).

In the general form of a model for a mixture given in (3.1), the closure problem immediately appears. Namely, system (3.1) needs constitutive equations for the pressure tensor $\mathbf{p}_i$ and the heat flux $\mathbf{q}_i$, as well as an expression of production terms $\mathbf{N}_i$, E_i in terms of field variables $\rho_i, \mathbf{u}_i, e_i$. This problem has been studied in the framework of extended thermodynamics. In this theory, it is required that a model satisfies two fundamental principles – the objectivity principle, that assumes invariance of the field equations with respect to Galilean transformations, and the entropy principle (or accordance with entropy inequality) for all thermodynamic processes.

We recall first that as far as (inviscid) fluids are considered, off-diagonal parts of the pressure tensor and the heat flux vector vanish. In other words,

(3.4)
$$\mathbf{p}_i = p_i \,\mathrm{Id}, \qquad \mathbf{q}_i = 0, \quad i = 1, \dots, s,$$

where p_i is the pressure of the constituent $\mathcal{A}_i$, and

$$p = \sum_{i=1}^{s} p_i$$

is the total pressure. Therefore, multivelocity and multitemperature Eulerian fluids obey the following set of equations

$$\partial_t \rho_i + \nabla_{\mathbf{x}} \cdot (\rho_i\,\mathbf{u}_i) = 0,$$

(3.5)
$$\partial_t (\rho_i\,\mathbf{u}_i) + \nabla_{\mathbf{x}} (\rho_i\,\mathbf{u}_i \otimes \mathbf{u}_i + p_i\,\mathrm{Id}) = \mathbf{N}_i,$$

$$\partial_t \left(\tfrac{1}{2}\rho_i\,|\mathbf{u}_i|^2 + \rho_i e_i \right) + \nabla_{\mathbf{x}} \cdot \left\{ \left(\tfrac{1}{2}\rho_i\,|\mathbf{u}_i|^2 + \rho_i e_i \right)\mathbf{u}_i + p_i\mathbf{u}_i \right\} = E_i, \quad i = 1, ..., s,$$

by means of (3.1) and assumption (3.4). It now remains to determine the production terms $\mathbf{N}_i$ and E_i.

Following [54], balance laws for the species $\mathcal{A}_s$ are replaced with the mixture conservation laws. In such a way, instead of (3.6), the following system of equations is considered:

$$\partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho \, \mathbf{u}) = 0,$$

$$\partial_t (\rho \, \mathbf{u}) + \nabla_{\mathbf{x}} (\rho \, \mathbf{u} \otimes \mathbf{u} + p \, \mathrm{Id}) = \mathbf{0},$$

$$\partial_t \left(\tfrac{1}{2} \rho \, |\mathbf{u}|^2 + \rho e \right) + \nabla_{\mathbf{x}} \cdot \left\{ \left(\tfrac{1}{2} \rho \, |\mathbf{u}|^2 + \rho e \right) \mathbf{u} + p\mathbf{u} \right\} = 0,$$

(3.6)

$$\partial_t \rho_i + \nabla_{\mathbf{x}} \cdot (\rho_i \, \mathbf{u}_i) = 0,$$

$$\partial_t (\rho_i \, \mathbf{u}_i) + \nabla_{\mathbf{x}} (\rho_i \, \mathbf{u}_i \otimes \mathbf{u}_i + p_i \, \mathrm{Id}) = \mathbf{N}_i,$$

$$\partial_t \left(\tfrac{1}{2} \rho_i \, |\mathbf{u}_i|^2 + \rho_i e_i \right) + \nabla_{\mathbf{x}} \cdot \left\{ \left(\tfrac{1}{2} \rho_i \, |\mathbf{u}_i|^2 + \rho_i e_i \right) \mathbf{u}_i + p_i\mathbf{u}_i \right\} = E_i, \quad i = 1, ..., s - 1,$$

As in [53], the objectivity principle is applied to general hyperbolic systems of balance type. It is required that the field equations are invariant with respect to the Galilean transformations:

$$t \mapsto t^*, \qquad \mathbf{x} \mapsto \mathbf{x}^* = \mathbf{x} + t \, \mathbf{c}, \qquad \mathbf{u} \mapsto \mathbf{u}^* = \mathbf{u} + \mathbf{c},$$

where $\mathbf{c}$ is some constant vector. This principle applied to the system (3.1) in the absence of chemical reactions implies the following structure of the production terms [54]:

(3.7)
$$\mathbf{N}_i = \hat{\mathbf{N}}_i,$$
$$E_i = \mathbf{u} \cdot \hat{\mathbf{N}}_i + \hat{E}_i, \quad i = 1, \dots, s - 1,$$

where $\hat{\ }$ denotes a quantity that does not depend on the velocity $\mathbf{u}$.

Another important restriction comes from the entropy principle that requires accordance with the entropy inequality, seen as an extra balance law. It is achieved through the following procedure. First, it is proved that the entropy density of the mixture is a convex function with respect to the variables related to a species $\mathcal{A}_i$ i.e. $(\rho_i, \rho_i \mathbf{u}_i, \tfrac{1}{2} \rho_i \, |\mathbf{u}_i|^2 + \rho_i e_i)$. Then, the production terms are determined through the application of the residual inequality: the internal parts of production terms are chosen in such a way that the entropy production is quadratic form [54]:

(3.8)
$$\hat{\mathbf{N}}_i = -\sum_{j=1}^{s-1} \alpha_{ij}(\boldsymbol{w}) \left(\frac{\mathbf{u}_j}{T_j} - \frac{\mathbf{u}_s}{T_s} - \mathbf{u} \left(\frac{1}{T_j} - \frac{1}{T_s} \right) \right),$$

$$\hat{E}_i = -\sum_{j=1}^{s-1} \beta_{ij}(\boldsymbol{w}) \left(-\frac{1}{T_j} + \frac{1}{T_s} \right), \qquad \forall \, i = 1, \dots, s - 1,$$

where $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are positive definite $(s-1) \times (s-1)$ matrix functions of the objective quantities $\boldsymbol{w}$. We recall that a quantity is objective if it is invariant with respect to Euclidean transformations that are more restrictive than Galilean ones: a Euclidean transformation is a time dependent rigid transformation of frame from $(t, \mathbf{x})$ to $(t^*, \mathbf{x}^*)$ defined by

(3.9)
$$t \mapsto t^*, \qquad \mathbf{x} \mapsto \mathbf{x}^* = Q(t) \, \mathbf{x} + \mathbf{c}(t),$$

where $Q(t)$ is an orthogonal tensor and $\mathbf{c}$ is a vector [50].

It will be useful in the sequel to reformulate production terms (3.8) in a such a way that the sum involves terms corresponding to species $\mathcal{A}_i$ and $\mathcal{A}_j$, rather than $\mathcal{A}_j$ and $\mathcal{A}_s$. We are thus led to add and subtract $(\mathbf{u}_i/T_i + \mathbf{u}/T_i)$ in the term $\hat{\mathbf{N}}_i$ and add and subtract $1/T_i$ in $\hat{E}_i$. Then, source terms (3.7) read

(3.10)

$$\mathbf{N}_i = -\sum_{\substack{j=1 \\ j \neq i}}^{s-1} \alpha_{ij}(\boldsymbol{w}) \left(\frac{\mathbf{u}_j}{T_j} - \frac{\mathbf{u}_i}{T_i} - \mathbf{u} \left(\frac{1}{T_j} - \frac{1}{T_i} \right) \right) + \left(\sum_{j=1}^{s-1} \alpha_{ij}(\boldsymbol{w}) \right) \left(\frac{\mathbf{u}_s}{T_s} - \frac{\mathbf{u}_i}{T_i} - \mathbf{u} \left(\frac{1}{T_s} - \frac{1}{T_i} \right) \right),$$

$$E_i = \mathbf{u} \cdot \mathbf{N}_i - \sum_{\substack{j=1 \\ j \neq i}}^{s-1} \beta_{ij}(\boldsymbol{w}) \left(-\frac{1}{T_j} + \frac{1}{T_i} \right) + \left(\sum_{j=1}^{s-1} \beta_{ij}(\boldsymbol{w}) \right) \left(-\frac{1}{T_s} + \frac{1}{T_i} \right),$$

for any $i = 1, \ldots, s-1$.

The coefficients $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are of phenomenological nature, and extended thermodynamics cannot determine them in the general case. They can be only compared with experimental data for some particular cases. Our aim is to obtain a system of equations describing mixture of Eulerian polyatomic gases starting from the kinetic theory, and to compare the obtained production terms with (3.10). In particular, the purpose is to compute the coefficients $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$.

Our contribution to the closure problem is based on a completely different approach, directly related to the kinetic theory of mixtures of polyatomic gases. Let us first recall that the approach to equilibrium for a mixture of gases is much more intricate than for a single component gas, because many different scales appear. Namely, the approach to equilibrium can be divided roughly into two processes [34]. One of the processes is the approach of each distribution function to a Maxwellian distribution which we call the Maxwellisation step of a species. Typically, it takes place on the scale on which the pressure tensor of that species becomes isotropic or, equivalently, the scale on which the heat conduction relaxes. The Maxwellisation step is followed by another process, namely the equilibration of the species, i.e. vanishing of differences in velocity and temperature among the species. Equilibration proceeds at the macroscopic scale without an ordered pattern: equalization of velocities and temperatures can occur on a different scale or on the same scale.

This Section aims at obtaining at the formal level a multivelocity and multitemperature model, as an asymptotic limit of the Boltzmann equations (1.98). For that purpose, we assume that the Maxwellisation steps for each species are of the same order. Moreover, we assume that this scale is much shorter than the equilibration scale between different species. This is achieved by assuming that the typical mean free path for collisions between molecules of the same species are much shorter than the mean free path for collisions between molecules of different species (which is assumed to be of the same order as the macroscopic scale). This scaling has also been proposed and studied in [16] in the case of mixtures of gases with discrete internal energy. Also, the multitemperature model is derived from the kinetic model in [15] within the framework of mixture of monatomic gases with possible chemical reactions, by assuming the dominance of non-reactive collisions between molecules of the same species. Therefore, if we introduce a small parameter ε that represents the Knudsen number for the fast processes, the Boltzmann equations take the following form:

$$\partial_t f_i^\varepsilon + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i^\varepsilon = \frac{1}{\varepsilon} Q_{ii}(f_i^\varepsilon, f_i^\varepsilon) + \sum_{\substack{j=1 \\ j \neq i}}^{s} Q_{ij}(f_i^\varepsilon, f_j^\varepsilon), \quad 1 \leq i \leq s.$$

As a consequence, when ε tends to zero, f_i^ε converges at the formal level towards the "mid-equilibrium" distribution function (1.119) with coefficients depending on t and $\mathbf{x}$:

$$(3.11) \qquad f_{E_i} = \frac{n_i}{\zeta_{0_i}(T_i)} \left(\frac{m}{2\pi k T_i} \right)^{N/2} e^{-\frac{1}{k T_i} \left(\frac{m_i}{2} |\mathbf{v} - \mathbf{u}_i|^2 + I \right)},$$

where

$$\zeta_{0_i}(T_i) = \int_{\mathbb{R}_+} \varphi_i(I) e^{-\frac{1}{k T_i} I} \, \mathrm{d}I,$$

and the number density $n_i(t, \mathbf{x}) =: n_i$, the velocity $\mathbf{u}_i(t, \mathbf{x}) =: \mathbf{u}_i$ and the temperature $T_i(t, \mathbf{x}) =: T_i$ of the component $\mathcal{A}_i$ satisfy the system (3.6)

$$\partial_t \rho_i + \nabla_{\mathbf{x}} \cdot (\rho_i \, \mathbf{u}_i) = 0,$$
$$\partial_t (\rho_i \, \mathbf{u}_i) + \nabla_{\mathbf{x}} (\rho_i \, \mathbf{u}_i \otimes \mathbf{u}_i + p_i \, \mathrm{Id}) = \mathbf{N}_i,$$
$$\partial_t \left(\tfrac{1}{2} \rho_i |\mathbf{u}_i|^2 + \rho_i e_i \right) + \nabla_{\mathbf{x}} \cdot \left\{ \left(\tfrac{1}{2} \rho_i |\mathbf{u}_i|^2 + \rho_i e_i \right) \mathbf{u}_i + p_i \mathbf{u}_i \right\} = E_i, \quad i = 1, \ldots, s,$$

with source terms $\mathbf{N}_i$ and E_i given by

$$\mathbf{N}_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} \iint_{\mathbb{R}^N \times \mathbb{R}_+} m_i \, \mathbf{v} \, Q_{ij}^b(f_{E_i}, f_{E_j})(\mathbf{v}, I) \, \varphi_i(I) \, \mathrm{d}\mathbf{v} \, \mathrm{d}I,$$

$$E_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} \iint_{\mathbb{R}^N \times \mathbb{R}_+} \left(\tfrac{m_i}{2} \, |\mathbf{v}|^2 + I \right) Q_{ij}^b(f_{E_i}, f_{E_j})(\mathbf{v}, I) \, \varphi_i(I) \, \mathrm{d}\mathbf{v} \, \mathrm{d}I.$$

We recall the special form of the internal energy (1.54) for the choice (3.11) and $\varphi_i(I) = I^{\alpha_i}$, with $\alpha_i > -1$ for every $i = 1, \ldots, s$:

$$\rho_i e_i|_{f_i = f_{E_i}} = \left(\alpha_i + \frac{5}{2} \right) k \, n_i \, T_i.$$

It remains to compute the production terms. To that end, we will use the modified VHS model for the cross section

$$(3.12) \qquad \mathcal{B}_{ij}\left(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R, \boldsymbol{\omega}\right) = 2^{N-1} K R^{s_{ij}} \left|\mathbf{v} - \mathbf{v}_*\right|^{2 s_{ij}} \left| \boldsymbol{\omega} \cdot \frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|} \right|^{N-2},$$

where the parameter s_{ij} satisfies $s_{ij} = s_{ji}$, and K is an appropriate dimensional constant. We will also assume that $N > 1$ and $s_{ij} > -\frac{N}{2}$. The interest of this model is that it depends on one unique parameter s_{ij} for each couple of species, which can be fitted by experiments involving only macroscopic quantities.

Let us mention that our computation of the production terms $\mathbf{N}_i$ et E_i is much alike the computation of the production terms obtained by the same hydrodynamic limit of the kinetic model with discrete energy levels [16].

1. Computation of the production term for the momentum exchange

The production term $\mathbf{N}_i$ that corresponds to the balance law of momentum of the species $\mathcal{A}_i$ for the Euler fluids and the choice (3.12) reads

$$\mathbf{N}_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_{\Omega} \int_{S^{N-1}} m_i \mathbf{v} \left(f_{E_i}\left(\mathbf{v}', I'\right) f_{E_j}\left(\mathbf{v}'_*, I'_*\right) - f_{E_i}\left(\mathbf{v}, I\right) f_{E_j}\left(\mathbf{v}_*, I_*\right) \right)$$

$$\times 2^{N-1} K (1 - R) R^{s_{ij} + \frac{N}{2} - 1} |\mathbf{v} - \mathbf{v}_*|^{2 s_{ij}} \left| \boldsymbol{\omega} \cdot \frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|} \right|^{N-2} \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}r \, \mathrm{d}R \, \mathrm{d}I_* \, \mathrm{d}\mathbf{v}_* \, \mathrm{d}I \, \mathrm{d}\mathbf{v}.$$

Performing the change of variables $(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R) \mapsto (\mathbf{v}', \mathbf{v}'_*, I', I'_*, r', R')$ for $\boldsymbol{\omega}$ fixed in the first integral, with Jacobian (1.102), we get

$$\mathbf{N}_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_{\Omega} \int_{S^{N-1}} m_i \left(\mathbf{v}' - \mathbf{v} \right) f_{E_i}\left(\mathbf{v}, I\right) f_{E_j}\left(\mathbf{v}_*, I_*\right)$$

$$\times 2^{N-1} K (1 - R) R^{s_{ij} + \frac{N}{2} - 1} |\mathbf{v} - \mathbf{v}_*|^{2 s_{ij}} \left| \boldsymbol{\omega} \cdot \frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|} \right|^{N-2} \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}r \, \mathrm{d}R \, \mathrm{d}I_* \, \mathrm{d}\mathbf{v}_* \, \mathrm{d}I \, \mathrm{d}\mathbf{v}.$$

Let us pass to the $\boldsymbol{\sigma}-$notation with Jacobian (1.37). Expressing

$$\mathbf{v}' - \mathbf{v} = \frac{m_j}{m_i + m_j} \left(-\mathbf{v} + \mathbf{v}_* + \sqrt{\frac{2 \, RE}{\mu_{ij}}} \boldsymbol{\sigma} \right),$$

we obtain

$$\mathbf{N}_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} K \frac{n_i n_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \left(\frac{m_i m_j}{4\pi^2 k^2 T_i T_j}\right)^{\frac{N}{2}} \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_{\Omega} \int_{S^{N-1}} \mu_{ij} \left(-\mathbf{v} + \mathbf{v}_* + \sqrt{\frac{2\,RE}{\mu_{ij}}}\,\boldsymbol{\sigma}\right)$$

$$\times\, e^{-\frac{1}{kT_i}\left(\frac{m_i}{2}|\mathbf{v}-\mathbf{u}_i|^2 + I\right)} e^{-\frac{1}{kT_j}\left(\frac{m_j}{2}|\mathbf{v}_*-\mathbf{u}_j|^2 + I_*\right)} (1-R) R^{s_{ij}+\frac{N}{2}-1} |\mathbf{v}-\mathbf{v}_*|^{2s_{ij}}\, d\boldsymbol{\sigma}\, dr\, dR\, dI_*\, d\mathbf{v}_*\, dI\, d\mathbf{v}.$$

Integration with respect to $\boldsymbol{\sigma}$, and then with respect to all variables except velocities $\mathbf{v}$ and $\mathbf{v}_*$ leads to:

$$(3.13)\quad \mathbf{N}_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} K \frac{n_i n_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \left(\frac{m_i m_j}{4\pi^2 k^2 T_i T_j}\right)^{\frac{N}{2}} \mu_{ij} \left|S^{N-1}\right| k^2 T_i T_j \frac{4}{(N+2s_{ij})(N+2s_{ij}+2)}$$

$$\times \iint_{\mathbb{R}^N \times \mathbb{R}^N} (-\mathbf{v} + \mathbf{v}_*)\, e^{-\frac{m_i}{2kT_i}|\mathbf{v}-\mathbf{u}_i|^2 - \frac{m_j}{2kT_j}|\mathbf{v}_*-\mathbf{u}_j|^2} |\mathbf{v}-\mathbf{v}_*|^{2s_{ij}}\, d\mathbf{v}\, d\mathbf{v}_*,$$

where

$$\left|S^{N-1}\right| = \int_{S^{N-1}} d\boldsymbol{\sigma}.$$

In order to obtain a final formula, which is as explicit as possible, we pass to the center of mass reference frame

$$(3.14)\qquad\qquad (\mathbf{v}, \mathbf{v}_*) \mapsto \left(\mathbf{g} := \mathbf{v} - \mathbf{v}_*, \mathbf{G} := \frac{m_i \mathbf{v} + m_j \mathbf{v}_*}{m_i + m_j}\right),$$

with unit Jacobian. Moreover, we seek the expression in the power of the exponential in (3.13) under the form

$$(3.15)\qquad\qquad -\left(a_{ij}\,|\mathbf{g} + \mathbf{b}_{ij}|^2 + c_{ij}\,|\mathbf{G} + d_{ij}\,\mathbf{g} + \mathbf{e}_{ij}|^2\right),$$

where $a_{ij}, \mathbf{b}_{ij}, c_{ij}, d_{ij}, \mathbf{e}_{ij}$ are coefficients to be determined with a_{ij} and c_{ij} positive. Inserting (3.14) into (3.15), and comparing the obtained formula with the expression in the power of the exponential (3.13), leads to the system of equations for coefficients:

$$a_{ij} + c_{ij}d_{ij}^2 + \frac{m_i^2}{(m_i+m_j)^2}c_{ij} + \frac{2\,m_i}{m_i+m_j}c_{ij}\,d_{ij} = \frac{m_i}{2kT_i},$$

$$2\,a_{ij}\mathbf{b}_{ij} + 2\,c_{ij}\,d_{ij}\,\mathbf{e}_{ij} + \frac{2\,m_i}{m_i+m_j}c_{ij}\,\mathbf{e}_{ij} = -\frac{m_i}{kT_i}\mathbf{u}_i,$$

$$a_{ij} + c_{ij}d_{ij}^2 + \frac{m_j^2}{(m_i+m_j)^2}c_{ij} - \frac{2\,m_j}{m_i+m_j}c_{ij}\,d_{ij} = \frac{m_j}{2kT_j},$$

$$-2\,a_{ij}\mathbf{b}_{ij} - 2\,c_{ij}\,d_{ij}\,\mathbf{e}_{ij} + \frac{2\,m_j}{m_i+m_j}c_{ij}\,\mathbf{e}_{ij} = -\frac{m_j}{kT_j}\mathbf{u}_j,$$

$$-a_{ij} - c_{ij}\,d_{ij}^2 + \frac{m_i m_j}{(m_i+m_j)^2}c_{ij} + \frac{m_j-m_i}{m_i+m_j}c_{ij}\,d_{ij} = 0,$$

$$a_{ij}\,\mathbf{b}_{ij}^2 + c_{ij}\mathbf{e}_{ij}^2 = \frac{m_i}{2kT_i}\,|\mathbf{u}_i|^2 + \frac{m_j}{2kT_j}\,|\mathbf{u}_j|^2.$$

This system is overdetermined ($(2N+4)$ equations for $(2N+3)$ unknowns), but consistent, and has the following solution:

(3.16)
$$a_{ij} = \left(\frac{2\,k\,T_i}{m_i} + \frac{2\,k\,T_j}{m_j} \right)^{-1},$$

$$\mathbf{b}_{ij} = \mathbf{u}_j - \mathbf{u}_i,$$

$$c_{ij} = \frac{m_i}{2\,k\,T_i} + \frac{m_j}{2\,k\,T_j},$$

$$d_{ij} = \mu_{ij} \left(\frac{m_i}{2\,k\,T_i} + \frac{m_j}{2\,k\,T_j} \right)^{-1} \left(\frac{1}{2\,k\,T_i} - \frac{1}{2\,k\,T_j} \right),$$

$$\mathbf{e}_{ij} = - \left(\frac{m_i}{2\,k\,T_i} + \frac{m_j}{2\,k\,T_j} \right)^{-1} \left(\frac{m_i}{2\,k\,T_i} \mathbf{u}_i + \frac{m_j}{2\,k\,T_j} \mathbf{u}_j \right).$$

Summarizing, (3.13) becomes

$$\mathbf{N}_i = - \sum_{\substack{j=1 \\ j \neq i}}^s K \frac{n_i n_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \left(\frac{m_i m_j}{4\,\pi^2\,k^2\,T_i T_j} \right)^{\frac{N}{2}} \mu_{ij} \left| S^{N-1} \right| k^2 T_i T_j \frac{4}{(N+2s_{ij})\,(N+2s_{ij}+2)}$$

$$\times \iint_{\mathbb{R}^N \times \mathbb{R}^N} \mathbf{g}\, e^{-a_{ij}|\mathbf{g}+\mathbf{b}_{ij}|^2 - c_{ij}|\mathbf{G}+d_{ij}\,\mathbf{g}+\mathbf{e}_{ij}|^2}\, |\mathbf{g}|^{2s_{ij}}\, \mathrm{d}\mathbf{g}\,\mathrm{d}\mathbf{G},$$

where coefficients are determined by (3.16). Note that

(3.17)
$$c_{ij}^{-1} = \frac{4\,k^2\,T_i\,T_j}{m_i\,m_j}\, a_{ij}.$$

Integration with respect to $\mathbf{G}$ yields integrals which only involve the relative velocity $\mathbf{g}$:

