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Contributions autour de l'équation de Boltzmann et certaines de ses variantes

Thèse dirigée par Laurent BOUDIN
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COLOPHON

Mémoire de thèse intitulé « Contributions autour de l'équation de Boltzmann et certaines de ses variantes », écrit par Thomas BORSONI, achevé le 13 juillet 2024, composé au moyen du système de préparation de document \LaTeX et de la classe `yathesis` dédiée aux thèses préparées en France.

À ma famille

À la mémoire de Pierre Ferrand

CONTRIBUTIONS AUTOUR DE L'ÉQUATION DE BOLTZMANN ET CERTAINES DE SES VARIANTES**Résumé**

Nous étudions certaines variantes de l'équation de Boltzmann, cette dernière décrivant via une approche classique les gaz raréfiés simples et monoatomiques à l'échelle mésoscopique. Dans un premier temps, nous proposons un cadre général de modélisation de Boltzmann des gaz polyatomiques, englobant une large classe de modèles pré-existants et permettant d'en construire de nouveaux. D'abord présenté pour un gaz simple, ce cadre est ensuite étendu aux mélanges gazeux, pour lesquels on autorise des réactions chimiques binaires. Dans un deuxième temps, nous nous intéressons à un type de gaz polyatomique singulier, au sein duquel les collisions sont résonantes. Nous prouvons une propriété de compacité pour l'opérateur linéarisé lié à ce modèle. Afin de rendre plus flexible le cadre résonant, nous proposons ensuite un formalisme de Boltzmann pour des collisions quasi-résonantes, étudions ses propriétés-clés et menons des expériences numériques pour étayer notre compréhension de celles-ci. Enfin, dans un troisième temps, nous nous tournons vers une équation de Boltzmann incluant le principe d'exclusion de Pauli, utile notamment pour la description de la distribution d'électrons dans les semi-conducteurs. Nous développons une méthode permettant de transférer certaines inégalités fonctionnelles, liées à l'entropie, connues dans le cas classique, vers ce cas quantique. Par suite, grâce à l'obtention de ces nouvelles inégalités, nous obtenons un taux explicite de relaxation à l'équilibre pour les solutions de l'équation de Boltzmann-Fermi-Dirac homogène pour les potentiels durs avec cut-off.

Mots clés : théorie cinétique, équation de Boltzmann, gaz polyatomiques, collisions résonantes, méthodes entropiques, équation de Nordheim, équation de Boltzmann-Fermi-Dirac

Abstract

We study some variants of the Boltzmann equation, the latter describing, via a classical approach, single and monatomic rarefied gases at the mesoscopic scale. First, we propose a general framework for Boltzmann modelling of polyatomic gases, encompassing a wide class of pre-existing models and allowing to build new ones. Primarily presented for a single gas, the framework is then extended to mixtures, within which we allow binary chemical reactions. Second, we focus on a singular type of polyatomic gas, the molecules of which undergo resonant collisions, and prove a compactness property of the linearized operator related to this model. In order to make the latter resonant framework more flexible, we then propose a Boltzmann formalism with quasi-resonant collisions, study its key properties and conduct numerical experiences to support our understanding of them. Third, we turn our attention towards a Boltzmann equation which includes Pauli's exclusion principle, notably used in the study of electron distributions in semi-conductors. We develop a method that allows to transfer some functional inequalities, related to entropy, which are known in the classical case, to this quantum case. As a consequence, we use these new inequalities to obtain an explicit rate of relaxation to equilibrium for solutions to the homogeneous Boltzmann-Fermi-Dirac equation with cut-off hard potentials.

Keywords: kinetic theory, Boltzmann equation, polyatomic gases, resonant collisions, entropy methods, Nordheim equation, Boltzmann-Fermi-Dirac equation

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Sommaire

Résumé	v
Remerciements	vii
Sommaire	ix
1 Introduction	5
1.1 Présentation de l'équation de Boltzmann	6
Quelques notations	21
1.2 Un cadre général de modèles de Boltzmann pour les gaz polyatomiques	22
1.3 Autour d'un modèle singulier : collisions résonantes et quasi-résonantes	37
1.4 Méthodes entropiques et relaxation vers l'équilibre pour l'équation de Boltzmann-Fermi-Dirac	47
I A general framework for Boltzmann models for polyatomic gases	63
Overview	65
2 A general framework for the kinetic modelling of polyatomic cases	67
2.1 Introduction	68
2.2 General setting and collision rules	70
2.3 Boltzmann model	73
2.4 H Theorem and collision equilibria	82
2.5 Euler limit	90
2.6 Equipartition Theorem	91
2.7 Models within the framework	93
2.8 Reduction to one real variable and comparison with Borgnakke-Larsen	103
2.9 Conclusions	108
Acknowledgements	111
3 An internal state kinetic model for chemically reacting mixtures of monatomic and polyatomic gases	115
3.1 Introduction	117
3.2 Setting	118
3.3 Collision model	120
3.4 The Boltzmann model	123
3.5 Equilibrium	131

3.6	Euler limit	140
3.7	Example of a computation of the rate of reaction	143
3.8	Reduced models and energy of reaction	144
3.9	Example of a three species gas mixture undergoing one chemical reaction	145
3.10	Conclusion	148
3.A	Auxiliary lemma	149
3.B	Physical and chemical quantities reminder	151
 II Around a singular polyatomic model: resonant and quasi-resonant collisions		157
Overview		159
 4 A compactness property of the linearized Boltzmann operator for a polyatomic gas undergoing resonant collisions		161
4.1	Introduction	162
4.2	Resonant collision model	163
4.3	Main result	168
4.4	Proof of the main result	168
4.A	Grad's proof revisited	180
4.B	A technical lemma	189
 5 A Boltzmann model for polyatomic gases undergoing quasi-resonant collisions		193
Introduction		194
5.1	A Boltzmann model with quasi-resonant collisions	194
5.2	Expected properties of the model, Landau-Teller equations	201
5.3	Numerical experiments	206
5.A	Technical lemmas	212
 III On relaxation towards equilibrium for the Boltzmann-Fermi-Dirac equation		217
Overview		219
 6 Extending Cercignani's conjecture results from Boltzmann to Boltzmann-Fermi-Dirac		221
6.1	Introduction	223
6.2	Main results	230
6.3	Proof of Theorem 6.1 and Proposition 6.2	234
6.4	Proof of Corollary 6.3	243
6.5	About the Landau-Fermi-Dirac equation	247
6.6	L^1 - L^2 weighted Csiszár-Kullback-Pinsker inequality	249
6.A	Similar results in the Bose-Einstein case	253
6.B	A general discussion about entropies and equilibria	255
6.C	Technical results	260
Acknowledgements		265

7 Quantitative relaxation towards equilibrium for solutions to the Boltzmann-Fermi-Dirac equation with cutoff hard potentials	269
7.1 Introduction and main results	271
7.2 Uniform-in- ε L^∞ bound: proof of Theorem 7.3	281
7.3 Explicit rate of convergence to equilibrium: proof of Theorem 7.4	295
7.A More physically relevant models	299
7.B Known results about (BFD Eq.) and the Fermi-Dirac entropy	301
7.C Explicit and uniform-in- ε bounds for Fermi-Dirac statistics	303
Acknowledgments	306
Table des matières	309
Bibliographie	313

Introduction

Préambule

Cette thèse s'articule autour de l'équation de Boltzmann. Cette dernière naquit au XIX^e siècle dans l'optique de fournir un modèle de description des *gaz raréfiés*, à l'échelle *mésoscopique*.

L'échelle *mésoscopique* se place en intermédiaire entre les visions microscopique (pour un gaz, description à l'échelle de la molécule) et macroscopique (description à l'échelle fluide). Considérant qu'un gaz est un système composé d'un « très grand » nombre de molécules, l'étude porte alors sur la *répartition statistique* de celles-ci. Cette approche présente l'intérêt formidable de pouvoir décrire un phénomène dans son ensemble en se basant sur les éléments le constituant.

Notons que cette approche statistique se trouve être pertinente dans bien d'autres situations que l'étude des gaz et plasmas, par exemple en neurosciences ou en dynamique des populations (phénomènes de foules). Les équations utilisées pour modéliser ces phénomènes sont couramment nommées *équations cinétiques*.

Je tiens à souligner qu'à mon sens, l'échelle mésoscopique peut être vue, non comme une échelle en soi, mais bien comme la description du *changement d'échelle*. Ces approches tentent en fait d'expliquer des comportements macroscopiques – évolution d'un fluide ou mouvements d'un banc de poissons – à partir des *caractéristiques individuelles* des éléments microscopiques le composant – molécules ou poissons – ainsi que des *interactions* entre ces éléments.

Le modèle de Boltzmann originel est bien adapté aux *gaz classiques* dits *simples* et *monoatomiques*, c'est-à-dire composés d'une seule espèce, et dont les molécules sont composées d'un seul atome – par exemple de l'hélium He. Plusieurs variantes ont depuis été développées pour couvrir plus de cas, par exemple en incluant des principes de *relativité restreinte* ou de *mécanique quantique*, en étendant le modèle à des gaz dits *polyatomiques* (molécules composées de plusieurs atomes comme le dioxyde de carbone CO₂) et à des *mélanges*.

Cette thèse se compose de trois parties. Dans la première, nous proposons un cadre général, non relativiste, de modélisation de Boltzmann pour les *gaz polyatomiques*, avec une extension aux *mélanges*. Dans la seconde partie, nous étudions des propriétés d'un modèle de gaz polyatomique dit *résonant*, et développons la notion de *quasi-résonance*. Enfin, la troisième et dernière partie sera dédiée à l'étude d'un modèle de Boltzmann pour les *fermions* incluant le *principe d'exclusion de Pauli*.

D'une partie à l'autre, certaines notations peuvent varier ; en particulier, la notation ε a un sens différent dans chacune d'elles.

Dans ce chapitre introductif, nous présentons d'abord l'équation de Boltzmann originelle, puis les diverses parties de cette thèse.

Introduction

Sommaire du présent chapitre

1.1 Présentation de l'équation de Boltzmann	6
1.1.1 Construction de l'équation de Boltzmann	6
1.1.2 Conservations, entropie et équilibre thermodynamique	12
1.1.3 Méthodes entropiques pour un taux de relaxation vers l'équilibre	17
1.1.4 Théorie proche équilibre et opérateur de Boltzmann linéarisé	18
Quelques notations	21
1.2 Un cadre général de modèles de Boltzmann pour les gaz polyatomiques	22
1.2.1 Présentation du cadre général pour un gaz simple	22
1.2.2 Réduction de modèle : approches basées sur l'énergie	26
1.2.3 Extension aux mélanges avec réactions chimiques	31
1.3 Autour d'un modèle singulier : collisions résonantes et quasi-résonantes	37
1.3.1 Propriété de compacité du linéarisé pour un gaz polyatomique avec collisions résonantes	37
1.3.2 Un modèle de gaz polyatomique avec collisions quasi-résonantes	41
1.4 Méthodes entropiques et relaxation vers l'équilibre pour l'équation de Boltzmann-Fermi-Dirac	47
1.4.1 L'équation de Boltzmann-Fermi-Dirac	47
1.4.2 Transfert d'inégalités entropiques depuis le cas classique vers le cas quantique	51
1.4.3 Relaxation vers l'équilibre avec un taux algébrique explicite	56

1.1 Présentation de l'équation de Boltzmann

Dans cette première section, nous présentons le modèle de Boltzmann pour un gaz dit *simple* et *monoatomique*. Les premiers travaux sur cette approche remontent à Maxwell [127] puis Boltzmann [34]. Bien qu'il y ait eu, sur le plan de la modélisation, de l'analyse mathématique, et des implémentations numériques, des avancées significatives depuis ces travaux, maintes questions restent ouvertes sur ce modèle, et ses variantes.

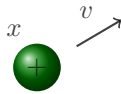
1.1.1 Construction de l'équation de Boltzmann

Ici, nous reconstruisons le modèle de description de Boltzmann, afin d'en présenter les divers acteurs. On décrit un gaz *simple*, c'est-à-dire composé d'une seule espèce de molécules, et *monoatomique*, c'est-à-dire que les molécules du gaz considéré ne sont composées que d'un seul atome – on peut penser par exemple à l'hélium He. En partie I de cette thèse, nous étudierons les gaz dits *polyatomiques*, dont les molécules sont composées de plusieurs atomes – par exemple l'eau H₂O ou le dioxyde de carbone CO₂ –, et nous verrons aussi les *mélanges gazeux* – par exemple un mélange de diazote N₂ et de dioxyde de carbone CO₂. Nous y reviendrons en section 1.2 de cette introduction.

1.1.1.1 Mise en place du modèle

Nous considérons le gaz étudié comme un ensemble composé d'une infinité de molécules, avec un point de vue *statistique* : nous étudions alors une *densité de molécules*.

Supposons que le gaz occupe l'espace \mathbb{R}^3 (on pourrait aussi se restreindre à un sous-domaine).



On caractérise, à un temps t , les molécules du gaz par leur position $x \in \mathbb{R}^3$ et leur vitesse $v \in \mathbb{R}^3$. En particulier, elles sont supposées être des points matériels. Il est possible de généraliser l'étude à $v \in \mathbb{R}^d$, $d \geq 2$ (le cas uni-dimensionnel étant singulier), mais nous nous focaliserons, dans cette thèse, sur le cas physique $d = 3$.

Notre objet d'étude est la densité de molécules du gaz $f \equiv f(t, x, v) \geq 0$, dépendant donc du temps t , de la position dans l'espace $x \in \mathbb{R}^3$ et de la vitesse $v \in \mathbb{R}^3$. En particulier, pour deux ouverts $\mathcal{X} \subset \mathbb{R}^3$ et $\mathcal{V} \subset \mathbb{R}^3$, la quantité de molécules du gaz ayant une position appartenant à \mathcal{X} et une vitesse appartenant à \mathcal{V} est donnée, à l'instant t , par

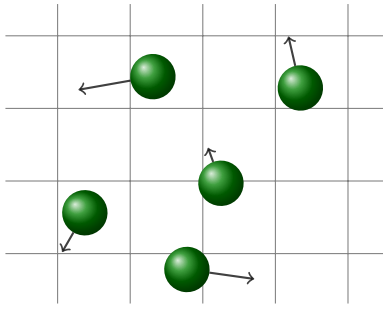
$$\iint_{\mathcal{X} \times \mathcal{V}} f(t, x, v) dx dv.$$

Le gaz sera supposé *raréfié* et *isolé*, ainsi ses molécules pourront :

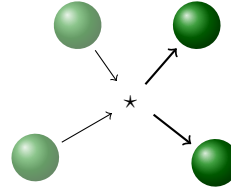
1. soit se déplacer librement en ligne droite à leur propre vitesse,
2. soit entrer en collision avec *une* autre molécule du gaz.

Nous représentons en figure 1.1 ces deux aspects. L'advection d'une molécule (sous-figure 1.1a) aura pour effet de *modifier sa position* x en gardant *constante sa vitesse* v , et une collision entre deux molécules (sous-figure 1.1b) a lieu à *position* x *fixée*, et aura pour effet de *modifier leurs vitesses*.

Ces considérations se traduisent sur la densité f comme suit. La variation temporelle de la densité, $\partial_t f$, est liée à un *terme traduisant l'effet de l'advection*, $v \cdot \nabla_x f$, et un *terme traduisant l'effet des collisions*, $Q(f, f)$.



(a) Advection dans l'espace des molécules à leur propre vitesse.



(b) Une collision entre deux molécules.

FIGURE 1.1 – Une représentation de l'advection et d'une collision.

La densité f satisfait donc à l'**équation de Boltzmann**, pour tout $(t, x, v) \in \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3$,

$$\partial_t f(t, x, v) + v \cdot \nabla_x f(t, x, v) = Q(f(t, x, \cdot), f(t, x, \cdot))(v). \quad (1.1)$$

Remarquons dès à présent que, puisque les collisions sont supposées survenir à *temps et position fixées*, l'opérateur Q , rendant compte de l'effet des collisions, agit sur des fonctions ne dépendant que de la variable de vitesse v .

L'équation (1.1) n'est complète qu'avec la donnée d'une densité initiale :

$$f(0, x, v) = f_{\text{in}}(x, v), \quad (x, v) \in \mathbb{R}^3 \times \mathbb{R}^3.$$

De plus, si le domaine d'espace considéré n'était pas \mathbb{R}^3 mais un domaine à bord, on ajouterait une condition au bord – les plus courantes étant la *réflexion spéculaire*, le *rebond* et la *diffusion de Maxwell*.

Équation de Boltzmann homogène en espace L'équation de Boltzmann (1.1) est plus communément appelée équation *inhomogène en espace*, puisqu'elle contient par construction une dépendance en la variable d'espace x . L'étude de cette équation sous cette forme, via la présence du terme de transport $v \cdot \nabla_x f$, est mathématiquement difficile (lemmes de moyenne, voir Bouchut [42], solutions renormalisées de DiPerna et Lions [79]). Ainsi, il est courant de se ramener au problème dit « homogène en espace », où l'on retire la dépendance de f en la variable d'espace x .

On obtient dans ce cas l'équation de Boltzmann *homogène en espace*, qui s'écrit alors, pour une densité de molécules $f \equiv f(t, v) \geq 0$ dépendant uniquement du temps t et de la vitesse v , et avec donnée initiale $f_{\text{in}} \equiv f_{\text{in}}(v) \geq 0$,

$$\begin{cases} \partial_t f(t, v) = Q(f(t, \cdot), f(t, \cdot))(v), & (t, v) \in \mathbb{R}_+ \times \mathbb{R}^3, \\ f(0, \cdot) = f_{\text{in}}. \end{cases} \quad (1.2)$$

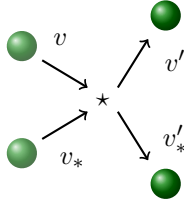
Bien que l'équation homogène soit à première vue seulement une simplification de l'équation inhomogène, elle présente tout de même un fort intérêt en soi. On peut la voir comme focalisée sur *l'effet des interactions*, et son étude permet déjà une certaine compréhension des comportements attendus pour les solutions de l'équation inhomogène, l'opérateur de collision Q n'agissant que sur la variable de vitesse v . De plus, on s'attend à ce qu'une solution de l'équation inhomogène qui serait *presque* homogène en espace conserve cette propriété dans le temps.

La théorie mathématique autour de l'équation de Boltzmann homogène en espace est aujourd'hui très avancée, en particulier dans le cas des potentiels durs avec cut-off (ces termes seront précisés plus loin) avec par exemple Arkeryd, Desvillettes, Pulvirenti, Mischler, Wennberg [17, 72, 143, 131].

1.1.1.2 L'opérateur de collision

Dans cette sous-section, nous présentons la construction de l'opérateur de collision Q . Il a pour rôle de *quantifier la variation instantanée de la répartition des vitesses due aux collisions*. Comme mentionné plus tôt, puisque les collisions sont supposées localisées en temps et espace, cet opérateur agit à temps et position fixés; ainsi, nous considérerons abusivement, dans le but de simplifier les notations, que la densité f ne dépend que de la variable v , c'est-à-dire $f \equiv f(v)$.

Conservations lors d'une collision Considérons une collision entre deux molécules, dont les vitesses pré- et post-collisionnelles sont respectivement v, v_* et v', v'_* .



Nous supposons le système à deux molécules *isolé* lors de la collision; il vient alors que la *quantité de mouvement totale* ainsi que l'*énergie totale* du système à deux molécules doivent être *conservés*. Ici, dans le cas de molécules monoatomiques, l'énergie totale du système correspond à l'énergie cinétique totale du système (dans le cas polyatomique, que nous verrons plus tard, s'y ajoutera une énergie interne). Nous concluons que les couples de vitesses pré- et post-collisionnelles doivent satisfaire aux *lois de conservations* microscopiques suivantes :

$$\begin{aligned} v + v_* &= v' + v'_* \\ |v|^2 + |v_*|^2 &= |v'|^2 + |v'_*|^2, \end{aligned} \quad (1.3)$$

où, dans (1.3), la première équation correspond à la conservation de la quantité de mouvement et la seconde à la conservation de l'énergie cinétique.

Paramétrisation sur la sphère. Nous constatons qu'au couple de vitesses pré-collisionnelles $(v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3$ fixé, l'équation (1.3) décrit une *sphère de dimension 2* dans l'espace $\mathbb{R}^3 \times \mathbb{R}^3$. En effet, un couple $(v', v'_*) \in \mathbb{R}^3 \times \mathbb{R}^3$ satisfera (1.3) si et seulement s'il existe un angle $\sigma \in \mathbb{S}^2$ (où \mathbb{S}^2 désigne la sphère de dimension 2) tel que

$$\begin{aligned} v' &= \frac{v + v_*}{2} + \frac{|v - v_*|}{2} \sigma, \\ v'_* &= \frac{v + v_*}{2} - \frac{|v - v_*|}{2} \sigma. \end{aligned} \quad (1.4)$$

Remarque 1.1. La paramétrisation (1.4) est communément appelée la « représentation en σ ». Il est aussi possible de paramétrer les vitesses post-collisionnelles via la « représentation en ω », par

$$\begin{aligned} v' &= v - ((v - v_*) \cdot \omega) \omega, \\ v'_* &= v_* + ((v - v_*) \cdot \omega) \omega, \end{aligned} \quad \omega \in \mathbb{S}^2. \quad (1.5)$$

Dans la suite de cette section, nous conservons la représentation en σ .

Noyau de collision Les lois de conservation (1.3) entraînent que l'on peut décrire les collisions grâce à une fonction

$$B : (v, v_*, \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2 \mapsto B(v, v_*, \sigma) \in \mathbb{R}_+,$$

appelée **noyau de collision** : ainsi, pour tous $\mathcal{V}, \mathcal{V}_*, \mathcal{V}'$ et \mathcal{V}'_* boréliens de \mathbb{R}^3 , la *quantité de collisions possibles* $(v, v_*) \mapsto (v', v'_*)$ telles que $(v, v_*) \in \mathcal{V} \times \mathcal{V}_*$ et $(v', v'_*) \in \mathcal{V}' \times \mathcal{V}'_*$ est donnée par

$$\iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} \mathbb{1}_{[(v, v_*) \in \mathcal{V} \times \mathcal{V}_*]} \times \mathbb{1}_{[(v', v'_*) \in \mathcal{V}' \times \mathcal{V}'_*]} B(v, v_*, \sigma) dv dv_* d\sigma,$$

où dans l'intégrale ci-dessus, v' et v'_* sont fonctions de v, v_* et σ , donnés par (1.4).

Symétrie et micro-réversibilité Le modèle de Boltzmann contient parmi ses hypothèses fondamentales, celle dite de *symétrie* et celle dite de *micro-réversibilité*. La première découle du fait que les molécules du gaz sont supposées être parfaitement *indiscernables* entre elles, et la deuxième de la *symétrie temporelle* des lois de la mécanique.