(3.18)
$$\mathbf{N}_i = - \sum_{\substack{j=1 \\ j \neq i}}^s K \mu_{ij}\, n_i\, n_j \frac{k^2\,T_i\,T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \frac{4\,|S^{N-1}|}{(N+2s_{ij})\,(N+2s_{ij}+2)} \left(\frac{a_{ij}}{\pi} \right)^{\frac{N}{2}}$$

$$\times \int_{\mathbb{R}^N} \mathbf{g}\, |\mathbf{g}|^{2s_{ij}}\, e^{-a_{ij}|\mathbf{g}-(\mathbf{u}_i-\mathbf{u}_j)|^2}\mathrm{d}\mathbf{g}.$$

In order to treat the scalar product of $\mathbf{g}$ and $\mathbf{u}_i - \mathbf{u}_j$, we consider the orthonormal basis $\left\{ \frac{\mathbf{u}_i-\mathbf{u}_j}{|\mathbf{u}_i-\mathbf{u}_j|}, \mathbf{y}_1, \ldots, \mathbf{y}_{N-1} \right\}$ and decompose the vector $\mathbf{g}$ with respect to this basis:

$$\mathbf{g} = \left(\mathbf{g} \cdot \frac{\mathbf{u}_i - \mathbf{u}_j}{|\mathbf{u}_i - \mathbf{u}_j|} \right) \frac{\mathbf{u}_i - \mathbf{u}_j}{|\mathbf{u}_i - \mathbf{u}_j|} + \sum_{m=1}^{N-1} (\mathbf{g} \cdot \mathbf{y}_m)\, \mathbf{y}_m.$$

Let φ_1 denotes the angle between $\mathbf{g}$ and $\frac{\mathbf{u}_i-\mathbf{u}_j}{|\mathbf{u}_i-\mathbf{u}_j|}$. Therefore, its cosine is

$$\cos \varphi_1 = \frac{\mathbf{g}}{|\mathbf{g}|} \cdot \frac{\mathbf{u}_i - \mathbf{u}_j}{|\mathbf{u}_i - \mathbf{u}_j|}.$$

Next, we pass from $\mathbb{R}^N$ to the spherical coordinate system, with angular coordinates denoted with $\varphi_1, \varphi_2, \ldots, \varphi_{N-1}$, where φ_{N-1} ranges over $[0, 2\pi)$ and all the others angles range over $[0, \pi]$. We express $\mathbf{g}$ in terms of its spherical coordinates with axis $\frac{\mathbf{u}_i-\mathbf{u}_j}{|\mathbf{u}_i-\mathbf{u}_j|}$ i.e. we choose the polar angle to be φ_1. Thus, we perform the following change of variables

(3.19)
$$\mathbf{g} \mapsto |\mathbf{g}| \begin{bmatrix} \cos \varphi_1 \\ \sin \varphi_1 \cos \varphi_2 \\ \sin \varphi_1 \sin \varphi_2 \cos \varphi_3 \\ \vdots \\ \sin \varphi_1 \sin \varphi_2 \cdots \sin \varphi_{N-2} \cos \varphi_{N-1} \\ \sin \varphi_1 \sin \varphi_2 \cdots \sin \varphi_{N-2} \sin \varphi_{N-1} \end{bmatrix} =: |\mathbf{g}| \begin{bmatrix} \cos \varphi_1 \\ \sin \varphi_1\, \tilde{\boldsymbol{\omega}} \end{bmatrix},$$

where $\tilde{\boldsymbol{\omega}}$ represents the element of sphere S^{N-2}. The computation of the Jacobian of this transformation gives (note that we do not need an absolute value since all sine functions are positive on the considered domain):

$$d\mathbf{g} = |\mathbf{g}|^{N-1} (\sin \varphi_1)^{N-2} (\sin \varphi_2)^{N-3} \cdots \sin \varphi_{N-2} \, d \, |\mathbf{g}| \, d\varphi_1 \, d\varphi_2 \ldots d\varphi_{N-1}$$

(3.20)
$$= |\mathbf{g}|^{N-1} (\sin \varphi_1)^{N-2} \, d \, |\mathbf{g}| \, d\varphi_1 \, d\tilde{\boldsymbol{\omega}},$$

where, according to the standard notation in kinetic theory, we denoted

$$d\tilde{\boldsymbol{\omega}} = (\sin \varphi_2)^{N-3} \cdots \sin \varphi_{N-2} \, d\varphi_2 \ldots d\varphi_{N-1}.$$

Finally, the integral (3.18) becomes

$$\mathbf{N}_i = -\sum_{\substack{j=1 \\ j \neq i}}^{s} K \mu_{ij} \, n_i \, n_j \, \frac{k^2 \, T_i \, T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \frac{4 \left| S^{N-1} \right|}{(N + 2s_{ij})(N + 2s_{ij} + 2)} \left(\frac{a_{ij}}{\pi} \right)^{\frac{N}{2}}$$

$$\times \int_{S^{N-2}} \int_0^\pi \int_{\mathbb{R}_+} \left(\cos \varphi_1 \frac{\mathbf{u}_i - \mathbf{u}_j}{|\mathbf{u}_i - \mathbf{u}_j|} + \sin \varphi_1 \sum_{m=1}^{N-1} \tilde{\omega}_m \mathbf{y}_m \right) e^{-a_{ij}\left(|\mathbf{g}|^2 - 2|\mathbf{g}||\mathbf{u}_i - \mathbf{u}_j| \cos \varphi_1 + |\mathbf{u}_i - \mathbf{u}_j|^2 \right)}$$

$$\times |\mathbf{g}|^{2s_{ij}+N} (\sin \varphi_1)^{N-2} \, d \, |\mathbf{g}| \, d\varphi_1 \, d\tilde{\boldsymbol{\omega}}.$$

Integration with respect to the element $\tilde{\boldsymbol{\omega}}$ of the sphere S^{N-2} yields

$$\mathbf{N}_i = -\sum_{\substack{j=1 \\ j \neq i}}^{s} K \mu_{ij} \, n_i \, n_j \, \frac{k^2 \, T_i \, T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \frac{4 \left| S^{N-1} \right| \left| S^{N-2} \right|}{(N + 2s_{ij})(N + 2s_{ij} + 2)} \left(\frac{a_{ij}}{\pi} \right)^{\frac{N}{2}} \frac{\mathbf{u}_i - \mathbf{u}_j}{|\mathbf{u}_i - \mathbf{u}_j|} e^{-a_{ij}|\mathbf{u}_i - \mathbf{u}_j|^2}$$

$$\times \int_{\mathbb{R}_+} |\mathbf{g}|^{2s_{ij}+N} e^{-a_{ij}|\mathbf{g}|^2} \int_0^\pi \cos \varphi_1 \, e^{2 \, a_{ij}|\mathbf{g}||\mathbf{u}_i - \mathbf{u}_j| \cos \varphi_1} (\sin \varphi_1)^{N-2} \, d\varphi_1 \, d \, |\mathbf{g}|.$$

Let us concentrate on the integral with respect to the angular variable φ_1. We change variable $\cos \varphi_1 \mapsto p$,

(3.21)
$$\int_0^\pi \cos \varphi_1 \, e^{2 \, a_{ij}|\mathbf{g}||\mathbf{u}_i - \mathbf{u}_j| \cos \varphi_1} (\sin \varphi_1)^{N-2} \, d\varphi_1 = \int_{-1}^1 p \left(1 - p^2 \right)^{\frac{N-3}{2}} e^{2 \, a_{ij}|\mathbf{g}||\mathbf{u}_i - \mathbf{u}_j|p} \, dp,$$

where we expressed $(\sin \varphi_1)^{N-3} = \left(\sin \varphi_1^2 \right)^{\frac{N-3}{2}} = \left(1 - p^2 \right)^{\frac{N-3}{2}}$, which is allowed since the sine function is positive on the considered interval. Next, we perform a partial integration with

$$u = e^{2a_{ij}|\mathbf{g}||\mathbf{u}_i - \mathbf{u}_j|p} \quad \Rightarrow \quad du = 2a_{ij} \, |\mathbf{g}| \, |\mathbf{u}_i - \mathbf{u}_j| \, e^{2a_{ij}|\mathbf{g}||\mathbf{u}_i - \mathbf{u}_j|p},$$

$$dv = p \left(1 - p^2 \right)^{\frac{N-3}{2}} dp \quad \Rightarrow \quad v = -\frac{1}{N-1} \left(1 - p^2 \right)^{\frac{N-1}{2}},$$

so that

$$\int_{-1}^1 p \left(1 - p^2 \right)^{\frac{N-3}{2}} e^{2 \, a_{ij}|\mathbf{g}||\mathbf{u}_i - \mathbf{u}_j|p} \, dp = \frac{2a_{ij} \, |\mathbf{g}| \, |\mathbf{u}_i - \mathbf{u}_j|}{N-1} \int_{-1}^1 \left(1 - p^2 \right)^{\frac{N-1}{2}} e^{2a_{ij}|\mathbf{g}||\mathbf{u}_i - \mathbf{u}_j|p} dp$$

$$= \frac{2a_{ij} \, |\mathbf{g}| \, |\mathbf{u}_i - \mathbf{u}_j|}{N-1} \sqrt{\pi} \, \Gamma \left[\frac{N+1}{2} \right] \, {}_0\tilde{F}_1 \left(; \frac{N}{2} + 1; a_{ij}^2 \, |\mathbf{g}|^2 \, |\mathbf{u}_i - \mathbf{u}_j|^2 \right)$$

$$= a_{ij} \, |\mathbf{g}| \, |\mathbf{u}_i - \mathbf{u}_j| \sqrt{\pi} \, \Gamma \left[\frac{N-1}{2} \right] \, {}_0\tilde{F}_1 \left(; \frac{N}{2} + 1; a_{ij}^2 \, |\mathbf{g}|^2 \, |\mathbf{u}_i - \mathbf{u}_j|^2 \right),$$

by means of comparison with the integral representation (15). Note that in the case when $N = 3$, the computation of the integral (3.21) is particulary simple and it can be done directly, without need for representation through special functions. Denoting $A_{ij} = 2 \, a_{ij} \, |\mathbf{u}_i - \mathbf{u}_j| \, |\mathbf{g}|$, for $N = 3$ we obtain the following result:

$$\int_{-1}^1 p \, e^{A_{ij}p} \, dp = \frac{2}{A_{ij}^2} \left(A_{ij} \cosh A_{ij} - \sinh A_{ij} \right).$$

Next, we focus on the integral

$$\int_{\mathbb{R}_+} |\mathbf{g}|^{2s_{ij}+N+1} e^{-a_{ij}|\mathbf{g}|^2} \, {}_0\tilde{F}_1\left(;\frac{N}{2}+1;a_{ij}^2\,|\mathbf{g}|^2\,|\mathbf{u}_i-\mathbf{u}_j|^2\right)\mathrm{d}\,|\mathbf{g}|.$$

We perform the following changes of variables: $|\mathbf{g}| \mapsto |\mathbf{g}|^2 =: x$ and $x \mapsto a_{ij}x =: \overline{x}$, that yield

$$\int_{\mathbb{R}_+} |\mathbf{g}|^{2s_{ij}+N+1} e^{-a_{ij}|\mathbf{g}|^2} \, {}_0\tilde{F}_1\left(;\frac{N}{2}+1;a_{ij}^2\,|\mathbf{u}_i-\mathbf{u}_j|^2\,|\mathbf{g}|^2\right)\mathrm{d}\,|\mathbf{g}|$$

$$= \frac{1}{2}\int_{\mathbb{R}_+} x^{s_{ij}+\frac{N}{2}} e^{-a_{ij}x} \, {}_0\tilde{F}_1\left(;\frac{N}{2}+1;a_{ij}^2\,|\mathbf{u}_i-\mathbf{u}_j|^2\,x\right)\mathrm{d}x$$

$$= \frac{1}{2\,a_{ij}^{s_{ij}+\frac{N}{2}+1}}\int_{\mathbb{R}_+} \overline{x}^{s_{ij}+\frac{N}{2}} e^{-\overline{x}} \, {}_0\tilde{F}_1\left(;\frac{N}{2}+1;a_{ij}\,|\mathbf{u}_i-\mathbf{u}_j|^2\,\overline{x}\right)\mathrm{d}\overline{x}$$

$$= \frac{1}{2\,a_{ij}^{s_{ij}+\frac{N}{2}+1}}\Gamma\left[s_{ij}+\frac{N}{2}+1\right] \, {}_1\tilde{F}_1\left(s_{ij}+\frac{N}{2}+1;\frac{N}{2}+1;a_{ij}\,|\mathbf{u}_i-\mathbf{u}_j|^2\right),$$

for $s_{ij} > -N/2$, where we used the representation (14). Therefore, we can write $\mathbf{N}_i$ in closed form as follows:

$$\mathbf{N}_i = -\sum_{\substack{j=1 \\ j \neq i}}^{s} (\mathbf{u}_i-\mathbf{u}_j)\,K\mu_{ij}\,n_i\,n_j\,\frac{k^2\,T_i\,T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)}\frac{2\left|S^{N-1}\right|\left|S^{N-2}\right|}{(N+2s_{ij})\,(N+2s_{ij}+2)}a_{ij}^{-s_{ij}}\pi^{\frac{1-N}{2}}e^{-a_{ij}|\mathbf{u}_i-\mathbf{u}_j|^2}$$

$$\times \Gamma\left[\frac{N-1}{2}\right]\Gamma\left[s_{ij}+\frac{N}{2}+1\right] \, {}_1\tilde{F}_1\left(s_{ij}+\frac{N}{2}+1;\frac{N}{2}+1;a_{ij}\,|\mathbf{u}_i-\mathbf{u}_j|^2\right).$$

Finally, the source term $\mathbf{N}_i$ corresponding to the balance law of momentum of the species $\mathcal{A}_i$ for Euler fluids in the case of the VHS model for cross section reads

$$(3.22)\quad \mathbf{N}_i = -\sum_{\substack{j=1 \\ j \neq i}}^{s} (\mathbf{u}_i-\mathbf{u}_j)\,K\mu_{ij}\,n_i\,n_j\,\frac{k^2\,T_i\,T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)}\frac{2\left|S^{N-1}\right|\left|S^{N-2}\right|}{(N+2s_{ij})\,(N+2s_{ij}+2)}$$

$$\times \left(\frac{2\,k\,T_i}{m_i}+\frac{2\,k\,T_j}{m_j}\right)^{s_{ij}}\pi^{\frac{1-N}{2}}e^{-\left(\frac{2\,k\,T_i}{m_i}+\frac{2\,k\,T_j}{m_j}\right)^{-1}|\mathbf{u}_i-\mathbf{u}_j|^2}\Gamma\left[\frac{N-1}{2}\right]\Gamma\left[s_{ij}+\frac{N}{2}+1\right]$$

$$\times \, {}_1\tilde{F}_1\left(s_{ij}+\frac{N}{2}+1;\frac{N}{2}+1;\left(\frac{2\,k\,T_i}{m_i}+\frac{2\,k\,T_j}{m_j}\right)^{-1}|\mathbf{u}_i-\mathbf{u}_j|^2\right).$$

2. Computation of the production term for the energy exchange

The full expression of the production term E_i corresponding to the energy balance law of the species $\mathcal{A}_i$ in the case of Euler fluids and model (3.12) for the cross section reads

$$E_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_{\Omega}\int_{S^{N-1}} \left(\frac{1}{2}m_i\,|\mathbf{v}|^2 + I\right)\left(f_{E_i}\left(\mathbf{v}',I'\right)f_{E_j}\left(\mathbf{v}'_*,I'_*\right) - f_{E_i}\left(\mathbf{v},I\right)f_{E_j}\left(\mathbf{v}_*,I_*\right)\right)$$

$$\times 2^{N-1}K(1-R)R^{s_{ij}+\frac{N}{2}-1}\,|\mathbf{v}-\mathbf{v}_*|^{2s_{ij}}\left|\boldsymbol{\omega}\cdot\frac{\mathbf{v}-\mathbf{v}_*}{|\mathbf{v}-\mathbf{v}_*|}\right|^{N-2}\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_*\,\mathrm{d}\mathbf{v}_*\,\mathrm{d}I\,\mathrm{d}\mathbf{v}.$$

Its computation resembles the computation of the production term $\mathbf{N}_i$.

The first step consists in the change of variables $(\mathbf{v}, \mathbf{v}_*, I, I_*, r, R) \mapsto (\mathbf{v}', \mathbf{v}'_*, I', I'_*, r', R')$ for $\boldsymbol{\omega}$ fixed with Jacobian (1.102). We obtain

$$E_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_\Omega \int_{S^{N-1}} \left(\frac{1}{2} m_i \left| \mathbf{v}' \right|^2 + I' - \frac{1}{2} m_i \left| \mathbf{v} \right|^2 - I \right) f_{E_i}(\mathbf{v}, I) f_{E_j}(\mathbf{v}_*, I_*)$$

$$\times 2^{N-1} K(1-R) R^{s_{ij} + \frac{N}{2} - 1} \left| \mathbf{v} - \mathbf{v}_* \right|^{2s_{ij}} \left| \boldsymbol{\omega} \cdot \frac{\mathbf{v} - \mathbf{v}_*}{\left| \mathbf{v} - \mathbf{v}_* \right|} \right|^{N-2} d\boldsymbol{\omega}\, dr\, dR\, dI_*\, d\mathbf{v}_*\, dI\, d\mathbf{v}.$$

The term in the first parenthesis can be expressed in terms of non-prime variables as follows:

$$\frac{1}{2} m_i \left| \mathbf{v}' \right|^2 + I' - \frac{1}{2} m_i \left| \mathbf{v} \right|^2 - I$$

$$= -\mu_{ij} (\mathbf{v} - \mathbf{v}_*) \cdot \left(\frac{m_i}{m_i + m_j} \mathbf{v} + \frac{m_j}{m_i + m_j} \mathbf{v}_* \right)$$

$$+ \sqrt{2\mu_{ij} R E} \left(\frac{m_i}{m_i + m_j} \mathbf{v} + \frac{m_j}{m_i + m_j} \mathbf{v}_* \right) \cdot T_{\boldsymbol{\omega}} \left[\frac{\mathbf{v} - \mathbf{v}_*}{\left| \mathbf{v} - \mathbf{v}_* \right|} \right]$$

$$+ \left| \mathbf{v} - \mathbf{v}_* \right|^2 \frac{\mu_{ij}}{2} (1-R) \left(-\frac{m_j}{(m_i + m_j)} + r \right)$$

$$+ I \left(\frac{m_j}{m_i + m_j} R + r(1-R) - 1 \right) + I_* \left(\frac{m_j}{m_i + m_j} R + r(1-R) \right).$$

We pass to the $\boldsymbol{\sigma}$ notation, and integration with respect to this variable yields

$$E_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} K \frac{n_i n_j}{\zeta_{0_i}(T_i) \zeta_{0_j}(T_j)} \left(\frac{m_i m_j}{4\, \pi^2\, k^2\, T_i T_j} \right)^{\frac{N}{2}} \left| S^{N-1} \right|$$

$$\times \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_\Omega e^{-\frac{1}{kT_i} \left(\frac{m_i}{2} |\mathbf{v} - \mathbf{u}_i|^2 + I \right)} e^{-\frac{1}{kT_j} \left(\frac{m_j}{2} |\mathbf{v}_* - \mathbf{u}_j|^2 + I_* \right)} \left| \mathbf{v} - \mathbf{v}_* \right|^{2s_{ij}} (1-R) R^{s_{ij} + \frac{N}{2} - 1}$$

$$\times \left\{ -\mu_{ij}(\mathbf{v} - \mathbf{v}_*) \cdot \left(\frac{m_i}{m_i + m_j} \mathbf{v} + \frac{m_j}{m_i + m_j} \mathbf{v}_* \right) \right.$$

$$+ \left| \mathbf{v} - \mathbf{v}_* \right|^2 \frac{\mu_{ij}}{2} (1-R) \left(-\frac{m_j}{(m_i + m_j)} + r \right)$$

$$\left. + I \left(\frac{m_j}{m_i + m_j} R + r(1-R) - 1 \right) + I_* \left(\frac{m_j}{m_i + m_j} R + r(1-R) \right) \right\} dr\, dR\, dI_*\, d\mathbf{v}_*\, dI\, d\mathbf{v}.$$

Next, we pass to the reference frame of the center of mass by means of the change of variables (3.14). We rewrite the part concerning velocities in the exponential as (3.15). The following integral is obtained

$$E_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} K \frac{n_i n_j}{\zeta_{0_i}(T_i) \zeta_{0_j}(T_j)} \left(\frac{m_i m_j}{4\, \pi^2\, k^2\, T_i T_j} \right)^{\frac{N}{2}} \left| S^{N-1} \right|$$

$$\times \iint_{\mathbb{R}^N \times \mathbb{R}_+} \int_\Omega e^{-a_{ij} |\mathbf{g} + \mathbf{b}_{ij}|^2 - \frac{1}{kT_i} I} e^{-c_{ij} |\mathbf{G} + d_{ij} \mathbf{g} + \mathbf{e}_{ij}|^2 - \frac{1}{kT_j} I_*} \left| \mathbf{g} \right|^{2s_{ij}} (1-R) R^{s_{ij} + \frac{N}{2} - 1}$$

$$\times \left\{ -\mu_{ij}\, \mathbf{g} \cdot \mathbf{G} + \left| \mathbf{g} \right|^2 \frac{\mu_{ij}}{2} (1-R) \left(-\frac{m_j}{(m_i + m_j)} + r \right) \right.$$

$$\left. + I \left(\frac{m_j}{m_i + m_j} R + r(1-R) - 1 \right) + I_* \left(\frac{m_j}{m_i + m_j} R + r(1-R) \right) \right\} dr\, dR\, dI_*\, d\mathbf{g}\, dI\, d\mathbf{G}.$$

Then, integration with respect to $\mathbf{G}$ in conjunction with (3.17) gives

$$
E_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} K \frac{n_i n_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \left| S^{N-1} \right| \left(\frac{a_{ij}}{\pi} \right)^{\frac{N}{2}} \int_{\mathbb{R}_+} \int_{\Omega} e^{-a_{ij}|\mathbf{g}+\mathbf{b}_{ij}|^2} e^{-\frac{1}{kT_i}I} e^{-\frac{1}{kT_j}I_*} \left| \mathbf{g} \right|^{2s_{ij}} (1-R) R^{s_{ij}+\frac{N}{2}-1}
$$

$$
\times \left\{ \mu_{ij}\, \mathbf{g} \cdot (d_{ij}\mathbf{g} + \mathbf{e}_{ij}) + |\mathbf{g}|^2 \frac{\mu_{ij}}{2}(1-R)\left(-\frac{m_j}{(m_i + m_j)} + r \right) \right.
$$

$$
\left. + I\left(\frac{m_j}{m_i + m_j}R + r(1-R) - 1 \right) + I_*\left(\frac{m_j}{m_i + m_j}R + r(1-R) \right) \right\} \, dr \, dR \, dI_* \, d\mathbf{g} \, dI.
$$

Integration with respect to I and I_*, and grouping coefficients of the same degree in $\mathbf{g}$, yields

$$
E_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} K n_i n_j \frac{k^2\, T_i\, T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \left| S^{N-1} \right| \left(\frac{a_{ij}}{\pi} \right)^{\frac{N}{2}} \int_{\mathbb{R}^N} \int_{[0,1]} \int_{[0,1]} |\mathbf{g}|^{2s_{ij}}\, e^{-a_{ij}|\mathbf{g}-(\mathbf{u}_i-\mathbf{u}_j)|^2}(1-R)R^{s_{ij}+\frac{N}{2}-1}
$$

$$
\times \left\{ \mu_{ij}\left(d_{ij} + \frac{1}{2}(1-R)\left(-\frac{m_j}{m_i + m_j} + r \right) \right) |\mathbf{g}|^2 \right.
$$

$$
+ \mu_{ij}\mathbf{e}_{ij} \cdot \mathbf{g}
$$

$$
\left. + k\, T_i\left(\frac{m_j}{m_i + m_j}R + r(1-R) - 1 \right) + k\, T_j\left(\frac{m_j}{m_i + m_j}R + r(1-R) \right) \right\} \, dr \, dR \, d\mathbf{g}.
$$

Next, integrating with respect to r, we get

$$
E_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} K n_i n_j \frac{k^2\, T_i\, T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \left| S^{N-1} \right| \left(\frac{a_{ij}}{\pi} \right)^{\frac{N}{2}} \int_{\mathbb{R}^N} \int_{[0,1]} |\mathbf{g}|^{2s_{ij}}\, e^{-a_{ij}|\mathbf{g}-(\mathbf{u}_i-\mathbf{u}_j)|^2}(1-R)R^{s_{ij}+\frac{N}{2}-1}
$$

$$
\times \left\{ \mu_{ij}\left(d_{ij} + \frac{m_i - m_j}{4\,(m_i + m_j)}(1-R) \right) |\mathbf{g}|^2 \right.
$$

$$
+ \mu_{ij}\mathbf{e}_{ij} \cdot \mathbf{g}
$$

$$
\left. + k\, T_i\left(\frac{m_j - m_i}{2\,(m_i + m_j)}R - \frac{1}{2} \right) + k\, T_j\left(\frac{m_j - m_i}{2\,(m_i + m_j)}R + \frac{1}{2} \right) \right\} \, dR \, d\mathbf{g}.
$$

Integration with respect to R gives

$$
E_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} K n_i n_j \frac{k^2\, T_i\, T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \frac{4\left| S^{N-1} \right|}{(N + 2s_{ij} + 2)} \left(\frac{a_{ij}}{\pi} \right)^{\frac{N}{2}} \int_{\mathbb{R}^N} |\mathbf{g}|^{2s_{ij}}\, e^{-a_{ij}|\mathbf{g}-(\mathbf{u}_i-\mathbf{u}_j)|^2}
$$

$$
\times \left\{ \frac{\mu_{ij}}{(N + 2s_{ij})}\left(d_{ij} + \frac{m_i - m_j}{(m_i + m_j)}\frac{1}{(N + 2s_{ij} + 4)} \right) |\mathbf{g}|^2 \right.
$$

$$
+ \frac{\mu_{ij}}{(N + 2s_{ij})}\mathbf{e}_{ij} \cdot \mathbf{g}
$$

$$
\left. + \frac{m_j - m_i}{2\,(m_i + m_j)}\frac{1}{(N + 2s_{ij} + 4)}(k\, T_i + k\, T_j) + \frac{1}{2\,(N + 2s_{ij})}(k\, T_j - k\, T_i) \right\} \, d\mathbf{g}.
$$

Comparing with (3.18), we recognize that the coefficient of $\mathbf{e}_{ij}$ is $-\tilde{\mathbf{N}}_{ij}$, where $-\tilde{\mathbf{N}}_{ij}$ is such that $\mathbf{N}_i = \sum_{\substack{j=1 \\ j \neq i}}^{s} \tilde{\mathbf{N}}_{ij}$. We are then led to write

$$
\begin{aligned}
E_i = & -\sum_{\substack{j=1 \\ j \neq i}}^{s} \mathbf{e}_{ij} \cdot \tilde{\mathbf{N}}_{ij} + \sum_{\substack{j=1 \\ j \neq i}}^{s} K n_i n_j \frac{k^2 T_i T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \frac{4\left|S^{N-1}\right|}{(N + 2s_{ij} + 2)} \left(\frac{a_{ij}}{\pi}\right)^{\frac{N}{2}} \int_{\mathbb{R}^N} |\mathbf{g}|^{2s_{ij}} e^{-a_{ij}|\mathbf{g} - (\mathbf{u}_i - \mathbf{u}_j)|^2} \\
& \times \left\{ \frac{\mu_{ij}}{(N + 2s_{ij})} \left(\mu_{ij} \frac{k T_j - k T_i}{m_i k T_j + m_j k T_i} + \frac{m_i - m_j}{(m_i + m_j)} \frac{1}{(N + 2s_{ij} + 4)} \right) |\mathbf{g}|^2 \right. \\
& \left. + \frac{m_j - m_i}{2(m_i + m_j)} \frac{1}{(N + 2s_{ij} + 4)} (k T_i + k T_j) + \frac{1}{2(N + 2s_{ij})} (k T_j - k T_i) \right\} \mathrm{d}\mathbf{g}.
\end{aligned}
$$

Next step consists in passing to spherical coordinates for $\mathbf{g}$, using the change of variable (3.19) with Jacobian (3.20), and expressing

$$
|\mathbf{g} - (\mathbf{u}_i - \mathbf{u}_j)|^2 = |\mathbf{g}|^2 - 2|\mathbf{u}_i - \mathbf{u}_j| |\mathbf{g}| \cos \varphi_1 + |\mathbf{u}_i - \mathbf{u}_j|^2.
$$

We obtain the following integral

$$
\begin{aligned}
E_i = & -\sum_{\substack{j=1 \\ j \neq i}}^{s} \mathbf{e}_{ij} \cdot \tilde{\mathbf{N}}_{ij} + \sum_{\substack{j=1 \\ j \neq i}}^{s} K n_i n_j \frac{k^2 T_i T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \frac{4\left|S^{N-1}\right|\left|S^{N-2}\right|}{(N + 2s_{ij} + 2)} \left(\frac{a_{ij}}{\pi}\right)^{\frac{N}{2}} e^{-a_{ij}|\mathbf{u}_i - \mathbf{u}_j|^2} \\
& \times \int_{\mathbb{R}_+} |\mathbf{g}|^{2s_{ij}+N-1} e^{-a_{ij}|\mathbf{g}|^2} \int_0^\pi e^{2a_{ij}|\mathbf{u}_i-\mathbf{u}_j||\mathbf{g}| \cos \varphi_1} (\sin \varphi_1)^{N-2} \mathrm{d}\varphi_1 \\
& \times \left\{ \frac{\mu_{ij}}{(N + 2s_{ij})} \left(\mu_{ij} \frac{k T_j - k T_i}{m_i k T_j + m_j k T_i} + \frac{m_i - m_j}{(m_i + m_j)} \frac{1}{(N + 2s_{ij} + 4)} \right) |\mathbf{g}|^2 \right. \\
& \left. + \frac{m_j - m_i}{2(m_i + m_j)} \frac{1}{(N + 2s_{ij} + 4)} (k T_i + k T_j) + \frac{1}{2(N + 2s_{ij})} (k T_j - k T_i) \right\} \mathrm{d}|\mathbf{g}|.
\end{aligned}
$$

The integral with respect to the angular variable φ_1 can easily be represented using (16), i.e.

$$
\int_0^\pi e^{2a_{ij}|\mathbf{u}_i-\mathbf{u}_j||\mathbf{g}| \cos \varphi_1} (\sin \varphi_1)^{N-2} \mathrm{d}\varphi_1 = \sqrt{\pi} \, \Gamma\left[\frac{N-1}{2}\right] \, {}_0\tilde{F}_1\left(; \frac{N}{2}; a_{ij}^2 |\mathbf{u}_i - \mathbf{u}_j|^2 |\mathbf{g}|^2 \right).
$$

In particular, when $N = 3$, the computation is quite simple: denoting $A_{ij} = 2a_{ij} |\mathbf{u}_i - \mathbf{u}_j| |\mathbf{g}|$, we use the change of variable $\cos \varphi_1 \mapsto p$, and obtain

$$
\int_0^\pi e^{A_{ij} \cos \varphi_1} \sin \varphi_1 \mathrm{d}\varphi_1 = \int_{-1}^1 e^{A_{ij} p} \mathrm{d}p = \frac{2}{A_{ij}} \sinh A_{ij}.
$$

In the general case, we write

$$
\begin{aligned}
E_i = & -\sum_{\substack{j=1 \\ j \neq i}}^{s} \mathbf{e}_{ij} \cdot \tilde{\mathbf{N}}_{ij} + \sum_{\substack{j=1 \\ j \neq i}}^{s} K n_i n_j \frac{k^2 T_i T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \frac{4\left|S^{N-1}\right|\left|S^{N-2}\right|}{(N + 2s_{ij} + 2)} \left(\frac{a_{ij}}{\pi}\right)^{\frac{N}{2}} e^{-a_{ij}|\mathbf{u}_i - \mathbf{u}_j|^2} \sqrt{\pi} \, \Gamma\left[\frac{N-1}{2}\right] \\
& \times \int_{\mathbb{R}_+} |\mathbf{g}|^{2s_{ij}+N-1} e^{-a_{ij}|\mathbf{g}|^2} \, {}_0\tilde{F}_1\left(; \frac{N}{2}; a_{ij}^2 |\mathbf{u}_i - \mathbf{u}_j|^2 |\mathbf{g}|^2 \right) \\
& \times \left\{ \frac{\mu_{ij}}{(N + 2s_{ij})} \left(\mu_{ij} \frac{k T_j - k T_i}{m_i k T_j + m_j k T_i} + \frac{m_i - m_j}{(m_i + m_j)} \frac{1}{(N + 2s_{ij} + 4)} \right) |\mathbf{g}|^2 \right. \\
& \left. + \frac{m_j - m_i}{2(m_i + m_j)} \frac{1}{(N + 2s_{ij} + 4)} (k T_i + k T_j) + \frac{1}{2(N + 2s_{ij})} (k T_j - k T_i) \right\} \mathrm{d}|\mathbf{g}|.
\end{aligned}
$$

We perform the following change of variable $a_{ij}\,|\mathbf{g}|^2 \mapsto x$, and get

$$
E_i = -\sum_{\substack{j=1 \\ j\neq i}}^{s} \mathbf{e}_{ij} \cdot \tilde{\mathbf{N}}_{ij} + \sum_{\substack{j=1 \\ j\neq i}}^{s} K n_i n_j \frac{k^2 T_i T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \frac{4\left|S^{N-1}\right|\left|S^{N-2}\right|}{(N+2s_{ij}+2)} \left(\frac{a_{ij}}{\pi}\right)^{\frac{N}{2}} e^{-a_{ij}|\mathbf{u}_i-\mathbf{u}_j|^2} \sqrt{\pi}\,\Gamma\left[\frac{N-1}{2}\right]
$$

$$
\times \int_{\mathbb{R}_+} e^{-x}\; {}_0\tilde{F}_1\left(;\frac{N}{2};a_{ij}\,|\mathbf{u}_i-\mathbf{u}_j|^2\,x\right)
$$

$$
\times \left\{ \frac{\mu_{ij}}{(N+2s_{ij})}\left(\mu_{ij}\frac{kT_j-kT_i}{m_i kT_j+m_j kT_i} + \frac{m_i-m_j}{(m_i+m_j)}\frac{1}{(N+2s_{ij}+4)}\right)\frac{1}{2} a_{ij}^{-\frac{N+2s_{ij}+2}{2}} x^{\frac{N+2s_{ij}+2}{2}-1} \right.
$$

$$
\left. + \left(\frac{m_j-m_i}{2(m_i+m_j)}\frac{1}{(N+2s_{ij}+4)}(kT_i+kT_j) + \frac{1}{2(N+2s_{ij})}(kT_j-kT_i)\right)\frac{1}{2} a_{ij}^{-\frac{N+2s_{ij}}{2}} x^{\frac{N+2s_{ij}}{2}-1} \right\} dx.
$$

Comparing these integrals with representation (14) yields

$$
E_i = -\sum_{\substack{j=1 \\ j\neq i}}^{s} \mathbf{e}_{ij} \cdot \tilde{\mathbf{N}}_{ij} + \sum_{\substack{j=1 \\ j\neq i}}^{s} K n_i n_j \frac{k^2 T_i T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \frac{4\left|S^{N-1}\right|\left|S^{N-2}\right|}{(N+2s_{ij}+2)} \left(\frac{a_{ij}}{\pi}\right)^{\frac{N}{2}} e^{-a_{ij}|\mathbf{u}_i-\mathbf{u}_j|^2} \sqrt{\pi}\,\Gamma\left[\frac{N-1}{2}\right]
$$

$$
\times \left\{ \frac{\mu_{ij}}{(N+2s_{ij})}\left(\mu_{ij}\frac{kT_j-kT_i}{m_i kT_j+m_j kT_i} + \frac{m_i-m_j}{(m_i+m_j)}\frac{1}{(N+2s_{ij}+4)}\right) \right.
$$

$$
\times \frac{1}{2} a_{ij}^{-\frac{N+2s_{ij}+2}{2}} \Gamma\left[\frac{N+2s_{ij}+2}{2}\right]\; {}_1\tilde{F}_1\left(\frac{N+2s_{ij}+2}{2};\frac{N}{2};a_{ij}\,|\mathbf{u}_i-\mathbf{u}_j|^2\right)
$$

$$
+ \left(\frac{m_j-m_i}{2(m_i+m_j)}\frac{1}{(N+2s_{ij}+4)}(kT_i+kT_j) + \frac{1}{2(N+2s_{ij})}(kT_j-kT_i)\right)
$$

$$
\left. \times \frac{1}{2} a_{ij}^{-\frac{N+2s_{ij}}{2}} \Gamma\left[\frac{N+2s_{ij}}{2}\right]\; {}_1\tilde{F}_1\left(\frac{N+2s_{ij}}{2};\frac{N}{2};a_{ij}\,|\mathbf{u}_i-\mathbf{u}_j|^2\right) \right\}.
$$

Substituting the coefficients, we get the final expression for the production term that corresponds to the energy balance law of the species $\mathcal{A}_i$ of Euler fluids, in the case of a cross section of VHS type:

$$
(3.23)\quad E_i = \sum_{\substack{j=1 \\ j\neq i}}^{s} \left(\frac{m_i}{2kT_i}+\frac{m_j}{2kT_j}\right)^{-1}\left(\frac{m_i}{2kT_i}\mathbf{u}_i+\frac{m_j}{2kT_j}\mathbf{u}_j\right)\cdot\tilde{\mathbf{N}}_{ij}
$$

$$
+ \sum_{\substack{j=1 \\ j\neq i}}^{s} K n_i n_j \frac{k^2 T_i T_j}{\zeta_{0_i}(T_i)\zeta_{0_j}(T_j)} \frac{2\left|S^{N-1}\right|\left|S^{N-2}\right|}{(N+2s_{ij}+2)}
$$

$$
\times \left(\frac{2kT_i}{m_i}+\frac{2kT_j}{m_j}\right)^{s_{ij}} \pi^{\frac{1-N}{2}} e^{-\left(\frac{2kT_i}{m_i}+\frac{2kT_j}{m_j}\right)^{-1}|\mathbf{u}_i-\mathbf{u}_j|^2} \Gamma\left[\frac{N-1}{2}\right]\Gamma\left[\frac{N+2s_{ij}}{2}\right]
$$

$$
\times \left\{ \left(\frac{m_j\,kT_i+m_i\,kT_j}{m_i+m_j}\right)\left(\mu_{ij}\frac{kT_j-kT_i}{m_i kT_j+m_j kT_i} + \frac{m_i-m_j}{(m_i+m_j)}\frac{1}{(N+2s_{ij}+4)}\right) \right.
$$

$$
\times\; {}_1\tilde{F}_1\left(\frac{N+2s_{ij}+2}{2};\frac{N}{2};\left(\frac{2kT_i}{m_i}+\frac{2kT_j}{m_j}\right)^{-1}|\mathbf{u}_i-\mathbf{u}_j|^2\right)
$$

$$
+ \left(\frac{m_j-m_i}{2(m_i+m_j)}\frac{1}{(N+2s_{ij}+4)}(kT_i+kT_j) + \frac{1}{2(N+2s_{ij})}(kT_j-kT_i)\right)
$$

$$
\left. \times\; {}_1\tilde{F}_1\left(\frac{N+2s_{ij}}{2};\frac{N}{2};\left(\frac{2kT_i}{m_i}+\frac{2kT_j}{m_j}\right)^{-1}|\mathbf{u}_i-\mathbf{u}_j|^2\right) \right\}.
$$

3. Comparison of the models built thanks to extended thermodynamics and those built thanks to kinetic theory

This Section aims at comparing the source terms (3.10) obtained by means of extended thermodynamics and the source terms (3.22) and (3.23) obtained with the help of kinetic theory. The comparison is motivated by the intrinsic limitations of extended thermodynamics – phenomenological coefficients cannot be completely determined within its framework. In that sense, kinetic theory seems to be more complete. Once the model of interaction is fixed, the structure of source terms can be completely determined in principle.

Comparison of source terms (3.10), obtained in extended thermodynamics, with the source terms (3.22) and (3.23) from kinetic theory, is not possible in general, since they have a completely different structure. Namely, (3.10) is proportional to $\mathbf{u}_i/T_i - \mathbf{u}_j/T_j$ and $1/T_i - 1/T_j$, while kinetic source terms are highly nonlinear with respect to macroscopic state variables. We can establish the relation between them only in the limit $\mathbf{u}_i \to \mathbf{u}$ and $T_i \to T$, for every $i = 1, \ldots, s$. More precisely, we are led to approximate the source terms $\mathbf{N}_i(\mathbf{u}_i, \mathbf{u}_j, T_i, T_j)$ and $E_i(\mathbf{u}_i, \mathbf{u}_j, T_i, T_j)$ around the point $(\mathbf{u}, \mathbf{u}, T, T)$ retaining the first order terms, i.e.

(3.24)
$$\mathbf{N}_i := \mathbf{N}_i(\mathbf{u}_i, \mathbf{u}_j, T_i, T_j) \approx \mathbf{N}_i(\mathbf{u}, \mathbf{u}, T, T) + \nabla \mathbf{N}_i(\mathbf{u}, \mathbf{u}, T, T) \cdot [\mathbf{u}_i - \mathbf{u} \quad \mathbf{u}_j - \mathbf{u} \quad T_i - T \quad T_j - T]^T,$$

$$E_i := E_i(\mathbf{u}_i, \mathbf{u}_j, T_i, T_j) \approx E_i(\mathbf{u}, \mathbf{u}, T, T) + \nabla E_i(\mathbf{u}, \mathbf{u}, T, T) \cdot [\mathbf{u}_i - \mathbf{u} \quad \mathbf{u}_j - \mathbf{u} \quad T_i - T \quad T_j - T]^T,$$

which holds when $(\mathbf{u}_i, \mathbf{u}_j, T_i, T_j)$ is close to $(\mathbf{u}, \mathbf{u}, T, T)$, for any $i, j = 1, \ldots, s$.

Regarding source terms (3.10) issuing from extended thermodynamics, such an approximation yields

(3.25)
$$\mathbf{N}_i \approx -\sum_{\substack{j=1 \\ j \neq i}}^{s-1} \alpha_{ij}(\boldsymbol{w}^0) \frac{1}{T} (\mathbf{u}_j - \mathbf{u}_i) + \left(\sum_{j=1}^{s-1} \alpha_{ij}(\boldsymbol{w}^0) \right) \frac{1}{T} (\mathbf{u}_s - \mathbf{u}_i),$$

$$E_i \approx -\sum_{\substack{j=1 \\ j \neq i}}^{s-1} \alpha_{ij}(\boldsymbol{w}^0) \frac{1}{T} \mathbf{u} \cdot (\mathbf{u}_j - \mathbf{u}_i) + \left(\sum_{j=1}^{s-1} \alpha_{ij}(\boldsymbol{w}^0) \right) \frac{1}{T} \mathbf{u} \cdot (\mathbf{u}_s - \mathbf{u}_i)$$

$$- \sum_{\substack{j=1 \\ j \neq i}}^{s-1} \beta_{ij}(\boldsymbol{w}^0) \frac{1}{T^2} (T_j - T_i) + \left(\sum_{j=1}^{s-1} \beta_{ij}(\boldsymbol{w}^0) \frac{1}{T^2} \right) (T_s - T_i),$$

where $\boldsymbol{w}^0 := \boldsymbol{w}(\mathbf{u}, \mathbf{u}, T, T)$ denotes an objective quantity $\boldsymbol{w}$ evaluated at the point $(\mathbf{u}, \mathbf{u}, T, T)$.