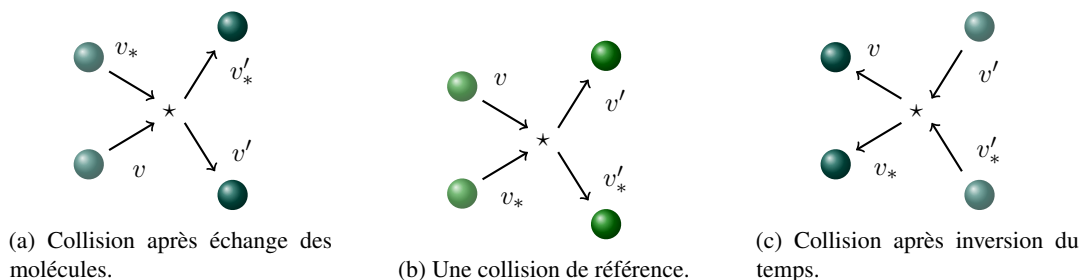


FIGURE 1.2 – Symétrie et micro-réversibilité des collisions.

Nous illustrons en figure 1.2 ci-dessus les principes annoncés de symétrie et de micro-réversibilité. Du point de vue des collisions,

1. le principe de symétrie indique que la collision $(v_*, v) \mapsto (v'_*, v')$ est tout aussi « probable » que $(v, v_*) \mapsto (v', v'_*)$ (équivalence après échange des molécules),
2. le principe de micro-réversibilité indique que la collision $(v', v'_*) \mapsto (v, v_*)$ est aussi « probable » que la collision $(v, v_*) \mapsto (v', v'_*)$ (équivalence après inversion du temps)

Cela se traduit sur le noyau B comme suit : pour $(v, v_*, \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2$,

$$(sym.) \quad B(v, v_*, \sigma) = B(v_*, v, -\sigma) \quad (1.6a)$$

$$(rev.) \quad B(v, v_*, \sigma) = B(v'_*, v', \sigma'), \quad (1.6b)$$

où, dans (1.6b), v' et v'_* sont définis par (1.4) et $\sigma' = \frac{v - v_*}{|v - v_*|}$. En particulier, introduisant θ l'angle de déviation de la collision, satisfaisant

$$\cos \theta = \sigma \cdot \sigma',$$

on observe que (1.6a)–(1.6b) implique que B ne dépend en fait que de

$$|v - v_*| \quad \text{et} \quad \cos \theta.$$

Remarque 1.2. Avec la représentation en ω (voir (1.5)), on considérera un noyau $\tilde{B} \equiv \tilde{B}(v, v_*, \omega)$ tel que

$$\tilde{B}(v, v_*, \omega) = B \left(v, v_*, T_\omega \left[\frac{v - v_*}{|v - v_*|} \right] \right), \quad (1.7)$$

où $T_\omega[V] = V - 2(V \cdot \omega)\omega$ est la symétrie par rapport à $\{\omega\}^\perp$, et pour lequel les équations (1.6a)–(1.6b) deviennent, pour $(v, v_*, \omega) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2$,

$$\begin{aligned} (\text{sym.}) \quad & \tilde{B}(v, v_*, \omega) = \tilde{B}(v_*, v, \omega) \\ (\text{rev.}) \quad & \tilde{B}(v, v_*, \omega) = \tilde{B}(v'_*, v', \omega), \end{aligned}$$

où v' et v'_* sont donnés par (1.5). Dans (1.7), nous ne prenons pas la peine de spécifier le cas $v = v_*$, puisque \tilde{B} est tout de même bien défini presque partout.

Types d'interaction Il n'est pas toujours possible d'explicitier la forme exacte du noyau de collision B . Néanmoins, Maxwell a montré dans [127] que, lorsque les molécules exercent entre elles une répulsion dont la force est proportionnelle à l'inverse de la distance les séparant à la puissance $s > 1$, il est possible d'écrire B sous la forme suivante :

$$B(v, v_*, \sigma) = |v - v_*|^\gamma b(\cos \theta), \quad (1.8)$$

où $\cos \theta = \sigma \cdot \frac{v - v_*}{|v - v_*|}$ et

$$\gamma = \frac{s - 5}{s - 1}. \quad (1.9)$$

Le cas limite $\gamma = 1$ (correspondant formellement à $s = +\infty$) et b constant est appelé *sphères dures*, où l'on décrit l'interaction entre les molécules comme des collisions élastiques entre des boules de billard. Le cas $\gamma \in (0, 1)$ est celui des *potentiels durs*, quand $\gamma \in (-3, 0)$ sera qualifié de *potentiels mous* – et même potentiels *très mous* quand $\gamma \in (-3, -2)$. Le cas particulier $\gamma = 0$ est appelé *cas des molécules de Maxwell*, et présente un intérêt avant tout mathématique : il permet de mener certains calculs de manière explicite. Enfin, le cas limite du potentiel de Coulomb, très intéressant du point de vue de la modélisation physique, correspondrait à $\gamma = -3$ et $b(\cos \theta)$ proportionnel à $|\sin(\theta/2)|^{-4}$, mais n'est cependant pas atteignable via la modélisation de Boltzmann. Pour traiter ce dernier cas, on passera par une équation cousine de Boltzmann : celle de Landau.

On trouve une discussion sur les noyaux de collision associés à des potentiels d'interaction plus généraux dans [156].

Le chaos moléculaire Le dernier ingrédient fondamental dans la construction du modèle de Boltzmann est l'*hypothèse de chaos moléculaire* (Stosszahlansatz). Cette notion est délicate et je tenterai dans les prochaines lignes de donner un aperçu de ce concept.

Imaginons, à un instant t fixé, un gaz dont on suppose que les molécules sont toutes *indépendantes*. À l'instant $t + dt$, les molécules ayant collisionné entre elles deviennent *corrélées*. L'hypothèse de chaos moléculaire stipule que, bien qu'il y ait techniquement corrélation, de par le très grand nombre de molécules présentes, on peut toujours supposer, *dans son ensemble*, que les molécules du gaz, à l'instant $t + dt$, sont indépendantes. Mathématiquement, cela implique que la *distribution à deux molécules* s'écrit comme le produit tensoriel de la *distribution à une molécule* f avec elle-même, c'est-à-dire, pour $(v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3$,

$$f(v)f(v_*).$$

À première vue, cette hypothèse peut sembler forcer l'indépendance de manière factice. Elle est en fait très raisonnable ; cela constitue l'objet de l'étude de la *propagation du chaos*, pour laquelle nous citons ici pour le lecteur curieux une revue de l'état de l'art (en deux parties) par Chaintron et Diez [65, 66]. Les travaux de ce domaine de recherche permettent d'observer, moralement, que le principe de chaos

moléculaire tend à être « de plus en plus vrai » à mesure que le nombre de molécules du système tend vers l'infini – bien qu'il soit techniquement incorrect à nombre fini de molécules. Le nombre de molécules du gaz étant effectivement supposé infini dans le cadre de la théorie cinétique, l'hypothèse du chaos est alors tout à fait raisonnable d'un point de vue de la modélisation physique.

Nous soulignons ici que cette hypothèse est *responsable* de l'apparition dans le modèle de la *flèche du temps* – rappelons qu'au niveau microscopique, tout est réversible en temps – et elle impliquera le *deuxième principe de la thermodynamique*, énonçant que dans un système isolé, l'entropie du système est une fonction croissante du temps. Cette notion d'*entropie* est un outil mathématique clé de notre étude, intimement lié à celle d'*équilibre thermodynamique*. Ce sera en particulier l'objet du chapitre 6.

L'opérateur de collision de Boltzmann Nous concluons que la variation de la densité f de molécules ayant pour vitesse $v \in \mathbb{R}^3$, due aux collisions binaires, est, en ne considérant ci-dessous pour f que sa dépendance en v ,

$$Q(f, f)(v) = \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \{f(v')f(v'_*) - f(v)f(v_*)\} B(v, v_*, \sigma) \, d\sigma \, dv_*, \quad (1.10)$$

avec, dans l'intégrale ci-dessus, v' et v'_* fonctions de v , v_* et σ , définis par (1.4). En effet, les collisions de molécules ayant pour vitesses pré- et post-collisionnelles respectivement v' , v'_* et v , v_* (voir la sous-figure 1.2c) nous font *gagner* des molécules à vitesse v , et les collisions de molécules ayant pour vitesses pré- et post-collisionnelles respectivement v , v_* et v' , v'_* (voir la sous-figure 1.2b) nous font *perdre* des molécules à vitesse v . Après avoir intégré sur toutes les collisions impliquant la vitesse v (donc en v_* et en σ), le principe de micro-réversibilité (figure 1.2, équation (1.6b)) permet alors d'obtenir (1.10).

La notion de cut-off Comme l'opérateur de collision de Boltzmann (1.10) contient une partie de *gain* et une partie de *perte*, on a envie de le décomposer, au moins formellement, comme

$$Q = Q^+ - Q^-,$$

avec, pour f une densité et $v \in \mathbb{R}^3$, notant pour simplifier $B \equiv B(v, v_*, \sigma)$,

$$Q^+(f, f)(v) = \iint_{\mathbb{R}^3 \times \mathbb{S}^2} f(v')f(v'_*) B \, d\sigma \, dv_*, \quad Q^-(f, f)(v) = f(v) \iint_{\mathbb{R}^3 \times \mathbb{S}^2} f(v_*) B \, d\sigma \, dv_*.$$

Cette décomposition présente de nombreux avantages dans l'étude mathématique de l'opérateur de Boltzmann. On mentionne en particulier que Q^+ aura, pour certains noyaux de collision, des propriétés assimilables à une convolution [102], de gain d'intégrabilité [9] et de diffusion [143]. D'un autre côté, puisque $Q^-(f, f)$ s'écrit comme le produit de f avec un opérateur linéaire appliqué en f , on pourra dans certaines situations appliquer la *formule de Duhamel* [143].

Toutefois, **cette décomposition n'a de sens que si** pour presque tous v, v_* ,

$$\int_{\mathbb{S}^2} B(v, v_*, \sigma) \, d\sigma < \infty. \quad (1.11)$$

On appelle (1.11) l'*hypothèse de cut-off angulaire*, et elle fut introduite initialement par Grad dans [94]. Néanmoins, (1.11) n'est vérifiée que lorsque le potentiel d'interaction entre les molécules est supposé à *portée finie* – typiquement dans le cas des sphères dures –, voir [156, équation (15)]. En pratique, les potentiels d'interaction à distance sont à portée infinie, et faire l'hypothèse de cut-off (1.11) revient alors à « couper » les interactions à très longue portée.

Dans le cas dit **sans cut-off**, c'est-à-dire lorsque l'on considère des interactions à portée infinie, le noyau B présente une *singularité non intégrable* en $\theta \sim 0$ – où l'on rappelle que $\cos \theta = \sigma \cdot \frac{v-v_*}{|v-v_*|}$. Dans ce cas où la décomposition de Q en $Q^+ - Q^-$ n'est pas possible, on peut tout de même donner un sens à Q , défini par (1.10), pour des densités f assez régulières et des singularités angulaires modérées. L'étude mathématique est dans ce cas *en général* plus complexe; néanmoins, l'opérateur devient alors *régularisant*, avec un comportement qu'on peut lier à celui d'un laplacien fractionnaire.

1.1.2 Conservations, entropie et équilibre thermodynamique

1.1.2.1 Forme faible et invariants de collision

Forme faible de l'opérateur de collision de Boltzmann Soit une fonction test $\psi : \mathbb{R}^3 \rightarrow \mathbb{R}$. Formellement (quand cela a un sens), intégrant $Q(f, f)$, dont la forme est donnée dans (1.10), contre ψ , il vient, pour une densité $f \equiv f(v)$, grâce aux propriétés de symétrie et de réversibilité du noyau de collision B données dans (1.6a)–(1.6b), que

$$\int_{\mathbb{R}^3} Q(f, f)(v) \psi(v) \, dv = -\frac{1}{4} \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} \{f' f'_* - f f_*\} (\psi' + \psi'_* - \psi - \psi_*) B \, dv \, dv_* \, d\sigma, \quad (1.12)$$

où nous avons, pour simplifier, utilisé ci-dessus les raccourcis $f \equiv f(v)$, $f_* \equiv f(v_*)$, $f' \equiv f(v')$, $f'_* \equiv f(v'_*)$, de même pour ψ , et $B \equiv B(v, v_*, \sigma)$. Aussi, v' et v'_* sont ci-dessus fonctions de v, v_* et σ , données par (1.4). L'équation (1.12) est appelée *forme faible de l'opérateur de collision*.

Invariants de collision On observe avec (1.12) que si ψ vérifie

$$\psi(v') + \psi(v'_*) = \psi(v) + \psi(v_*) \quad (1.13)$$

pour presque tout $(v, v_*, \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2$, avec v' et v'_* définis par (1.4), on a alors, au moins formellement,

$$\int_{\mathbb{R}^3} Q(f, f)(v) \psi(v) \, dv = 0. \quad (1.14)$$

Une fonction ψ vérifiant (1.13) est appelée *invariant de collision*, et on constate que satisfaire (1.14) signifie être une *quantité conservée* par l'opérateur de collision.

Par construction, la masse, la quantité de mouvement et l'énergie sont conservées durant les collisions, et on vérifie aisément que les fonctions

$$\psi_0(v) = 1, \quad \psi_i(v) = v_i, \quad i = 1, 2, 3, \quad \text{et} \quad \psi_4(v) = |v|^2$$

satisfont bien (1.13). Il est alors naturel de chercher à *caractériser* les invariants de collision, afin de s'assurer que le modèle ne conserve pas a priori (involontairement) d'autres quantités. On peut montrer – sous des hypothèses de régularité très faibles et moralement uniquement techniques – que **tout invariant de collision** est combinaison linéaire de la masse, de la quantité de mouvement et de l'énergie, c'est-à-dire

$$\psi \text{ invariant de collision} \iff \psi \in \text{Vect} \{ \psi_i \}_{0 \leq i \leq 4}. \quad (1.15)$$

Conservations Les considérations précédentes concernant la masse, la quantité de mouvement et l'énergie se traduisent par

$$\int_{\mathbb{R}^3} Q(f, f)(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = 0.$$

On en conclut que si $f \equiv f(t, v)$ est solution de l'équation homogène (1.2), on aura pour tout temps t que

$$\int_{\mathbb{R}^3} f(t, v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = \int_{\mathbb{R}^3} f_{\text{in}}(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv, \quad (1.16)$$

c'est-à-dire que la masse, la quantité de mouvement et l'énergie du système à un temps t quelconque sont égaux à ceux du système au temps initial.

1.1.2.2 L'entropie de Boltzmann

La dissipation d'entropie Nous introduisons ici la notion d'*entropie* de manière rétrograde, en partant de la *dissipation d'entropie*. On choisit cette approche car elle permet de comprendre en quoi la forme de la fonctionnelle d'entropie est *déterminée par celle de l'opérateur de collision* – cela nous sera utile plus tard lorsque nous étudierons des variantes de l'équation de Boltzmann. Considérons, toujours formellement et pour une densité strictement positive $f \equiv f(v) > 0$, la fonction test $\psi = \log f$ dans la forme faible de l'opérateur de collision, équation (1.12). Nous avons alors, par la propriété de morphisme du log,

$$\int_{\mathbb{R}^3} Q(f, f)(v) \log f(v) dv = -\mathcal{D}_0(f),$$

où l'on a introduit la fonctionnelle de *dissipation d'entropie* \mathcal{D}_0 , définie par

$$\mathcal{D}_0(f) := \frac{1}{4} \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} \{f' f'_* - f f_*\} \log \left(\frac{f' f'_*}{f f_*} \right) B dv dv_* d\sigma, \quad (1.17)$$

avec, pour alléger les notations, $f \equiv f(v)$, $f_* \equiv f(v_*)$, $f' \equiv f(v')$, $f'_* \equiv f(v'_*)$, v' , v'_* donnés par (1.4) et $B \equiv B(v, v_*, \sigma)$. Par (stricte) croissance du log et positivité de B , nous constatons deux propriétés fondamentales que sont

1. la positivité de \mathcal{D}_0 ,

$$\mathcal{D}_0(f) \geq 0, \quad (1.18)$$

2. le lien avec les invariants de collision (supposant B strictement positif presque partout)

$$\mathcal{D}_0(f) = 0 \iff \log f \text{ est un invariant de collision.} \quad (1.19)$$

Considérons alors une solution de l'équation de Boltzmann *homogène en espace* (1.2), que l'on suppose strictement positive, notée $f \equiv f_t(v) > 0$ (dépendant donc du temps t et de la vitesse v). Nous avons alors, à tout temps t fixé,

$$\int_{\mathbb{R}^3} \partial_t f_t(v) \log f_t(v) dv = \int_{\mathbb{R}^3} Q(f_t, f_t)(v) \log f_t(v) dv = -\mathcal{D}_0(f_t).$$

Par suite, si l'on considère une *primitive* du log notée Φ_0 , on obtient, au moins formellement, que pour tout temps t ,

$$\frac{d}{dt} \int_{\mathbb{R}^3} \Phi_0(f_t(v)) \, dv = -\mathcal{D}_0(f_t).$$

L'entropie de Boltzmann Des considérations précédentes émerge donc naturellement, puisque $x \mapsto x \log x - x$ est une primitive du log, la fonctionnelle d'*entropie de Boltzmann* H_0 définie par, pour toute densité $g \equiv g(v) \geq 0$ telle que cela ait un sens,

$$H_0(g) := \int_{\mathbb{R}^3} \{g \log g - g\} \, dv. \quad (1.20)$$

Remarque 1.3. *Puisque la masse est conservée durant la dynamique, on peut de manière équivalente se baser sur la définition suivante de l'entropie :*

$$g \mapsto \int g \log g \, dv,$$

qui est en fait plus communément utilisée. Dans une optique de généralité et de cohérence, il est toutefois plus judicieux dans notre étude de garder en mémoire, dans la définition de l'entropie, la notion de primitive du log.

1.1.2.3 Le théorème H et l'équilibre thermodynamique

Nous venons de conclure que, pour f solution de l'équation de Boltzmann homogène en espace (1.2), on a pour tout temps t ,

$$\frac{d}{dt} H_0(f_t) = -\mathcal{D}_0(f_t). \quad (1.21)$$

Notons ρ , u et T respectivement les masse, vitesse globale et température du système (identiques en tout temps par (1.16)), définies par

$$\int_{\mathbb{R}^3} f_{\text{in}}(v) \begin{pmatrix} 1 \\ v \\ |v-u|^2 \end{pmatrix} \, dv = \begin{pmatrix} \rho \\ \rho u \\ 3\rho T \end{pmatrix}. \quad (1.22)$$

La combinaison de (1.21) avec (1.18)–(1.19) donne le résultat suivant, appelé « théorème H ». Il contient deux parties ; la première correspond au *second principe de la thermodynamique*, et le second à la *caractérisation de l'équilibre thermodynamique*.

Théorème 1.1

Théorème H de Boltzmann.

1. Formellement, le long d'une solution de l'équation de Boltzmann (1.2), l'entropie du système est dissipée.

2. La dissipation d'entropie d'une densité f s'annule si et seulement si $f = M_0$, où M_0 est donnée par, pour tous $v \in \mathbb{R}^3$,

$$M_0(v) = \rho (2\pi T)^{-\frac{3}{2}} \exp\left(-\frac{|v-u|^2}{2T}\right), \quad (1.23)$$

avec ρ , u et T respectivement la densité, la vitesse globale et la température associées à f et définies comme dans (1.22).

Le théorème ci-dessus suggère que, durant la dynamique de Boltzmann, le système devrait avoir tendance à tendre vers un *équilibre*, qui aura la forme donnée par (1.23). Ces distributions sont appelées *maxwelliennes*, et il est à noter qu'il s'agit en réalité de *distributions de Gibbs* – c'est-à-dire des densités proportionnelles à l'exponentielle de l'opposé de l'énergie divisée par la température. On peut aussi les comprendre comme des gaussiennes en la vitesse v , de masse ρ , centrées en u et de variance T .

Il est alors naturel de se demander s'il est possible de *quantifier* le taux de cette supposée convergence vers l'équilibre : cela sera le rôle des *méthodes entropiques*, qu'on verra un peu plus loin en sous-section 1.1.3, et un aspect de la théorie proche équilibre, voir sous-section 1.1.4.

1.1.2.4 Interlude : considérations générales sur les entropies et équilibres thermodynamiques

Je tiens à souligner dès maintenant que, dans le cadre de l'équation de Boltzmann monoatomique, bien que (1.23) soit l'écriture usuelle des distributions d'équilibre, car pertinente d'un point de vue physique, il convient de remarquer qu'elle peut s'écrire sous la forme plus générale

$$M_0 = (\Phi'_0)^{-1} \left(\sum_{i=0}^4 \alpha_i \psi_i \right),$$

où les α_i , $i = 0, 1, 2, 3$ sont des réels et $\alpha_4 < 0$. Nous rappelons que $(\Phi'_0)^{-1} = \exp$ puisque Φ_0 est une primitive du log, et que les ψ_i sont les fonctions $v \mapsto 1$, $v \mapsto v_i$, $i = 1, 2, 3$ et $v \mapsto |v|^2$ – ce sont les *invariants de collision*. L'avantage de l'écriture ci-dessus réside en sa *généralité* et le fait qu'elle lie de manière claire les *équilibres thermodynamiques*, l'*entropie* et les *invariants de collision*.

Entropie, quantités conservées et équilibre thermodynamique dans un cadre général Pour alléger la lecture et ne pas introduire de notations utilisées ici uniquement, nous ne spécifierons ici ni les espaces ni les mesures d'intégration – ce qui est avancé tient en fait dans un cadre très général. Pour plus de précision, je renvoie à l'annexe 6.B du chapitre 6. Considérons une fonction réelle Φ définie sur un intervalle, *deux fois dérivable* et *strictement convexe*. On définit la fonctionnelle d'entropie associée à Φ , pour une densité f définie sur un certain espace mesuré et telle que cela ait un sens, par

$$H(f) := \int \Phi(f). \quad (1.24)$$

Considérons une famille (finie) de fonctions (ψ_i) , que nous appelons *quantités conservées*, définies sur le même espace que f , et supposons qu'il existe une famille (α_i) de réels tels que, pour un f fixé

$$M^f := (\Phi')^{-1} \left(\sum_i \alpha_i \psi_i \right) \quad (1.25)$$

est une densité bien définie et telle que, pour tout i ,

$$\int M^f \psi_i = \int f \psi_i. \quad (1.26)$$

Alors M^f est l'unique minimiseur de H sous les contraintes imposées par les quantités $\int f \psi_i$ (au sens de (1.26)).

Cet énoncé, apparemment purement théorique (et peut-être un peu obscur) a néanmoins la claire interprétation physique suivante, que je tiens à souligner, dans lequel H et $M^{f_{\text{in}}}$ correspondent aux définitions ci-dessus :

Pour un système en interaction libre, lors desquelles les quantités (ψ_i) sont conservées, avec donnée initiale f_{in} et où l'entropie associée est H , on s'attend à une relaxation du système vers l'équilibre $M^{f_{\text{in}}}$.

L'intérêt de la généralisation présentée ici réside en deux points. Dans un premier temps, nous avons vu que la forme de l'entropie naturelle associée à un problème physique dépend de la nature des interactions ; nous verrons en particulier que, lors d'interactions entre fermions, l'entropie à considérer diffère de celle de Boltzmann. Dans un second temps, les quantités conservées peuvent varier : en se plaçant par exemple dans un cadre relativiste, ou en considérant, comme nous le verrons plus tard, des molécules possédant une énergie interne. La forme de la distribution d'équilibre (1.25) permet donc une *unification* vis-à-vis de possibles variantes.