Approximating source terms (3.22) and (3.23) coming from kinetic theory, we obtain

(3.26)
$$\mathbf{N}_i \approx \sum_{\substack{j=1 \\ j \neq i}}^{s} K \mu_{ij}^{1-s_{ij}} n_i n_j \frac{2^{s_{ij}} 64\pi^{1/2}}{3(2s_{ij}+3)(2s_{ij}+5)} \frac{\Gamma[s_{ij} + \frac{5}{2}]}{\Gamma[\alpha_i + 1]\Gamma[\alpha_j + 1]} (kT)^{-(\alpha_i+\alpha_j)+s_{ij}} (\mathbf{u}_j - \mathbf{u}_i)$$

$$E_i \approx \sum_{\substack{j=1 \\ j \neq i}}^{s} K \mu_{ij}^{1-s_{ij}} n_i n_j \frac{2^{s_{ij}} 64\pi^{1/2}}{3(2s_{ij}+3)(2s_{ij}+5)} \frac{\Gamma[s_{ij} + \frac{5}{2}]}{\Gamma[\alpha_i + 1]\Gamma[\alpha_j + 1]} (kT)^{-(\alpha_i+\alpha_j)+s_{ij}} \mathbf{u} \cdot (\mathbf{u}_j - \mathbf{u}_i)$$

$$+ \sum_{\substack{j=1 \\ j \neq i}}^{s} K k \mu_{ij}^{-s_{ij}} n_i n_j \frac{2^{s_{ij}} 16\pi^{1/2}}{(2s_{ij}+5)} \frac{\Gamma[s_{ij} + \frac{3}{2}]}{\Gamma[\alpha_i + 1]\Gamma[\alpha_j + 1]} (kT)^{-(\alpha_i+\alpha_j)+s_{ij}}$$

$$\times \frac{(m_i - m_j)^2(2s_{ij}+3) + (m_i + m_j)^2(2s_{ij}+7) + 2(2s_{ij}+3)(2s_{ij}+7)m_i m_j}{(m_i + m_j)^2(2s_{ij}+3)(2s_{ij}+7)} (T_j - T_i).$$

Then (3.25) and (3.26) can be directly compared to obtain explicit expressions for matrices $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ in equilibrium. First, we obtain the off-diagonal terms:

$$\alpha_{ij}(\boldsymbol{w}^0) = -K\mu_{ij}^{1-s_{ij}} n_i n_j \frac{2^{s_{ij}} 64\pi^{1/2}}{3(2s_{ij}+3)(2s_{ij}+5)} \frac{\Gamma[s_{ij}+\frac{5}{2}]}{\Gamma[\alpha_i+1]\Gamma[\alpha_j+1]} (kT)^{-(\alpha_i+\alpha_j)+s_{ij}} T,$$

$$\beta_{ij}(\boldsymbol{w}^0) = -K\mu_{ij}^{-s_{ij}} n_i n_j \frac{2^{s_{ij}} 16\pi^{1/2}}{(2s_{ij}+5)} \frac{\Gamma[s_{ij}+\frac{3}{2}]}{\Gamma[\alpha_i+1]\Gamma[\alpha_j+1]} (kT)^{-(\alpha_i+\alpha_j)+s_{ij}} kT^2$$
$$\times \frac{(m_i-m_j)^2(2s_{ij}+3) + (m_i+m_j)^2(2s_{ij}+7) + 2(2s_{ij}+3)(2s_{ij}+7)m_i m_j}{(m_i+m_j)^2(2s_{ij}+3)(2s_{ij}+7)},$$

for any $i = 1, \ldots, s-1$ and for $1 \leq j \leq s-1$ such that $j \neq i$. Next, we get the diagonal terms:

$$\alpha_{ii}(\boldsymbol{w}^0) = K\mu_{is}^{1-s_{is}} n_i n_s \frac{2^{s_{is}} 64\pi^{1/2}}{3(2s_{is}+3)(2s_{is}+5)} \frac{\Gamma[s_{is}+\frac{5}{2}]}{\Gamma[\alpha_i+1]\Gamma[\alpha_s+1]} (kT)^{-(\alpha_i+\alpha_s)+s_{is}} T$$
$$+ \sum_{\substack{j=1 \\ j \neq i}}^{s-1} K\mu_{ij}^{1-s_{ij}} n_i n_j \frac{2^{s_{ij}} 64\pi}{3(2s_{ij}+3)(2s_{ij}+5)} \frac{\Gamma[s_{ij}+2]}{\Gamma[\alpha_i+1]\Gamma[\alpha_j+1]} (kT)^{-(\alpha_i+\alpha_j)+s_{ij}} T,$$

$$\beta_{ii}(\boldsymbol{w}^0) = K\mu_{is}^{-s_{is}} n_i n_s \frac{2^{s_{is}} 16\pi^{1/2}}{(2s_{is}+5)} \frac{\Gamma[s_{is}+\frac{3}{2}]}{\Gamma[\alpha_i+1]\Gamma[\alpha_s+1]} (kT)^{-(\alpha_i+\alpha_s)+s_{is}} kT^2$$
$$\times \frac{(m_i-m_s)^2(2s_{is}+3) + (m_i+m_s)^2(2s_{is}+7) + 2(2s_{is}+3)(2s_{is}+7)m_i m_s}{(m_i+m_s)^2(2s_{is}+3)(2s_{is}+7)}$$
$$+ \sum_{\substack{j=1 \\ j \neq i}}^{s-1} K\mu_{ij}^{-s_{ij}} n_i n_j \frac{2^{s_{ij}} 16\pi^{1/2}}{(2s_{ij}+5)} \frac{\Gamma[s_{ij}+\frac{3}{2}]}{\Gamma[\alpha_i+1]\Gamma[\alpha_j+1]} (kT)^{-(\alpha_i+\alpha_j)+s_{ij}} kT^2$$
$$\times \frac{(m_i-m_j)^2(2s_{ij}+3) + (m_i+m_j)^2(2s_{ij}+7) + 2(2s_{ij}+3)(2s_{ij}+7)m_i m_j}{(m_i+m_j)^2(2s_{ij}+3)(2s_{ij}+7)},$$

where $i = 1, \ldots, s-1$.

In conclusion to this analysis, which has mostly formal character, we have to say that kinetic theory model of VHS yielded the source terms of macroscopic balance laws of momentum and energy at Euler level. Both thermodynamic (3.10) and kinetic (3.22), (3.23) source terms describe the rate of change of momentum and energy of the constituents due to mutual interaction with other constituents. Even though we restricted the attention to the hydrodynamic limit at the Euler level, both source terms are nonlinear, but different in structure, and their explicit comparison is not possible in general. However, they can be reduced to considerably simpler form, (3.25) and (3.26), if we restrict the attention to processes which occur in the neighborhood of the average velocity $\mathbf{u}$ and the average temperature T of the mixture. Under this assumption, we can linearize the source terms (3.10), (3.22), (3.23) and determine the phenomenological coefficients $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ of extended thermodynamics for $\mathbf{u}_i = \mathbf{u}$ and $T_i = T$, $i = 1, \ldots, s$, from the source terms provided by the kinetic theory. Although rather restrictive at first sight, these assumptions lead to important results for thermodynamic model, since extended thermodynamics, regarded as macroscopic theory, does not provide any mean for explicit determination of phenomenological coefficients.

CHAPTER 4

Diffusion asymptotics of a kinetic model for the mixtures of monatomic gases

The interest about the derivation of macroscopic equations starting from kinetic theory goes back to Hilbert [**41**] in his lecture at ICM in 1900. He pointed out the importance of developing "mathematically the limiting processes which lead from the atomistic view to the laws of motion of continua". This problem has been a very active field of research, and many results have been obtained, both at a formal level and in the context of rigorous limits. We tackle, in this Chapter, the asymptotic behavior of Boltzmann equations for mixtures.

The main tools are based on asymptotic (Hilbert, Chapman-Enskog) expansions with respect to the mean free path, see for instance [**25**]. The translation in a rigorous mathematical language has been performed in a series of pioneering papers by Bardos, Golse and Levermore [**10, 11, 12**]. The authors derive formal limits from the kinetic equation towards the compressible Euler and the incompressible Navier-Stokes equations. These results led to significant articles, such as [**36**], where Golse and Saint-Raymond established a Navier-Stokes limit for the Boltzmann equation considered over the infinite spatial domain $\mathbb{R}^3$: appropriately scaled families of DiPerna-Lions renormalized solutions are shown to have fluctuations whose limit points are governed by Leray solutions of the limiting Navier-Stokes equations.

Apart from the research concerning the classical Boltzmann equation (see [**28**] as a review article), which can be seen as a model describing a mono-species, monatomic and ideal gas, one can focus on the study, at a kinetic level, of gaseous mixtures. In such a framework, the models are much more intricate. It is indeed necessary to treat systems of Boltzmann-like equations, rather than one single equation, with multi-species kernels and cross interactions between the different distribution functions describing each component of the mixture [**56**]. The complexity of the models grows dramatically if exchanges of internal energy and chemical reactions are allowed [**56, 22, 52, 40, 13, 14**].

The derivation of macroscopic equations from kinetic models remains crucial for mixtures, both at a mathematical level and for deducing relevant macroscopic equations based on the modelling of microscopic binary interactions. In this spirit, in [**30**], the authors propose a model describing a reacting mixture of polyatomic gases and recover in the limit, via the appropriate scaling $(t, \mathbf{x}) \to (t/\varepsilon, \mathbf{x}/\varepsilon)$ for $\varepsilon > 0$, the reactive Euler equations. We refer also to Chapter 3 of this thesis, where a multivelocity and multitemperature model for mixture of Eulerian polyatomic gases is derived.

Our aim is to investigate diffusive scaling, i.e. $(t, \mathbf{x}) \to (t/\varepsilon^2, \mathbf{x}/\varepsilon)$, $\varepsilon > 0$, for the mixture of several different non reactive and monatomic gases, which evolves in time via the classical Boltzmann system for non-reacting multicomponent mixtures. We study the formal Hilbert expansion for each distribution function, following Grad's strategy [**38, 39**], who studied the formal small free path limit for the Boltzmann equation in the monatomic and mono-species case. The formal asymptotics of this model, investigated in [**21**], leads to the so-called Maxwell-Stefan equations, which are a standard diffusion model for multicomponent mixtures.

Putting the Hilbert expansions into the Boltzmann equations leads to various equalities at each order of the small mean free path ε. The first one allows to identify the zero order term of the expansions to Maxwellian functions, thanks to the H−theorem. The second one is a functional equation that involves a linear operator $\mathcal{L} = \mathcal{K} - \nu \,\mathrm{Id}$, where $\nu > 0$, only acting on the velocity variable. To solve this functional equation, we use the Fredholm alternative on the operator $\mathcal{L}$. In general, the alternative deals with the equation $(\mathrm{T} - \lambda \,\mathrm{Id}) \, u = f$, where T is a compact operator on a Hilbert space E, and $\lambda \in \mathbb{C}$.

THEOREM 4.1 (Fredholm Alternative). *Let* T *be a compact operator on* E, *and assume* $\lambda \neq 0$. *Then one of the two following alternatives holds:*

(i) *The homogeneous equation has only the zero solution, in which case* $(T - \lambda\,\text{Id})^{-1}$ *is bounded, and the inhomogeneous equation has exactly one solution* $u = (T - \lambda\,\text{Id})^{-1} f$, *for each* $f \in E$.

(ii) *The homogeneous equation has a non-zero solution, in which case the inhomogeneous equation has a solution (necessarily not unique) if and only if* $f \in (\text{Ker}(T^* - \lambda\,\text{Id}))^{\perp}$.

We first study the kernel of the operator $\mathcal{L}$ and state that $\ker \mathcal{L} \neq \{0\}$. Afterwards, we compute the adjoint operator $\mathcal{L}^*$ ($\mathcal{L}^*$ is different from $\mathcal{L}$ in the multispecies case, whereas it equals $\mathcal{L}$ in the monospecies case) and find $\ker \mathcal{L}^*$. Finally, the Fredholm alternative, statement (ii), ensures the existence of a solution to the functional equation involving $\mathcal{L}$ with an assumption on the total macroscopic density of the mixture.

The main difficulty lies in the proof of compactness of the operator $\mathcal{K}$. To that purpose, the following characterization of compact operators is used.

THEOREM 4.2. *A bounded subset* K *of* $L^p(\mathbb{R}^N)$, $1 \leq p < \infty$, *is relatively compact if and only if the two following properties hold*

(i) $\displaystyle\int_{\mathbb{R}^N} |u(\mathbf{v} + \mathbf{w}) - u(\mathbf{v})|^p \, d\mathbf{v} \to 0$, *as* $\mathbf{w} \to 0$ *uniformly for* u *in* K,

(ii) $\displaystyle\int_{|\mathbf{v}| > R} |u(\mathbf{v})|^p \, d\mathbf{v} \to 0$ *as* $R \to \infty$ *uniformly for* u *in* K.

On the one hand, when molecular masses are equal, the techniques introduced by Grad [38, 39] can be extended to the multispecies case. On the other hand, when masses are different, the proof requires a new approach. Indeed, Grad's arguments do not hold anymore. To overcome this issue, we prove that, thanks to a change of variables in velocities, the operator can be written under a kernel form, that allows to recover the compactness property. Note that this last approach only holds when molecular masses are different, so that it is necessary to keep Grad's approach for collisions of molecules with the same mass.

1. Statement of the problem

1.1. Diffusion asymptotics. In this work, we focus on the diffusion limit of the following Boltzmann equations for mixtures (1.38)

$$\partial_t f_i + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = \sum_{j=1}^{s} Q_{ij}(f_i, f_j), \quad \forall i = 1, \dots, s,$$

where $f_i := f_i(t, \mathbf{x}, \mathbf{v})$. That limit is obtained from the framework of the classical diffusive scaling, where the scaling parameter is the mean free path $\varepsilon > 0$. The diffusive scaling reads

$$t \mapsto t^{\varepsilon} = \varepsilon^2 t, \quad \mathbf{x} \mapsto \mathbf{x}^{\varepsilon} = \varepsilon \mathbf{x}.$$

This corresponds to a slow dynamics in space and an even slower one in time. We introduce new distribution functions with scaled arguments:

$$f_i\left(\frac{t^{\varepsilon}}{\varepsilon^2}, \frac{\mathbf{x}^{\varepsilon}}{\varepsilon}, \mathbf{v}\right) =: f_i^{\varepsilon}\left(t^{\varepsilon}, \mathbf{x}^{\varepsilon}, \mathbf{v}\right), \quad \forall i = 1, \dots, s.$$

The substitution of the scaled variables t and $\mathbf{x}$ into the Boltzmann equations (1.38) yields

$$\left(\varepsilon^2 \, \partial_{t^{\varepsilon}} + \varepsilon \, \mathbf{v} \cdot \nabla_{\mathbf{x}^{\varepsilon}}\right) f_i^{\varepsilon}\left(t^{\varepsilon}, \mathbf{x}^{\varepsilon}, \mathbf{v}\right) = \sum_{j=1}^{s} Q_{ij}\left(f_i^{\varepsilon}, f_j^{\varepsilon}\right)\left(t^{\varepsilon}, \mathbf{x}^{\varepsilon}, \mathbf{v}\right), \quad \forall i = 1, \dots, s.$$

From now on, we drop the index ε in the notations t^{ε} and $\mathbf{x}^{\varepsilon}$.

Hence, for any i, each distribution function f_i^{ε} solves the following scaled Boltzmann equation:

$$(4.1) \qquad \varepsilon \, \partial_t f_i^{\varepsilon} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i^{\varepsilon} = \frac{1}{\varepsilon} \sum_{j=1}^{I} Q_{ij}(f_i^{\varepsilon}, f_j^{\varepsilon}), \quad t > 0, \, \mathbf{x} \in \mathbb{R}^3, \, \mathbf{v} \in \mathbb{R}^3.$$

1.2. Solution as Hilbert formal series. We look for f_i^ε as a formal power series in ε:

$$(4.2) \qquad f_i^\varepsilon(t, \mathbf{x}, \mathbf{v}) = \sum_{k \geq 0} \varepsilon^k f_{i_{(k)}}(t, \mathbf{x}, \mathbf{v}), \quad \forall\, i = 1, \ldots, s.$$

It should be noticed that this series does not converge in general for any value of $\varepsilon > 0$. We however only study the first few terms of this series.

Supposing that f_i^ε in (4.2) is a solution of the scaled Boltzmann equation (4.1), we identify the coefficients of the same power in ε.

We only focus on the first two terms in series (4.2). We focus on the following two equations:

Order ε^{-1} :

$$(4.3) \qquad \sum_{j=1}^s Q_{ij}(f_{i_{(0)}}, f_{j_{(0)}}) = 0\,;$$

Order ε^0 :

$$(4.4) \qquad \sum_{j=1}^s \Big(Q_{ij}(f_{i_{(0)}}, f_{j_{(1)}}) + Q_{ij}(f_{i_{(1)}}, f_{j_{(0)}}) \Big) = \mathbf{v} \cdot \nabla_{\mathbf{x}} f_{i_{(0)}}.$$

Thanks to Proposition 1.5, (4.3) allows to find the zero-th order term of the series: those are the Maxwell functions (1.48):

$$f_{i_{(0)}}(\mathbf{v}) = n_i \left(\frac{m_i}{2\,\pi\,k\,T} \right)^{3/2} e^{-\frac{m_i}{2kT}|\mathbf{v} - \mathbf{u}|^2}.$$

Therefore, each distribution function f_i^ε, $1 \leq i \leq s$, can be seen as a perturbation of the equilibrium (1.48). Consistently with the diffusion asymptotics, we set $\mathbf{u} = 0$ (diffusion limit) and $kT = 1$. Furthermore, we allow the macroscopic density functions to depend on the time and the space variable, $n_i := n_i(t, \mathbf{x})$, and therefore $f_{i_{(0)}}$ takes the following form

$$f_{i_{(0)}} := f_{i_{(0)}}(t, \mathbf{x}, \mathbf{v}) = M_i(\mathbf{v})\, n_i(t, \mathbf{x}),$$

where $M_i(\mathbf{v})$ is the normalized, centered Maxwell function

$$(4.5) \qquad M_i(\mathbf{v}) = \left(\frac{m_i}{2\pi} \right)^{3/2} e^{-\frac{m_i}{2}|\mathbf{v}|^2}, \quad \forall\, \mathbf{v} \in \mathbb{R}^3.$$

Moreover, we denote

$$f_{i_{(1)}} := f_{i_{(1)}}(t, \mathbf{x}, \mathbf{v}) = M_i(\mathbf{v})^{1/2} g_i(t, \mathbf{x}, \mathbf{v}).$$

We choose to put $M_i(\mathbf{v})^{1/2}$ within the first-order term of f_i^ε since it allows us to work in a plain L^2 framework in the variable $\mathbf{v}$ for g_i.

Finally, we can rewrite f_i^ε from (4.2) as

$$(4.6) \qquad f_i^\varepsilon(t, \mathbf{x}, \mathbf{v}) = M_i(\mathbf{v})\, n_i(t, \mathbf{x}) + \varepsilon\, M_i(\mathbf{v})^{1/2}\, g_i(t, \mathbf{x}, \mathbf{v}) + ..., \quad \forall\, t \geq 0,\ \forall\, \mathbf{x}, \mathbf{v} \in \mathbb{R}^3.$$

We then focus on (4.4), the zero-th order in ε. We obtain the following equation, holding for any $1 \leq i \leq s$,

$$(4.7) \qquad M_i^{-1/2} \sum_{j=1}^s \Big(n_i\, Q_{ij}(M_i, M_j^{1/2} g_j) + n_j\, Q_{ij}(M_i^{1/2} g_i, M_j) \Big) = M_i^{1/2}\, (\mathbf{v} \cdot \nabla_{\mathbf{x}} n_i).$$

In this work, we investigate the existence of $\mathbf{g} = (g_1, \ldots, g_s)$. satisfying (4.7). Note that the dependence of (4.7) with respect to t and $\mathbf{x}$ is not crucial, in the sense that t, $\mathbf{x}$, (n_i) and $(\nabla_{\mathbf{x}} n_i)$ can be seen as parameters.

For any function $\mathbf{g} \in L^2(\mathbb{R}^3)^s$ of $\mathbf{v}$, we shall write the L^2 norm of $\mathbf{g}$:

$$\|\mathbf{g}\|_{L^2}^2 = \sum_{j=1}^s \|g_j\|_{L^2}^2 = \sum_{j=1}^s \int_{\mathbb{R}^3} g_j(\mathbf{v})^2\, d\mathbf{v}.$$

Observing that $M_i(\mathbf{v}')M_j(\mathbf{v}'_*) = M_i(\mathbf{v})M_j(\mathbf{v}_*)$, we can write the left-hand side of (4.7) in a more suitable form if we introduce the operator $\mathcal{K}$, where the i-th component of $\mathcal{K}\mathbf{g}$ is given by

$$(4.8) \quad [\mathcal{K}\mathbf{g}]_i(\mathbf{v}) = \sum_{j=1}^{s} \left(\frac{m_j}{2\pi}\right)^{3/4} \iint_{\mathbb{R}^3 \times S^2} \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, e^{-\frac{1}{4}m_i|\mathbf{v}|^2} \, e^{-\frac{1}{2}m_j|\mathbf{v}_*|^2}$$

$$\times \left[n_i \left(\frac{m_i}{2\pi}\right)^{3/4} \left(e^{\frac{1}{4}m_j|\mathbf{v}'_*|^2} g_j(\mathbf{v}'_*) - e^{\frac{1}{4}m_j|\mathbf{v}_*|^2} g_j(\mathbf{v}_*) \right) \right.$$

$$\left. + n_j \left(\frac{m_j}{2\pi}\right)^{3/4} e^{\frac{1}{4}m_i|\mathbf{v}'|^2} g_i(\mathbf{v}') \right] \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*,$$

for any i, and the positive function $\nu = \nu(\mathbf{v})$, whose i-th component is

$$(4.9) \qquad \nu_i(\mathbf{v}) = \sum_{j=1}^{s} n_j \left(\frac{m_j}{2\pi}\right)^{3/2} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{2}m_j|\mathbf{v}_*|^2} \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*.$$

Let us point out an abuse of notation that we made. In this Section, we denote the cross section by $\mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*)$, instead of $\mathcal{B}_{ij}\left(|\mathbf{v} - \mathbf{v}_*|, \left|\boldsymbol{\omega} \cdot \frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|}\right|\right)$, as in (1.42).

After introducing (4.8) and (4.9), (4.7) can be written as a functional equation in the variable $\mathbf{v}$:

$$(4.10) \qquad (\mathcal{K} - \nu\,\mathrm{Id})\,\mathbf{g} = \left(M_i^{1/2}(\mathbf{v} \cdot \nabla_\mathbf{x} n_i) \right)_{1 \leq i \leq s}.$$

1.3. Assumption on the cross section. In this work, we assume that the cross sections $\mathcal{B}_{ij}$ satisfy a quite general condition

$$(4.11) \qquad \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{V}) \leq a\,|\sin\theta|\,|\cos\theta|\,\left(|\mathbf{V}| + \frac{1}{|\mathbf{V}|^{1-\delta}}\right), \quad \forall\,\boldsymbol{\omega} \in S^2,\ \forall\,\mathbf{V} \in \mathbb{R}^3,$$

where $a > 0$, $0 < \delta < 1$ and θ is the angle between $\boldsymbol{\omega}$ and $\mathbf{V} := \mathbf{v} - \mathbf{v}_*$. As emphasized in [39], this corresponds to intermolecular potentials with finite range and it means that $\mathcal{B}_{ij}$ linearly approaches 0 near $\theta = 0$ and $\theta = \pi/2$, and is of restricted growth for both small and large $|\mathbf{V}|$.

Condition (4.11) is, for instance, satisfied by hard spheres of diameter $\sigma_{ij} > 0$:

$$\mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{V}) = \sigma_{ij}^2\,|\mathbf{V}|\,\sin\theta\,\cos\theta,$$

and by all cutoff power-law (hard or moderately soft) potentials:

$$\mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{V}) = |\mathbf{V}|^{\gamma_{ij}}\,\beta_{ij}(\theta), \quad \gamma_{ij} = \frac{s_{ij} - 5}{s_{ij} - 1},$$

where $\beta_{ij}(\theta)$ is a bounded function which linearly approaches 0 when θ tends to $\pi/2$, and $s_{ij} > 3$.

Let us now state the main result of this Chapter.

THEOREM 4.3. *Suppose that the cross sections $(\mathcal{B}_{ij})_{1 \leq i,j \leq s}$ are positive functions satisfying (4.11). If we assume that*

$$(4.12) \qquad \sum_{i=1}^{s} n_i(t, \mathbf{x}) \text{ does not depend on } \mathbf{x},$$

then, for any t, $\mathbf{x}$, there exists $\mathbf{g}(t, \mathbf{x}, \cdot) \in L^2(\mathbb{R}_\mathbf{v}^3)^s$ satisfying (4.10), where $\mathcal{K}$ and ν are given by (4.8)–(4.9).

Condition (4.12) means that we consider a situation where the total number density of molecules is uniform in space. This Theorem is based on the following Proposition.

PROPOSITION 4.4. *The operator $\mathcal{K}$, defined by (4.8), is compact from $L^2(\mathbb{R}_\mathbf{v}^3)^s$ to $L^2(\mathbb{R}_\mathbf{v}^3)^s$.*

The proof of Proposition 4.4 is given in Section 3. Let us emphasize again that, in Proposition 4.4, t, $\mathbf{x}$ and (n_i) are considered as parameters and the compactness is only related to the variable $\mathbf{v}$. Since $\mathcal{K}$ is compact, we can apply the Fredholm alternative to the operator $\mathcal{K} - \nu\,\mathrm{Id}$. This is explained in the next Section. We also observe that the Proposition does not hold when non cutoff power law potentials are considered.

2. Proof of Theorem 4.3

This Section is devoted to the proof of Theorem 4.3, assuming that the compactness in L^2 of the operator $\mathcal{K}$ is known. Let us denote $\mathcal{L} = \mathcal{K} - \nu\,\mathrm{Id}$, and study the null space of $\mathcal{L}$, as required by the Fredholm alternative.