Représentation de Taylor de l'entropie relative à l'équilibre La raison pour laquelle la distribution (1.25) minimise la fonctionnelle (1.24) sous les contraintes (1.26) vient de ce qui suit. Nous introduisons la notion d'*entropie relative* entre deux densités f et g comme

$$H[f|g] := H(f) - H(g).$$

Pour deux densités quelconques, cette quantité n'est pas particulièrement signée ; toutefois, on verra dans la proposition 6.15 du chapitre 6 que, pour une densité f quelconque, en supposant que la densité M^f satisfaisant (1.25) et (1.26) existe bien, on a

$$H[f|M^f] := \int_0^1 (1-\tau) \left\{ \int (f - M^f)^2 \Phi'' \left((1-\tau)M^f + \tau f \right) \right\} d\tau. \quad (1.27)$$

Cette écriture de l'*entropie relative à l'équilibre* sera nommée *représentation de Taylor de l'entropie relative à l'équilibre* – tout simplement car elle provient d'un développement de Taylor de Φ à l'ordre 1 avec reste intégral. Cette forme avait déjà été observée, notamment par Lu [121] dans le cadre d'une entropie bosonique, Jünger [111] et Villani dans le cas de l'entropie classique.

Puisque l'on a supposé Φ strictement convexe, (1.27) implique immédiatement que $H[f|M^f] \geq 0$, et donc que M^f minimise H sous les contraintes imposées par f .

L'entropie relative sera l'outil principal des *méthodes entropiques*, auxquelles nous revenons un peu plus loin.

Inégalités de Csiszár-Kullback-Pinsker généralisées Les inégalités de Csiszár-Kullback-Pinsker permettent, dans leur forme originelle, de lier la distance en norme 1 entre une densité et son équilibre associé et l'entropie de Boltzmann relative à l'équilibre de cette densité – plus précisément la variation totale et la divergence Kullback de deux probabilités à densité. Elles permettent alors de transformer une « convergence » en entropie relative en une *vraie* convergence en norme 1.

Plusieurs extensions de ces inégalités ont été proposées [33, 111, 55]. Nous en donnons une généralisation à toute entropie de la forme (1.24), et aux normes L^p à poids, $1 \leq p \leq 2$, un peu plus générale et

optimale que les précédentes. Dans la proposition suivante, pour alléger les notations, nous ne spécifions pas les espaces et mesures d'intégration, qui sont libres. Pour sa formulation précise, nous renvoyons à la proposition 6.16.

Proposition 1.2

Inégalité de Csiszár-Kullback-Pinsker généralisée. Soit f une densité et un poids positif ϖ défini sur le même espace mesuré que f , on a pour tout $p \in [1, 2]$, en supposant que ce qui suit ait un sens,

$$\|f - M^f\|_{L^p_\varpi}^2 \leq \left(\int_0^1 (1-\tau) \left\| \Phi''((1-\tau)M^f + \tau f)^{-1} \right\|_{L^{\frac{p}{2-p}}_\varpi}^{-1} d\tau \right)^{-1} H[f|M^f], \quad (1.28)$$

où l'on a supposé l'existence de M^f satisfaisant (1.25) et (1.26), et les normes L^p_ϖ sont définies en (1.36).

Dans le cas $p = 2$, $L^{\frac{p}{2-p}}$ s'interprète comme L^∞ . Je mentionne que ce résultat tient pour n'importe quel espace mesuré (sur lequel serait définie f), sous réserve que toutes les quantités soient bien définies et aient un sens.

Dans le cas de l'entropie de Boltzmann À titre d'exemple significatif, nous présentons la forme que prennent ces inégalités (en fait, une forme simplifiée sous-optimale, voir l'annexe 6.B pour un résultat optimisé) dans le cas de l'entropie usuelle de Boltzmann. Nous rappelons que nous notons H_0 la fonctionnelle d'entropie de Boltzmann, et qu'elle est associée à la fonction $\Phi_0 : x \mapsto x \log x - x$; ainsi, dans ce cas, $\Phi_0'' : x \mapsto \frac{1}{x}$.

Considérons une densité $0 \leq f \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3)$ (ces espaces sont définis par (1.35) et (1.37)), et notons M_0 sa maxwellienne associée (distribution de la forme (1.23)). Alors pour tout poids $\varpi : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ et $p \in [1, 2]$ on a

$$\|f - M_0\|_{L^p_\varpi}^2 \leq 2 \max \left(\|f\|_{L^{\frac{p}{2-p}}_\varpi}, \|M_0\|_{L^{\frac{p}{2-p}}_\varpi} \right) H_0[f|M_0]. \quad (1.29)$$

L'inégalité de Csiszár-Kullback-Pinsker originelle correspond au cas $\varpi = 1$, $p = 1$.

1.1.3 Méthodes entropiques pour un taux de relaxation vers l'équilibre

Les méthodes entropiques ont pour objectif de fournir un taux explicite de convergence des solutions de l'équation de Boltzmann (homogène en espace) (1.2) vers leur équilibre thermodynamique associé – les maxwelliennes (1.23). Cette méthode a notamment été appliquée par Toscani et Villani dans [153]. Le point de départ est le suivant. Pour $f \equiv f_t(v)$ une solution de (1.2), rappelant que l'on a nommé H_0 la fonctionnelle d'entropie de Boltzmann et \mathcal{D}_0 la fonctionnelle de dissipation d'entropie de Boltzmann, on a, par (1.21) et puisque $H_0(M_0^{f_{\text{in}}})$ ne dépend pas du temps,

$$\frac{d}{dt} H_0[f_t|M_0^{f_{\text{in}}}] = -\mathcal{D}_0(f_t). \quad (1.30)$$

La quantité $H_0[f_t|M_0^{f_{\text{in}}}]$ est positive et représente (mais n'est pas au sens strict) une distance entre la distribution du système au temps t et son équilibre associé. Elle nous permettra de *quantifier la convergence* vers l'équilibre; par suite, nous utiliserons les inégalités de Csiszár-Kullback-Pinsker présentées plus haut pour obtenir une réelle convergence en norme dans un espace de Lebesgue.

La méthode d'obtention du taux de décroissance de l'entropie relative à l'équilibre $H_0[f_t|M_0^{f_{\text{in}}}]$ est la suivante :

1. on prouve une **inégalité fonctionnelle** entre l'entropie relative et la dissipation d'entropie, de la forme

$$\mathcal{D}_0(f) \gtrsim H_0[f|M_0^f]^{1+\delta}, \quad (1.31)$$

2. on combine (1.31) avec (1.30), ce qui fournit, par un argument de type Grönwall, une décroissance de $t \mapsto H_0[f_t|M_0^{f_{\text{in}}}]$ avec taux explicite, en $\mathcal{O}(t^{-\frac{1}{\delta}})$ si $\delta > 0$ et exponentiel si $\delta = 0$,
3. on utilise une inégalité de Csiszár-Kullback-Pinsker pour obtenir un taux de décroissance temporelle d'une distance (liée à un espace de Lebesgue) entre la solution et son équilibre associé.

La force de cette méthode réside en ce qu'elle fournit un taux explicite de convergence, *même en partant loin de l'équilibre*; ce taux n'est néanmoins généralement *pas optimal*, et l'on obtient une estimation plus précise du réel taux de convergence (toutefois, pas toujours explicite) via une étude dite « proche équilibre », que nous présentons dans les grandes lignes dans la sous-section suivante.

Des inégalités fonctionnelles du type conjecture de Cercignani Les premiers résultats d'inégalités de type (1.31) on en fait été obtenus pour l'équation de Landau (équation cousine de Boltzmann) par Desvillettes et Villani, voir [78, 156, 77] avec encore récemment de nouvelles avancées [71, 73].

En ce qui concerne l'équation de Boltzmann, il fut émis par Cercignani la conjecture que, pour la plupart des noyaux de collision B , on ait pour une large classe de fonctions f

$$\mathcal{D}_0(f) \geq \lambda_f H_0[f|M_0^f],$$

avec $\lambda_f > 0$ dépendant uniquement des masses et température associées à f et d'une borne supérieure sur son entropie. Ainsi, les inégalités fonctionnelles du type (1.31) sont couramment appelées *conjectures de Cercignani*. Divers contre-exemples ont depuis été obtenus, par exemple dans [31]. Toutefois, Villani a montré dans [157] que cette conjecture est « parfois vraie et toujours presque vraie »; ainsi, pour certains noyaux de collision B (non physiques), la conjecture de Cercignani est effectivement vérifiée, et pour une classe très générale de noyaux de collision B elle est presque vérifiée, au sens où l'on a plutôt

$$\mathcal{D}_0(f) \geq C_\delta(f) H_0[f|M_0^f]^{1+\delta},$$

avec $\delta > 0$ et $C_\delta(f)$ dépendant de diverses quantités associées à f – typiquement des normes L^p à poids et H^k .

1.1.4 Théorie proche équilibre et opérateur de Boltzmann linéarisé

Nous présentons dans cette dernière sous-section l'idée de l'étude dite proche équilibre. Considérons une densité $f \equiv f(v)$ et son équilibre maxwellien associé M . Nous décomposons f comme

$$f = M + \sqrt{M}g, \quad (1.32)$$

où g représente alors une *perturbation de l'équilibre*. Nous avons défini plus haut (dans (1.10)) l'opérateur de collision $Q(f, f)$ appliqué à une densité f , mais l'on peut étendre naturellement sa définition à des

couples de densités (f_1, f_2) par

$$Q(f_1, f_2)(v) = \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \{f_1(v') f_2(v'_*) - f_1(v) f_2(v_*)\} B(v, v_*, \sigma) \, d\sigma \, dv_*,$$

Ainsi, Q est un opérateur bilinéaire et il vient de (1.32) que

$$Q(f, f) = Q(M, M) + Q(\sqrt{M}g, M) + Q(M, \sqrt{M}g) + Q(\sqrt{M}g, \sqrt{M}g).$$

On définit alors l'opérateur *linéarisé* de Boltzmann \mathcal{L} , sur un ensemble de fonctions h sur \mathbb{R}^3 adaptées, par

$$\mathcal{L}h := \frac{1}{\sqrt{M}} \left[Q(\sqrt{M}h, M) + Q(M, \sqrt{M}h) \right],$$

qui est lui *linéaire*, par bilinéarité de Q . Puisque M est une distribution d'équilibre, on a $Q(M, M) = 0$, ainsi

$$Q(f, f) = \sqrt{M} \mathcal{L}g + Q(\sqrt{M}g, \sqrt{M}g). \quad (1.33)$$

Une approche perturbative L'idée centrale de l'approche dite perturbative ou proche-équilibre est la suivante. Affirmer que f est proche de l'équilibre M est équivalent à affirmer que la fonction g , introduite dans (1.32), soit petite – dans des sens que l'on peut rendre rigoureux.

Ainsi, pour g petite, (1.33) implique moralement que

$$Q(f, f) = \sqrt{M} \mathcal{L}g + \mathcal{O}(\|g\|^2).$$

On comprend donc que, proche de l'équilibre, la dynamique est majoritairement pilotée par l'opérateur linéarisé \mathcal{L} . En conséquence, l'étude de \mathcal{L} permettra notamment d'apprécier

1. l'existence et unicité de solutions à l'équation de Boltzmann lorsque la condition initiale est proche de l'équilibre,
2. la relaxation du système vers son équilibre associé, via l'étude du *spectre* de \mathcal{L} .

L'élément crucial, pour ces deux points, est de montrer la *compacité* d'un opérateur lié à \mathcal{L} .

1.1.4.1 Étude du linéarisé

Nous faisons à présent l'*hypothèse de cut-off angulaire* (1.11), qui, rappelons-nous, permet de *scinder* l'opérateur de collision.

Décomposition de \mathcal{L} Il est possible de décomposer l'opérateur \mathcal{L} de la manière suivante :

$$\mathcal{L} = K - \bar{\nu} \text{Id},$$

où Id représente l'opérateur identité, $\bar{\nu} \equiv \bar{\nu}(v)$ est appelée *fréquence de collision*, donnée par

$$\bar{\nu}(v) := \iint_{\mathbb{R}^3 \times \mathbb{S}^2} M(v_*) B(v, v_*, \sigma) \, dv_* \, d\sigma, \quad v \in \mathbb{R}^3,$$

et pour toute fonction h de \mathbb{R}^3 telle que ce qui suit ait un sens, Kh est donné pour tous $v \in \mathbb{R}^3$ par

$$Kh(v) := M^{\frac{1}{2}}(v) \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \left([M^{-\frac{1}{2}}h](v') + [M^{-\frac{1}{2}}h](v'_*) - [M^{-\frac{1}{2}}h](v_*) \right) M(v_*) B(v, v_*, \sigma) \, dv_* \, d\sigma. \quad (1.34)$$

En montrant la *compacité* de l'opérateur K , on pourra appliquer l'*alternative de Fredholm* pour obtenir un résultat d'existence et unicité de solutions à l'équation de Boltzmann proche de l'équilibre. Avec de plus une étude de la fréquence de collision $\bar{\nu}$, il sera possible d'en déduire des propriétés sur le spectre de l'opérateur \mathcal{L} . Des travaux à ce sujet pour le cas monoatomique, des mélanges, et polyatomique ont notamment été effectués dans [93, 46, 52, 20, 21]. Nous mentionnons aussi [87] qui traite un cas général.

Compacité de K La preuve de la compacité de l'opérateur K , relativement à un espace de fonctions adapté et pour une certaine famille de noyaux de collision B , fut initialement obtenue par Grad [93] (voir aussi [92]). Nous proposons, dans l'annexe 4.A du chapitre 4, une variante de cette preuve faisant intervenir un changement de variables légèrement différent, ayant une claire interprétation géométrique. Cela nous permet d'étendre le résultat de compacité à une famille de noyaux de collisions un peu plus large et, là où la preuve dans [93] est spécifique au cas monoatomique, la variante que nous proposons semble s'étendre naturellement à d'autres cas (comme le cas polyatomique).

La clé de la preuve réside en le changement de variables, bien défini presque partout, et représenté géométriquement en figure 1.3 ci-dessous,

$$(\sigma_1, \sigma_2) \in \mathbb{S}^2 \times \mathbb{S}^2 \quad \mapsto \quad (z, A) \in \mathcal{B}_{\mathbb{R}^3}(0, 1) \times \mathbb{S}^1,$$

où $\mathcal{B}_{\mathbb{R}^3}(0, 1)$ désigne la boule unité de \mathbb{R}^3 et l'angle $A \in \mathbb{S}^1$ ne sera pas directement explicité.

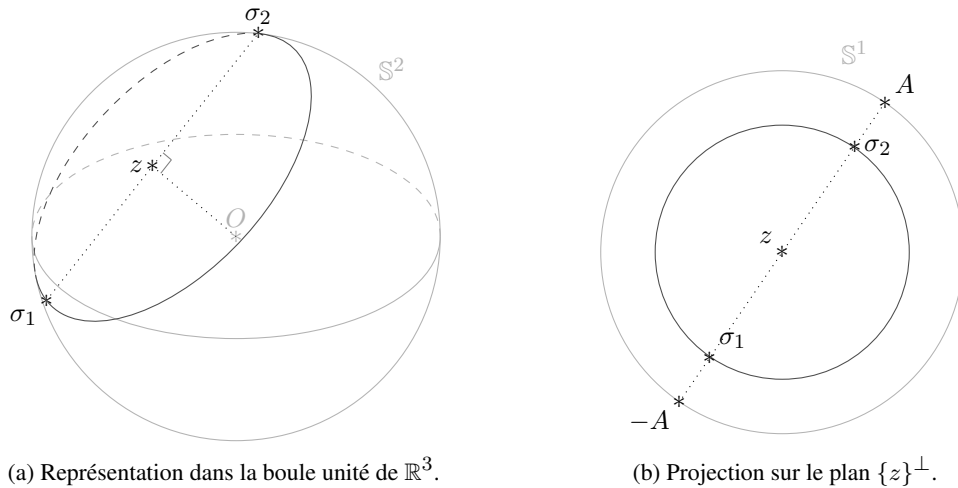


FIGURE 1.3 – Configuration géométrique de σ_1 , σ_2 , z et A .

Quelques notations

Nous introduisons ici nos notations d'espaces fonctionnels en nous basant sur \mathbb{R}^3 ; elles s'étendent naturellement à tout espace mesuré.

Espaces de Lebesgue. Pour $p \geq 1$, on note $L^p(\mathbb{R}^3)$ l'espace de Lebesgue défini par

$$L^p(\mathbb{R}^3) := \left\{ f : \mathbb{R}^3 \rightarrow \mathbb{R} \text{ mesurable} \mid \int_{\mathbb{R}^3} |f(v)|^p \, dv < \infty \right\},$$

muni de sa norme naturelle

$$\|f\|_p := \left(\int_{\mathbb{R}^3} |f(v)|^p \, dv \right)^{\frac{1}{p}}.$$

On note $L^\infty(\mathbb{R}^3)$ l'espace des fonctions de \mathbb{R}^3 essentiellement bornées (relativement à la mesure de Lebesgue sur \mathbb{R}^3), avec

$$\|f\|_\infty := \sup_{\mathbb{R}^3} \text{ess } f.$$

Crochet japonais. Pour tout $v \in \mathbb{R}^3$, on note $\langle v \rangle$ le crochet japonais de v , défini par

$$\langle v \rangle = (1 + |v|^2)^{\frac{1}{2}}.$$

Espace de Lebesgue à poids. Pour tout $p \geq 1$ et $k \in \mathbb{R}$, on note $L_k^p(\mathbb{R}^3)$ l'espace de Lebesgue à poids défini par

$$L_k^p(\mathbb{R}^3) := \left\{ f : \mathbb{R}^3 \rightarrow \mathbb{R} \text{ mesurable} \mid \int_{\mathbb{R}^3} |f(v)|^p \langle v \rangle^{kp} \, dv < \infty \right\},$$

muni de sa norme naturelle

$$\|f\|_{L_k^p} := \left(\int_{\mathbb{R}^3} |f(v)|^p \langle v \rangle^{kp} \, dv \right)^{\frac{1}{p}}. \quad (1.35)$$

Pour un poids $\varpi : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ mesurable, on notera aussi

$$\|f\|_{L_\varpi^p} := \left(\int_{\mathbb{R}^3} |f(v)|^p \varpi(v)^p \, dv \right)^{\frac{1}{p}}. \quad (1.36)$$

Espace $L^p \log L$. Pour $p \geq 1$, nous noterons $L^p \log L(\mathbb{R}^3)$ l'espace défini par

$$L^p \log L(\mathbb{R}^3) := \left\{ f : \mathbb{R}^3 \rightarrow \mathbb{R}_+ \text{ mesurable} \mid \int_{\mathbb{R}^3} f(v)^p |\log f(v)| \, dv < \infty \right\}. \quad (1.37)$$

Nous noterons aussi la quantité (qui n'est pas une norme),

$$\|f\|_{L^p \log L} := \int_{\mathbb{R}^3} f(v)^p |\log f(v)| \, dv.$$

Dans le cas $p = 1$, nous notons cet espace simplement $L \log L$.

Remarque 1.4. La définition (1.37) de $L^p \log L$ n'est pas exactement celle usuelle.

1.2 Un cadre général de modèles de Boltzmann pour les gaz polyatomiques

Le modèle de Boltzmann que nous avons présenté dans la section 1.1 est, comme mentionné, bien adapté à la description des gaz *simples* composés de molécules *monoatomiques* (c'est-à-dire n'étant composées que d'un seul atome). Nous présentons ici une *variante* de ce modèle, dont l'objectif est de l'étendre à la description de gaz composés de molécules *polyatomiques* (composées de plusieurs atomes). La différence entre mono- et polyatomique réside en la présence, pour les molécules polyatomiques, d'une *structure interne* que nous souhaitons prendre en compte : typiquement, la *structure géométrique* de la molécule induira un moment *angulaire* ainsi que des modes de *vibration* intra-moléculaires non négligeables.

L'extension du modèle de Boltzmann aux molécules polyatomiques remonte aux années 1950 avec des travaux de Wang Chang et Uhlenbeck [161], décrivant la structure interne par une variable d'énergie *discrète*, relative aux modes de vibration. Le modèle dit « à énergie discrète » a été extensivement étudié par Spiga, Groppi et Bisi [100, 25, 29] autour des années 2000. D'un autre côté, Taxman proposa dans [150] une modélisation classique, reprise plus tard par Borgnakke et Larsen [35] avec une approche orientée vers la simulation numérique, où dans cette dernière la structure interne est décrite par une variable d'énergie *continue* $I \in \mathbb{R}_+$. Ce cadre fut complété par Desvilletes [75, 76], nous apprenant que la structure interne est en fait précisée par le choix de la *mesure* sur \mathbb{R}_+ (associée à la variable I).

En collaboration avec M. Bisi et M. Groppi, nous avons alors proposé un cadre de modélisation plus général, permettant de

1. généraliser les approches existantes,
2. créer des modèles « ab initio » avec sens physique clair,
3. pouvoir naviguer entre différentes approches selon les besoins,
4. combiner des modèles.

Cela a donné lieu aux deux articles [37, 24] figurant dans la partie I de cette thèse, correspondant aux chapitres 2 et 3, et dont nous donnons ci-après les idées principales.

1.2.1 Présentation du cadre général pour un gaz simple

Cette sous-section est dédiée à l'introduction du chapitre 2, dans lequel nous proposons un cadre de modélisation pour un gaz polyatomique *simple* (c'est-à-dire composé d'une seule espèce).

1.2.1.1 Niveau microscopique

Nous considérons que les molécules du gaz, ayant pour masse $m > 0$, sont décrites, à tout instant, par leur position $x \in \mathbb{R}^3$, leur vitesse $v \in \mathbb{R}^3$ et leur état interne, que nous nommons ζ . En toute généralité, ζ appartient à l'*espace des états internes*, que nous appelons \mathcal{E} , et qui est déterminé par l'*espèce* ainsi que le *modèle moléculaire* considéré. Nous supposons que l'espace \mathcal{E} est muni d'une tribu, et d'une mesure positive, appelée μ .

Nous considérons de plus une application mesurable¹ (mesurabilité associée à la tribu sur \mathcal{E} et aux boréliens sur \mathbb{R})

$$\varepsilon : \mathcal{E} \rightarrow \mathbb{R},$$

1. Dans cette section, la notation ε désigne la fonction d'énergie interne.

que nous appelons *fonction d'énergie interne*, qui, à chaque état interne ζ associe une énergie $\varepsilon(\zeta)$. Nous faisons l'hypothèse que ε est *essentiellement minorée* et appelons ε^0 son infimum essentiel² (relativement à la mesure μ), soit

$$\varepsilon^0 := \inf_{\text{ess}_\mu} \varepsilon,$$

correspondant au *niveau d'énergie fondamental* de la molécule (une *énergie potentielle de configuration*). Nous appelons par suite *fonction d'énergie ajustée* l'application

$$\bar{\varepsilon} := \varepsilon - \varepsilon^0,$$

qui est donc telle que $\inf_{\text{ess}_\mu} \bar{\varepsilon} = 0$. Enfin, nous supposons la finitude de la *fonction de partition*,

$$\forall \beta > 0, \quad Z(\beta) := \int_{\mathcal{E}} \exp(-\beta \bar{\varepsilon}(\zeta)) \, d\mu(\zeta) < \infty. \quad (1.38)$$

Ce cadre est très général, et les hypothèses (existence d'un niveau d'énergie fondamental, finitude de la fonction de partition) sont pertinentes d'un point de vue physique.

Exemple 1.1. *Nous donnons ici deux exemples pertinents afin de fixer les idées.*

1. *On peut, pour décrire la rotation de manière classique (non quantique), considérer comme états internes la vitesse angulaire $z \in \mathbb{R}^3$, (ou \mathbb{R}^2 si la molécule est linéaire) avec comme énergie associée l'énergie cinétique de rotation. On aurait alors, avec $\zeta = z$,*

$$(\mathcal{E}, \mu) = (\mathbb{R}^3, \text{Lebesgue}), \quad \varepsilon(z) = \sum_{i=1}^3 \frac{1}{2} \mathcal{J}_i z_i^2,$$

où $\mathcal{J}_i > 0$ est le moment d'inertie dans la direction i . Ici, on aurait alors $\varepsilon^0 = 0$.

2. *Pour une molécule dont on souhaite décrire une vibration entre deux atomes, on peut utiliser par exemple le modèle de l'oscillateur harmonique quantique, ce qui donnerait, avec $\zeta = n \in \mathbb{N}$ le mode de la vibration, le modèle*

$$(\mathcal{E}, \mu) = (\mathbb{N}, \text{comptage}), \quad \varepsilon(n) = \left(n + \frac{1}{2}\right) \Delta E,$$

où $\Delta E > 0$ est le gap entre deux niveaux d'énergie consécutifs. Ici, le niveau fondamental vaut $\varepsilon^0 = \frac{1}{2} \Delta E$.

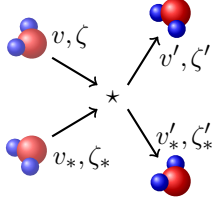
On remarquera en particulier que notre cadre permet le traitement autant de modèles continus que de modèles discrets.

Remarque 1.5. *Soulignons que le cas de la molécule monoatomique (sans structure interne) est bien inclus dans le cadre général : il suffit pour cela de considérer l'espace des états réduit à un seul élément (par exemple $\{0\}$) muni de la mesure de comptage, et une valeur d'énergie interne fixée ε^0 .*

Finalement, une molécule ayant pour vitesse v et pour état interne ζ aura pour énergie totale la somme son énergie cinétique de translation et de son énergie interne, c'est-à-dire

$$\frac{1}{2} m |v|^2 + \varepsilon(\zeta).$$

2. Je tiens à faire remarquer dès à présent que la valeur de ε^0 n'interviendra que dans l'étude de *réactions chimiques*, que nous verrons plus loin.



Concentrons nous à présent sur une collision entre deux molécules, représentée sur le schéma ci contre. Étant localisée en temps et espace, la collision n'affecte que les variables dites microscopiques, v et ζ . Notons $((v, \zeta), (v_*, \zeta_*))$ le couple d'états pré-collisionnels et $((v', \zeta'), (v'_*, \zeta'_*))$ le couple d'états post-collisionnels. Supposant isolé le système à deux molécules, nous avons donc, par conservation de la quantité de mouvement et de l'énergie totale,

$$\begin{aligned} v' + v'_* &= v + v_*, \\ \frac{1}{2}m|v'|^2 + \varepsilon(\zeta') + \frac{1}{2}m|v'_*|^2 + \varepsilon(\zeta'_*) &= \frac{1}{2}m|v|^2 + \varepsilon(\zeta) + \frac{1}{2}m|v_*|^2 + \varepsilon(\zeta_*). \end{aligned} \quad (1.39)$$

Si l'on note alors

$$\Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*) := \frac{1}{4}|v - v_*|^2 + \frac{1}{m}(\varepsilon(\zeta) + \varepsilon(\zeta_*) - \varepsilon(\zeta') - \varepsilon(\zeta'_*)), \quad (1.40)$$

on peut remarquer que la collision n'est possible que lorsque $\Delta \geq 0$. Dans ce cas, il existe un angle $\omega \in \mathbb{S}^2$ tel que

$$\begin{aligned} v' &= \frac{v + v_*}{2} + \sqrt{\Delta} T_\omega \begin{bmatrix} v - v_* \\ |v - v_*| \end{bmatrix}, \\ v'_* &= \frac{v + v_*}{2} - \sqrt{\Delta} T_\omega \begin{bmatrix} v - v_* \\ |v - v_*| \end{bmatrix}. \end{aligned} \quad (1.41)$$

Remarque 1.6. Nous prenons ici la convention de la représentation en ω , qui est celle considérée au chapitre 2. Il est aussi possible d'utiliser la représentation en σ , dans laquelle $T_\omega \begin{bmatrix} v - v_* \\ |v - v_*| \end{bmatrix}$ deviendrait σ .

1.2.1.2 Niveau mésoscopique

Au niveau mésoscopique, nous étudierons la densité de molécules du gaz $f \equiv f(t, x, v, \zeta) \geq 0$, qui dépend du temps t , de la position x , la vitesse v et l'état interne ζ . On retrouve en particulier les quantités macroscopiques que sont la *densité massique* ρ , la *vitesse globale* u et la *température* T via les formules suivantes

$$\rho(t, x) := \iint_{\mathbb{R}^3 \times \mathcal{E}} m f(t, x, v, \zeta) \, dv \, d\mu(\zeta), \quad (1.42)$$

$$u(t, x) := \frac{1}{\rho(t, x)} \iint_{\mathbb{R}^3 \times \mathcal{E}} m v f(t, x, v, \zeta) \, dv \, d\mu(\zeta), \quad (1.43)$$

$$T(t, x) := \Theta^{-1} \left(\frac{1}{\rho(t, x)} \iint_{\mathbb{R}^3 \times \mathcal{E}} \left(\frac{m}{2} |v - u|^2 + \bar{\varepsilon}(\zeta) \right) f(t, x, v, \zeta) \, dv \, d\mu(\zeta) \right), \quad (1.44)$$

où Θ^{-1} est la réciproque de Θ définie pour tout $T > 0$ par

$$\Theta(T) := \frac{3 + \delta(T)}{2} T,$$

et δ , appelé le *nombre de degrés de liberté internes*, est donné, pour tout $T > 0$, par

$$\delta(T) := \frac{2}{T} Z \left(\frac{1}{T} \right)^{-1} \int_{\mathcal{E}} \bar{\varepsilon}(\zeta) \exp \left(-\frac{\bar{\varepsilon}(\zeta)}{T} \right) d\mu(\zeta). \quad (1.45)$$

Modèle de Boltzmann On suppose à présent que la densité f satisfait à l'équation de Boltzmann suivante, pour presque tous $t \geq 0$, $x \in \mathbb{R}^3$, $v \in \mathbb{R}^3$ et $\zeta \in \mathcal{E}$,

$$\partial_t f(t, x, v, \zeta) + v \cdot \nabla_x f(t, x, v, \zeta) = Q(f(t, x, \cdot, \cdot), f(t, x, \cdot, \cdot))(v, \zeta), \quad (1.46)$$

où l'opérateur de collision Q agit toujours à temps et positions fixées, donc uniquement sur les variables v et ζ . Formellement, Q s'écrit sous une forme similaire au cas monoatomique, avec cette fois l'ajout de l'intégration sur les variables internes, pour une densité $f \equiv f(v, \zeta) \geq 0$ et tous $v \in \mathbb{R}^3$, $\zeta \in \mathcal{E}$,

$$Q(f, f)(v, \zeta) := \iiint_{\mathcal{E}^3} \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \{f(v', \zeta') f(v'_*, \zeta'_*) - f(v, \zeta) f(v, \zeta_*)\} B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) d\omega dv_* d\mu^{\otimes 3}(\zeta_*, \zeta', \zeta'_*), \quad (1.47)$$

où B est le noyau de collision, tel que, rappelant que Δ est défini dans (1.40),

$$\Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*) < 0 \implies B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \cdot) = 0,$$

et (v', v'_*) sont définis par (1.41). On suppose de plus que le noyau B satisfait des propriétés de *symétrie* et *micro-réversibilité* adaptées à ce cadre, que nous ne détaillons pas plus ici. Définissons enfin la fonctionnelle d'entropie, pour des densités $f \equiv f(v, \zeta) \geq 0$,

$$H_0(f) := \iint_{\mathbb{R}^3 \times \mathcal{E}} \{f \log f - f\} dv d\mu(\zeta). \quad (1.48)$$

Si la densité dépend aussi de la position dans l'espace x , on intégrera aussi en x .

La validité, du point de vue de la modélisation, de notre cadre pour le modèle de Boltzmann est assurée par le théorème suivant (voir théorème 2.3 au chapitre 2).

Théorème 1.3

Théorème H.

1. Formellement, le long d'une solution de l'équation de Boltzmann (1.46) (ou homogène), l'entropie est dissipée.

2. La dissipation d'entropie d'une densité $f \equiv f(v, \zeta) \geq 0$ s'annule si et seulement si $f = \mathcal{M}[\rho, u, T]$, où ρ , u et T sont respectivement la densité, la vitesse globale et la température associées à f définis comme dans (1.42)–(1.44) et, pour tout $(v, \zeta) \in \mathbb{R}^3 \times \mathcal{E}$,

$$\mathcal{M}[\rho, u, T](v, \zeta) = \frac{\rho}{m} \left(\frac{2\pi T}{m} \right)^{-3/2} Z \left(\frac{1}{T} \right)^{-1} \exp \left(-\frac{m|v-u|^2}{2T} - \frac{\bar{\varepsilon}(\zeta)}{T} \right). \quad (1.49)$$

Nous soulignons que les distributions d'équilibre de la forme (1.49), nommées « maxwelliennes généralisées », sont ici encore des *distributions de Gibbs*.

Équations d'Euler Nous retrouvons formellement les équations d'Euler, pour un gaz parfait dont le nombre de degrés de liberté est $3 + \delta(T)$, en insérant la maxwellienne (1.49) dans l'équation de Boltzmann (1.46). Ces équations sont données en (2.32) dans le chapitre 2.

1.2.2 Réduction de modèle : approches basées sur l'énergie

Dans cette sous-section, nous tentons de fournir des clarifications et intuitions pour comprendre les possibilités de modélisation, et comment choisir parmi celles-ci. Bien que n'étant pas associées à un chapitre en particulier, ces réflexions sont initiées en section 2.8 du chapitre 2, et sous-jacentes dans toute la partie II de cette thèse.

L'idée de réduction de modèle est de construire, pour un modèle donné, un modèle équivalent *plus simple* que le premier. Nous verrons plus loin cette réduction, dont l'idée est de ne garder que l'information de l'énergie interne en oubliant les états.

Il émerge que l'on peut adopter trois points de vue principaux pour la description de la structure interne, dont nous donnons une représentation schématique dans la figure 1.4.

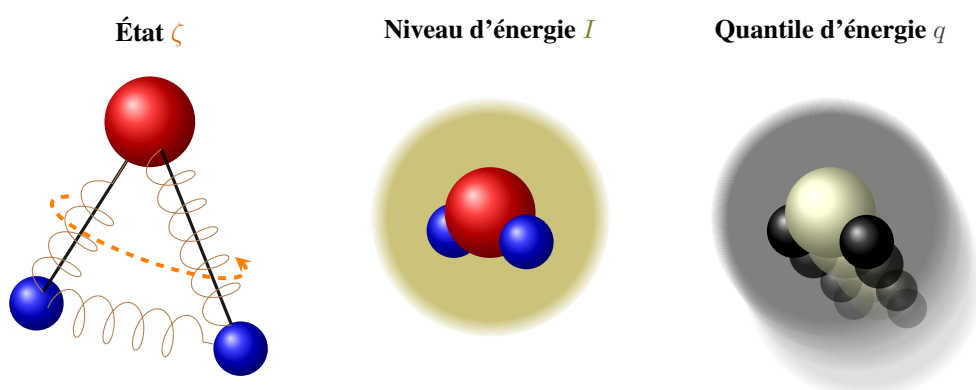


FIGURE 1.4 – Représentation schématique des trois points de vue principaux pour la description de la structure interne d'une molécule polyatomique, dans un contexte cinétique.

Le premier point de vue est de considérer l'*état interne* ζ comme variable de description de la structure interne, en considérant qu'à chaque état est associé une énergie, comme dans le cadre général. Le deuxième consiste à oublier les états internes pour ne considérer que le *niveau d'énergie* I , en prenant en compte, via une mesure sur \mathbb{R}_+ , la répartition des niveaux d'énergie – il y a donc moins d'information dans cette approche que dans la première. Le troisième point de vue se base sur la notion de quantiles d'énergie, et, d'interprétation plus délicate, ne sera détaillé qu'un peu plus loin. L'approche basée sur les états étant exactement l'*interprétation physique* de notre cadre général présenté plus tôt, nous nous focalisons dans ce qui suit sur les deux approches liées à l'énergie.

Soulignons que les points de vue basés sur les niveaux ou les quantiles d'énergie sont des cas particuliers du cadre général.

1.2.2.1 Approche basée sur les niveaux d'énergie

Nous présentons ici l'approche basée sur l'énergie interne en la *construisant* depuis un modèle général. Considérons donc un modèle dont l'espace des états est \mathcal{E} , muni d'une mesure μ et d'une fonction d'énergie interne ε , satisfaisant aux hypothèses du cadre général.

Nous allons construire un nouveau modèle à partir du premier, d'une forme adaptée au cadre général, pour lequel l'espace des états sera *unidimensionnel*, et qui décrit le même modèle moléculaire que le premier – avec toutefois une perte d'information au niveau de la molécule.

Puisque la fonction d'énergie interne ajustée $\bar{\varepsilon}$ est mesurable, relativement à la tribu de \mathcal{E} et aux boréliens de \mathbb{R}_+ , on peut définir la **loi d'énergie** comme la *mesure image*, sur \mathbb{R}_+ , de μ par $\bar{\varepsilon}$:

$$\mu_{\bar{\varepsilon}}(A) := \mu(\bar{\varepsilon} \in A), \quad A \in \text{Bor}(\mathbb{R}_+). \quad (1.50)$$

On a alors, pour toute fonction mesurable $\phi : \mathbb{R} \rightarrow \mathbb{R}_+$,

$$\int_{\mathcal{E}} \phi(\bar{\varepsilon}(\zeta)) \, d\mu(\zeta) = \int_{\mathbb{R}_+} \phi(I + \varepsilon^0) \, d\mu_{\bar{\varepsilon}}(I).$$

Cette simple égalité, provenant de la définition même de la mesure image, nous permet, par identification, de conclure immédiatement que le modèle dit « basé sur l'énergie interne » dans lequel

1. on considère la variable I , le *niveau d'énergie interne*, dans l'espace des états $(\mathbb{R}_+, \mu_{\bar{\varepsilon}})$,
2. l'énergie interne de la molécule ayant pour niveau d'énergie I est $I + \varepsilon^0$,

décrit bien le même modèle moléculaire que le modèle initial – à une perte d'information près.

Remarque 1.7. *Nous remarquons que, lorsque $\mu_{\bar{\varepsilon}}$ est une mesure à densité (que l'on appelle alors φ) par rapport à la mesure de Lebesgue, on retrouve le modèle avec énergie continue [150, 47, 75, 76]. Nous mentionnons en particulier que (1.50) indique très simplement comment calculer φ à partir du modèle moléculaire; nous y reviendrons plus tard avec des exemples. Dans le cas où $\mu_{\bar{\varepsilon}}$ est une mesure discrète (typiquement, une somme de mesures de Dirac), on retrouve alors les modèles à énergie discrète de [161, 100].*

L'intérêt majeur de cette approche réside en ce que **l'espace de la variable considérée est unidimensionnel**, donc très simple, et que **la fonction d'énergie interne est (presque) triviale**. Nous avons résumé toute l'information sur la structure interne de la molécule dans la mesure $\mu_{\bar{\varepsilon}}$.

1.2.2.2 Approche basée sur les quantiles d'énergie

La dernière approche, basée sur les quantiles d'énergie, étant moins intuitive d'un point de vue de son interprétation immédiate, nous proposons pour la comprendre, dans le tableau 1.1 ci-dessous, un parallèle entre notre cadre polyatomique général et un cadre général en théorie des probabilités. La notation *Leb* y désigne la mesure de Lebesgue.

On comprend qu'en réalité, la seule différence entre notre cadre et un cadre d'étude probabiliste réside en le fait qu'ici, la mesure μ n'est pas contrainte à être une *probabilité*; elle ne le sera d'ailleurs pas en général, pouvant être typiquement la mesure de Lebesgue sur \mathbb{R}^2 . Ceci mis à part, le parallèle est flagrant : l'espace des états internes (\mathcal{E}, μ) peut être interprété comme un espace d'*événements*, la fonction d'énergie interne ε interprétée comme une *variable aléatoire* sur cet espace, et $\mu_{\bar{\varepsilon}}$ comme la *loi* de $\bar{\varepsilon}$ (l'énergie interne ajustée), de manière à ce qu'on interprète $(\mathbb{R}_+, \mu_{\bar{\varepsilon}})$ comme un espace de *réalisations*.

De la même manière que l'on peut définir un espace de *quantiles* en probabilités, on comprend par analogie qu'il est possible de faire de même dans notre cas. Néanmoins, puisque μ ne somme pas nécessairement à 1, il se peut que nos quantiles soient définis sur $]0, +\infty[$, rendant le terme *quantile* inexact, bien que donnant une bonne intuition.

Par analogie, définissons la fonction de répartition d'énergie $F_{\mu_{\bar{\varepsilon}}}$ par

$$F_{\mu_{\bar{\varepsilon}}}(I) = \mu_{\bar{\varepsilon}}([0, I]), \quad I \in \mathbb{R}_+, \quad (1.51)$$

et la *fonction quantile d'énergie* comme l'inverse généralisé à gauche de $F_{\mu_{\bar{\varepsilon}}}$, c'est-à-dire

$$F_{\mu_{\bar{\varepsilon}}}^{\leftarrow}(q) = \inf \{I \in \mathbb{R}_+ \text{ tel que } F_{\mu_{\bar{\varepsilon}}}(I) \geq q\}, \quad q \in (0, \mu(\mathcal{E})), \quad (1.52)$$

Cadre polyatomique général	En théorie des probabilités
(\mathcal{E}, μ) espace des états internes ε fonction d'énergie interne	(Ω, \mathbb{P}) espace des événements X variable aléatoire réelle
$(\mathbb{R}_+, \mu_{\bar{\varepsilon}})$ espace des niveaux d'énergie $\mu_{\bar{\varepsilon}}$ loi d'énergie	$(\mathbb{R}, \mathbb{P}_X)$ espace des réalisations \mathbb{P}_X loi de X
$((0, \mu(\mathcal{E})), \text{Leb})$ espace des quantiles d'énergie $F_{\mu_{\bar{\varepsilon}}}^{\leftarrow}$ fonction quantile d'énergie	$((0, 1), \text{Leb})$ espace des quantiles $F_{\mathbb{P}_X}^{\leftarrow}$ fonction quantile

TABLEAU 1.1 – Parallèle entre le cadre général polyatomique un cadre général en probabilités

où l'on a remarqué que $\mu(\mathcal{E}) = \mu_{\bar{\varepsilon}}(\mathbb{R}_+)$. Bien sûr, lorsque $F_{\mu_{\bar{\varepsilon}}}$ est inversible, $F_{\mu_{\bar{\varepsilon}}}^{\leftarrow} = F_{\mu_{\bar{\varepsilon}}}^{-1}$.

Alors, pour toute fonction mesurable $\phi : \mathbb{R} \rightarrow \mathbb{R}_+$, on a

$$\int_{\mathbb{R}_+} \phi(I + \varepsilon^0) d\mu_{\bar{\varepsilon}}(I) = \int_0^{\mu(\mathcal{E})} \phi(F_{\mu_{\bar{\varepsilon}}}^{\leftarrow}(q) + \varepsilon^0) dq.$$

On peut par suite définir le modèle annoncé, où

1. on considère la variable q , le *quantile* d'énergie interne, dans l'espace des états $((0, \mu(\mathcal{E})), \text{Leb})$,
2. l'énergie interne d'une molécule du quantile q est $F_{\mu_{\bar{\varepsilon}}}^{\leftarrow}(q) + \varepsilon^0$,

et conclure qu'il est complètement équivalent (et avec la même quantité d'information) que l'approche basée sur les niveaux d'énergie.

L'intérêt de cette approche réside en le fait que, comme précédemment, **l'espace de la variable considérée est unidimensionnel**, mais cette fois **la mesure sur l'espace des états est uniforme**. Ici, à l'inverse de l'approche basée sur les niveaux d'énergie, on a résumé toute l'information sur la structure interne de la molécule dans la fonction quantile d'énergie $F_{\mu_{\bar{\varepsilon}}}^{\leftarrow}$, et rendu triviale la mesure d'intégration.

Ce modèle est pertinent dans le cadre de *simulations numériques* particulières – typiquement, les simulations de type Monte Carlo (DSMC) – par l'*unidimensionnalité* de l'espace d'états et le fait qu'il soit muni d'une *mesure uniforme*. En effet, imaginons un modèle dans lequel la mesure sur l'espace des états ne serait *pas* uniforme. Alors, lors d'une simulation, changer l'état d'une particule impliquerait, involontairement, un changement de son poids numérique : ainsi, les conservations seraient perdues (et la simulation invalide). Ce problème est donc évité uniquement lorsque l'espace d'états est muni d'une mesure *uniforme*. Dans les simulations que nous avons menées, dans le chapitre 5 de cette thèse, nous nous sommes effectivement basés sur cette approche.

1.2.2.3 Résumé et comparaison des différentes approches

Résumons dans le tableau 1.2 les caractéristiques de chaque approche, et donnons dans quels cas il nous semble judicieux d'utiliser l'une ou l'autre.

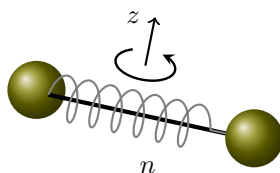
	État ζ	Niveau I	Quantile q
<i>Points forts</i>	dérive directement de la physique, général	espace 1-D, fonction d'énergie triviale	espace 1-D, mesure uniforme
<i>Difficultés</i>	« gros » espace, mesure et fonction d'énergie non triviales	mesure non uniforme	fonction d'énergie non triviale
<i>Information microscopique</i>	complète	réduite à l'énergie interne	réduite à l'énergie interne
Adapté à	Modélisation et preuves générales	Calculs et preuves techniques	Simulations particulières

TABLEAU 1.2 – Un résumé des divers points de vue.

1.2.2.4 Combinaison de modèles

Présentons à présent comment construire un modèle par combinaison de modèles simples, de manière indépendante, et les propriétés immédiates qui découlent de cette combinaison, via un exemple, à partir duquel on déduit aisément le procédé pour le cas général.