Step 1 – Study of ker $\mathcal{L}$. Using (4.8), (4.9) with notation (4.5) we can write down the i-th component of $\mathcal{L}\mathbf{g}$

$$[\mathcal{L}\mathbf{g}]_i(\mathbf{v}) = \sum_{j=1}^{s} \iint_{\mathbb{R}^3 \times S^2} M_i(\mathbf{v})^{1/2} M_j(\mathbf{v}_*)$$

$$\times \Big[n_j M_i(\mathbf{v}')^{-1/2} g_i(\mathbf{v}') + n_i M_j(\mathbf{v}_*')^{-1/2} g_j(\mathbf{v}_*')$$

$$- n_j M_i(\mathbf{v})^{-1/2} g_i(\mathbf{v}) - n_i M_j(\mathbf{v}_*)^{-1/2} g_j(\mathbf{v}_*) \Big]$$

$$\times \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*)\, d\boldsymbol{\omega}\, d\mathbf{v}_*.$$

Thanks to the H-theorem 1.5, $\mathbf{g} \in \ker \mathcal{L}$ if and only if there exist $\boldsymbol{\alpha} \in \mathbb{R}^s$, $\boldsymbol{\beta} \in \mathbb{R}^3$, $\gamma \in \mathbb{R}$ such that, for any i,

$$g_i(t, \mathbf{x}, \mathbf{v}) = n_i(t, \mathbf{x})\, M_i(\mathbf{v})^{1/2} \left(\alpha_i + m_i\, \boldsymbol{\beta} \cdot \mathbf{v} + \gamma \frac{m_i}{2} |\mathbf{v}|^2 \right), \quad \forall\, t > 0,\, \mathbf{x},\, \mathbf{v} \in \mathbb{R}^3.$$

Consequently, $\ker \mathcal{L} \neq \{0\}$, and the Fredholm alternative implies that (4.10) has a solution if and only if

(4.13)
$$\left(M_i^{1/2} (\mathbf{v} \cdot \nabla_{\mathbf{x}} n_i) \right)_{i=1,\dots,s} \in (\ker \mathcal{L}^*)^\perp, \quad \forall\, t > 0,\, \mathbf{x} \in \mathbb{R}^3.$$

Step 2 – Computation of $\mathcal{L}^*$. Let us compute the adjoint operator $\mathcal{L}^*$ by studying the inner product between $\mathcal{L}\mathbf{g}$ and a vector $h \in L^2(\mathbb{R}^3_{\mathbf{v}})^s$. We successively write, using the change of variables $(\mathbf{v}, \mathbf{v}_*) \mapsto (\mathbf{v}', \mathbf{v}_*')$ and $(\mathbf{v}, \mathbf{v}_*) \mapsto (\mathbf{v}_*, \mathbf{v})$

$$\sum_{i=1}^{s} \int_{\mathbb{R}^3} [\mathcal{L}\mathbf{g}]_i(\mathbf{v})\, h_i(\mathbf{v})\, d\mathbf{v}$$

$$= \sum_{i,j=1}^{s} \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times S^2} h_i(\mathbf{v})\, M_i(\mathbf{v})^{-1/2} \Big[n_i\, M_i(\mathbf{v}') M_j(\mathbf{v}_*')^{1/2} g_j(\mathbf{v}_*')$$

$$- n_i M_i(\mathbf{v}) M_j(\mathbf{v}_*)^{1/2} g_j(\mathbf{v}_*) + n_j M_j(\mathbf{v}_*') M_i(\mathbf{v}')^{1/2} g_i(\mathbf{v}')$$

$$- n_j M_j(\mathbf{v}_*) M_i(\mathbf{v})^{1/2} g_i(\mathbf{v}) \Big] \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*)\, d\boldsymbol{\omega}\, d\mathbf{v}_*\, d\mathbf{v}$$

$$= \sum_{i,j=1}^{s} \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times S^2} g_i(\mathbf{v})\, n_j\, M_i(\mathbf{v})^{-1/2} \Big[M_i(\mathbf{v}') M_j(\mathbf{v}_*')^{1/2} h_j(\mathbf{v}_*')$$

$$- M_i(\mathbf{v}) M_j(\mathbf{v}_*)^{1/2} h_j(\mathbf{v}_*) + M_j(\mathbf{v}_*') M_i(\mathbf{v}')^{1/2} h_i(\mathbf{v}')$$

$$- M_j(\mathbf{v}_*) M_i(\mathbf{v})^{1/2} h_i(\mathbf{v}) \Big] \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*)\, d\boldsymbol{\omega}\, d\mathbf{v}_*\, d\mathbf{v}.$$

Consequently, we have

$$[\mathcal{L}^* h]_i = M_i^{-1/2} \sum_{j=1}^{s} n_j \left(Q_{ij}(M_i, M_j^{1/2} h_j) + Q_{ij}(M_i^{1/2} h_i, M_j) \right).$$

Thanks to the H-theorem, $h \in \ker \mathcal{L}^*$ if and only if there exist $\mathbf{a} \in \mathbb{R}^s$, $\mathbf{b} \in \mathbb{R}^3$, $c \in \mathbb{R}$ such that, for any i,

$$(4.14) \qquad h_i(\mathbf{v}) = M_i(\mathbf{v})^{1/2} \left(a_i + m_i \, \mathbf{b} \cdot \mathbf{v} + c \frac{m_i}{2} \, |\mathbf{v}|^2 \right), \quad \forall \, \mathbf{v} \in \mathbb{R}^3.$$

Step 3 – Conclusion. Now, taking (4.14) into account, condition (4.13) can be rewritten as

$$\sum_{i=1}^{s} \sum_{k=1}^{3} \frac{\partial n_i}{\partial x_k} \int_{\mathbb{R}^3} \begin{pmatrix} v_k \\ m_i v_k \, v_j \\ m_i v_k \, |\mathbf{v}|^2 / 2 \end{pmatrix} M_i(\mathbf{v}) \, \mathrm{d}\mathbf{v} = 0, \quad 1 \le j \le 3.$$

Using parity arguments, the first and third conditions are immediately satisfied, as well as the second ones if $k \ne j$. In the case when $k = j$, the condition $\nabla_\mathbf{x} \sum n_i = 0$, which is assumed in (4.12), allows to complete the proof.

3. Proof of Proposition 4.4

We still have to prove that $\mathcal{K}$ is compact. In this section, $(n_i)_{1 \le i \le s}$ are assumed to be nonnegative constants. Let $\mathbf{g} \in L^2(\mathbb{R}^3)^s$. First, we write $\mathcal{K}$ as the sum of four operators $\mathcal{K}_1, ..., \mathcal{K}_4$. For any i, the i-th component of each $\mathcal{K}_\ell \, \mathbf{g}$, $1 \le \ell \le 4$, is given by

$$[\mathcal{K}_1 \mathbf{g}]_i (\mathbf{v}) = -n_i \sum_{j=1}^{s} \left(\frac{m_i m_j}{4\pi^2} \right)^{3/4} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4} m_i |\mathbf{v}|^2} e^{-\frac{1}{4} m_j |\mathbf{v}_*|^2} g_j(\mathbf{v}_*)$$
$$\times \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*,$$

$$[\mathcal{K}_2 \mathbf{g}]_i (\mathbf{v}) = n_i \sum_{j \notin \mathcal{M}_i} \left(\frac{m_i m_j}{4\pi^2} \right)^{3/4} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4} m_i |\mathbf{v}|^2} e^{-\frac{1}{2} m_j |\mathbf{v}_*|^2} e^{\frac{1}{4} m_j |\mathbf{v}_*'|^2} g_j(\mathbf{v}_*')$$
$$\times \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*,$$

$$[\mathcal{K}_3 \mathbf{g}]_i (\mathbf{v}) = \sum_{j \in \mathcal{M}_i} \left(\frac{m_i}{2\pi} \right)^{3/2} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4} m_i |\mathbf{v}|^2} e^{-\frac{1}{2} m_i |\mathbf{v}_*|^2}$$
$$\times \left[n_i \, e^{\frac{1}{4} m_i |\mathbf{v}_*'|^2} g_j(\mathbf{v}_*') + n_j \, e^{\frac{1}{4} m_i |\mathbf{v}'|^2} g_i(\mathbf{v}') \right] \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*,$$

$$[\mathcal{K}_4 \mathbf{g}]_i (\mathbf{v}) = \sum_{j \notin \mathcal{M}_i} n_j \left(\frac{m_j}{2\pi} \right)^{3/2} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4} m_i |\mathbf{v}|^2} e^{-\frac{1}{2} m_j |\mathbf{v}_*|^2} e^{\frac{1}{4} m_i |\mathbf{v}'|^2} g_i(\mathbf{v}')$$
$$\times \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{v}_*.$$

We denoted, for any i,

$$\mathcal{M}_i := \{ 1 \le j \le s \mid m_j = m_i \},$$

which is non empty since $i \in \mathcal{M}_i$. It is crucial to dissociate the cases when $m_i \ne m_j$ on the one hand, and $m_i = m_j$ on the other hand, because the proofs are quite different.

We successively prove that $\mathcal{K}_\ell$, $1 \le \ell \le 4$, is compact. To this end, we use Theorem 4.2. More precisely, we obtain the following properties for $\ell = 1, \dots, 4$:

- a uniform decay at infinity

$$(4.15) \qquad \|\mathcal{K}_\ell \, \mathbf{g}\|_{L^2(B(0,R)^c)} \le \sigma(R) \, \|\mathbf{g}\|_{L^2(\mathbb{R}^3)}, \qquad \forall R > 0,$$

   where $B(0, R)$ denotes the open ball of $\mathbb{R}^3_\mathbf{v}$ centred at 0 and of radius R, and $\sigma(R)$ goes to 0 when R goes to $+\infty$;

- an equiintegrability in L^2 property, i.e., for any $\varepsilon > 0$, there exists $\varrho > 0$ such that, for all $\mathbf{w} \in B(0, \varrho)$,

$$(4.16) \qquad \|(\tau_\mathbf{w} - \mathrm{Id})\mathcal{K}_\ell \, \mathbf{g}\|_{L^2(\mathbb{R}^3)} \le \varepsilon \|\mathbf{g}\|_{L^2(\mathbb{R}^3)},$$

   where $\tau_\mathbf{w}$ denotes the translation operator, i.e.

$$\tau_\mathbf{w} \mathcal{K}_\ell \, \mathbf{g}(\mathbf{v}) = \mathcal{K}_\ell \, \mathbf{g}(\mathbf{v} + \mathbf{w}), \qquad \forall \mathbf{v}, \mathbf{w} \in \mathbb{R}^3.$$

3.1. Compactness of $\mathcal{K}_1$. Let us denote, for any i, j,

$$k_1^{ij}(\mathbf{v}, \mathbf{v}_*) = \int_{S^2} e^{-\frac{1}{4}m_i|\mathbf{v}|^2} e^{-\frac{1}{4}m_j|\mathbf{v}_*|^2} \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, \mathrm{d}\boldsymbol{\omega}, \quad \forall \mathbf{v}, \mathbf{v}_* \in \mathbb{R}^3.$$

We immediately have, for any i,

$$[\mathcal{K}_1 \mathbf{g}]_i(\mathbf{v}) = -n_i \sum_{j=1}^{s} \left(\frac{m_i m_j}{4\pi^2}\right)^{3/4} \int_{\mathbb{R}^3} g_j(\mathbf{v}_*) k_1^{ij}(\mathbf{v}, \mathbf{v}_*) \, \mathrm{d}\mathbf{v}_*, \quad \forall \mathbf{v} \in \mathbb{R}^3.$$

Properties of k_1^{ij}. First of all, note that $k_1^{ij}(\mathbf{v}, \mathbf{v}_*)$ is invariant under the exchange of species:

(4.17) $$k_1^{ij}(\mathbf{v}, \mathbf{v}_*) = k_1^{ji}(\mathbf{v}_*, \mathbf{v}),$$

for any i, j and $\mathbf{v}$, $\mathbf{v}_*$, thanks to (1.43).

In order to prove the uniform decay at infinity and the equiintegrability for $\mathcal{K}_1$ (i.e. inequalities (4.15) and (4.16)), we need to establish some preliminary properties of k_1^{ij}.

LEMMA 4.5. *There exists $C > 0$ such that, for any i, j,*

(4.18) $$\int_{\mathbb{R}^3} k_1^{ij}(\mathbf{v}, \mathbf{v}_*) \mathrm{d}\mathbf{v}_* \le C \, e^{-\frac{1}{4}m_i|\mathbf{v}|^2} \left(1 + |\mathbf{v}|\right), \quad \forall \mathbf{v} \in \mathbb{R}^3.$$

PROOF. Thanks to (4.11), and using the change of variables $\mathbf{v}_* \mapsto \mathbf{V}_* = \mathbf{v}_* - \mathbf{v}$, we can write

$$\int_{\mathbb{R}^3} k_1^{ij}(\mathbf{v}, \mathbf{v}_*) \mathrm{d}\mathbf{v}_* \le C \int_{\mathbb{R}^3} e^{-\frac{1}{4}m_i|\mathbf{v}|^2} e^{-\frac{1}{4}m_j|\mathbf{V}_*+\mathbf{v}|^2} \left(|\mathbf{V}_*| + |\mathbf{V}_*|^{\delta-1}\right) \mathrm{d}\mathbf{V}_*.$$

Splitting the range of integration into $\{|\mathbf{V}_*| \le 1\}$ and $\{|\mathbf{V}_*| \ge 1\}$, we get

$$\int_{\mathbb{R}^3} k_1^{ij}(\mathbf{v}, \mathbf{v}_*) \mathrm{d}\mathbf{v}_* \le C \int_{\mathbb{R}^3} e^{-\frac{1}{4}m_i|\mathbf{v}|^2} e^{-\frac{1}{4}m_j|\mathbf{V}_*+\mathbf{v}|^2} \left(|\mathbf{V}_*| + |\mathbf{V}_*|^{\delta-1}\right) \mathrm{d}\mathbf{V}_*$$

$$= C \, e^{-\frac{1}{4}m_i|\mathbf{v}|^2} \int_{|\mathbf{V}_*|\le 1} e^{-\frac{1}{4}m_j|\mathbf{V}_*+\mathbf{v}|^2} \left(|\mathbf{V}_*| + |\mathbf{V}_*|^{\delta-1}\right) \mathrm{d}\mathbf{V}_*$$

$$+ C \, e^{-\frac{1}{4}m_i|\mathbf{v}|^2} \int_{|\mathbf{V}_*|\ge 1} e^{-\frac{1}{4}m_j|\mathbf{V}_*+\mathbf{v}|^2} \left(|\mathbf{V}_*| + |\mathbf{V}_*|^{\delta-1}\right) \mathrm{d}\mathbf{V}_*$$

$$\le C \, e^{-\frac{1}{4}m_i\mathbf{v}^2} \left[\int_{|\mathbf{V}_*|\le 1} \left(|\mathbf{V}_*| + |\mathbf{V}_*|^{\delta-1}\right) \mathrm{d}\mathbf{V}_* \right.$$

$$\left. + \int_{|\mathbf{V}_*|\ge 1} (|\mathbf{V}_*| + 1) \, e^{-\frac{1}{4}m_j(\mathbf{V}_*+\mathbf{v})^2} \mathrm{d}\mathbf{V}_* \right].$$

Since $\delta - 1 \in (-1, 0)$, the first integral is integrable and we get

$$\int_{|\mathbf{V}_*|\le 1} \left(|\mathbf{V}_*| + |\mathbf{V}_*|^{\delta-1}\right) \mathrm{d}\mathbf{V}_* \le C.$$

For the second integral we obtain

$$\int_{|\mathbf{V}_*|\ge 1} (|\mathbf{V}_*| + 1) \, e^{-\frac{1}{4}m_j(\mathbf{V}_*+\mathbf{v})^2} \mathrm{d}\mathbf{V}_* \le C \left(1 + |\mathbf{v}|\right).$$

Summarizing, we obtain the required result (4.18).

$$\int_{\mathbb{R}^3} k_1^{ij}(\mathbf{v}, \mathbf{v}_*) \mathrm{d}\mathbf{v}_* \le C \, e^{-\frac{1}{4}m_i\mathbf{v}^2} \left(1 + |\mathbf{v}|\right), \quad \forall \mathbf{v} \in \mathbb{R}^3.$$

$\square$

LEMMA 4.6. *For any i, j, k_1^{ij} belongs to $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$.*

PROOF. The proof follows the same strategy as the previous one, using (4.11) and the same change of variables. We can write

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} k_1^{ij}(\mathbf{v}, \mathbf{v}_*)^2 \mathrm{d}\mathbf{v}_* \, \mathrm{d}\mathbf{v} \leq C \iint_{\mathbb{R}^3 \times \mathbb{R}^3} e^{-\frac{1}{2}m_i|\mathbf{v}|^2} e^{-\frac{1}{2}m_j|\mathbf{v}_*|^2}$$
$$\times \left(|\mathbf{v} - \mathbf{v}_*|^2 + |\mathbf{v} - \mathbf{v}_*|^{2\delta - 2} \right) \mathrm{d}\mathbf{v}_* \, \mathrm{d}\mathbf{v}$$
$$\leq C \int_{\mathbb{R}^3} e^{-\frac{1}{2}m_i|\mathbf{v}|^2} \left(1 + |\mathbf{v}|^2 \right) \mathrm{d}\mathbf{v},$$

which is clearly finite. □

Uniform decay. The L^2 norm of $\mathcal{K}_1\mathbf{g}$ decreases at infinity. More precisely, the following proposition holds.

PROPOSITION 4.7. *Let* $\mathbf{g} \in L^2(\mathbb{R}^3)^s$. *For any* $R > 0$ *and any* i, *we have*

(4.19)
$$\| [\mathcal{K}_1\mathbf{g}]_i \|_{L^2(B(0,R)^c)} \leq \frac{C \, n_i}{R} \|\mathbf{g}\|_{L^2(\mathbb{R}^3)},$$

where $C > 0$ *is a constant.*

PROOF. Let $1 \leq i \leq s$ and write

$$\int_{\mathbb{R}^3} |\mathbf{v}|^2 \, [\mathcal{K}_1\mathbf{g}]_i (\mathbf{v})^2 \mathrm{d}\mathbf{v} \leq C n_i^2 \sum_{j=1}^{s} \int_{\mathbb{R}^3} |\mathbf{v}|^2 \left[\int_{\mathbb{R}^3} k_1^{ij}(\mathbf{v}, \mathbf{v}_*) \, g_j(\mathbf{v}_*) \, \mathrm{d}\mathbf{v}_* \right]^2 \mathrm{d}\mathbf{v}.$$

Thanks to the Cauchy-Schwarz inequality, the previous inequality becomes

$$\int_{\mathbb{R}^3} |\mathbf{v}|^2 \, [\mathcal{K}_1\mathbf{g}]_i (\mathbf{v})^2 \mathrm{d}\mathbf{v} \leq C n_i^2 \sum_{j=1}^{s} \int_{\mathbb{R}^3} |\mathbf{v}|^2 \left[\int_{\mathbf{v}_* \in \mathbb{R}^3} g_j(\mathbf{v}_*)^2 \, k_1^{ij}(\mathbf{v}, \mathbf{v}_*) \mathrm{d}\mathbf{v}_* \right]$$
$$\times \left[\int_{\mathbb{R}^3} k_1^{ij}(\mathbf{v}, \mathbf{v}_*) \mathrm{d}\mathbf{v}_* \right] \mathrm{d}\mathbf{v}.$$

Using Lemma 4.5 and Fubini's theorem, we get

$$\int_{\mathbb{R}^3} |\mathbf{v}|^2 \, [\mathcal{K}_1\mathbf{g}]_i (\mathbf{v})^2 \mathrm{d}\mathbf{v} \leq C n_i^2 \sum_{j=1}^{s} \int_{\mathbb{R}^3} g_j(\mathbf{v}_*)^2 \left[\int_{\mathbb{R}^3} k_1^{ij}(\mathbf{v}, \mathbf{v}_*) \phi_i(\mathbf{v}) \mathrm{d}\mathbf{v} \right] \mathrm{d}\mathbf{v}_*,$$

where $\phi_i(\mathbf{v}) = |\mathbf{v}|^2 (1 + |\mathbf{v}|) \, e^{-\frac{1}{4}m_i|\mathbf{v}|^2}$ is clearly bounded. Consequently, since $k_1^{ij}(\mathbf{v}, \mathbf{v}_*) = k_1^{ji}(\mathbf{v}_*, \mathbf{v})$, we have

$$\int_{\mathbb{R}^3} |\mathbf{v}|^2 \, [\mathcal{K}_1\mathbf{g}]_i (\mathbf{v})^2 \mathrm{d}\mathbf{v} \leq C n_i^2 \sum_{j=1}^{s} \int_{\mathbb{R}^3} g_j(\mathbf{v}_*)^2 \left(\int_{\mathbb{R}^3} k_1^{ji}(\mathbf{v}_*, \mathbf{v}) \mathrm{d}\mathbf{v} \right) \mathrm{d}\mathbf{v}_*.$$

Using Lemma 4.5 again, we obtain

$$\int_{\mathbb{R}^3} |\mathbf{v}|^2 \, [\mathcal{K}_1\mathbf{g}]_i (\mathbf{v})^2 \mathrm{d}\mathbf{v} \leq C n_i^2 \|\mathbf{g}\|_{L^2}^2.$$

Besides, we can deduce, for any $R > 0$,

$$\int_{\mathbb{R}^3} |\mathbf{v}|^2 \, [\mathcal{K}_1\mathbf{g}]_i (\mathbf{v})^2 \mathrm{d}\mathbf{v} \geq \int_{|\mathbf{v}| \geq R} |\mathbf{v}|^2 \, [\mathcal{K}_1\mathbf{g}]_i (\mathbf{v})^2 \mathrm{d}\mathbf{v} \geq R^2 \int_{|\mathbf{v}| \geq R} [\mathcal{K}_1\mathbf{g}]_i (\mathbf{v})^2 \mathrm{d}\mathbf{v}.$$

It is then easy to recover (4.19). □

L^2 *Equiintegrability.* The following property of L^2 equiintegrability of $\mathcal{K}_1$ holds.

PROPOSITION 4.8. *For any* $\mathbf{w} \in \mathbb{R}^3$, *set*

$$\varrho_1(\mathbf{w}) = C \max_{i,j} \left[n_i \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \left(k_1^{ij}(\mathbf{v} + \mathbf{w}, \mathbf{v}_*) - k_1^{ij}(\mathbf{v}, \mathbf{v}_*) \right)^2 d\mathbf{v}_* d\mathbf{v} \right]^{1/2},$$

where C is a suitable nonnegative constant. Then, for any i, we have

(4.20) $$\| \left[(\tau_{\mathbf{w}} - \mathrm{Id}) \mathcal{K}_1 \mathbf{g} \right]_i \|_{L^2(\mathbb{R}^3_{\mathbf{v}})} \leq \varrho_1(\mathbf{w}) \|\mathbf{g}\|_{L^2(\mathbb{R}^3_{\mathbf{v}})}, \quad \forall \mathbf{w} \in \mathbb{R}^3,$$

and $\varrho_1(\mathbf{w})$ tends to 0 when $\mathbf{w}$ tends to 0.