Exemple pour une molécule diatomique Considérons, comme dans le schéma qui suit, une molécule composée de deux atomes, pour laquelle on souhaite prendre en compte la rotation de la molécule ainsi que la vibration entre les deux atomes.



Dans cet exemple, nous choisissons (mais d'autres choix sont possibles) de décrire la rotation via une approche *classique*, en considérant la *vitesse angulaire* $z \in \mathbb{R}^2$ (qui ici n'a que deux composantes car la molécule est linéaire, voir la discussion dans « Semi-classical description of the internal structure » en sous-section 2.7.3 du chapitre 2), et la vibration par le modèle de l'oscillateur *quantique* harmonique, avec $n \in \mathbb{N}$ le mode de vibration. Si l'on suppose la rotation et la vibration indépendantes, l'énergie interne associée à l'état (z, n) s'écrit alors comme la somme de l'énergie cinétique de rotation et de l'énergie de vibration :

$$\frac{1}{2} \mathcal{J} |z|^2 + \left(n + \frac{1}{2} \right) \Delta E,$$

où \mathcal{J} est le moment d'inertie et ΔE le gap d'énergie entre deux modes de vibration.

On a alors construit un modèle qui prend en compte la rotation *et* la vibration en *combinant* un modèle décrivant la rotation et un modèle décrivant la vibration. Nous donnons dans le tableau la configuration de ces modèles dans le cadre général ainsi que certaines propriétés typiques.

Dans le tableau 1.3 ci-dessus, Leb désigne la mesure de Lebesgue, compt la mesure de comptage, δ_x la mesure de Dirac en x et $\lceil \cdot \rceil$ la partie entière supérieure. De plus, dans la dernière ligne, $T > 0$ désigne une température, et nous rappelons que le nombre de degrés de liberté internes est défini par (1.45).

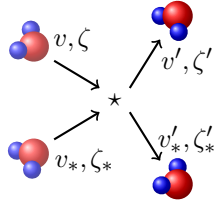
	Rotation	Vibration	Rotation et vibration
Espace d'états internes	$(\mathbb{R}^2, \text{Leb}_{\mathbb{R}^2})$	$(\mathbb{N}, \text{compt})$	$(\mathbb{R}^2 \times \mathbb{N}, \text{Leb}_{\mathbb{R}^2} \otimes \text{compt})$
Fonction d'énergie interne	$\frac{1}{2} \mathcal{J} z ^2$	$\left(n + \frac{1}{2}\right) \Delta E$	$\frac{1}{2} \mathcal{J} z ^2 + \left(n + \frac{1}{2}\right) \Delta E$
Niveau d'énergie fondamental	0	$\frac{1}{2} \Delta E$	$\frac{1}{2} \Delta E$
Loi d'énergie interne	$\frac{2\pi}{\mathcal{J}} \text{Leb}_{\mathbb{R}_+}$	$\sum_{k \in \mathbb{N}} \delta_{k \Delta E}$	$\frac{2\pi}{\mathcal{J}} \left[\frac{I}{\Delta E} \right] dI$
Nb. de degrés de liberté interne	2	$2 \frac{\Delta E/T}{e^{\Delta E/T} - 1}$	$2 + 2 \frac{\Delta E/T}{e^{\Delta E/T} - 1}$

TABLEAU 1.3 – Un exemple de modèle combinant rotation et vibration.

1.2.2.5 Modèle basé sur les états et modèle réduit : y a-t-il équivalence au niveau mésoscopique ?

Cette question se reformule de la manière suivante : est-ce que la *perte d'information* au niveau microscopique lors du processus de réduction – le fait d'oublier les états internes pour ne garder que la répartition des niveaux d'énergie – a une répercussion sur le modèle au niveau *mésoscopique* ? La réponse courte est : cela dépend.

Pour y répondre, nous devons nous tourner vers l'élément-clé du modèle que sont les *collisions*.



Rappelons que lors d'une collision, représentée sur le schéma ci-contre, les lois de conservation s'écrivent

$$v' + v'_* = v + v_*,$$

$$\frac{1}{2} m |v'|^2 + \varepsilon(\zeta') + \frac{1}{2} m |v'_*|^2 + \varepsilon(\zeta'_*) = \frac{1}{2} m |v|^2 + \varepsilon(\zeta) + \frac{1}{2} m |v_*|^2 + \varepsilon(\zeta_*).$$

Dans l'équation ci-dessus, on remarque que l'état interne ζ n'intervient que via son énergie $\varepsilon(\zeta)$. Ainsi, *en ce qui concerne les lois de conservation*, on peut oublier l'état interne et garder uniquement l'énergie *sans perte d'information*. De plus, comme les distributions d'équilibre (maxwelliennes) sont complètement déterminées par les quantités conservées, il n'y a pas non plus de perte d'information les concernant. Ainsi, du point de vue de l'équilibre *thermodynamique*, il est absolument *équivalent* de considérer un modèle complet, basé sur les états internes, ou un modèle réduit, basé uniquement sur l'énergie.

Toutefois, pour qu'il y ait équivalence des deux approches sur la description complète de Boltzmann (et pas uniquement au niveau de l'équilibre thermodynamique), il faudrait que la *section efficace*, caractérisant la répartition des états post-collisionnels en fonction des états pré-collisionnels, *ne dépende elle-même des états internes que via leur énergie*. Si tel est le cas, alors tous les éléments du modèle de Boltzmann ne dépendent des états internes que via leur énergie, et donc considérer directement l'énergie ne représente pas de perte d'information.

Dans le cas contraire, *il n'y a pas équivalence* des approches car ne considérer que l'énergie représente une réelle perte d'information au niveau du modèle de Boltzmann.

Enfin, reprenons à titre d'exemple le modèle décrivant la rotation et la vibration d'une molécule diatomique présenté plus haut, et considérons le modèle de Boltzmann associé à ce modèle moléculaire. Imaginons que la section efficace dépende, en ce qui concerne les états internes, distinctement de l'énergie de rotation et de l'énergie de vibration. Alors, l'information interne ne pouvant être réduite à l'énergie interne totale, il n'est pas possible (au sens où l'on perdrait de l'information au niveau des collisions) de réduire complètement ce modèle. Cependant, *on peut réduire séparément* la partie du modèle associée à la rotation et la partie associée à la vibration, puisque, au niveau des collisions, toute l'information de la rotation peut être réduite à son énergie, et de même pour la vibration. Le modèle correspondant serait donc à deux énergies internes $(I_{\text{rot}}, I_{\text{vib}})$, dont l'espace des états serait $\mathbb{R}_+ \times \mathbb{R}_+$, et sur lequel la mesure serait le produit tensoriel entre la loi d'énergie associée à la rotation et la loi d'énergie associée à la vibration.

1.2.3 Extension aux mélanges avec réactions chimiques

Dans ce qui précède, nous avons construit un cadre de Boltzmann général pour l'étude de gaz polyatomiques simples. Il convient d'étendre à présent la modélisation aux mélanges de gaz avec (ou non) réactions chimiques : c'est l'objet du chapitre 3, correspondant à la publication [24].

1.2.3.1 Présentation du cadre microscopique

On considère un gaz composé de $N \in \mathbb{N}^*$ espèces. Pour chaque espèce $i = 1, \dots, N$, on note $m_i > 0$ la masse d'une molécule, (\mathcal{E}_i, μ_i) l'espace des états internes et ε_i la fonction d'énergie internes. Notons en particulier que ε_i^0 désigne l'énergie fondamentale d'une molécule de l'espèce i et que Z_i désigne la fonction de partition associée à l'espèce i , toujours définie par (1.38).

Nous ne considérons dans ce qui suit que les interactions *binaires*, mais il est possible d'étendre assez naturellement ce cadre pour qu'il prenne en compte des interactions entre un nombre arbitraire de molécules (voir [89]). S'il y a réaction de l'espèce i avec j pour donner k et ℓ , on notera cette réaction $\{(i, j) \rightarrow (k, \ell)\}$. On appelle Ω l'ensemble des réactions possibles. En toute généralité, *il n'est pas nécessaire*, dans notre approche, *de distinguer les collisions mécaniques et les réactions chimiques*. Le terme « réaction » sera donc employé pour désigner ou une collision ou une réaction chimique. Puisque, a minima, les molécules peuvent entrer en collision entre elles, on a par défaut que

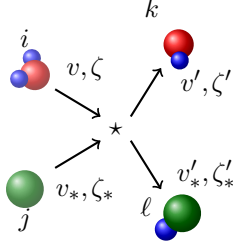
$$\{(i, j) \rightarrow (i, j)\} \in \Omega, \quad \forall 1 \leq i, j \leq N.$$

De plus, les molécules étant supposées indiscernables au sein d'une même espèce on a

$$\{(i, j) \rightarrow (k, \ell)\} \in \Omega \quad \iff \quad \{(j, i) \rightarrow (\ell, k)\} \in \Omega.$$

Pour assurer la réversibilité des interactions au niveau microscopique, on suppose que les réactions chimiques sont à double sens, c'est-à-dire

$$\{(i, j) \rightarrow (k, \ell)\} \in \Omega \quad \iff \quad \{(k, \ell) \rightarrow (i, j)\} \in \Omega.$$

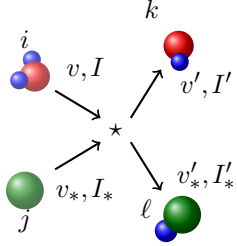


Intéressons nous à présent à une réaction $\{(i, j) \rightarrow (k, \ell)\} \in \Omega$, représentée sur le schéma ci-contre. Soulignons qu'ici, $\zeta \in \mathcal{E}_i$, $\zeta_* \in \mathcal{E}_j$, $\zeta' \in \mathcal{E}_k$ et $\zeta'_* \in \mathcal{E}_\ell$. En supposant *isolé* le système à deux molécules, nous avons donc conservation de la masse (l'équation ci-dessus), de la quantité de mouvement et de l'énergie totale, donc

$$\begin{aligned} m_k v' + m_\ell v'_* &= m_i v + m_j v_*, \\ \frac{1}{2} m_k |v'|^2 + \varepsilon_k(\zeta') + \frac{1}{2} m_\ell |v'_*|^2 + \varepsilon_\ell(\zeta'_*) &= \frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) + \frac{1}{2} m_j |v_*|^2 + \varepsilon_j(\zeta_*). \end{aligned} \quad (1.53)$$

On peut paramétrer (1.53) de manière similaire au cas du gaz simple (1.41), et obtenir que (1.53) implique qu'il existe un angle $\omega \in \mathbb{S}^2$ tel que v' et v'_* sont des fonctions (explicites) de $v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*$ et ω . La formule étant un peu plus technique que précédemment, nous ne la détaillons pas ici et renvoyons au chapitre 3, équation (3.14).

Énergie de réaction Dans le cas des réactions chimiques, nous n'avons pas présupposé l'existence d'une *énergie de réaction*. En effet, ce n'est pas un paramètre du modèle, mais elle apparaît naturellement. Reconsidérons la réaction décrite précédemment, mais en nous basant cette fois sur les *modèles réduits* (basés sur les niveaux d'énergie).



Ici, $(I, I_*) \in \mathbb{R}_+^2$ sont les niveaux d'énergie interne du couple de molécules pré-collisionnel, dont l'énergie interne totale est $I + I_* + \varepsilon_i^0 + \varepsilon_j^0$. De la même façon, (I', I'_*) sont les niveaux d'énergie interne du couple de molécules post-collisionnel, dont l'énergie totale est $I' + I'_* + \varepsilon_k^0 + \varepsilon_\ell^0$. Ainsi, la conservation de l'énergie du système à deux molécules s'écrit ici

$$\frac{1}{2} m_k |v'|^2 + I' + \frac{1}{2} m_\ell |v'_*|^2 + I'_* = \frac{1}{2} m_i |v|^2 + I + \frac{1}{2} m_j |v_*|^2 + I_* - (\Delta\varepsilon^0)_{ij}^{k\ell}, \quad (1.54)$$

où

$$(\Delta\varepsilon^0)_{ij}^{k\ell} := \varepsilon_k^0 + \varepsilon_\ell^0 - \varepsilon_i^0 - \varepsilon_j^0$$

peut donc s'interpréter comme l'*énergie consommée par la réaction* : cette dernière est dite *endothermique* si $(\Delta\varepsilon^0)_{ij}^{k\ell} > 0$ et *exothermique* si $(\Delta\varepsilon^0)_{ij}^{k\ell} < 0$.

Dans notre cadre de modélisation, l'**énergie de réaction n'est pas un paramètre du modèle** mais **apparaît** à partir des modèles moléculaires.

Je souligne que (1.53) et (1.54) décrivent strictement la même information, mais différent dans leur écriture : en particulier,

1. (1.53) a la même forme pour les collisions mécaniques que pour les réactions chimiques (on peut voir une collision comme un cas particulier de réaction chimique),
2. (1.53) est complètement microscopique et l'on considère bien que le système est isolé, à l'inverse de (1.54) qui inclut un échange avec l'environnement, une notion non microscopique,

3. (1.53) est symétrique.

État de transition et énergie d'activation Afin de reproduire fidèlement la cinétique des réactions chimiques, nous incluons au modèle la notion d'*état de transition*, introduite dans les années 1930 [83, 82]. On peut comprendre l'état de transition de la réaction chimique $\{(i, j) \rightarrow (k, \ell)\}$ comme une configuration particulière des atomes du système durant la transformation de (i, j) en (k, ℓ) , et dont l'énergie potentielle associée est maximale, relativement à la coordonnée de réaction. Une représentation schématique clarifiant ce propos est donnée en figure 1.5.

L'état de transition ayant une durée de vie extrêmement courte, il n'est pas nécessaire, au niveau cinétique, de le prendre directement en compte. Son existence se traduira simplement par l'introduction d'une *barrière d'énergie potentielle*. Ainsi, pour chaque réaction $\{(i, j) \rightarrow (k, \ell)\} \in \Omega$, nous supposons la donnée d'une quantité, $\kappa_{ij}^{k\ell} \in \mathbb{R}$, qui représente l'*énergie potentielle de configuration associée à l'état de transition* de la réaction $\{(i, j) \rightarrow (k, \ell)\}$.

On définit alors l'*énergie d'activation* E_a de la réaction chimique $\{(i, j) \rightarrow (k, \ell)\}$ comme la différence entre l'énergie potentielle de configuration de l'état de transition et l'énergie potentielle de configuration des réactifs. Dans notre formalisme, cela s'écrit

$$E_a := \kappa_{ij}^{k\ell} - \varepsilon_i^0 - \varepsilon_j^0.$$

La cinétique de la réaction dépend fortement de la valeur de cette énergie E_a : moralement, plus E_a est grand, plus la réaction sera lente. Mentionnons la *loi d'Arrhenius*, principe proposé empiriquement à la fin du XIX^e siècle, établissant une dépendance entre la cinétique de la réaction, l'énergie d'activation et la température du système ; nous retrouvons théoriquement sur un cas-test une forme proche de la loi d'Arrhenius, voir la section 3.7 du chapitre 3.

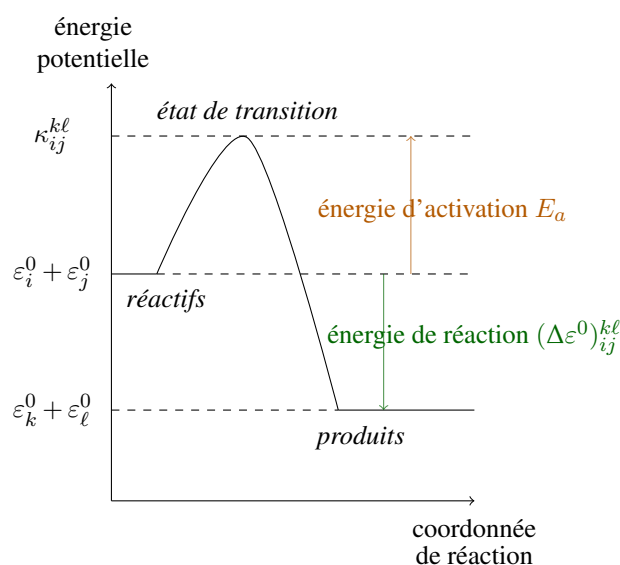


FIGURE 1.5 – Diagramme d'une réaction chimique $\{(i, j) \rightarrow (k, \ell)\}$

Sur la figure 1.5, on retrouve que l'énergie potentielle des réactifs s'écrit comme la somme des énergies fondamentales des deux espèces réactives, et similairement pour les produits. L'énergie consommée par la réaction correspond à la différence d'énergie potentielle entre les produits et les réactifs (sur cet exemple,

la réaction est exothermique), et l'énergie d'activation est bien la différence entre l'énergie potentielle de l'état de transition et de celle des réactifs.

Afin de préserver la réversibilité des interactions au niveau microscopique, nous supposons que l'énergie potentielle de l'état de transition de la réaction $\{(i, j) \rightarrow (k, \ell)\}$ est identique à celle de la réaction $\{(k, \ell) \rightarrow (i, j)\}$, c'est-à-dire

$$\kappa_{ij}^{k\ell} = \kappa_{k\ell}^{ij}.$$

Notons toutefois que l'énergie d'activation associée à $\{(k, \ell) \rightarrow (i, j)\}$ vaut $\kappa_{ij}^{k\ell} - \varepsilon_k^0 - \varepsilon_\ell^0$ et diffère donc de l'énergie d'activation associée à $\{(i, j) \rightarrow (k, \ell)\}$.

Enfin, puisqu'il n'y a pas d'état de transition pour les collisions, on prend la convention $\kappa_{ij}^{ij} = \varepsilon_i^0 + \varepsilon_j^0$.

1.2.3.2 Niveau mésoscopique

Au niveau mésoscopique, nous étudierons la famille des densités de molécules de chaque espèce, $f \equiv (f_i(t, x, v_i, \zeta_i))$, qui dépend du temps t , de la position x , la vitesse v_i et l'état interne $\zeta_i \in \mathcal{E}_i$. On note ρ_i et n_i , u_i et T_i respectivement la *densité massique* et *densité molaire*, la *vitesse moyenne molaire* (d'autres types de moyenne pourraient être considérées) et la *température* associées à l'espèce i , données comme précédemment par

$$\rho_i(t, x) := \iint_{\mathbb{R}^3 \times \mathcal{E}_i} m_i f_i(t, x, v, \zeta) \, dv \, d\mu_i(\zeta), \quad n_i = \frac{\rho_i}{m_i}, \quad (1.55)$$

$$u_i(t, x) := \frac{1}{\rho_i(t, x)} \iint_{\mathbb{R}^3 \times \mathcal{E}_i} m_i v f_i(t, x, v, \zeta) \, dv \, d\mu_i(\zeta), \quad (1.56)$$

$$T_i(t, x) := \Theta_i^{-1} \left(\frac{1}{n_i(t, x)} \iint_{\mathbb{R}^3 \times \mathcal{E}_i} \left(\frac{m_i}{2} |v - u_i|^2 + \bar{\varepsilon}_i(\zeta) \right) f_i(t, x, v, \zeta) \, dv \, d\mu_i(\zeta) \right), \quad (1.57)$$

où, pour tout $T > 0$,

$$\Theta_i(T) := \frac{3 + \delta_i(T)}{2} T,$$

avec δ_i le *nombre de degrés de liberté internes* associé à l'espèce i , défini dans (1.45). On définit de plus $\bar{\rho}$ et \bar{n} , \bar{u} et \bar{T} respectivement la *densité massique*, la *densité molaire*, la *vitesse globale* et la *température* du mélange, donnés par

$$\bar{\rho} = \sum_{i=1}^N \rho_i, \quad \bar{n} = \sum_{i=1}^N n_i, \quad \bar{u} = \sum_{i=1}^N \frac{n_i}{\bar{n}} u_i, \quad (1.58)$$

et

$$\bar{T}(t, x) = \bar{\Theta} \left[\left(\frac{n_i}{\bar{n}} \right) \right]^{-1} \left(\frac{1}{\bar{n}} \sum_{i=1}^N \iint_{\mathbb{R}^3 \times \mathcal{E}_i} \left(\frac{1}{2} m_i |v - u_i|^2 + \bar{\varepsilon}_i(\zeta) \right) f_i(v, \zeta) \, dv \, d\mu_i(\zeta) \right), \quad (1.59)$$

avec

$$\bar{\Theta} \left[\left(\frac{n_i}{\bar{n}} \right) \right] (T) := \sum_{i=1}^N \frac{n_i}{\bar{n}} \Theta_i(T).$$

Modèle de Boltzmann Construisons à présent le modèle de Boltzmann. On suppose alors que pour tout i , chaque densité f_i satisfait l'équation suivante, pour presque tout $t \geq 0$, $x, v \in \mathbb{R}^3$ et $\zeta \in \mathcal{E}_i$,

$$\partial_t f_i(t, x, v, \zeta) + v \cdot \nabla_x f_i(t, x, v, \zeta) = Q_i(f(t, x, \cdot, \cdot), f(t, x, \cdot, \cdot))(v, \zeta), \quad (1.60)$$

où l'opérateur Q_i prend en compte toutes les réactions binaires – collisions mécaniques et réactions chimiques – qui impliquent l'espèce i , et est défini, pour une famille de densités $f \equiv (f_j(v_j, \zeta_j))_j$ et $(v, \zeta) \in \mathbb{R}^3 \times \mathcal{E}_i$ tels que ce qui suit ait un sens, par

$$Q_i(f, f)(v, \zeta) := \sum_{\substack{j, k, \ell \\ \{(i, j) \rightarrow (k, \ell)\} \in \Omega}} \iiint_{\mathcal{E}_j \times \mathcal{E}_k \times \mathcal{E}_\ell} \iint_{\mathbb{R}^3 \times \mathbb{S}^2} (f'_k f'_{\ell_*} - f_i f_{j_*}) B_{ij}^{k\ell} dv_* d\sigma d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_\ell(\zeta'_*). \quad (1.61)$$

Dans l'intégrale (1.61), on utilise les notations contractées $f'_k \equiv f_k(v', \zeta')$, $f'_{\ell_*} \equiv f_\ell(v'_*, \zeta'_*)$, $f_i \equiv f_i(v, \zeta)$, $f_{j_*} \equiv f_j(v_*, \zeta_*)$, et

$$B_{ij}^{k\ell} \equiv B_{ij}^{k\ell}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega)$$

est le noyau de collision associé à la réaction $\{(i, j) \rightarrow (k, \ell)\}$. De plus, dans (1.61), v' et v'_* sont des fonctions de $v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*$ et ω (définies par (3.14) au chapitre 3).

Le noyau B est supposé satisfaire aux propriétés de *symétrie* et *micro-réversibilité* (donnés en (3.23) et (3.24) au chapitre 3). L'information des réactions possibles étant donnée par le *support* du noyau B , on inclut dans le modèle la notion d'état de transition et d'énergie d'activation détaillée plus haut via une *condition* sur ce support, traduisant l'idée d'une barrière de potentiel.

1.2.3.3 Équilibre réactionnel

Définissons enfin la fonctionnelle d'entropie, pour des familles de densités $f \equiv (f_i(v_i, \zeta_i))$,

$$H_0^{\text{mélange}}(f) := \sum_{i=1}^N \iint_{\mathbb{R}^3 \times \mathcal{E}_i} \left\{ f_i \log \frac{f_i}{m_i^3} - f_i \right\} dv d\mu_i(\zeta).$$

Si la densité dépend aussi de la position dans l'espace x , on intégrera aussi en x .