PROOF. First, thanks to Lemma 4.6, it is clear that ϱ_1 is a continuous function of $\mathbf{w}$, and goes to 0 when $\mathbf{w}$ goes to zero. Let us now focus on (4.20). For any i, using the Cauchy–Schwarz inequality, we have

$$\| \left[(\tau_{\mathbf{w}} - \mathrm{Id}) \mathcal{K}_1 \mathbf{g} \right]_i \|^2_{L^2(\mathbb{R}^3)} \leq C n_i^2 \sum_{j=1}^s \|g_j\|^2_{L^2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \left(k_1^{ij}(\mathbf{v} + \mathbf{w}, \mathbf{v}_*) - k_1^{ij}(\mathbf{v}, \mathbf{v}_*) \right)^2 d\mathbf{v}_* d\mathbf{v}.$$

Estimate (4.20) is an immediate consequence of the previous inequality. $\square$

3.2. Compactness of $\mathcal{K}_2$. As in Section 3.1, we first write $\mathcal{K}_2$ in a more convenient form. Indeed, thanks to (1.39), we have

$$-\frac{1}{4} m_i \, |\mathbf{v}|^2 - \frac{1}{2} m_j \, |\mathbf{v}_*|^2 + \frac{1}{4} m_j \, |\mathbf{v}'_*|^2 = -\frac{1}{4} m_j \, |\mathbf{v}_*|^2 - \frac{1}{4} m_i \, |\mathbf{v}'|^2.$$

Hence, $[\mathcal{K}_2]_i$ becomes

(4.21) $$[\mathcal{K}_2 \mathbf{g}]_i (\mathbf{v}) = \sum_{j \notin \mathcal{M}_i} n_i \left(\frac{m_i m_j}{4\pi^2} \right)^{3/4} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4} m_j |\mathbf{v}_*|^2} e^{-\frac{1}{4} m_i |\mathbf{v}'|^2} g_j(\mathbf{v}'_*) \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \, d\boldsymbol{\omega} \, d\mathbf{v}_*.$$

The next step consists in writing (4.21) in a form that allows to apply the same strategy as the one used for $\mathcal{K}_1$.

In order to get this particular form, we need the following lemma.

LEMMA 4.9. *There exists $b > 0$ such that, for any i, j satisfying $m_i \neq m_j$,*

(4.22) $$m_i \left| \mathbf{v}' \right|^2 + m_j \left| \mathbf{v}_* \right|^2 \geq b \left(m_i \, |\mathbf{v}|^2 + m_j \left| \mathbf{v}'_* \right|^2 \right)$$

for any $\mathbf{v}$, $\mathbf{v}_* \in \mathbb{R}^3$ and $\mathbf{v}'$, $\mathbf{v}'_*$ given by (1.40).

Remark. The assumption that the masses are different is crucial here, as we shall see in the proof. Indeed, (4.22) somehow gives a property of norm equivalence in $\mathbb{R}^3 \times \mathbb{R}^3$, linking $(\mathbf{v}, \mathbf{v}'_*)$ and $(\mathbf{v}', \mathbf{v}_*)$. Such a property does not hold when we deal with molecules having the same mass.

PROOF. Choose $j \notin \mathcal{M}_i$. Equation (1.40) can be rewritten as

(4.23) $$\mathbf{v}' = \left(\mathrm{I}_3 - 2 \frac{m_j}{m_i + m_j} \boldsymbol{\omega} \, \boldsymbol{\omega}^T \right) \mathbf{v} + 2 \frac{m_j}{m_i + m_j} \boldsymbol{\omega} \, \boldsymbol{\omega}^T \mathbf{v}_*,$$

(4.24) $$\mathbf{v}'_* = \left(\mathrm{I}_3 - 2 \frac{m_i}{m_i + m_j} \boldsymbol{\omega} \, \boldsymbol{\omega}^T \right) \mathbf{v}_* + 2 \frac{m_i}{m_i + m_j} \boldsymbol{\omega} \, \boldsymbol{\omega}^T \mathbf{v},$$

where I_3 is the identity matrix of $\mathbb{R}^3$. Then, from (4.24), we get

$$\left(\mathrm{I}_3 - 2 \frac{m_i}{m_i + m_j} \boldsymbol{\omega} \, \boldsymbol{\omega}^T \right) \mathbf{v}_* = \mathbf{v}'_* - 2 \frac{m_i}{m_i + m_j} \boldsymbol{\omega} \, \boldsymbol{\omega}^T \mathbf{v}.$$

Let us now set

$$\mathrm{A} = \mathrm{I}_3 - 2 \frac{m_i}{m_i + m_j} \boldsymbol{\omega} \, \boldsymbol{\omega}^T.$$

This matrix A is invertible, since $\det \mathrm{A} = (m_j - m_i) / (m_i + m_j)$ and $j \notin \mathcal{M}_i$. Consequently, we can write

(4.25) $$\mathbf{v}_* = \left(\mathrm{I}_3 - \mathrm{A}^{-1} \right) \mathbf{v} + \mathrm{A}^{-1} \mathbf{v}'_*,$$

where we used the equality

$$-2\frac{m_i}{m_i + m_j}\,\mathrm{A}^{-1}\,\boldsymbol{\omega}\,\boldsymbol{\omega}^T = \mathrm{I}_3 - \mathrm{A}^{-1}\,.$$

Then we put (4.25) in (4.23) to obtain

$$\mathbf{v}' = \left(\frac{m_i + m_j}{m_i}\,\mathrm{I}_3 - \frac{m_j}{m_i}\,\mathrm{A}^{-1}\right)\mathbf{v} - \frac{m_j}{m_i}\left(\mathrm{I}_3 - \mathrm{A}^{-1}\right)\mathbf{v}'_*.$$

Consider now the following block matrix

$$\mathbb{A} = \begin{bmatrix} \frac{m_i + m_j}{m_i}\,\mathrm{I}_3 - \frac{m_j}{m_i}\,\mathrm{A}^{-1} & -\sqrt{\frac{m_j}{m_i}}\left(\mathrm{I}_3 - \mathrm{A}^{-1}\right) \\ \sqrt{\frac{m_j}{m_i}}\left(\mathrm{I}_3 - \mathrm{A}^{-1}\right) & \mathrm{A}^{-1} \end{bmatrix},$$

which is invertible: $\det \mathbb{A} = -1$ and $\mathbb{A}^{-1} = \mathbb{A}$. The following vector equality holds:

$$\begin{bmatrix} \sqrt{m_i}\,\mathbf{v}' \\ \sqrt{m_j}\,\mathbf{v}_* \end{bmatrix} = \mathbb{A}\begin{bmatrix} \sqrt{m_i}\,\mathbf{v} \\ \sqrt{m_j}\,\mathbf{v}'_* \end{bmatrix}.$$

In fact, (4.22) is obtained by finding a lower bound of

$$\frac{\left|\mathbb{A}\begin{bmatrix} \sqrt{m_i}\,\mathbf{v} & \sqrt{m_j}\,\mathbf{v}'_* \end{bmatrix}^T\right|^2}{\left|\begin{bmatrix} \sqrt{m_i}\,\mathbf{v} & \sqrt{m_j}\,\mathbf{v}'_* \end{bmatrix}^T\right|^2},$$

which is $\|\mathbb{A}^{-1}\|_2^{-2} = \|\mathbb{A}\|_2^{-2}$. In order to determine the matrix 2-norm of $\mathbb{A}$, we compute eigenvalues of $\mathbb{A}^T\mathbb{A}$. Indeed, the eigenvalues in increasing order are

$$\frac{m_i^2 + 6m_im_j + m_j^2 - 4(m_i + m_j)\sqrt{m_im_j}}{(m_i - m_j)^2},\ 1,\ \frac{m_i^2 + 6m_im_j + m_j^2 + 4(m_i + m_j)\sqrt{m_im_j}}{(m_i - m_j)^2},$$

where eigenvalue 1 has multiplicity 4. Choosing

$$b = \min_{i,j}\frac{(m_i - m_j)^2}{m_i^2 + 6m_im_j + m_j^2 + 4(m_i + m_j)\sqrt{m_im_j}}$$

leads to the required estimate (4.22). □

Using (4.11) and Lemma 4.9, we obtain the upper bound

$$[\mathcal{K}_2\mathbf{g}]_i(\mathbf{v}) \leq C\,n_i\sum_{j\notin\mathcal{M}_i} e^{-\frac{b}{4}m_i|\mathbf{v}|^2}\int_{\mathbb{R}^3} e^{-\frac{b}{4}m_j|\mathbf{v}'_*|^2}\,g_j(\mathbf{v}'_*)\left(|\mathbf{v} - \mathbf{v}_*| + |\mathbf{v} - \mathbf{v}_*|^{\delta-1}\right)\,d\mathbf{v}_*.$$

Let us then perform the change of variable $\mathbf{v}_* \mapsto \mathbf{v}'_*$, whose Jacobian is $1/\det \mathrm{A}$. Since

$$\mathbf{v} - \mathbf{v}_* = \mathrm{A}^{-1}\left(\mathbf{v} - \mathbf{v}'_*\right)\quad\text{and}\quad \|\mathrm{A}\|_2^{-1} \leq \frac{\left|\mathrm{A}^{-1}\left(\mathbf{v} - \mathbf{v}'_*\right)\right|}{|(\mathbf{v} - \mathbf{v}'_*)|} \leq \|\mathrm{A}^{-1}\|_2,$$

we can write

$$|\mathbf{v} - \mathbf{v}_*| + |\mathbf{v} - \mathbf{v}_*|^{\delta-1} \leq \|\mathrm{A}^{-1}\|_2\,|\mathbf{v} - \mathbf{v}'_*| + \|\mathrm{A}\|_2^{1-\delta}\,|\mathbf{v} - \mathbf{v}'_*|^{\delta-1}\,.$$

Finally, we obtain

$$[\mathcal{K}_2\mathbf{g}]_i(\mathbf{v}) \leq C\,n_i\sum_{j\notin\mathcal{M}_i}\iint_{\mathbb{R}^3\times S^2} e^{-\frac{b}{4}m_i|\mathbf{v}|^2}\,e^{-\frac{b}{4}m_j|\mathbf{v}'_*|^2}\,g_j(\mathbf{v}'_*)\left(|\mathbf{v} - \mathbf{v}'_*| + |\mathbf{v} - \mathbf{v}'_*|^{\delta-1}\right)\,d\boldsymbol{\omega}\,d\mathbf{v}'_*.$$

The upper bound in the previous equality has exactly a kernel form, which allows us to conclude on the compactness of $\mathcal{K}_2$ in the same way as in Section 3.1.

3.3. Compactness of $\mathcal{K}_3$. This operator describes interactions between molecules with the same mass. Note that assuming the same mass of molecules of species $\mathcal{A}_i$ and $\mathcal{A}_j$ does not imply that species $\mathcal{A}_i$ and $\mathcal{A}_j$ are the same, since $\mathcal{B}_{ii}$, $\mathcal{B}_{ij}$ and $\mathcal{B}_{jj}$ can be different. In order to treat the case of $\mathcal{K}_3$, it is sufficient to adapt ideas from [39] and [23] used in the monospecies case.

Obtaining a kernel form. Note that if $m_i = m_j$, (1.40) becomes

(4.26) $$\mathbf{v}' = \mathbf{v} - (\boldsymbol{\omega} \cdot (\mathbf{v} - \mathbf{v}_*))\,\boldsymbol{\omega}, \quad \mathbf{v}'_* = \mathbf{v}_* + (\boldsymbol{\omega} \cdot (\mathbf{v} - \mathbf{v}_*))\,\boldsymbol{\omega}.$$

Symmetry properties allow us to write $[\mathcal{K}_3 \mathbf{g}]_i$ in terms of $\mathbf{v}$, $\mathbf{v}_*$ and $\mathbf{v}'$, and not $\mathbf{v}'_*$ anymore. More precisely, we have the following lemma.

LEMMA 4.10. *For any i, there exist nonnegative functions $\left(\tilde{\mathcal{B}}_{ij}\right)_{1 \leq j \leq s}$ satisfying (4.11), such that*

(4.27) $$[\mathcal{K}_3 \mathbf{g}]_i (\mathbf{v}) = \sum_{j \in \mathcal{M}_i} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4} m_i |\mathbf{v}|^2 - \frac{1}{2} m_j |\mathbf{v}_*|^2 + \frac{1}{4} m_i |\mathbf{v}'|^2}\, g_j(\mathbf{v}')\, \tilde{\mathcal{B}}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*)\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}\mathbf{v}_*,$$

$$\forall \mathbf{v} \in \mathbb{R}^3.$$

PROOF. The key idea of the proof lies in (4.26). Indeed, if we consider the relative velocity $\mathbf{V} = \mathbf{v} - \mathbf{v}_*$, we can choose one unit vector $\boldsymbol{\omega}^\perp \in \mathrm{Span}(\mathbf{V}, \boldsymbol{\omega})$ orthogonal to $\boldsymbol{\omega}$ (the choice of either $\boldsymbol{\omega}^\perp$ or $-\boldsymbol{\omega}^\perp$ is irrelevant, but must be performed in a continuous way with respect to $\boldsymbol{\omega}$, and not randomly). Consequently, we can write

$$\mathbf{V} = \boldsymbol{\omega}(\boldsymbol{\omega} \cdot \mathbf{V}) + \boldsymbol{\omega}^\perp(\boldsymbol{\omega}^\perp \cdot \mathbf{V}),$$

from which we immediately get

(4.28) $$\mathbf{v} - (\boldsymbol{\omega} \cdot \mathbf{V})\boldsymbol{\omega} = \mathbf{v}_* + (\boldsymbol{\omega}^\perp \cdot \mathbf{V})\boldsymbol{\omega}^\perp, \qquad \mathbf{v}_* + (\boldsymbol{\omega} \cdot \mathbf{V})\boldsymbol{\omega} = \mathbf{v} - (\boldsymbol{\omega}^\perp \cdot \mathbf{V})\boldsymbol{\omega}^\perp.$$

We can see that, if we look for the post-collisional velocities corresponding to the pre-collisional $\mathbf{v}$ and $\mathbf{v}_*$, but with respect to $\boldsymbol{\omega}^\perp$ instead of $\boldsymbol{\omega}$, we exchange the velocities $\mathbf{v}'$ and $\mathbf{v}'_*$: for instance, comparing (4.26) and (4.28) we can see that the new $\mathbf{v}'_*$, depending on $\boldsymbol{\omega}^\perp$ – let it be denoted with $\mathbf{v}'_{*\,\boldsymbol{\omega}^\perp}$ – will be the old $\mathbf{v}'$, depending on $\boldsymbol{\omega}$ – denoted with $\mathbf{v}'_{\boldsymbol{\omega}}$, i.e. (4.28) becomes

$$\mathbf{v}'_{\boldsymbol{\omega}} = \mathbf{v}'_{*\,\boldsymbol{\omega}^\perp}, \qquad \mathbf{v}'_{*\,\boldsymbol{\omega}} = \mathbf{v}'_{\boldsymbol{\omega}^\perp}.$$

Hence, it is clear that $\boldsymbol{\omega} \mapsto \boldsymbol{\omega}^\perp$ corresponds to $\mathbf{v}' \mapsto \mathbf{v}'_*$ and $\mathbf{v}'_* \mapsto \mathbf{v}'$.

Consequently, if we replace $\boldsymbol{\omega}$ by $\boldsymbol{\omega}^\perp$ in the integral

$$\iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{2} m_i |\mathbf{v}_*|^2}\, e^{\frac{1}{4} m_i |\mathbf{v}_* + (\boldsymbol{\omega} \cdot \mathbf{V})\boldsymbol{\omega}|^2}\, g_j(\mathbf{v}_* + (\boldsymbol{\omega} \cdot \mathbf{V})\boldsymbol{\omega})\, \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{V})\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}\mathbf{v}_*,$$

it becomes

$$\iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{2} m_i |\mathbf{v}_*|^2}\, e^{\frac{1}{4} m_i |\mathbf{v}_* + (\boldsymbol{\omega}^\perp \cdot \mathbf{V})\boldsymbol{\omega}^\perp|^2}\, g_j(\mathbf{v}_* + (\boldsymbol{\omega}^\perp \cdot \mathbf{V})\boldsymbol{\omega}^\perp)\, \mathcal{B}_{ij}(\boldsymbol{\omega}^\perp, \mathbf{V})\, \mathrm{d}\boldsymbol{\omega}^\perp\, \mathrm{d}\mathbf{v}_*.$$

The change of variable $\boldsymbol{\omega} \mapsto \boldsymbol{\omega}^\perp$ can be done thanks to a rotation, so $\mathrm{d}\boldsymbol{\omega}^\perp = \mathrm{d}\boldsymbol{\omega}$. Hence, using (4.28), the previous integral becomes

$$\iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{2} m_i |\mathbf{v}_*|^2}\, e^{\frac{1}{4} m_i |\mathbf{v}'|^2}\, g_j(\mathbf{v}')\, \mathcal{B}_{ij}(\boldsymbol{\omega}^\perp, \mathbf{V})\, \mathrm{d}\boldsymbol{\omega}^\perp\, \mathrm{d}\mathbf{v}_*$$

$$= \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{2} m_i |\mathbf{v}_*|^2}\, e^{\frac{1}{4} m_i |\mathbf{v}'|^2}\, g_j(\mathbf{v}')\, \mathcal{B}_{ij}(\boldsymbol{\omega}^\perp, \mathbf{V})\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}\mathbf{v}_*.$$

Summarizing, we can rewrite $[\mathcal{K}_3 \mathbf{g}]_i$:

$$[\mathcal{K}_3 \mathbf{g}]_i (\mathbf{v}) = \sum_{j \in \mathcal{M}_i} \left(\frac{m_i}{2\pi}\right)^{3/2} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4} m_i |\mathbf{v}|^2}\, e^{-\frac{1}{2} m_i |\mathbf{v}_*|^2}$$

$$\times \left[n_i\, e^{\frac{1}{4} m_i |\mathbf{v}'_*|^2}\, g_j(\mathbf{v}'_*) + n_j\, e^{\frac{1}{4} m_i |\mathbf{v}'|^2}\, g_i(\mathbf{v}') \right] \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*)\, \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}\mathbf{v}_*$$

$$= \left(\frac{m_i}{2\pi}\right)^{3/2} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4} m_i |\mathbf{v}|^2}\, e^{-\frac{1}{2} m_i |\mathbf{v}_*|^2} e^{\frac{1}{4} m_i |\mathbf{v}'_*|^2}$$

$$\times \left[n_i \left(\sum_{j \in \mathcal{M}_i} \mathcal{B}_{ij}(\boldsymbol{\omega}^\perp, \mathbf{v} - \mathbf{v}_*)\, g_j(\mathbf{v}'_*) \right) + \left(\sum_{j \in \mathcal{M}_i} n_j\, \mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{v} - \mathbf{v}_*) \right) g_i(\mathbf{v}') \right] \mathrm{d}\boldsymbol{\omega}\, \mathrm{d}\mathbf{v}_*.$$

Let us set

$$\tilde{\mathcal{B}}_{ij}(\boldsymbol{\omega}, \mathbf{V}) = \left(\frac{m_i}{2\pi}\right)^{3/2} \begin{cases} n_i \, \mathcal{B}_{ij}(\boldsymbol{\omega}^\perp, \mathbf{V}) & \text{if } i \neq j, \\ n_i \, \mathcal{B}_{ii}(\boldsymbol{\omega}^\perp, \mathbf{V}) + \displaystyle\sum_{k \in \mathcal{M}_i} n_k \, \mathcal{B}_{ik}(\boldsymbol{\omega}, \mathbf{V}) & \text{if } i = j. \end{cases}$$

Assumption (4.11) on both $\mathcal{B}_{ij}(\boldsymbol{\omega}, \mathbf{V})$ and $\mathcal{B}_{ij}(\boldsymbol{\omega}^\perp, \mathbf{V})$ ensures that, for any i, j

$$(4.29) \qquad \tilde{\mathcal{B}}_{ij}(\boldsymbol{\omega}, \mathbf{V}) \leq 2\, a \left(\frac{m_i}{2\pi}\right)^{3/2} \left(\max_{k \in \mathcal{M}_i} n_k\right) |\sin\theta| \, |\cos\theta| \left(|\mathbf{V}| + |\mathbf{V}|^{\delta-1}\right),$$

as well as (4.27). □

Lemma 4.10 allows to obtain the kernel form of $\mathcal{K}_3$. More precisely, we have

PROPOSITION 4.11. *Denote, for any i, j,*

$$(4.30) \qquad k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) = e^{-\frac{1}{8} m_i (\boldsymbol{\eta} - \mathbf{v})^2 - \frac{1}{8} m_i \frac{(|\boldsymbol{\eta}|^2 - |\mathbf{v}|^2)^2}{|\boldsymbol{\eta} - \mathbf{v}|^2}} |\boldsymbol{\eta} - \mathbf{v}|^{-1} \varphi_3^{ij}(\boldsymbol{\eta} - \mathbf{v}), \quad \forall \boldsymbol{\eta}, \mathbf{v} \in \mathbb{R}^3,$$

where

$$(4.31) \qquad \varphi_3^{ij}(\mathbf{p}) = \frac{2}{|\mathbf{p}|} \int_{\{\mathbf{p}\}^\perp} e^{-\frac{1}{2} m_i |\mathbf{q} + \mathbf{z}_2|^2} \tilde{\mathcal{B}}_{ij}(\mathbf{p}, \mathbf{q}) \, |\sin(\mathbf{p}, \mathbf{p} + \mathbf{q})|^{-1} \, \mathrm{d}\mathbf{q}, \quad \forall \mathbf{p} \in \mathbb{R}^3.$$

Then we have

$$(4.32) \qquad [\mathcal{K}_3 \mathbf{g}]_i (\mathbf{v}) = \sum_{j \in \mathcal{M}_i} \int_{\mathbb{R}^3} g_j(\boldsymbol{\eta}) \, k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) \mathrm{d}\boldsymbol{\eta}, \quad \forall \mathbf{v} \in \mathbb{R}^3.$$

PROOF. We perform the change of variable $\mathbf{v}_* \mapsto \mathbf{V}_* = \mathbf{v}_* - \mathbf{v}$ in (4.27), whose Jacobian equals 1, and get

$$(4.33) \qquad [\mathcal{K}_3 \mathbf{g}]_i (\mathbf{v}) = \sum_{j \in \mathcal{M}_i} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4} m_i |\mathbf{v}|^2} e^{-\frac{1}{2} m_i |\mathbf{V}_* + \mathbf{v}|^2} e^{\frac{1}{4} m_i |\mathbf{v}'|^2} g_j(\mathbf{v}') \, \tilde{\mathcal{B}}_{ij}(\boldsymbol{\omega}, \mathbf{V}_*) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\mathbf{V}_*.$$

Next, we consider the following orthogonal basis in $\mathbb{R}^3$: we choose $\boldsymbol{\omega}$ and a plane Π orthogonal to $\boldsymbol{\omega}$. Then we decompose $\mathbf{V}_*$ in this basis: we consider the components of $\mathbf{V}_*$ respectively parallel and orthogonal to $\boldsymbol{\omega}$, i.e. we write $\mathbf{V}_* = \mathbf{p} + \mathbf{q}$, where $\mathbf{p} = \boldsymbol{\omega}(\boldsymbol{\omega} \cdot \mathbf{V}_*)$, $\mathbf{q} = \mathbf{V}_* - \boldsymbol{\omega}(\boldsymbol{\omega} \cdot \mathbf{V}_*)$. The component $\mathbf{q}$ which is orthogonal to $\boldsymbol{\omega}$ belongs to the plane $\Pi = \{\boldsymbol{\omega}\}^\perp = \{\mathbf{p}\}^\perp$.
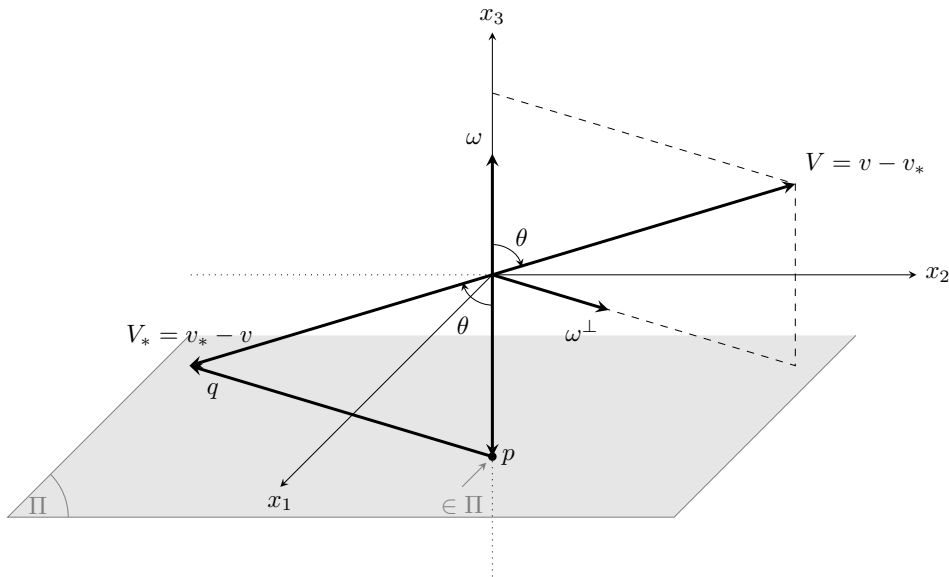

FIGURE 4.1. Geometrical situation for the change of variables (4.34)

We now perform the change of variables (see Figure 4.1)

$$(4.34) \qquad (\mathbf{V}_*, \boldsymbol{\omega}) \mapsto (\mathbf{p}, \mathbf{q}), \qquad \mathbb{R}^3 \times S^2 \to \mathbb{R}^3 \times \Pi,$$

such that two components of $\mathbf{V}_*$ give the plane vector $\mathbf{q}$, and the third component combined with two angles gives a vector $\mathbf{p} \in \mathbb{R}^3$. Let us compute its Jacobian. For $\boldsymbol{\omega}$ fixed, the replacement of $\mathbf{V}_*$ by $\mathbf{p}$ and $\mathbf{q}$ has unit Jacobian. Note that $\mathbf{V}_*$ and $\boldsymbol{\omega}$ are independent of each other, which is not the case with $\mathbf{p}$ and $\mathbf{q}$: to obtain $\mathbf{p}$ and $\mathbf{q}$ we should look simultaneously at $\mathbf{V}_*$ and $\boldsymbol{\omega}$! The key lies in the following observation: when one changes $\boldsymbol{\omega}$ for fixed $\mathbf{V}_*$, both $\mathbf{p}$ and $\mathbf{q}$ are changed. Therefore, the integration order is crucial. Hence we first integrate with respect to $\mathbf{q}$ since $\Pi = \{\mathbf{p}\}^\perp$. Then we combine the one-dimensional integration in the direction $\boldsymbol{\omega}$ with the integral of $\boldsymbol{\omega}$ over the unit sphere to give a three-dimensional integration over the three rectangular components of $|\mathbf{p}| \boldsymbol{\omega}$. We have to introduce the factor 2, since $\mathbf{p} = \pm |\mathbf{p}| \boldsymbol{\omega}$. The Jacobian from $\mathbf{p}$ to $(|\mathbf{p}|, \boldsymbol{\omega})$ (Cartesian to spherical coordinates) is $|\mathbf{p}|^2 \sin(\mathbf{p}, \mathbf{p} + \mathbf{q})$. Consequently, we can write

$$\mathrm{d}\mathbf{V}_* \, \mathrm{d}\boldsymbol{\omega} = \frac{2}{|\mathbf{p}|^2 \sin(\mathbf{p}, \mathbf{p} + \mathbf{q})} \mathrm{d}\mathbf{p} \, \mathrm{d}\mathbf{q}.$$

Eventually, it is clear that

$$\mathbf{v}' = \mathbf{v} - \boldsymbol{\omega}(\boldsymbol{\omega} \cdot (\mathbf{v} - \mathbf{v}_*)) = \mathbf{v} + \boldsymbol{\omega}(\boldsymbol{\omega} \cdot \mathbf{V}_*) = \mathbf{v} + \mathbf{p}.$$

Hence, (4.33) becomes

$$(4.35) \quad [\mathcal{K}_3 \mathbf{g}]_i (\mathbf{v}) = 2 \sum_{j \in \mathcal{M}_i} \int_{\mathbb{R}^3} \int_\Pi e^{-\frac{1}{4} m_i |\mathbf{v}|^2 - \frac{1}{2} m_i |\mathbf{p} + \mathbf{q} + \mathbf{v}|^2 + \frac{1}{4} m_i |\mathbf{v} + \mathbf{p}|^2} g_j(\mathbf{v} + \mathbf{p})$$

$$\times \tilde{\mathcal{B}}_{ij}(\mathbf{p}, \mathbf{q}) |\mathbf{p}|^{-2} |\sin(\mathbf{p}, \mathbf{p} + \mathbf{q})|^{-1} \mathrm{d}\mathbf{q} \, \mathrm{d}\mathbf{p}.$$

Since $\mathbf{p} \cdot \mathbf{q} = 0$, we can deduce

$$-\frac{1}{4} |\mathbf{v}|^2 + \frac{1}{4} |\mathbf{v} + \mathbf{p}|^2 - \frac{1}{2} |\mathbf{p} + \mathbf{q} + \mathbf{v}|^2 = -\frac{1}{8} |\mathbf{p}|^2 - \frac{1}{2} \left[\mathbf{q} + \frac{1}{2}(2\mathbf{v} + \mathbf{p}) \right]^2.$$

Consequently, we obtain

$$[\mathcal{K}_3 \mathbf{g}]_i (\mathbf{v}) = 2 \sum_{j \in \mathcal{M}_i} \int_{\mathbb{R}^3} \int_\Pi e^{-\frac{1}{8} m_i |\mathbf{p}|^2 - \frac{1}{2} m_i \left| \mathbf{q} + \frac{1}{2}(2\mathbf{v} + \mathbf{p}) \right|^2} g_j(\mathbf{v} + \mathbf{p})$$

$$\times \tilde{\mathcal{B}}_{ij}(\mathbf{p}, \mathbf{q}) |\mathbf{p}|^{-2} |\sin(\mathbf{p}, \mathbf{p} + \mathbf{q})|^{-1} \mathrm{d}\mathbf{q} \, \mathrm{d}\mathbf{p}.$$

Furthermore, let us set

$$\mathbf{z} = \frac{1}{2}(2\mathbf{v} + \mathbf{p}),$$

and denote by $\mathbf{z}_1$ the component of $\mathbf{z}$ which is parallel to $\boldsymbol{\omega}$ and $\mathbf{z}_2 = \mathbf{z} - \mathbf{z}_1 \in \Pi$. Then we can write

$$\left| \mathbf{q} + \frac{1}{2}(2\mathbf{v} + \mathbf{p}) \right|^2 = |\mathbf{q} + \mathbf{z}_1 + \mathbf{z}_2|^2 = |\mathbf{z}_1|^2 + |\mathbf{q} + \mathbf{z}_2|^2,$$

and $[\mathcal{K}_3 \mathbf{g}]_i$ becomes

$$[\mathcal{K}_3 \mathbf{g}]_i = 2 \sum_{j \in \mathcal{M}_i} \int_{\mathbb{R}^3} e^{-\frac{1}{8} m_i |\mathbf{p}|^2 - \frac{1}{2} m_i |\mathbf{z}_1|^2} g_j(\mathbf{v} + \mathbf{p}) |\mathbf{p}|^{-2}$$

$$\times \int_\Pi e^{-\frac{1}{2} m_i |\mathbf{q} + \mathbf{z}_2|^2} \tilde{\mathcal{B}}_{ij}(\mathbf{p}, \mathbf{q}) |\sin(\mathbf{p}, \mathbf{p} + \mathbf{q})|^{-1} \mathrm{d}\mathbf{q} \, \mathrm{d}\mathbf{p}.$$

Finally, we perform the change of variable $\mathbf{p} \mapsto \boldsymbol{\eta} = \mathbf{p} + \mathbf{v}$, and write

$$\mathbf{z}_1{}^2 = \left(\mathbf{z} \cdot \frac{\boldsymbol{\eta} - \mathbf{v}}{|\boldsymbol{\eta} - \mathbf{v}|} \right)^2 = \left(\frac{1}{2}(\boldsymbol{\eta} + \mathbf{v}) \cdot \frac{(\boldsymbol{\eta} - \mathbf{v})}{|\boldsymbol{\eta} - \mathbf{v}|} \right)^2 = \frac{1}{4} \frac{(|\boldsymbol{\eta}|^2 - |\mathbf{v}|^2)^2}{|\boldsymbol{\eta} - \mathbf{v}|^2}.$$
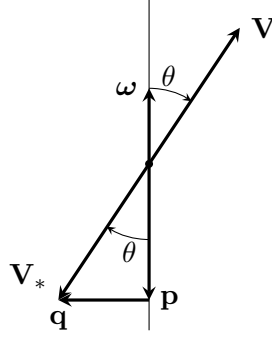
This completes the proof. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

Figure 4.2. Geometrical explanation

Properties of k_3^{ij}. Let us first prove the following lemma, and then investigate some properties of k_3^{ij}.

LEMMA 4.12. *The function $\varphi_3^{ij} : \mathbb{R}^3 \to \mathbb{R}_+$, defined by (4.31) for any i, j, belongs to $L^\infty(\mathbb{R}^3)$.*

PROOF. Let $1 \leq i, j \leq s$, and choose $\mathbf{p} \in \mathbb{R}^3$ and $\mathbf{q} \in \{\mathbf{p}\}^\perp$. From (4.29), we obtain

$$0 \leq \frac{\tilde{\mathcal{B}}_{ij}(\mathbf{p}, \mathbf{q})}{|\sin(\mathbf{p}, \mathbf{p} + \mathbf{q})|} \leq 2\,a \left(\frac{m_i}{2\pi}\right)^{3/2} \left(\max_{k \in \mathcal{M}_i} n_k\right) |\cos(\mathbf{p}, \mathbf{p} + \mathbf{q})| \left(|\mathbf{p} + \mathbf{q}| + |\mathbf{p} + \mathbf{q}|^{\delta-1}\right)$$

$$= 2\,a \left(\frac{m_i}{2\pi}\right)^{3/2} \left(\max_{k \in \mathcal{M}_i} n_k\right) |\cos(\mathbf{p}, \mathbf{p} + \mathbf{q})| \left[(|\mathbf{p}|^2 + |\mathbf{q}|^2)^{\frac{1}{2}} + (|\mathbf{p}|^2 + |\mathbf{q}|^2)^{\frac{\delta-1}{2}}\right].$$

The cosine function can be rewritten as follows

$$|\cos(\mathbf{p}, \mathbf{p} + \mathbf{q})| = \left(\frac{1}{\cos(\mathbf{p}, \mathbf{p} + \mathbf{q})^2}\right)^{1/2} = \left(\frac{\cos(\mathbf{p}, \mathbf{p} + \mathbf{q})^2 + \sin(\mathbf{p}, \mathbf{p} + \mathbf{q})^2}{\cos(\mathbf{p}, \mathbf{p} + \mathbf{q})^2}\right)^{1/2}$$

$$= \left(1 + \tan(\mathbf{p}, \mathbf{p} + \mathbf{q})^2\right)^{1/2}.$$

As it can be seen on Figure 4.2, $|\tan(\mathbf{p}, \mathbf{p} + \mathbf{q})| = |\mathbf{q}|/|\mathbf{p}|$, so that we can write

$$0 \leq \frac{\tilde{\mathcal{B}}_{ij}(\mathbf{p}, \mathbf{q})}{|\sin(\mathbf{p}, \mathbf{p} + \mathbf{q})|} \leq C_i \left(\max_{k \in \mathcal{M}_i} n_k\right) \left(1 + \frac{|\mathbf{q}|^2}{|\mathbf{p}|^2}\right)^{-\frac{1}{2}} \left[(|\mathbf{p}|^2 + |\mathbf{q}|^2)^{\frac{1}{2}} + (|\mathbf{p}|^2 + |\mathbf{q}|^2)^{\frac{\delta-1}{2}}\right]$$

$$= C_i \left(\max_{k \in \mathcal{M}_i} n_k\right) |\mathbf{p}| \left[1 + (|\mathbf{p}|^2 + |\mathbf{q}|^2)^{\frac{\delta}{2}-1}\right],$$

where $C_i = 2\,a\,(m_i/2\pi)^{3/2} > 0$. In what follows, C_i will denote any nonnegative constant only depending on m_i. This implies

$$0 \leq \frac{\tilde{\mathcal{B}}_{ij}(\mathbf{p}, \mathbf{q})}{|\mathbf{p}|\,|\sin(\mathbf{p}, \mathbf{p} + \mathbf{q})|} \leq C_i \left(\max_{k \in \mathcal{M}_i} n_k\right) \left[1 + |\mathbf{q}|^{\delta-2}\right],$$

using the fact that $\delta < 1$.

Coming back to the original form of (4.31) and using the above inequality, we obtain

$$\varphi_3^{ij}(\mathbf{p}) = \frac{2}{|\mathbf{p}|} \int_{\{\mathbf{p}\}^\perp} e^{-\frac{1}{2}m_i|\mathbf{q}+\mathbf{z}_2|^2}\, \tilde{\mathcal{B}}_{ij}(\mathbf{p}, \mathbf{q}) |\sin(\mathbf{p}, \mathbf{p} + \mathbf{q})|^{-1}\, d\mathbf{q}$$

$$\leq C_i \left(\max_{k \in \mathcal{M}_i} n_k\right) \int_{\{\mathbf{p}\}^\perp} e^{-\frac{1}{2}m_i|\mathbf{q}+\mathbf{z}_2|^2} \left[1 + |\mathbf{q}|^{\delta-2}\right] d\mathbf{q},$$

for every $\mathbf{p} \in \mathbb{R}^3$. Now, we split the range of integration into $|\mathbf{q}| \leq 1$ and $|\mathbf{q}| \geq 1$, and finally get

$$0 \leq \varphi_3^{ij}(\mathbf{p}) \leq C_i \max_{k \in \mathcal{M}_i} n_k \left(\int_{|\mathbf{q}| \leq 1} (1 + |\mathbf{q}|^{\delta-2}) \mathrm{d}\mathbf{q} + \int_{|\mathbf{q}| \geq 1} e^{-\frac{1}{2}|\mathbf{q} + \mathbf{z}_2|^2} \mathrm{d}\mathbf{q} \right)$$
$$\leq C_i \max_{k \in \mathcal{M}_i} n_k.$$

This ends the proof of Lemma 4.12. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

Let us now investigate two properties of k_3^{ij}, which are related to Lemmas 4.5–4.6 for k_1^{ij}.

LEMMA 4.13. *There exists $C > 0$ such that, for any i, j,*

$$\int_{\mathbb{R}^3} k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) \, \mathrm{d}\boldsymbol{\eta} \leq \frac{C}{|\mathbf{v}|}, \quad \forall \mathbf{v} \in \mathbb{R}^3 \setminus \{0\}, \qquad \int_{\mathbb{R}^3} k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) \, \mathrm{d}\boldsymbol{\eta} \leq C, \quad \forall \mathbf{v} \in \mathbb{R}^3.$$

PROOF. Let $1 \leq i, j \leq s$. The Lemma will be proved if we show that

$$\left(1 + |\mathbf{v}|^2\right)^{1/2} \int_{\mathbb{R}^3} k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) \, \mathrm{d}\boldsymbol{\eta} \leq C, \quad \forall \mathbf{v} \in \mathbb{R}^3,$$

since k_3^{ij} is a positive function, and the following estimates hold:

$$1 \leq \left(1 + |\mathbf{v}|^2\right)^{1/2}, \qquad |\mathbf{v}| \leq \left(1 + |\mathbf{v}|^2\right)^{1/2}, \qquad \forall \mathbf{v} \in \mathbb{R}^3.$$

We first integrate (4.30) with respect to $\boldsymbol{\eta}$ and perform the change of variable $\boldsymbol{\eta} \mapsto \mathbf{p} = \boldsymbol{\eta} - \mathbf{v}$:

$$\left(1 + |\mathbf{v}|^2\right)^{1/2} \int_{\mathbb{R}^3} k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) \, \mathrm{d}\boldsymbol{\eta} = \left(1 + |\mathbf{v}|^2\right)^{1/2} \int_{\mathbb{R}^3} e^{-\frac{1}{8} m_i |\mathbf{p}|^2 - \frac{1}{8} m_i \frac{(|\mathbf{p}|^2 + 2\mathbf{p} \cdot \mathbf{v})^2}{|\mathbf{p}|^2}} \frac{1}{|\mathbf{p}|} \varphi_3^{ij}(\mathbf{p}) \, \mathrm{d}\mathbf{p}, \quad \forall \mathbf{v} \in \mathbb{R}^3.$$

Using Lemma 4.12, we get

$$\left(1 + |\mathbf{v}|^2\right)^{1/2} \int_{\mathbb{R}^3} k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) \, \mathrm{d}\boldsymbol{\eta} \leq C \left(1 + |\mathbf{v}|^2\right)^{1/2} \int_{\mathbb{R}^3} e^{-\frac{1}{8} m_i |\mathbf{p}|^2 - \frac{1}{8} m_i \frac{(|\mathbf{p}|^2 + 2\mathbf{p} \cdot \mathbf{v})^2}{|\mathbf{p}|^2}} \frac{1}{|\mathbf{p}|} \, \mathrm{d}\mathbf{p}, \quad \forall \mathbf{v} \in \mathbb{R}^3.$$

We split the right-hand integral into $I_1 + I_2$, where I_1 refers to $\{|\mathbf{p}| \geq |\mathbf{v}|\}$ and I_2 to $\{|\mathbf{p}| \leq |\mathbf{v}|\}$. On the one hand, we have

$$I_1 = \left(1 + |\mathbf{v}|^2\right)^{1/2} \int_{|\mathbf{p}| \geq |\mathbf{v}|} e^{-\frac{1}{8} m_i |\mathbf{p}|^2 - \frac{1}{8} m_i \frac{(|\mathbf{p}|^2 + 2\mathbf{p} \cdot \mathbf{v})^2}{|\mathbf{p}|^2}} \frac{1}{|\mathbf{p}|} \, \mathrm{d}\mathbf{p}$$

$$\leq \left(1 + |\mathbf{v}|^2\right)^{1/2} \int_{|\mathbf{p}| \geq |\mathbf{v}|} e^{-\frac{1}{8} m_i |\mathbf{p}|^2} \frac{1}{|\mathbf{p}|} \, \mathrm{d}\mathbf{p} \leq C \left(1 + |\mathbf{v}|^2\right)^{1/2} e^{-\frac{1}{8} m_i |\mathbf{v}|^2} \leq C, \quad \forall \mathbf{v} \in \mathbb{R}^3.$$

On the other hand, for the second integral

$$I_2 = \left(1 + |\mathbf{v}|^2\right)^{1/2} \int_{|\mathbf{p}| \leq |\mathbf{v}|} e^{-\frac{1}{8} m_i |\mathbf{p}|^2 - \frac{1}{8} m_i \frac{(|\mathbf{p}|^2 + 2\mathbf{p} \cdot \mathbf{v})^2}{|\mathbf{p}|^2}} \frac{1}{|\mathbf{p}|} \, \mathrm{d}\mathbf{p}.$$

We have to consider two situations: $\{|\mathbf{v}| \leq 1\}$ and $\{|\mathbf{v}| \geq 1\}$. In the first case, we can simply write

$$I_2 \leq \sqrt{2} \int_{|\mathbf{p}| \leq 1} \frac{1}{|\mathbf{p}|} \, \mathrm{d}\mathbf{p} = C.$$

In the second case, with spherical coordinates, we have

$$I_2 = \left(1 + |\mathbf{v}|^2\right)^{1/2} \int_{|\mathbf{p}| \leq |\mathbf{v}|} e^{-\frac{1}{8} m_i |\mathbf{p}|^2 - \frac{1}{8} m_i \frac{(|\mathbf{p}|^2 + 2\mathbf{p} \cdot \mathbf{v})^2}{|\mathbf{p}|^2}} \frac{1}{|\mathbf{p}|} \, \mathrm{d}\mathbf{p}$$

$$= \left(1 + |\mathbf{v}|^2\right)^{1/2} \int_0^{|\mathbf{v}|} \int_0^{2\pi} \int_0^{\pi} e^{-\frac{1}{8} m_i r^2 - \frac{1}{8} m_i (r + 2|\mathbf{v}| \cos \psi_1)^2} r \sin \psi_1 \, \mathrm{d}\psi_1 \, \mathrm{d}\psi_2 \, \mathrm{d}r$$

$$= 2\pi \left(1 + |\mathbf{v}|^2\right)^{1/2} \int_0^{|\mathbf{v}|} r e^{-\frac{1}{8} m_i r^2} \int_0^{\pi} e^{-\frac{1}{8} m_i (r + 2|\mathbf{v}| \cos \psi_1)^2} \sin \psi_1 \, \mathrm{d}\psi_1 \, \mathrm{d}r,$$

where ψ_1 corresponds to the angle between $\mathbf{p}$ and $\mathbf{v}$. We perform the change of variable $\psi_1 \mapsto s = r + 2|\mathbf{v}|\cos\psi_1$, that yields

$$I_2 = \pi \frac{1}{|\mathbf{v}|} \left(1 + |\mathbf{v}|^2\right)^{1/2} \int_0^{|\mathbf{v}|} r e^{-\frac{1}{8}m_i r^2} \int_{r-2|\mathbf{v}|}^{r+2|\mathbf{v}|} e^{-\frac{1}{8}m_i s^2} \mathrm{d}s \, \mathrm{d}r.$$

Since $|\mathbf{v}| \geq 1$, we get

$$I_2 \leq \frac{C}{|\mathbf{v}|} \left(1 + |\mathbf{v}|^2\right)^{1/2} \int_0^{+\infty} r \, e^{-\frac{1}{8}m_i r^2} \mathrm{d}r \int_{-\infty}^{+\infty} e^{-\frac{1}{8}m_i s^2} \mathrm{d}s = \frac{C_i}{|\mathbf{v}|} \left(1 + |\mathbf{v}|^2\right)^{1/2} \leq C_i.$$

This completes the proof. $\qquad\square$

Using the same strategy as above, the following lemma can also be proved.