La validité, du point de vue de la modélisation, de notre cadre pour le modèle de Boltzmann est assurée par le théorème suivant (voir théorème 3.1 au chapitre 3).

Théorème 1.4

Théorème H et loi d'action de masse.

1. Formellement, le long d'une solution de l'équation de Boltzmann (1.60) (ou homogène), l'entropie est dissipée.

2. La dissipation d'entropie de $f \equiv (f_i(v_i, \zeta_i))$ s'annule si et seulement si $f_i = \mathcal{M}_i[n_i, \underline{u}, \bar{T}]$ pour tout $i = 1, \dots, N$, où n_i est la densité associée à l'espèce i définie comme dans (1.55), \underline{u} et \bar{T} respectivement la vitesse globale et la température du mélange, définis respectivement dans (1.58) et (1.59), avec pour tout $i = 1, \dots, N$ et $(v, \zeta) \in \mathbb{R}^3 \times \mathcal{E}_i$,

$$\mathcal{M}_i[n_i, \underline{u}, \bar{T}](v, \zeta) = n_i \left(\frac{2\pi\bar{T}}{m_i} \right)^{-3/2} Z_i \left(\frac{1}{\bar{T}} \right)^{-1} \exp \left(-\frac{m_i |v - \underline{u}|^2}{2\bar{T}} - \frac{\bar{\varepsilon}_i(\zeta)}{\bar{T}} \right), \quad (1.62)$$

et où les (n_i) satisfont la loi d'action de masse, pour tout i, j, k, ℓ tels que $\{(i, j) \rightarrow (k, \ell)\} \in \Omega$,

$$\frac{n_k n_\ell}{n_i n_j} = \mathcal{K}_{ij}^{k\ell}(T), \quad (1.63)$$

où $\mathcal{K}_{ij}^{k\ell}$ est la constante de réaction de $\{(i, j) \rightarrow (k, \ell)\}$, donnée par

$$\mathcal{K}_{ij}^{k\ell}(T) := \prod_{p \in \{i, j, k, \ell\}} \left\{ (2\pi m_p T)^{3\sigma_p/2} Z_p \left(\frac{1}{T} \right)^{\sigma_p} \right\} \exp \left(- \frac{(\Delta\varepsilon^0)_{ij}^{k\ell}}{T} \right), \quad (1.64)$$

avec $\sigma_k = \sigma_\ell = -\sigma_i = -\sigma_j = 1$.

Soulignons qu'à l'équilibre réactionnel, décrit ci-dessus, la vitesse globale est la même pour toutes les espèces, et de même pour la température. Les densités molaires sont toutefois différentes.

1.2.3.4 Équilibre mécanique et réactions relativement lentes

Un cadre d'étude intéressant est celui d'un mélange pour lequel les réactions chimiques sont dites *relativement lentes*. Dans ce cas, on considère que *la relaxation vers l'équilibre induite par les collisions mécaniques est beaucoup plus rapide que celle induite par les réactions chimiques*. On choisit alors de distinguer les collisions mécaniques et les réactions chimiques en partitionnant l'ensemble des réactions :

$$\Omega = \Omega_{\text{méca}} \cup \Omega_{\text{chim}}.$$

Sans rentrer dans plus de détails ici, on peut alors écrire la dissipation d'entropie comme la somme d'une dissipation liée aux collisions mécaniques et une dissipation liée aux réactions chimiques :

$$\mathcal{D}_0^{\text{mélange}} = \mathcal{D}_0^{\text{méca}} + \mathcal{D}_0^{\text{chim}}.$$

Ainsi, il nous est possible de considérer un « équilibre » intermédiaire, pour lequel seule la dissipation d'entropie liée aux collisions mécaniques s'annule : nous parlerons donc d'*équilibre mécanique*.

Théorème 1.5

Équilibre mécanique.

La dissipation d'entropie associée aux collisions mécaniques de $f \equiv (f_i(v_i, \zeta_i))$ s'annule si et seulement si $f_i = \mathcal{M}_i[n_i, u_i, T_i]$ pour tout $i = 1, \dots, N$, où ρ_i , u_i et T_i sont respectivement la densité, la vitesse globale et la température associées à l'espèce i , définis dans (1.55)–(1.57), et \mathcal{M}_i est la maxwellienne généralisée associée à l'espèce i , définie dans (1.62).

Je souligne qu'à l'équilibre mécanique, les vitesses globales et températures associées à chaque espèce ne sont pas identiques. De plus, la loi d'action de masse ne tient pas.

Équations d'Euler Nous retrouvons formellement les équations d'Euler, pour un mélange de gaz parfaits dont le nombre de degrés de liberté de chaque espèce i est $3 + \delta_i(T)$ et faisant intervenir les réactions chimiques caractérisées par Ω , en insérant la famille de maxwelliennes $(\mathcal{M}_i[n_i, u_i, T_i])$ dans l'équation de Boltzmann (1.60). Ces équations sont données dans le théorème 3.3 au chapitre 3.

1.3 Autour d'un modèle singulier : collisions résonantes et quasi-résonantes

Cette section est dédiée à l'introduction de la partie II de cette thèse, ayant trait à l'étude d'un gaz polyatomique au sein duquel les collisions sont *résonantes* ou *quasi-résonantes*. En chapitre 4, qui est une amélioration de [38], nous montrons une propriété de compacité de l'opérateur de Boltzmann linéarisé associé au modèle polyatomique résonant; le chapitre 5 est quant à lui consacré à la modélisation de la notion de *quasi-résonance*, une étude qualitative des propriétés attendues, et quelques expériences numériques.

1.3.1 Propriété de compacité du linéarisé pour un gaz polyatomique avec collisions résonantes

Dans cette sous-section, nous introduisons le chapitre 4, dont l'objet est la preuve de la compacité de la partie non-multiplicative du linéarisé de l'opérateur de Boltzmann associé. Nous présentons ci-après le modèle résonant, explicitons notre théorème et discutons l'approche de notre démonstration.

1.3.1.1 Modèle polyatomique résonant

Le modèle de Boltzmann pour un gaz simple polyatomique résonant a été proposé pour la première fois dans [44]. Dans ce qui suit, nous le présentons en nous basant sur l'approche des *niveaux d'énergie* présentée en sous-section 1.2.2. Le formalisme utilisé dans [44] fait intervenir un paramètre $r \in [0, 1]$ à la place de la variable $I' \in \mathbb{R}_+$ dans notre formalisme : les deux sont en fait équivalents (lorsque la mesure sur l'espace des niveaux d'énergie est absolument continue par rapport à la mesure de Lebesgue) via un changement de variable.

On considère donc un gaz polyatomique simple. On choisit le modèle moléculaire des *niveaux d'énergie* : ainsi (mettant de côté la variable macroscopique de la position x), l'état d'une molécule sera décrit par sa vitesse $v \in \mathbb{R}^3$ et son niveau d'énergie interne $I \in \mathbb{R}_+$. Puisque la valeur de l'énergie fondamentale n'a pas d'importance dans le cas du gaz simple (voir la section précédente), nous la fixons à zéro ; ainsi, l'énergie d'une molécule dans l'état (v, I) est

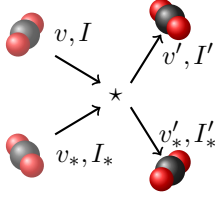
$$\frac{1}{2}m|v|^2 + I,$$

où $m > 0$ est la masse d'une molécule.

La mesure d'intégration sur \mathbb{R}_+ — la *loi d'énergie* — sera dénommée μ . Aussi, nous la supposons *absolument continue par rapport à la mesure de Lebesgue*, de telle sorte qu'il existe une fonction $\varphi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$, mesurable (et strictement positive presque partout), telle que

$$d\mu(I) = \varphi(I) dI, \quad I \in \mathbb{R}_+.$$

Collisions résonantes Il a été constaté que certaines molécules exhibent un comportement collisionnel singulier; nous renvoyons à [120] explicitant ce phénomène pour les molécules de CO_2 .



Lors d'une collision entre deux molécules polyatomiques, représentée ci-contre, dont les états pré- et post-collisionnels sont respectivement désignés par (v, I) , (v_*, I_*) et (v', I') , (v'_*, I'_*) , la quantité de mouvement et l'énergie totale du système à deux molécules sont conservés. La collision est dite **résonante** lorsque, de surcroît, l'énergie cinétique et l'énergie interne du système à deux molécules sont *séparément conservées*. Cela se traduit alors par les lois de conservation suivantes :

$$\begin{aligned} v' + v'_* &= v + v_*, \\ |v'|^2 + |v'_*|^2 &= |v|^2 + |v_*|^2, \\ I' + I'_* &= I + I_*. \end{aligned} \quad (1.65)$$

On observe dans (1.65) une *décorrélation complète* entre la vitesse et l'énergie interne. Elle se retrouvera plus tard sur les distributions d'équilibre. En particulier, les équations sur les variables de vitesses sont identiques au cas monoatomique. On peut en déduire, en utilisant la représentation en σ , que v , v_* , v' , v'_* satisfont aux équations de conservation (1.65) si et seulement s'il existe un angle $\sigma \in \mathbb{S}^2$ tel que

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

D'un autre côté, l'équation de conservation de l'énergie interne est trivialement équivalente à

$$I' \in [0, I + I_*], \quad I'_* = I + I_* - I'. \quad (1.66)$$

Mesure d'intégration associée à la variable post-collisionnelle Dans ce cadre, à la différence du modèle polyatomique usuel, dans lequel, dans l'opérateur de Boltzmann, l'intégration porte notamment sur les deux variables internes post-collisionnelles I' et I'_* (voir (1.46)), l'intégration ne porte, dans le cas résonant, que sur *une seule variable* post-collisionnelle, disons I' pour la suite, puisque l'autre est, par (1.66), complètement déterminée par la première et les variables internes pré-collisionnelles. Toutefois, il faut prendre en compte *les deux molécules*. Ainsi la mesure d'intégration associée à la variable interne post-collisionnelle I' doit être une loi d'énergie relative à *deux molécules* : elle aura la forme d'une convolution de μ avec elle-même — μ étant la loi d'énergie d'une molécule. Pour $I, I_* \geq 0$ nous définissons alors la mesure $\mu_2[I + I_*]$ définie sur $[0, I + I_*]$ par

$$d\mu_2[I + I_*](I') := \varphi(I + I_* - I') \varphi(I') dI', \quad I' \in [0, I + I_*]. \quad (1.67)$$

Dans [44], où le modèle résonant a été proposé, l'utilisation de la paramétrisation permet de contourner cette difficulté. Je mentionne par ailleurs que le chapitre 4 est une version mise à jour de [38], qui prend en compte la bonne mesure μ_2 . Une justification de (1.67) peut être apportée via un passage à la limite depuis le modèle *quasi-résonant* — voir la sous-section 5.1.3 du chapitre 5.

Opérateur de collision Boltzmann Définissons à présent l'opérateur de Boltzmann associé à ce cadre. Puisque la singularité du modèle n'est présente que dans les collisions, l'équation de Boltzmann correspondante aura la même forme que décrit précédemment dans le cadre polyatomique usuel — voir (1.46) — ainsi nous ne la détaillerons pas de nouveau.

On définit l'opérateur de Boltzmann résonant, pour une densité $f \equiv f(v, I) \geq 0$ et tout $v \in \mathbb{R}^3$, $I \in \mathbb{R}_+$, par

$$Q(f, f)(v, I) := \iint_{(\mathbb{R}_+)^2} \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \{f(v', I') f(v'_*, I'_*) - f(v, I) f(v, I_*)\}$$

$$\times B^{\text{res}}(v, v_*, I, I_*, I', \sigma) d\sigma dv_* d\mu_2[I + I_*](I') d\mu(I_*), \quad (1.68)$$

où v' et v'_* sont donnés par (1.5) (comme dans le cas monoatomique), $I'_* = I + I_* - I'$ et $B^{\text{res}} \geq 0$ est le noyau de collision. Ce dernier satisfait les propriétés de *symétrie* et *micro-réversibilité* (données explicitement dans (4.12)–(4.13) au chapitre 4), ainsi que la condition d'être non nul uniquement lorsque la collision est possible, c'est-à-dire, pour tout $(v, v_*, I, I_*, I', \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{S}^2$,

$$B^{\text{res}}(v, v_*, I, I_*, I', \sigma) > 0 \quad \iff \quad 0 \leq I' \leq I + I_*,$$

permettant d'assurer que (1.68) ait bien un sens — rappelons que $d\mu_2[I + I_*](I')$ n'a de sens que quand $0 \leq I' \leq I + I_*$.

Températures cinétique et interne Soit une densité de molécules $f \equiv f(v, I)$. Dans ce cadre, il est pertinent d'étudier, non pas la température globale T (donnée par 1.44), mais *les températures cinétique et interne* T_k et T_i , définies par

$$T_k := \frac{2}{3\rho} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \frac{m}{2} |v - u|^2 f(v, I) dv d\mu(I), \quad (1.69)$$

$$T_i := \Theta_i^{-1} \left(\frac{1}{\rho} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} I f(v, I) dv d\mu(I) \right), \quad (1.70)$$

avec ρ la densité associée à f , u sa vitesse moyenne et Θ_i défini par, pour tout $T > 0$,

$$\Theta_i(T) := \frac{\delta(T)}{2} T,$$

où δ est le nombre de degrés de liberté internes, donné dans (1.45).

Équilibre thermodynamique et maxwellienne à deux températures Considérons à présent la fonctionnelle d'entropie, définie comme dans (1.48), où l'on remplace \mathcal{E} par \mathbb{R}_+ et ζ par I . Nous avons, grâce à [44], le théorème suivant.

Théorème 1.6

Théorème H. [Polyatomique résonant]

1. Formellement, le long d'une solution de l'équation de Boltzmann polyatomique résonante, l'entropie est dissipée.

2. La dissipation d'entropie *résonante* d'une densité $f \equiv f(v, I) \geq 0$ s'annule si et seulement si $f = \mathcal{M}[\rho, u, T_i, T_k]$, où ρ , u , T_i et T_k sont respectivement la densité, la vitesse globale, la température interne et la température cinétique associées à f définis dans (1.42)–(1.43) et (1.69)–(1.70) et, pour tout $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$,

$$\mathcal{M}[\rho, u, T_i, T_k](v, I) = \frac{\rho}{m} \left(\frac{2\pi T_k}{m} \right)^{-3/2} Z \left(\frac{1}{T_i} \right)^{-1} \exp \left(-\frac{m|v - u|^2}{2T_k} - \frac{I}{T_i} \right), \quad (1.71)$$

où nous rappelons que Z est la fonction de partition, définie en (1.38).

On retrouve dans le théorème ci-dessus la particularité fondamentale du modèle résonant : à l'équilibre thermodynamique, les températures cinétique et interne sont a priori *distinctes*. En effet, comme il n'y

a pas d'échange entre les énergies cinétique et interne, les températures correspondantes n'ont aucune raison d'être confondues.

1.3.1.2 Étude du linéarisé et théorème de compacité

Une étude au voisinage de l'équilibre peut être conduite ici en considérant l'opérateur de Boltzmann polyatomique résonant *linéarisé*. De manière similaire au cas monoatomique (voir sous-section 1.1.4), considérant une distribution d'équilibre \mathcal{M} (ici, une maxwellienne à deux températures), on peut définir \mathcal{L} l'opérateur linéarisé de l'opérateur de Boltzmann polyatomique résonant, associé à \mathcal{M} et au noyau de collision B^{res} , par

$$\mathcal{L} := K - \bar{\nu} \text{Id},$$

où $\bar{\nu} \equiv \bar{\nu}(v, I)$ est la *fréquence de collision*, Id l'opérateur identité et K s'écrit, pour toute fonction $g \equiv g(v, I)$ telle que ce qui suit ait un sens, et tout $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$,

$$Kg(v, I) = \mathcal{M}(v, I)^{1/2} \int_{\mathbb{R}^3 \times (\mathbb{R}_+)^2 \times \mathbb{S}^2} \left([\mathcal{M}^{-1/2}g](v', I') + [\mathcal{M}^{-1/2}g](v'_*, I'_*) - [\mathcal{M}^{-1/2}g](v_*, I_*) \right) \times \mathcal{M}(v_*, I_*) B^{\text{res}}(v, v_*, I, I_*, I', \sigma) dv_* d\mu_2[I + I_*(I')] d\mu(I_*) d\sigma. \quad (1.72)$$

Compacité de K Comme expliqué en sous-section 1.1.4, la propriété clé à obtenir dans l'étude du linéarisé est la *compacité* de K . Ainsi, au chapitre 4, nous montrons le théorème suivant.

Théorème 1.7

Compacité de K . On suppose que la densité φ de la mesure μ se comporte comme une fonction puissance aux voisinages de 0 et de l'infini (voir (4.2)–(4.3)) et que le noyau de collision B^{res} satisfait certaines hypothèses de bornes supérieures (voir (4.15)–(4.17)). Alors K est **compact** comme opérateur de $L^2(\mathbb{R}^3 \times \mathbb{R}_+, dv d\mu(I))$ dans lui-même.

Soulignons que l'espace L^2 que l'on considère dans le théorème est effectivement celui qui a du sens dans notre cadre, puisque la mesure associée à \mathbb{R}_+ est bien μ .

Éléments de preuve du théorème 1.7 Donnons un rapide aperçu de la preuve de ce théorème, faisant l'objet du chapitre 4. La spécificité du modèle *résonant*, dans lequel on observe, au niveau des lois de conservation, la *séparation* entre les variables v et I , nous permet, dans la preuve de la compacité de K de *scinder* de la même manière l'étude en deux parties, une portant sur la variable de vitesse v et l'autre sur celle du niveau d'énergie interne I .

D'un côté, la partie en la variable de vitesse v se ramène exactement au cas monoatomique. Ainsi, nous utilisons majoritairement des résultats existants [93, 46]. D'un autre côté, la partie en la variable de niveau d'énergie interne I requiert un traitement spécifique, faisant l'objet principal de la démonstration. Enfin, la structure de la preuve du théorème 1.7 suit la méthode proposée dans [46], en montrant la compacité via des propriétés de décroissance à l'infini et d'équicontinuité.

Nous proposons de plus en annexe une variante à la preuve originale de Grad, apportant une interprétation géométrique et une extension du résultat à une classe un peu plus large de noyaux de collision (et qui pourrait se généraliser au cas polyatomique non résonant).

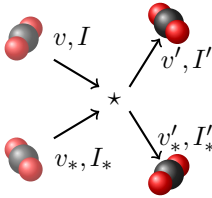
1.3.2 Un modèle de gaz polyatomique avec collisions quasi-résonantes

Le chapitre 5 de cette thèse est dédié à la construction d'un modèle pour un gaz polyatomique dans lequel les collisions sont *quasi-résonantes*. On discutera aussi *qualitativement* certaines propriétés attendues, en appuyant nos arguments par des *expériences numériques*. Ce faisant, nous avons proposé une approche pour obtenir, depuis Boltzmann, des équations de type « Landau-Teller » sur la relaxation des températures.

1.3.2.1 Le modèle

On se place dans le même cadre que dans la sous-section précédente (traitant du modèle polyatomique résonant), et utilisons les mêmes notations – en particulier, la mesure μ désigne la loi d'énergie. L'idée du modèle *quasi-résonant* est de rendre *un peu plus flexible* le modèle *résonant*, de la manière suivante.

Notion de quasi-résonance



Reprenons une collision entre deux molécules polyatomiques, représentée ci-contre, dont les états pré- et post-collisionnels sont respectivement désignés par (v, I) , (v_*, I_*) et (v', I') , (v'_*, I'_*) . La quantité de mouvement et l'énergie totale du système à deux molécules sont conservés. La collision sera dite **quasi-résonante** lorsque, de surcroît, l'énergie cinétique et l'énergie interne du système à deux molécules sont *à peu près séparément conservées*. Cela se traduit donc par les lois de conservation polyatomiques usuelles

$$\begin{aligned} v' + v'_* &= v + v_*, \\ \frac{1}{2}m|v'|^2 + I' + \frac{1}{2}m|v'_*|^2 + I'_* &= \frac{1}{2}m|v|^2 + I + \frac{1}{2}m|v_*|^2 + I_*, \end{aligned} \quad (1.73)$$

ainsi qu'une condition de quasi-résonance de la collision, demandant moralement que

$$|v'|^2 + |v'_*|^2 \approx |v|^2 + |v_*|^2,$$

ou de manière équivalente (d'après (1.73)),

$$I' + I'_* \approx I + I_*.$$

Il s'agit donc de *donner un sens mathématique rigoureux* à cet *à peu près*, et d'en traduire un comportement physique interprétable.

La résonance comme singularité, approximation du Dirac Pour commencer, nous allons représenter le cas *résonant* comme une variante *singulière* du cas polyatomique usuel. Rappelons les mesures d'intégration intervenant dans l'opérateur de Boltzmann dans chaque cas. Dans le cas polyatomique usuel, cette mesure s'écrit – on rappelle que φ est la densité de la mesure μ par rapport à la mesure de Lebesgue sur \mathbb{R}_+ –

$$B(v, v_*, I, I_*, I', I'_*, \sigma) d\sigma dv_* \varphi(I_*) \varphi(I') \varphi(I'_*) dI_* dI' dI'_*, \quad (1.74)$$

tandis que dans le cas résonant, cette mesure s'écrit

$$B^{\text{res}}(v, v_*, I, I_*, I', \sigma) d\sigma dv_* \varphi(I_*) \varphi(I') \varphi(I + I_* - I'_*) dI_* dI', \quad (1.75)$$

où l'on a considéré deux noyaux de collision, B dans le cas polyatomique usuel et B^{res} dans le cas résonant. Supposons à présent, pour fixer les idées, que B est continu et que $B = B^{\text{res}}$ sur l'ensemble $\{I'_* = I + I_* - I'\}$, dans le sens où

$$B(v, v_*, I, I_*, I', I + I_* - I', \sigma) = B^{\text{res}}(v, v_*, I, I_*, I', \sigma). \quad (1.76)$$

On constate qu'alors, on peut formellement réécrire (1.75) comme

$$B(v, v_*, I, I_*, I', I'_*, \sigma) \times \delta_{\{I+I_*\}}(I' + I'_*) \times d\sigma dv_* \varphi(I_*) \varphi(I') \varphi(I'_*) dI_* dI' dI'_*,$$

où $\delta_{\{x\}}$ désigne la mesure de Dirac en $x \in \mathbb{R}$. On retrouve alors (1.74), multiplié par une mesure de Dirac. On conclut que **le cas résonant s'interprète comme un cas polyatomique dans lequel le noyau de collision est supporté sur un ensemble de dimension inférieure à l'ensemble usuel.**

Bien que cette interprétation soit formelle, il en découle un moyen très naturel de définir la notion de *quasi-résonance*, via l'*approximation* de la mesure de Dirac $\delta_{\{I+I_*\}}(I' + I'_*)$. Ainsi, dans le cas *quasi-résonant*, on considérera un noyau de collision supporté sur un ensemble *de même dimension que dans le cas polyatomique usuel*, mais qui est « proche » (dans un certain sens) d'un noyau concentré sur l'ensemble correspondant au cas résonant, de dimension inférieure.