LEMMA 4.14. *For any i, j, k_3^{ij} belongs to $L_{\mathrm{loc}}^2 \left(\mathbb{R}_{\mathbf{v}}^3; L^2 \left(\mathbb{R}_{\boldsymbol{\eta}}^3\right)\right)$.*

PROOF. The Lemma will be proved if we show that k_3^{ij} belongs to $L^\infty \left(\mathbb{R}_{\mathbf{v}}^3; L^2 \left(\mathbb{R}_{\boldsymbol{\eta}}^3\right)\right)$ for any i, j. Equivalently, we must show the following property for any i, j

$$\int_{\mathbb{R}^3} k_3^{ij}(\boldsymbol{\eta}, \mathbf{v})^2 \mathrm{d}\boldsymbol{\eta} \in L^\infty \left(\mathbb{R}_{\mathbf{v}}^3\right).$$

Following the same idea as in the previous proof, we perform the change of variable $\boldsymbol{\eta} \mapsto \mathbf{p} = \boldsymbol{\eta} - \mathbf{v}$. Using Lemma 4.12, we get

$$\int_{\mathbb{R}^3} k_3^{ij}(\boldsymbol{\eta}, \mathbf{v})^2 \, \mathrm{d}\boldsymbol{\eta} \leq C_i \int_{\mathbb{R}^3} e^{-\frac{1}{4}m_i|\mathbf{p}|^2 - \frac{1}{4}m_i \frac{(|\mathbf{p}|^2 + 2\mathbf{p}\cdot\mathbf{v})^2}{|\mathbf{p}|^2}} \frac{1}{|\mathbf{p}|^2} \, \mathrm{d}\mathbf{p}, \quad \forall \mathbf{v} \in \mathbb{R}^3.$$

As before, the integral is split into I_1 and I_2, corresponding to $\{|\mathbf{p}| \geq |\mathbf{v}|\}$ and $\{|\mathbf{p}| \leq |\mathbf{v}|\}$, respectively. For I_1, using spherical coordinates, we have

$$I_1 = \int_{|\mathbf{p}| \geq |\mathbf{v}|} e^{-\frac{1}{4}m_i|\mathbf{p}|^2 - \frac{1}{4}m_i \frac{(|\mathbf{p}|^2 + 2\mathbf{p}\cdot\mathbf{v})^2}{|\mathbf{p}|^2}} \frac{1}{|\mathbf{p}|^2} \, \mathrm{d}\mathbf{p}$$

$$\leq \int_{|\mathbf{p}| \geq |\mathbf{v}|} e^{-\frac{1}{4}m_i|\mathbf{p}|^2} \frac{1}{|\mathbf{p}|^2} \, \mathrm{d}\mathbf{p} = 4\pi \int_{|\mathbf{v}|}^{+\infty} e^{-\frac{1}{8}m_i r^2} \, \mathrm{d}r \leq C_i.$$

We further look at two cases for I_2 – when $|\mathbf{v}| \leq 1$ and when $|\mathbf{v}| \geq 1$. In the first case, the result is straightforward:

$$I_2 = \int_{|\mathbf{p}| \leq |\mathbf{v}|} e^{-\frac{1}{8}m_i|\mathbf{p}|^2 - \frac{1}{8}m_i \frac{(|\mathbf{p}|^2 + 2\mathbf{p}\cdot\mathbf{v})^2}{|\mathbf{p}|^2}} \frac{1}{|\mathbf{p}|^2} \, \mathrm{d}\mathbf{p} \leq \int_{|\mathbf{p}| \leq 1} \frac{1}{|\mathbf{p}|^2} \, \mathrm{d}\mathbf{p} \leq C.$$

In the second case, using spherical coordinates, we get

$$I_2 = \int_{|\mathbf{p}| \leq |\mathbf{v}|} e^{-\frac{1}{8}m_i|\mathbf{p}|^2 - \frac{1}{8}m_i \frac{(|\mathbf{p}|^2 + 2\mathbf{p}\cdot\mathbf{v})^2}{|\mathbf{p}|^2}} \frac{1}{|\mathbf{p}|^2} \, \mathrm{d}\mathbf{p}$$

$$= \int_0^{|\mathbf{v}|} \int_0^{2\pi} \int_0^\pi e^{-\frac{1}{8}m_i r^2 - \frac{1}{8}m_i(r+2|\mathbf{v}|\cos\psi_1)^2} \sin\psi_1 \, \mathrm{d}\psi_1 \, \mathrm{d}\psi_2 \, \mathrm{d}r$$

$$= 2\pi \int_0^{|\mathbf{v}|} e^{-\frac{1}{8}m_i r^2} \int_0^\pi e^{-\frac{1}{8}m_i(r+2|\mathbf{v}|\cos\psi_1)^2} \sin\psi_1 \, \mathrm{d}\psi_1 \, \mathrm{d}r,$$

where ψ_1 corresponds to the angle between $\mathbf{p}$ and $\mathbf{v}$. We perform the change of variable $\psi_1 \mapsto s = r + 2|\mathbf{v}|\cos\psi_1$, that yields

$$I_2 = \pi \frac{1}{|\mathbf{v}|} \int_0^{|\mathbf{v}|} e^{-\frac{1}{8}m_i r^2} \int_{r-2|\mathbf{v}|}^{r+2|\mathbf{v}|} e^{-\frac{1}{8}m_i s^2} \mathrm{d}s \, \mathrm{d}r$$

$$\leq \frac{C}{|\mathbf{v}|} \int_0^{+\infty} e^{-\frac{1}{8}m_i r^2} \mathrm{d}r \int_{-\infty}^{+\infty} e^{-\frac{1}{8}m_i s^2} \mathrm{d}s = \frac{C_i}{|\mathbf{v}|} \leq C_i.$$

Summarizing, we proved that there exists a constant $C \geq 0$ such that

$$\int_{\mathbb{R}^3} k_3^{ij}(\boldsymbol{\eta}, \mathbf{v})^2 \mathrm{d}\boldsymbol{\eta} \leq C, \quad \forall \, \mathbf{v} \in \mathbb{R}^3,$$

which completes the proof. $\qquad\square$

Uniform decay. Let us now prove the uniform decay property at infinity.

PROPOSITION 4.15. *Let* $\mathbf{g} \in L^2(\mathbb{R}^3)^s$. *For any* $R > 0$ *and any* i, *we have*

$$\| \, [\mathcal{K}_3\mathbf{g}]_i \, \|_{L^2(B(0,R)^c)} \leq \frac{C}{\sqrt{R}} \, \|\mathbf{g}\|_{L^2(\mathbb{R}^3)},$$

where $C > 0$ *is a constant.*

PROOF. Using the Cauchy-Schwarz inequality and Lemma 4.13, we can write

$$\| \, [\mathcal{K}_3\mathbf{g}]_i \, \|_{L^2(B(0,R)^c)}^2 \leq C \int_{|\mathbf{v}| \geq R} \sum_{j \in \mathcal{M}_i} \left[\int_{\mathbb{R}^3} g_j(\boldsymbol{\eta})^2 k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) \, \mathrm{d}\boldsymbol{\eta} \right] \left[\int_{\mathbb{R}^3} k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) \, \mathrm{d}\boldsymbol{\eta} \right] \, \mathrm{d}\mathbf{v}$$

$$\leq \frac{C}{R} \sum_{j \in \mathcal{M}_i} \int_{\mathbb{R}^3} \left[\int_{\mathbb{R}^3} k_3^{ij}(\mathbf{v}, \boldsymbol{\eta}) \, \mathrm{d}\mathbf{v} \right] g_j(\boldsymbol{\eta})^2 \mathrm{d}\boldsymbol{\eta} = \frac{C}{R} \|\mathbf{g}\|_{L^2(\mathbb{R}^3)}^2,$$

where we also used the fact that $k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) = k_3^{ij}(\mathbf{v}, \boldsymbol{\eta})$. This ends the proof. $\qquad\square$

Equiintegrability. This property is described in the following proposition.

PROPOSITION 4.16. *For all* $\varepsilon > 0$, *there exists* $\alpha > 0$ *(not depending on* $\mathbf{g}$ *or* i*) such that*

$$(4.36) \qquad \| \, [(\tau_{\mathbf{w}} - \mathrm{Id})\mathcal{K}_3\mathbf{g}]_i \, \|_{L^2(\mathbb{R}^3)} \leq \varepsilon \|\mathbf{g}\|_{L^2(\mathbb{R}^3)}, \quad \forall \, \mathbf{w} \in B(0, \alpha).$$

PROOF. Let $\varepsilon > 0$ be given. For any $R > 0$ we can split the range of integration:
$$(4.37)$$
$$\| \, [(\tau_{\mathbf{w}} - \mathrm{Id}) \mathcal{K}_3\mathbf{g}]_i \, \|_{L^2(\mathbb{R}^3)}^2 = \int_{B(0,2R)} [(\tau_{\mathbf{w}} - \mathrm{Id}) \mathcal{K}_3\mathbf{g}]_i (\mathbf{v})^2 \, \mathrm{d}\mathbf{v} + \int_{B(0,2R)^c} [(\tau_{\mathbf{w}} - \mathrm{Id}) \mathcal{K}_3\mathbf{g}]_i (\mathbf{v})^2 \, \mathrm{d}\mathbf{v}.$$

Let us choose $\mathbf{w} \in B(0, R)$.

For the second integral in (4.37), we have

$$\int_{B(0,2R)^c} [(\tau_{\mathbf{w}} - \mathrm{Id}) \mathcal{K}_3\mathbf{g}]_i (\mathbf{v})^2 \, \mathrm{d}\mathbf{v} = \int_{B(0,2R)^c} ([\mathcal{K}_3\mathbf{g}]_i (\mathbf{v} + \mathbf{w}) - [\mathcal{K}_3\mathbf{g}]_i (\mathbf{v}))^2 \, \mathrm{d}\mathbf{v}$$

$$\leq 2 \left(\int_{B(0,2R)^c} [\mathcal{K}_3\mathbf{g}]_i (\mathbf{v} + \mathbf{w})^2 \, \mathrm{d}\mathbf{v} + \int_{B(0,2R)^c} [\mathcal{K}_3\mathbf{g}]_i (\mathbf{v})^2 \, \mathrm{d}\mathbf{v} \right).$$

Now, in the first integral, we perform the change of variable $\mathbf{v} \mapsto \tilde{\mathbf{v}} = \mathbf{v} + \mathbf{w}$ with the range of integration obtained by means of the following consideration. On one hand, we have $|\mathbf{w}| < R$ by assumption, and on the other hand, we have $|\mathbf{v}| \geq 2R$, since we integrate over $B(0, R)^c$. Therefore, by the triangle inequality $|\mathbf{v} + \mathbf{w}| \geq |\mathbf{v}| - |\mathbf{w}| \geq R$, and we can conclude that $\tilde{\mathbf{v}} \in B(0, R)^c$. For the second integral, we simply notice that $B(0, R) \subset B(0, 2R)$ and thus $B(0, 2R)^c \subset B(0, R)^c$. Finally,

$$\int_{B(0,2R)^c} [(\tau_{\mathbf{w}} - \mathrm{Id}) \mathcal{K}_3\mathbf{g}]_i (\mathbf{v})^2 \, \mathrm{d}\mathbf{v} \leq 2 \left(\int_{B(0,R)^c} [\mathcal{K}_3\mathbf{g}]_i (\tilde{\mathbf{v}})^2 \, \mathrm{d}\tilde{\mathbf{v}} + \int_{B(0,R)^c} [\mathcal{K}_3\mathbf{g}]_i (\mathbf{v})^2 \, \mathrm{d}\mathbf{v} \right)$$

$$\leq \frac{4C^2}{R} \|\mathbf{g}\|_{L^2(\mathbb{R}^3)}^2,$$

by means of Proposition 4.15. We now can choose R such that $4C^2/R < \varepsilon^2/2$, which yields

$$(4.38) \qquad \int_{B(0,2R)^c} [(\tau_{\mathbf{w}} - \mathrm{Id}) \mathcal{K}_3\mathbf{g}]_i (\mathbf{v})^2 \, \mathrm{d}\mathbf{v} < \frac{\varepsilon^2}{2} \|\mathbf{g}\|_{L^2(\mathbb{R}^3)}^2.$$

Regarding the first integral in the right-hand side of (4.37), thanks to the kernel form (4.32) and using the Cauchy-Schwarz inequality, it can be written

$$\int_{B(0,2R)} [(\tau_{\mathbf{w}} - \mathrm{Id}) \mathcal{K}_3 \mathbf{g}]_i (\mathbf{v})^2 \, \mathrm{d}\mathbf{v} \le \sum_{j \in \mathcal{M}_i} \int_{B(0,2R)} \left(\int_{\mathbb{R}^3} g_j(\boldsymbol{\eta}) \left(k_3^{ij}(\boldsymbol{\eta}, \mathbf{v} + \mathbf{w}) - k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) \right) \mathrm{d}\boldsymbol{\eta} \right)^2 \mathrm{d}\mathbf{v}$$

$$\le \sum_{j \in \mathcal{M}_i} \|g_j\|_{L^2(\mathbb{R}^3)}^2 \int_{B(0,2R)} \int_{\mathbb{R}^3} \left(k_3^{ij}(\boldsymbol{\eta}, \mathbf{v} + \mathbf{w}) - k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) \right)^2 \mathrm{d}\boldsymbol{\eta} \, \mathrm{d}\mathbf{v}.$$

Furthermore, Lemma 4.14, in conjunction with the continuity properties of translational operator $\tau_{\mathbf{w}}$ [6], yields that for every $\tilde{\varepsilon} > 0$ and so also for $\tilde{\varepsilon} = \varepsilon/\sqrt{2}$, there exists $\tilde{\alpha} > 0$ such that

$$|\mathbf{w}| < \tilde{\alpha} \quad \Rightarrow$$

$$\| (\tau_{\mathbf{w}} - \mathrm{Id}) k_3^{ij} \|_{L^2(B(0,2R)_{\mathbf{v}}; L^2(\mathbb{R}_{\boldsymbol{\eta}}^3))}^2 = \int_{B(0,2R)} \int_{\mathbb{R}^3} \left(k_3^{ij}(\boldsymbol{\eta}, \mathbf{v} + \mathbf{w}) - k_3^{ij}(\boldsymbol{\eta}, \mathbf{v}) \right)^2 \mathrm{d}\boldsymbol{\eta} \, \mathrm{d}\mathbf{v} < \tilde{\varepsilon}^2 = \frac{\varepsilon^2}{2}.$$

This inequality ensures that for $|\mathbf{w}| < \tilde{\alpha}$,

$$(4.39) \qquad \int_{B(0,2R)} [(\tau_{\mathbf{w}} - \mathrm{Id}) \mathcal{K}_3 \mathbf{g}]_i (\mathbf{v})^2 \, \mathrm{d}\mathbf{v} < \frac{\varepsilon^2}{2} \|\mathbf{g}\|_{L^2(\mathbb{R}^3)}^2.$$

Finally, (4.38) and (4.39) together with (4.37) imply that for a given $\varepsilon > 0$, we choose $\alpha = \min\{R, \tilde{\alpha}\} > 0$ such that whenever $|\mathbf{w}| < \alpha$, the required estimate (4.36) holds. $\qquad \square$

3.4. Compactness of $\mathcal{K}_4$. The proof of the compactness of $\mathcal{K}_4$ is very similar to the final part of the proof for $\mathcal{K}_3$. The main difficulty is to obtain a kernel form of $\mathcal{K}_4$. Once it is done, (4.15)–(4.16) can easily be proven as in Section 3.3. Using the same change of variables as the one leading to (4.35), we can write

$$[\mathcal{K}_4 \mathbf{g}]_i (\mathbf{v}) = 2 \sum_{j \notin \mathcal{M}_i} n_j \left(\frac{m_j}{2\pi} \right)^{3/2} \int_{\mathbb{R}^3} \int_{\Pi} e^{-\frac{1}{4} m_i |\mathbf{v}|^2 - \frac{1}{2} m_j |\mathbf{p} + \mathbf{q} + \mathbf{v}|^2 + \frac{1}{4} m_i \left| \mathbf{v} + 2 \frac{m_j}{m_i + m_j} \mathbf{p} \right|^2}$$

$$\times g_i \left(\mathbf{v} + 2 \frac{m_j}{m_i + m_j} \mathbf{p} \right) \mathcal{B}_{ij}(\mathbf{p}, \mathbf{q}) \, |\mathbf{p}|^{-2} \, |\sin(\mathbf{p}, \mathbf{p} + \mathbf{q})|^{-1} \, \mathrm{d}\mathbf{q} \, \mathrm{d}\mathbf{p}.$$

The exponential term can be modified thanks to the following relation

$$-\frac{1}{4} m_i |\mathbf{v}|^2 - \frac{1}{2} m_j |\mathbf{p} + \mathbf{q} + \mathbf{v}|^2 + \frac{1}{4} m_i \left| \mathbf{v} + 2 \frac{m_j}{m_i + m_j} \mathbf{p} \right|^2$$

$$= -\frac{m_j m_i^2}{2 (m_i + m_j)^2} |\mathbf{p}|^2 - \frac{m_j}{2} \left| \mathbf{q} + \mathbf{v} + \frac{m_j}{m_i + m_j} \mathbf{p} \right|^2.$$

If we denote

$$\mathbf{z} = \mathbf{v} + \frac{m_j}{m_i + m_j} \mathbf{p},$$

and decompose it into the component $\mathbf{z}_1$ parallel to $\boldsymbol{\omega}$ and the component $\mathbf{z}_2$ orthogonal to $\boldsymbol{\omega}$ ($\mathbf{z}_2 \in \Pi$), we obtain the new form of $[\mathcal{K}_4 \mathbf{g}]_i$:

$$[\mathcal{K}_4 \mathbf{g}]_i (\mathbf{v}) = 2 \sum_{j \notin \mathcal{M}_i} n_j \left(\frac{m_j}{2\pi} \right)^{3/2} \int_{\mathbb{R}^3} e^{-\frac{m_j m_i^2}{2(m_i + m_j)^2} |\mathbf{p}|^2 - \frac{1}{2} m_j \mathbf{z}_1^2} g_i \left(\mathbf{v} + 2 \frac{m_j}{m_i + m_j} \mathbf{p} \right)$$

$$\times |\mathbf{p}|^{-2} \int_{\Pi} e^{-\frac{1}{2} m_j |\mathbf{q} + \mathbf{z}_2|^2} \mathcal{B}_{ij}(\mathbf{p}, \mathbf{q}) \, |\sin(\mathbf{p}, \mathbf{p} + \mathbf{q})|^{-1} \, \mathrm{d}\mathbf{q} \, \mathrm{d}\mathbf{p}.$$

Next, we perform the change of variables

$$\mathbf{p} \mapsto \boldsymbol{\eta} = \mathbf{v} + 2 \frac{m_j}{m_i + m_j} \mathbf{p}, \text{ whose Jacobian equals } \left(2 \frac{m_j}{m_i + m_j} \right)^3,$$

and write $\mathbf{z}_1{}^2$ in the following form

$$\mathbf{z}_1{}^2 = \left(\mathbf{z} \cdot \frac{\boldsymbol{\eta} - \mathbf{v}}{|\boldsymbol{\eta} - \mathbf{v}|}\right)^2 = \frac{1}{4}\frac{\left(|\boldsymbol{\eta}|^2 - |\mathbf{v}|^2\right)^2}{|\boldsymbol{\eta} - \mathbf{v}|^2}.$$

Thus, $[\mathcal{K}_4\mathbf{g}]_i$ becomes

$$[\mathcal{K}_4\mathbf{g}]_i(\mathbf{v}) = \frac{1}{4}\sum_{j \notin \mathcal{M}_i} n_j \left(\frac{m_j}{2\pi}\right)^{3/2}\left(\frac{m_i + m_j}{m_j}\right)$$

$$\times \int_{\mathbb{R}^3} e^{-\frac{1}{8}\frac{m_i{}^2}{m_j}|\boldsymbol{\eta}-\mathbf{v}|^2 - \frac{1}{8}m_j\frac{(|\boldsymbol{\eta}|^2-|\mathbf{v}|^2)^2}{|\boldsymbol{\eta}-\mathbf{v}|^2}} g_i(\boldsymbol{\eta})\,|\boldsymbol{\eta} - \mathbf{v}|^{-2}$$

$$\times \int_{\Pi} e^{-\frac{1}{2}m_j|\mathbf{q}+\mathbf{z}_2|^2} \mathcal{B}_{ij}\left(\frac{m_i + m_j}{2m_j}(\boldsymbol{\eta} - \mathbf{v}), \mathbf{q}\right)$$

$$\times \left|\sin\left(\frac{m_i + m_j}{2m_j}(\boldsymbol{\eta} - \mathbf{v}), \frac{m_i + m_j}{2m_j}(\boldsymbol{\eta} - \mathbf{v}) + \mathbf{q}\right)\right|^{-1}\,\mathrm{d}\mathbf{q}\,\mathrm{d}\boldsymbol{\eta}.$$

To write $[\mathcal{K}_4\mathbf{g}]_i$ into the convenient kernel form, we introduce the function

$$\varphi_4^{ij}(\mathbf{p}) = \left(\frac{m_j}{2\pi}\right)^{3/2}\frac{m_i + m_j}{2m_j\,|\mathbf{p}|}\int_{\Pi} e^{-m_j\frac{1}{2}|\mathbf{q}+\mathbf{z}_2|^2} \mathcal{B}_{ij}(\mathbf{p}, \mathbf{q})\,|\sin(\mathbf{p}, \mathbf{p} + \mathbf{q})|^{-1}\,\mathrm{d}\mathbf{q}.$$

It is easy to prove, in the same way as in Lemma 4.12, that there exists $C > 0$ such that $\|\varphi_4^{ij}\|_{L^\infty(\mathbb{R}^3)} \le C$ for any i, j. The i-th component of $\mathcal{K}_4\mathbf{g}$ can be written in the kernel form

$$[\mathcal{K}_4\mathbf{g}]_i(\mathbf{v}) = \sum_{j \notin \mathcal{M}_i} n_j \int_{\mathbb{R}^3} k_4^{ij}(\boldsymbol{\eta}, \mathbf{v})g_i(\boldsymbol{\eta})\,\mathrm{d}\boldsymbol{\eta},$$

where $k_4^{ij}(\boldsymbol{\eta}, \mathbf{v})$ is given by

$$k_4^{ij}(\boldsymbol{\eta}, \mathbf{v}) = \frac{1}{4}\,e^{-\frac{1}{8}\frac{m_i{}^2}{m_j}|\boldsymbol{\eta}-\mathbf{v}|^2 - \frac{1}{8}m_j\frac{(|\boldsymbol{\eta}|^2-|\mathbf{v}|^2)^2}{|\boldsymbol{\eta}-\mathbf{v}|^2}}\,|\boldsymbol{\eta} - \mathbf{v}|^{-1}\,\varphi_4^{ij}\left(\frac{m_i + m_j}{2m_j}(\boldsymbol{\eta} - \mathbf{v})\right).$$

The form of each k_4^{ij} is exactly the same as in (4.30). Consequently, k_4^{ij} inherits the same properties as k_3^{ij} (see Lemmas 4.12 and 4.13), which allows to obtain (4.15)–(4.16) as in Propositions 4.15 and 4.16, and the compactness of $\mathcal{K}_4$.

Publications of Milana Pavić

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Short biography

Milana Pavić was born in 1986 in Zrenjanin. She finished the Elementary and Grammar School in Novi Sad. In 2005 she entered the Faculty of Sciences within the University of Novi Sad. On the Department of Mathematics and Informatics, she studied applied mathematics, more precisely technomathematics, and finished the studies in 4 years with the average note 9.37/10. She continued with master studies of the same study program, and finished them in 1 year with the average note 9.87/10. She started PhD studies in 2010 within the joint doctorate program of University of Novi Sad and Ecole Normale Supérieure de Cachan under the supervision of professor Srboljub Simić and professor Laurent Desvillettes.

From 2011–2013, she was engaged as a research assistant at the Faculty of Sciences in Novi Sad within the project "Mechanics of non-linear and dissipative systems – contemporary models, analysis and applications", n°ON174016, of Ministry of Education and Science of Serbia. From 2014, she is employed at the same Faculty as a teaching assistant.

Novi Sad, 6 June 2014 Milana Pavić

УНИВЕРЗИТЕТ У НОВОМ САДУ
ПРИРОДНО-МАТЕМАТИЧКИ ФАКУЛТЕТ

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