Une proposition de modélisation de la quasi-résonance Dans notre approche, nous considérerons un *noyau de collision* polyatomique usuel

$$B \equiv B(v, v_*, I, I_*, I', I'_*, \sigma),$$

que nous appellerons *noyau de référence*. Rappelons que le cas résonant revient moralement à considérer le noyau $B \times \delta_{\{I+I_*\}}(I' + I'_*)$.

Soit $(\chi_\varepsilon)_{\varepsilon>0}$ une famille de fonctions sur \mathbb{R}^2 positives et non totalement nulles³, permettant d'approcher $\delta_{\{I+I_*\}}(I' + I'_*)$. Nous définissons la *famille* de noyaux $(B_\varepsilon)_{\varepsilon>0}$ par

$$B_\varepsilon := B \times \chi_\varepsilon, \quad (1.77)$$

où nous détaillerons plus loin les arguments de la fonction χ_ε . Le paramètre $\varepsilon > 0$ est ici appelé *paramètre de quasi-résonance*.

Il semble alors que l'on a bien modélisé la notion de *quasi-résonance* : en effet, dans la limite $\varepsilon \rightarrow 0$ on retrouve formellement le cas résonant, et pour tout $\varepsilon > 0$, le noyau B_ε autorise bien (au moins un peu) des échanges d'énergie entre les parties cinétique et interne.

Un choix de modélisation Il convient à présent de faire un choix de modélisation : quelle famille $(\chi_\varepsilon)_{\varepsilon>0}$ serait-il le plus judicieux de considérer ?

Dans ce qui suit, on utilisera les notations usuelles E, R, R' , ainsi que les notations E_k, E'_k et E_i, E'_i , définies par, pour tous $v, v_* \in \mathbb{R}^3, \sigma \in \mathbb{S}^2$ et $I, I_*, I', I'_* \in \mathbb{R}_+$ tels que $I' + I'_* \leq \frac{m}{4}|v - v_*|^2 + I + I_*$,

$$E_k := \frac{m}{4}|v - v_*|^2, \quad E_i := I + I_*, \quad E'_k := \frac{m}{4}|v' - v'_*|^2, \quad E'_i := I' + I'_*, \quad E := E_k + E_i,$$

3. Dans cette section, la notation ε désigne le paramètre de quasi-résonance.

où v' et v'_* sont définis comme dans (1.41) (mais en représentation en σ), et

$$R := \frac{E'_k}{E}, \quad R' := \frac{E_k}{E}. \quad (1.78)$$

On remarque qu'avec ces notations, *la collision est résonante si et seulement si*

$$R = R'.$$

Ainsi, nous allons approcher le Dirac en $\{R = R'\}$ par une famille de fonctions indicatrices d'un « petit » ensemble de $(0, 1)^2$ autour de $\{R = R'\}$, lesquelles seront convenablement normalisées.

Nous choisissons la famille de fonctions suivante, pour $\varepsilon > 0$ et $R, R' \in (0, 1)$,

$$\chi_\varepsilon(R, R') = \frac{c_\eta(R, R')}{2\varepsilon} \mathbb{1}_{\left[|\eta(R) - \eta(R')| \leq \varepsilon\right]}, \quad (1.79)$$

où η est un \mathcal{C}^1 -difféomorphisme de $(0, 1)$ dans \mathbb{R} et c_η est une fonction de normalisation (continue) pouvant être choisie librement, du moment qu'elle vérifie

$$c_\eta(R, R') = c_\eta(R', R), \quad R, R' \in (0, 1), \quad (1.80)$$

$$c_\eta(R, R) = \eta'(R), \quad R \in (0, 1). \quad (1.81)$$

Ci-dessus, nous avons introduit la fonction η , \mathcal{C}^1 -difféomorphisme de $(0, 1)$ dans \mathbb{R} . La raison de ce choix – au lieu de considérer simplement $\mathbb{1}_{\left[|R - R'| \leq \varepsilon\right]}$ – est double :

1. en passant dans \mathbb{R} , nous éviterons des *effets de bord*,
2. cela offre une plus grande *flexibilité* de modélisation.

La condition de symétrie (1.80) sur la constante de normalisation permettra d'assurer la *micro-réversibilité* du noyau de collision quasi-résonant défini par (1.77), et la condition diagonale (1.81) permet d'assurer la *validité de l'approximation*.

Opérateur de Boltzmann et théorème H On définit l'opérateur de Boltzmann correspondant au modèle quasi-résonant, pour un certain $\varepsilon > 0$, une densité $f \equiv f(v, I)$ et $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$, par

$$Q_\varepsilon(f, f)(v, I) := \iiint_{(\mathbb{R}_+)^3} \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \left\{ f(v', I') f(v'_*, I'_*) - f(v, I) f(v, I_*) \right\} \times \\ B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) d\sigma dv_* d\mu(I_*) d\mu(I') d\mu(I'_*), \quad (1.82)$$

où dans l'intégrale, v' et v'_* sont définis comme dans (1.41) (mais en représentation en σ),

$$B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) := B(v, v_*, I, I_*, I', I'_*, \sigma) \times \chi_\varepsilon(R, R'),$$

et les notations R et R' étaient introduites en (1.78).

Puisqu'on autorise (même si c'est en faible quantité) des échanges entre l'énergie cinétique et l'énergie interne, on obtient sans surprise le théorème suivant, donnant un résultat identique au cas polyatomique usuel (où tous les échanges possibles sont autorisés) :

Théorème 1.8**Théorème H. [Polyatomique quasi-résonant]**

1. Formellement, le long d'une solution de l'équation de Boltzmann polyatomique quasi-résonante, l'entropie est dissipée.
2. La dissipation d'entropie polyatomique quasi-résonante d'une densité $f \equiv f(v, I) \geq 0$ s'annule si et seulement si $f = \mathcal{M}[\rho, u, T]$, où ρ , u et T sont respectivement la densité, la vitesse globale et la température associées à f définis comme dans (1.42)–(1.44) et, pour tous $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$,

$$\mathcal{M}[\rho, u, T](v, I) = \frac{\rho}{m} \left(\frac{2\pi T}{m} \right)^{-3/2} Z \left(\frac{1}{T} \right)^{-1} \exp \left(-\frac{m|v-u|^2}{2T} - \frac{I}{T} \right). \quad (1.83)$$

Soulignons qu'à l'équilibre (1.83), il y a, contrairement au cas résonant, *une seule température*.

Discussion qualitative sur les propriétés attendues du modèle Dans ce paragraphe, nous discutons de manière informelle les propriétés qu'il semble raisonnable d'attendre du modèle.

Moralement, on peut comprendre l'opérateur de Boltzmann quasi-résonant (1.82) comme la somme de l'opérateur résonant correspondant – dont le noyau associé serait B^{res} que l'on définirait comme dans (1.76) – et qui serait « d'ordre 1 », et une partie autorisant les échanges entre énergies, et qui elle serait « d'ordre ε » (nous n'avancions rien ici sur l'ordre précis). Ainsi, la dynamique devrait être *très largement* conduite par la partie résonante, et *faiblement* altérée par la partie contenant les échanges.

Ainsi, on peut s'attendre à ce que la dynamique quasi-résonante se déroule en deux temps :

1. en temps court, la dynamique se rapproche d'une maxwellienne à deux températures,
2. une fois ce temps passé, en temps long, la dynamique reste *proche de la forme maxwellienne à deux températures*, et les deux températures T_k et T_i relaxent l'une vers l'autre.

Nous soulignons que le premier temps « court » ne devrait pas (en première approximation) dépendre du paramètre de quasi-résonance ε , mais uniquement du noyau résonant B^{res} . Nous soulignons aussi que dans le cas polyatomique usuel, il n'y a aucune raison que, pour une donnée initiale maxwellienne à deux températures, la dynamique reste proche de cette forme ; c'est faux en général. Cette propriété peut apparaître dans le cas quasi-résonant car le « dérangement de la forme de la distribution » causé par la partie non-résonante est très faible comparé à l'effet de retour vers la maxwellienne à deux températures causé par la partie résonante.

1.3.2.2 Dérivation d'équations de type Landau-Teller

De la discussion précédente émerge une question : étant proche de l'équilibre de temps court intermédiaire (la maxwellienne à deux températures), sachant que la dynamique reste approximativement proche de cette forme et que seules les températures T_k et T_i évolueront dans le temps, peut-on obtenir une équation simple décrivant la relaxation de ces températures l'une vers l'autre ? Dans la littérature, ce type d'équation est communément appelé « équation de Landau-Teller », voir [137].

La forme maxwellienne permettant de mener des calculs explicites, à un instant $t > 0$ où la distribution est *exactement* une maxwellienne à deux températures, on peut trouver, pour une large classe de noyaux de collision, des équations différentielles ordinaires simples que vérifient localement les températures cinétiques et internes – de la forme des équations de Landau-Teller. On obtient alors la proposition suivante.

Proposition 1.9

Équation de Landau-Teller locale pour certains noyaux. Considérons un noyau de collision quasi-résonant B_ε d'une forme spécifique donnée dans (5.30), et considérons Q_ε l'opérateur de Boltzmann associé (1.82). Soient $\rho > 0$, $u \in \mathbb{R}^3$, $T_i^0, T_k^0 > 0$, considérons $f \equiv f(t, v, I)$ une solution de l'équation de Boltzmann homogène associée, avec comme condition initiale une maxwellienne à deux températures,

$$\partial_t f = Q_\varepsilon(f, f), \quad f(t=0) = \mathcal{M}[\rho, u, T_i^0, T_k^0]. \quad (1.84)$$

Alors, en notant $T_i(t)$ la température interne associée à $f(t, \cdot, \cdot)$, définie dans (1.70), on a

$$\left. \frac{dT_i(t)}{dt} \right|_{t=0} = \varepsilon^2 C(T_i^0, T_k^0) (T_k^0 - T_i^0) + \mathcal{O}(\varepsilon^4), \quad (1.85)$$

où $C(\cdot, \cdot)$ ne dépend, outre ses arguments, que de η et du noyau de collision de référence associé B , et est tel que

$$C(T, T) > 0, \quad T > 0.$$

Dans la proposition ci-dessus, l'équation de Landau-Teller (1.85) est obtenue à un temps où la distribution est exactement maxwellienne à deux températures. Il est attendu que la distribution *ne reste pas de cette forme durant la dynamique*, néanmoins, comme expliqué plus tôt, il est aussi attendu dans le cas quasi-résonant que la distribution *reste proche de cette forme durant la dynamique* (plus ε est petit, plus cela sera vérifié). Ainsi, cela nous conduit à émettre la conjecture suivante.

Conjecture. Si f est solution de (1.84), alors on a, pour ε assez petit, que pour tout $t \geq 0$,

$$(T_i(t), T_k(t)) \approx (\bar{T}_i(t), \bar{T}_k(t)).$$

où

$$\begin{aligned} \frac{d\bar{T}_i}{dt} &= \varepsilon^2 C(\bar{T}_i, \bar{T}_k) (\bar{T}_k - \bar{T}_i), & \bar{T}_i(t=0) &= T_i^0, \\ \frac{d\bar{T}_k}{dt} &= -\frac{2}{3} \frac{d}{dt} (\Theta_i(\bar{T}_i)), & \bar{T}_k(t=0) &= T_k^0. \end{aligned} \quad (1.86)$$

Rappelons que Θ_i est défini, pour tout $T > 0$, par

$$\Theta_i(T) := \frac{\delta(T)}{2} T,$$

où δ est le nombre de degrés de liberté internes, donné dans (1.45).

1.3.2.3 Expériences numériques et discussions finales

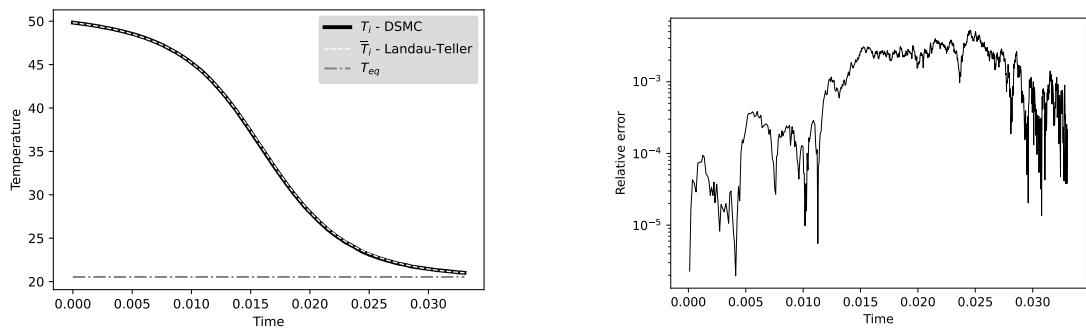
Enfin, nous menons des expériences numériques pour tester la validité de la conjecture annoncée ci dessus (1.86). D'une part, nous simulons l'équation de Boltzmann homogène 3D associée à certains noyaux de collision quasi-résonants et une condition initiale maxwellienne à deux températures, et comparons la température interne T_i de la solution en fonction du temps avec la solution \bar{T}_i du système

d'EDO (1.86), que nous résolvons numériquement. Cela nous fournit alors une *validation numérique* de la conjecture – dans le sens où l'on pourra affirmer non qu'elle est vraie mais qu'elle est au moins raisonnable.

Simulation de Boltzmann homogène par méthode DSMC Une approche standard pour simuler l'équation de Boltzmann est la méthode DSMC (Direct Simulation Monte Carlo). Nous renvoyons aux écrits de Bird à ce sujet, notamment à [22]. Il s'agit d'une approche *stochastique* où l'on simule un *système de particules représentatives*, avec une interprétation physique immédiate : on peut par ailleurs comprendre cette méthode *non comme une approximation de l'équation de Boltzmann, mais comme une modélisation différente du même phénomène*. L'avantage formidable de cette méthode réside en son *faible coût* d'un point de vue numérique. Sa limite réside en son aspect stochastique, pouvant amener, dans certaines situations, à devoir considérer un grand nombre de particules pour pallier au bruit dû à l'aléa.

Implémentation Nous avons implémenté la méthode DSMC en `python`, ce langage étant simple d'utilisation et flexible, notamment grâce aux bibliothèques disponibles comme `numpy`, `matplotlib`, `scipy` et `numba`, cette dernière palliant à la lenteur de `python` lors de l'utilisation de boucles, via la possibilité de compiler des fonctions et de paralléliser les calculs. D'un autre côté, on résout le système d'EDO (1.86) avec le solveur `solve_ivp` implémenté dans la bibliothèque `scipy`. Tout cela considéré, des résultats significatifs peuvent être obtenus en quelques minutes sur mon propre ordinateur.

Résultats numériques et discussion Nous donnons en figure 1.6 un résultat numérique que nous avons obtenu. Les températures initiales sont $T_k^0 = 1$ et $T_i^0 = 50$, la température d'équilibre associée est $T_{eq} = 20.6$, et l'ensemble des autres paramètres est donné en sous-section 5.3.2.



(a) Tracé des courbes de température interne via la simulation DSMC, T_i , et la résolution de (1.86), \bar{T}_i .

(b) Tracé de l'erreur relative $|T_i - \bar{T}_i|/\bar{T}_i$ en fonction du temps.

FIGURE 1.6 – Résultats numériques : test de la conjecture.

On constate sur la figure 1.6 que le système d'EDO (1.86) reproduit très fidèlement le comportement des températures internes et cinétiques (on montre ici seulement la température interne), validant la conjecture avancée pour notre ensemble de paramètres.

1.4 Méthodes entropiques et relaxation vers l'équilibre pour l'équation de Boltzmann-Fermi-Dirac

Dans cette dernière section, nous introduisons la partie III de cette thèse, dont l'objet d'étude est l'équation de Boltzmann-Fermi-Dirac, en particulier le comportement en temps long de ses solutions. Dans le chapitre 6, qui est une reproduction de [36], nous dresserons, via l'obtention d'une inégalité fonctionnelle, un pont entre les cas de Boltzmann classique et quantique (fermionique). Grâce à ce dernier, nous montrerons, dans le chapitre 7, reproduction de [39], la convergence des solutions de Boltzmann-Fermi-Dirac homogène (potentiels durs avec cut-off) vers leur équilibre associé, avec un *taux algébrique explicite*.

1.4.1 L'équation de Boltzmann-Fermi-Dirac

L'équation de Boltzmann-Fermi-Dirac, aussi appelée équation de Nordheim pour les fermions, proposée dans les années 1930 par Nordheim [138], Uehling et Uhlenbeck [154], se retrouve en physique notamment dans l'étude de *la distribution d'électrons au sein de semi-conducteurs*. Pour reprendre les termes de Villani [156, chapitre 5.3] (ici, en français), ce modèle « ne repose pas sur le formalisme quantique traditionnel, [...] il s'agit plutôt d'une description classique de particules en interaction avec des caractéristiques quantiques ». Nous modélisons le comportement de la distribution des fermions comme *celui d'un gaz raréfié simple*, composé de particules ayant une spécificité de nature quantique. Pour être plus précis, nous ajoutons au modèle de Boltzmann classique, présenté en section 1.1 de ce chapitre, le **principe d'exclusion de Pauli**, satisfait par les fermions.

1.4.1.1 Modélisation

Dans ce qui suit, une particule (un fermion) sera décrite, à un instant t , par sa position $x \in \mathbb{R}^3$ et sa vitesse $v \in \mathbb{R}^3$. Notant $m > 0$ sa masse, les quantité de mouvement et énergie cinétique d'une particule ayant pour vitesse v seront donnés respectivement par

$$mv \quad \text{et} \quad \frac{1}{2}m|v|^2.$$

Il est d'intérêt d'étudier la densité de fermions $f \equiv f(t, x, v) \geq 0$, dépendant donc du temps t , de la position x et de la vitesse v . Nous laissons dans la suite de côté la variable d'espace x – nous plaçant ainsi dans le cas *homogène* – et étudions donc une densité $f \equiv f(t, v)$. Il sera courant, lorsque nous nous concentrerons sur les opérateurs en jeu, que nous laissons aussi de côté la variable temporelle t .

Principe d'exclusion de Pauli Le principe d'exclusion de Pauli, énoncé à la fin des années 1930, affirme que *deux fermions ne peuvent pas se trouver simultanément dans le même état quantique*. Dans notre cadre, cela implique que *la densité de fermions f est bornée supérieurement*. La **densité maximale** sera donnée par la constante

$$\frac{1}{\varepsilon}$$

où $\varepsilon > 0$ est appelé le *paramètre quantique*,⁴ et dépend en particulier de la constante de Planck et de l'espèce de fermions considérés. Dans le cas des électrons, ε est de l'ordre de 10^{-10} , voir [3, 4]. On considérera alors généralement que ε est petit.

4. Dans cette section, la notation ε désigne le paramètre quantique.

On propose en figure 1.7 ci-dessous une représentation de ce principe. Considérant un certain état $v \in \mathbb{R}^3$, la densité $f(v)$ de fermions en v sera comprise entre 0 – l'état est *inoccupé* – et $1/\varepsilon$ – l'état est dit *saturé*. Ainsi, la proportion d'occupation de v vaut $\varepsilon f(v)$, et la proportion d'états encore disponibles (au niveau microscopique) est $1 - \varepsilon f(v)$.

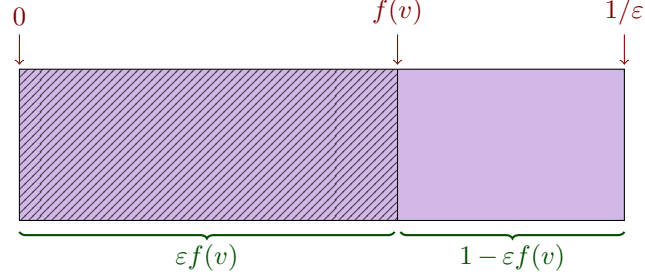
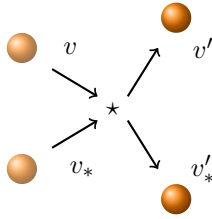


FIGURE 1.7 – Représentation de l'occupation de l'état $v \in \mathbb{R}^3$.

Collision entre fermions Considérons une collision entre deux particules devant satisfaire au principe de Pauli.



On note comme précédemment (v, v_*) et (v', v'_*) les couples de vitesses pré- et post-collisionnels. Les principes de conservation de la quantité de mouvement et de l'énergie sont toujours vérifiés ici, menant, comme dans le cas de Boltzmann classique monoatomique, à

$$\begin{aligned} v' + v'_* &= v + v_* \\ |v'|^2 + |v'_*|^2 &= |v|^2 + |v_*|^2. \end{aligned}$$

Ici, néanmoins, on doit préciser que **la probabilité d'une collision dépend aussi du taux de disponibilité de chaque état**. À titre d'illustration, avec les notations ci-dessus, on voudra implémenter que plus v', v'_* sont occupés, moins la collision $(v, v_*) \mapsto (v', v'_*)$ sera probable – car plus faible sera la proportion d'états (microscopiques) disponibles.

1.4.1.2 L'opérateur de collision de Boltzmann-Fermi-Dirac

Considérons un noyau de collision B , satisfaisant aux hypothèses de *symétrie* (1.6a) et de *micro-réversibilité* (1.6b). On définit alors l'opérateur de **Boltzmann-Fermi-Dirac** Q_ε , pour tout $f \equiv f(v) \in [0, 1/\varepsilon]$ tel que ce qui suit ait un sens et tout $v \in \mathbb{R}^3$, par

$$Q_\varepsilon(f, f)(v) = \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \{f' f'_* (1 - \varepsilon f)(1 - \varepsilon f_*) - f f_* (1 - \varepsilon f')(1 - \varepsilon f'_*)\} B(v, v_*, \sigma) d\sigma dv_*, \quad (1.87)$$

où l'on a utilisé les raccourcis $f \equiv f(v)$, $f_* \equiv f(v_*)$, $f' \equiv f(v')$ et $f'_* \equiv f(v'_*)$, et où v' et v'_* sont fonctions de v, v_* et σ , définis dans (1.4).

Nous soulignons que la différence entre Q_ε et l'opérateur de Boltzmann monoatomique classique Q_0 réside en la présence des termes en $(1 - \varepsilon f)$. Comme expliqué plus tôt, ceux-ci rendent compte du principe d'exclusion de Pauli, et quantifient le nombre d'états (microscopiques) encore disponibles. Choisissons

formellement $\varepsilon = 0$ (correspondant à prendre la constante de Planck égale à 0) dans (1.87), on retrouve exactement l'opérateur de Boltzmann classique, d'où l'appellation Q_0 de ce dernier.

On observe la *forme faible de l'opérateur* Q_ε : pour tout $f \equiv f(v) \in [0, 1/\varepsilon]$ et $\psi \equiv \psi(v)$ une fonction test telle que ce qui suit ait un sens, on a

$$\begin{aligned} & \int_{\mathbb{R}^3} Q_\varepsilon(f, f)(v) \psi(v) \, dv = \\ & -\frac{1}{4} \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} \{f' f'_* (1 - \varepsilon f)(1 - \varepsilon f_*) - f f_* (1 - \varepsilon f')(1 - \varepsilon f'_*)\} (\psi' + \psi'_* - \psi - \psi_*) B \, dv dv_* d\sigma, \end{aligned} \quad (1.88)$$

qui nous sera utile plus loin.

Équation homogène de Boltzmann-Fermi-Dirac Dans ce qui suit, nous nous plaçons dans le *cadre homogène en espace*, c'est-à-dire que l'équation à laquelle nous nous intéressons est

$$\begin{aligned} \partial_t f^\varepsilon(t, v) &= Q_\varepsilon(f^\varepsilon(t), f^\varepsilon(t))(v), & (t, v) \in \mathbb{R}_+ \times \mathbb{R}^3, \\ f^\varepsilon(0) &= f_{\text{in}}, \end{aligned} \quad (1.89)$$

où $f_{\text{in}} \equiv f_{\text{in}}(v) \geq 0$ est une condition initiale adaptée. Afin d'éviter les confusions dans ce qui suit, nous noterons $f^\varepsilon \equiv f^\varepsilon(t, v) \geq 0$ une solution de (1.89), et $f \equiv f(v) \geq 0$ des fonctions génériques sur \mathbb{R}^3 (non liées à l'équation (1.89)).

Conservation de la masse, de la quantité de mouvement et de l'énergie De manière similaire à l'opérateur de Boltzmann classique Q_0 , l'opérateur quantique Q_ε satisfait bien les propriétés attendues de conservation de la masse, de la quantité de mouvement et de l'énergie, au sens où, en utilisant (1.88),

$$\int_{\mathbb{R}^3} Q_\varepsilon(f, f)(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \, dv = 0.$$

Ainsi, les solutions f^ε de (1.89) sont telles que pour tout temps t , les masse, quantité de mouvement et énergie de $f^\varepsilon(t)$ sont identiques à celles de la condition initiale f_{in} .

Équilibres à la dynamique de Boltzmann-Fermi-Dirac Les distributions dites « d'équilibre » de la dynamique (homogène en espace) de Boltzmann-Fermi-Dirac se décomposent en deux familles, *selon la température du système*. Fixons une masse $\rho > 0$ et un $\varepsilon > 0$. On définit la **température de Fermi** associée à ρ et ε par

$$T(\rho, \varepsilon) := \frac{1}{2} \left(\frac{3\varepsilon\rho}{4\pi} \right)^{\frac{2}{3}}. \quad (1.90)$$

On trouve dans [123] que, pour tout $f = f(v) \geq 0$ tel que

$$\int_{\mathbb{R}^3} f(v) \begin{pmatrix} 1 \\ v \\ |v - u|^2 \end{pmatrix} \, dv = \begin{pmatrix} \rho \\ \rho u \\ 3\rho T \end{pmatrix}, \quad (1.91)$$

on a

$$f \leq \frac{1}{\varepsilon} \implies T \geq \frac{2}{5} \mathbf{T}(\varrho, \varepsilon), \quad (1.92)$$

et

$$f \leq \frac{1}{\varepsilon} \implies \left(T = \frac{2}{5} \mathbf{T}(\varrho, \varepsilon) \iff f = F_\varepsilon := \frac{1}{\varepsilon} \mathbb{1}_{\mathcal{B}(u, R_\varepsilon^\rho)} \right), \quad (1.93)$$

où $\mathcal{B}(u, R_\varepsilon^\rho)$ désigne la boule ouverte de \mathbb{R}^3 centrée en u et de rayon $R_\varepsilon^\rho := \left(\frac{3\varepsilon\rho}{4\pi}\right)^{\frac{1}{3}}$. On déduit de (1.92)–(1.93) que F_ε , appelé **état saturé**, est, à ρ et ε fixés, la distribution *la plus froide* possible. C'est un équilibre de la dynamique de Boltzmann-Fermi-Dirac, au sens où

$$Q_\varepsilon(F_\varepsilon, F_\varepsilon) = 0.$$

D'un autre côté, lorsque $T > \frac{2}{5} \mathbf{T}(\varrho, \varepsilon)$, il existe une unique (voir [123]) **statistique de Fermi-Dirac** associée à ε , ρ , u et T , notée \mathcal{M}_ε , donnée pour tous $v \in \mathbb{R}^3$ par

$$\mathcal{M}_\varepsilon(v) = \frac{e^{a_\varepsilon + b_\varepsilon |v-u|^2}}{1 + \varepsilon e^{a_\varepsilon + b_\varepsilon |v-u|^2}} \quad (1.94)$$

et $a_\varepsilon \in \mathbb{R}$, $b_\varepsilon < 0$ sont uniquement déterminés (de manière implicite) de telle sorte à ce que \mathcal{M}_ε puisse satisfaire à la même normalisation que f , équation (1.91). Ces statistiques sont des équilibres de la dynamique de Boltzmann-Fermi-Dirac, au sens où

$$Q_\varepsilon(\mathcal{M}_\varepsilon, \mathcal{M}_\varepsilon) = 0.$$

Notons que, pour une solution f^ε de (1.89), puisque les masse, quantité de mouvement et énergie sont conservées durant la dynamique, on sait que pour tout temps t , la distribution \mathcal{M}_ε associée à $f^\varepsilon(t)$ est la même que celle associée à la condition initiale f_{in} .

Entropie de Fermi-Dirac Nous donnons à présent la définition de l'entropie de Fermi-Dirac. Pour tous $\varepsilon > 0$, on pose

$$\Phi_\varepsilon(x) := \int_0^x \log\left(\frac{y}{1 - \varepsilon y}\right) dy, \quad x \in [0, 1/\varepsilon]. \quad (1.95)$$

Notons que Φ_ε est bien définie et continue sur $[0, 1/\varepsilon]$, strictement convexe et \mathcal{C}^2 sur $(0, 1/\varepsilon)$. On définit alors la **fonctionnelle d'entropie de Fermi-Dirac** H_ε , pour tout $f \equiv f(v) \in [0, 1/\varepsilon]$ telle que ce qui suit ait un sens, par

$$H_\varepsilon(f) := \int_{\mathbb{R}^3} \Phi_\varepsilon(f(v)) dv. \quad (1.96)$$

Explicitement,

$$H_\varepsilon(f) = \int_{\mathbb{R}^3} \{f \log f + \varepsilon^{-1}(1 - \varepsilon f) \log(1 - \varepsilon f)\} dv.$$

Remarque 1.8. En prenant $\varepsilon = 0$ dans (1.95), on retrouve $\Phi_0 : x \in \mathbb{R}_+ \mapsto x \log x - x$, ainsi H_0 correspond effectivement à l'entropie classique.

Remarque 1.9. Je souligne que l'on retrouve bien en la statistique de Fermi-Dirac la forme d'équilibre générale (1.25) discutée en sous-section 1.1.2.4 : remarquant que

$$(\Phi'_\varepsilon)^{-1} = \frac{\exp}{1 + \varepsilon \exp},$$

il vient, pour un certain $(\alpha, \beta, \gamma) \in \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}$, que l'on a, pour tout $v \in \mathbb{R}^3$,

$$\mathcal{M}_\varepsilon(v) = (\Phi_\varepsilon^t)^{-1} (\alpha \cdot 1 + \beta \cdot v + \gamma \cdot |v|^2),$$

qui, rappelons nous, est le fruit direct de la fonctionnelle d'entropie et des quantités conservées. Cette remarque permettra en fait d'aboutir naturellement au théorème 1.14.

1.4.1.3 Relaxation à l'équilibre et méthodes entropiques

Dissipation d'entropie Formellement, pour une solution $f^\varepsilon \equiv f^\varepsilon(t, v) \in (0, 1/\varepsilon)$ de (1.89), on a pour tout temps t

$$\frac{d}{dt} H_\varepsilon(f^\varepsilon(t)) = -\mathcal{D}_\varepsilon(f^\varepsilon(t)),$$

où \mathcal{D}_ε est la fonctionnelle de *dissipation d'entropie de Fermi-Dirac* – explicitée en (6.29). Il a été obtenu dans [123] le théorème suivant :

Théorème 1.10

Théorème H. [Boltzmann-Fermi-Dirac]

1. Formellement, le long d'une solution de l'équation de Boltzmann-Fermi-Dirac (1.89), l'entropie de Fermi-Dirac est dissipée.
2. La dissipation d'entropie d'une densité $f \equiv f(v) \in (0, 1/\varepsilon)$ s'annule si et seulement si f est une statistique de Fermi-Dirac (associée au paramètre ε), dont la forme est donnée en (1.94).

On remarquera que dans le point 2. du théorème ci-dessus, la condition $0 < f(v) < 1/\varepsilon$ implique en particulier que f n'est *pas* la distribution d'équilibre saturée.

Entropie relative à l'équilibre On notera dans ce qui suit, pour une densité $f \equiv f(v)$ adaptée,

$$H_\varepsilon[f|\mathcal{M}_\varepsilon^f] := H_\varepsilon(f) - H_\varepsilon(\mathcal{M}_\varepsilon^f)$$

l'entropie de Fermi-Dirac de f relative à son équilibre associé. Cette quantité est positive, car $\mathcal{M}_\varepsilon^f$ minimise H_ε sous les contraintes de masse, quantité de mouvement et énergie cinétique imposée par f – nous renvoyons à la discussion générale de la sous-section 1.1.2.4.

1.4.2 Transfert d'inégalités entropiques depuis le cas classique vers le cas quantique

Dans le chapitre 6 de la partie III, nous obtiendrons des inégalités de type conjecture de Cercignani (comme dans [78, 153, 157, 3, 4]) dans le cas Fermi-Dirac – c'est-à-dire une minoration de la dissipation d'entropie de Fermi-Dirac par une puissance de l'entropie de Fermi-Dirac relative à l'équilibre.

1.4.2.1 Stratégie générale et théorème principal

Au lieu d'essayer de montrer directement ces inégalités, nous basons notre approche sur une idée de « transfert ». Ainsi, nous prouverons en fait que **si une inégalité de type conjecture de Cercignani tient dans le cas classique, la même inégalité** (avec une constante légèrement différente) **tient dans le cas Fermi-Dirac**. Ayant obtenu cette méthode de transfert, on déduira des résultats obtenus dans le cas classique [78, 153, 157, 73, 71] toute une famille d'inégalités dans le cas Fermi-Dirac.

Un lien entre les dissipations d'entropie classique et quantique Établissons à présent le lien entre les cas quantique et classique au niveau de la dissipation d'entropie. Rappelons que nous notons \mathcal{D}_ε la dissipation d'entropie de Fermi-Dirac (associée au noyau B fixé et à ε) et \mathcal{D}_0 la dissipation d'entropie classique (associée au même noyau).

On peut en fait aisément observer que, pour tout $\kappa_0 \in (0, 1)$ et $f \equiv f(v) \in [0, 1/\varepsilon]$, on a

$$1 - \varepsilon f \geq \kappa_0 \quad \implies \quad \mathcal{D}_\varepsilon(f) \geq \kappa_0^4 \mathcal{D}_0\left(\frac{f}{1 - \varepsilon f}\right). \quad (1.97)$$

Cela établit un premier lien entre les cas quantique et classique.

Principe de transfert Le point clé de notre stratégie est le suivant – nous le donnons ici de manière informelle. Supposons connue une inégalité dans le cas classique, par exemple

$$\mathcal{D}_0(g) \gtrsim H_0[g | \mathcal{M}_0^g]^{1+\delta}. \quad (1.98)$$

Nous voulons obtenir la même inégalité dans le cas quantique, c'est-à-dire

$$\mathcal{D}_\varepsilon(f) \gtrsim H_\varepsilon[f | \mathcal{M}_\varepsilon^f]^{1+\delta}. \quad (1.99)$$

L'idée est de *transiter par le cas classique* : on passe de la dissipation d'entropie quantique à la classique en appliquant (1.97), puis on passe de la dissipation d'entropie classique à l'entropie classique relative à l'équilibre avec (1.98), et pour conclure, on cherchera alors à passer de l'entropie classique relative à l'équilibre à l'entropie de Fermi-Dirac relative à l'équilibre. Pour clarifier,

$$\mathcal{D}_\varepsilon(f) \gtrsim \mathcal{D}_0\left(\frac{f}{1 - \varepsilon f}\right) \gtrsim H_0\left[\frac{f}{1 - \varepsilon f} \middle| \mathcal{M}_0^{\frac{f}{1 - \varepsilon f}}\right]^{1+\delta} \gtrsim H_\varepsilon[f | \mathcal{M}_\varepsilon^f]^{1+\delta} ?$$

On constate que (1.99) se déduit alors immédiatement de (1.98) si la dernière inégalité ci-dessus est vraie. Nous affirmons qu'elle tient effectivement, via le théorème principal de ce chapitre :

Théorème 1.11

Comparaison des entropies relatives à l'équilibre.

Pour tous $\varepsilon > 0$ et $f \equiv f(v) \in [0, 1/\varepsilon]$ tels que tous les termes suivants aient un sens, on a

$$H_0\left[\frac{f}{1 - \varepsilon f} \middle| \mathcal{M}_0^{\frac{f}{1 - \varepsilon f}}\right] \geq H_\varepsilon[f | \mathcal{M}_\varepsilon^f]. \quad (1.100)$$

Cette inégalité fonctionnelle nous permet donc de transférer toutes les inégalités reliant entropie et dissipation d'entropie du cas de Boltzmann classique à Boltzmann quantique. Nous mentionnons aussi qu'il en est alors de même pour l'équation de Landau (équation cousine à celle de Boltzmann) – bien que des inégalités entropie/dissipation d'entropie étaient déjà connues dans le cas de Landau-Fermi-Dirac [3, 4], notre méthode de transfert en offre de nouvelles, avec une preuve simple. Nous donnons ci-dessous un corollaire majeur au théorème 1.11, adaptant (via la méthode de transfert) le résultat de Villani [157, théorème 4.1], donné pour Boltzmann classique, au cas Boltzmann-Fermi-Dirac. Certaines dépendances ne sont pas explicitées ici, nous renvoyons au corollaire 6.3 du chapitre 6 pour le résultat détaillé.

Corollaire 1.12

Inégalité entropique dans le cas Fermi-Dirac pour des noyaux généraux. Supposons l'existence de $B_0 > 0$ et $\beta_+, \beta_- \geq 0$ tels que pour tous $v, v_* \in \mathbb{R}^3$ et $\sigma \in \mathbb{S}^2$,

$$B(v, v_*, \sigma) \geq B_0 \min \left(|v - v_*|^{\beta_+}, |v - v_*|^{-\beta_-} \right),$$

et B satisfait les hypothèses de symétrie (1.6a) et micro-réversibilité (1.6b). Soit $\kappa_0 \in (0, 1)$, $0 \leq f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ et $\varepsilon \geq 0$ tels que $1 - \varepsilon f \geq \kappa_0$ et f soit *minorée par une gaussienne en vitesse*. Alors pour tout $\alpha \in (0, 1)$ il existe un $K_\alpha(f) > 0$ explicite, dépendant de α , B_0 , β_\pm et diverses quantités liées à f , tel que

$$\mathcal{D}_\varepsilon(f) \geq K_\alpha(f) H_\varepsilon[f | \mathcal{M}_\varepsilon^f]^{1+\alpha}. \quad (1.101)$$

1.4.2.2 Comparaison des entropies relatives à l'équilibre

Présentons à présent les éléments clés de la preuve du théorème 1.11, dont certains ont leur propre intérêt en soi. Puisque notre attention se porte sur une comparaison de différentes *entropies relatives à l'équilibre*, nous commençons par réécrire ces dernières sous une forme plus facilement manipulable. En effet, si l'on partait directement des formules explicites, nous devrions comparer

$$\begin{aligned} H_0 \left[\frac{f}{1 - \varepsilon f} \middle| \mathcal{M}_0^{\frac{f}{1 - \varepsilon f}} \right] &= \int_{\mathbb{R}^3} \left\{ \frac{f}{1 - \varepsilon f} \log \left(\frac{f}{1 - \varepsilon f} \right) - \frac{f}{1 - \varepsilon f} \right\} dv \\ &\quad - \int_{\mathbb{R}^3} \left\{ \frac{\mathcal{M}_0^{\frac{f}{1 - \varepsilon f}}}{1 - \varepsilon \mathcal{M}_0^{\frac{f}{1 - \varepsilon f}}} \log \left(\frac{\mathcal{M}_0^{\frac{f}{1 - \varepsilon f}}}{1 - \varepsilon \mathcal{M}_0^{\frac{f}{1 - \varepsilon f}}} \right) - \frac{\mathcal{M}_0^{\frac{f}{1 - \varepsilon f}}}{1 - \varepsilon \mathcal{M}_0^{\frac{f}{1 - \varepsilon f}}} \right\} dv \end{aligned}$$

et

$$\begin{aligned} H_\varepsilon[f | \mathcal{M}_\varepsilon^f] &= \int_{\mathbb{R}^3} \left\{ f \log f + \varepsilon^{-1} (1 - \varepsilon f) \log(1 - \varepsilon f) \right\} dv \\ &\quad - \int_{\mathbb{R}^3} \left\{ \mathcal{M}_\varepsilon^f \log \mathcal{M}_\varepsilon^f + \varepsilon^{-1} (1 - \varepsilon \mathcal{M}_\varepsilon^f) \log(1 - \varepsilon \mathcal{M}_\varepsilon^f) \right\} dv, \end{aligned}$$

qui apparaît, à première vue, être une tâche bien ardue. Il se trouve qu'à l'inverse de l'entropie relative à une densité quelconque, l'entropie relative à l'équilibre peut s'écrire sous une forme très simple, que nous avons explicitée dans un cadre général en sous-sous-section 1.1.2.4.

Représentation de Taylor de l'entropie relative à l'équilibre Définissons, pour tout $\varepsilon \geq 0$, la fonction

$$\varphi_\varepsilon(x) := \frac{x}{1 - \varepsilon x}, \quad x \in [0, 1/\varepsilon), \quad (1.102)$$

où l'on prend la convention que φ_0 soit l'identité sur \mathbb{R}_+ . Alors, pour tout $\varepsilon \geq 0$ (donc aussi dans le cas classique), et tout $f \equiv f(v) \in [0, 1/\varepsilon)$, on a

$$H_\varepsilon[f | \mathcal{M}_\varepsilon^f] = \int_{\mathbb{R}^3} \int_{\mathcal{M}_\varepsilon^f(v)}^{f(v)} \frac{f(v) - x}{\varphi_\varepsilon(x)} \varphi'_\varepsilon(x) dx dv. \quad (1.103)$$

Nous dénommons (1.103) la « représentation de Taylor de l'entropie relative à l'équilibre » en raison de sa provenance d'un développement de Taylor de Φ_ε à l'ordre 1 avec reste intégral. Il est clair que cette formulation, outre présenter des avantages en soi, comme son évidente positivité et son utilité dans la preuve d'inégalités de type Csiszár-Kullback, est bien plus aisément manipulable que les formules explicites données plus haut. Elle fournit de plus une uniformité entre les cas classique et quantique, qui simplifiera notre étude.

Proposition centrale de la preuve Donnons la proposition centrale à la preuve du théorème 1.11, dont cette fois nous explicitons les hypothèses précisément.

Proposition 1.13

Monotonie d'une fonctionnelle d'entropie relative à l'équilibre.

Soit $0 \leq g \in L_2^1(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3)$. On définit, pour tout $\varepsilon \in \mathbb{R}_+$,

$$R_g(\varepsilon) := H_\varepsilon \left[\varphi_\varepsilon^{-1}(g) \left| \mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}(g)} \right. \right]. \quad (1.104)$$

Alors la fonction R_g est décroissante sur \mathbb{R}_+ .

Voyons en quoi la proposition 1.13 fournit bien le résultat annoncé par le théorème 1.11. Prenons $\varepsilon > 0$ et $0 \leq f \equiv f(v)$ telle que $\frac{f}{1-\varepsilon f} \in L_2^1(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3)$ – il s'agit bien là des hypothèses minimales pour que tous les termes du théorème 1.11 aient un sens – et posons $g = \frac{f}{1-\varepsilon f}$. Puisque, par la proposition 1.13, R_g est décroissante sur \mathbb{R}_+ , on a en particulier que

$$R_g(0) \geq R_g(\varepsilon).$$

Comme $\varphi_0^{-1}(g) = g = \frac{f}{1-\varepsilon f}$ et $\varphi_\varepsilon^{-1}(g) = f$, l'inégalité ci-dessus est bien celle annoncée au théorème 1.11.

Arguments Notre méthode consiste à montrer la négativité de la dérivée de R_g sur \mathbb{R}_+^* . Sans rentrer dans trop de détails, les arguments principaux utilisés pour prouver la proposition 1.13 sont de nature très générale :

1. la représentation de Taylor de l'entropie relative (1.103),
2. le fait que l'équilibre s'écrive sous la forme $(\Phi'_\varepsilon)^{-1}$ d'une combinaison linéaire de quantités conservées, donnée dans le cas général en (1.25),
3. le fait que pour tout $\varepsilon > 0$, $x \mapsto \partial_\varepsilon \varphi_\varepsilon(x)$ soit décroissante.

Les spécificités du cas Fermi-Dirac ne seront utilisées, outre le point 3 ci-dessus, que pour les points techniques que sont :

4. la dérivabilité de R_g sur \mathbb{R}_+^* ,
5. la continuité de R_g en $\varepsilon = 0$.

Notre méthode est donc formellement directement généralisable à d'autres cas (à la preuve de dérivabilité et de continuité près), si le besoin d'un tel résultat venait à se manifester.

1.4.2.3 Quelques autres résultats

Du quantique au classique, ou résultats négatifs Via la méthode présentée précédemment, on peut en fait aussi obtenir des inégalités « dans l'autre sens ». En effet, on trouve aisément que

$$\mathcal{D}_\varepsilon(f) \leq \mathcal{D}_0\left(\frac{f}{1-\varepsilon f}\right).$$

On prouve aussi en Proposition 6.2 du chapitre 6, que pour tout $\kappa_0 \in (0, 1)$, $\varepsilon > 0$ et $0 \leq f \in L^1_2(\mathbb{R}^3)$ telle que $1 - \varepsilon f \geq \kappa_0$, on a

$$H_0\left[\frac{f}{1-\varepsilon f} \middle| \mathcal{M}_0^{\frac{f}{1-\varepsilon f}}\right] \leq \exp(16(\kappa_0^{-1} - 1)) H_\varepsilon[f | \mathcal{M}_\varepsilon^f].$$

Ainsi, la méthodologie peut aussi être appliquée pour obtenir que si une inégalité d'entropie / dissipation d'entropie est vraie dans le cas quantique, elle le sera aussi dans le cas classique. Cela implique que l'on peut aussi étendre les *contre-exemples* du cas classique (par exemple de [31]) : si une inégalité présente des contre-exemples, dans le cas classique, alors la même inégalité en présentera dans le cas quantique.

Équation de Boltzmann-Bose-Einstein Là où le formalisme de Boltzmann-Fermi-Dirac ajoute à celui de Boltzmann une propriété quantique satisfaite par les *fermions*, celui de Boltzmann-Bose-Einstein y ajoute une propriété quantique satisfaite par les *bosons*. Elle a une forme très similaire à l'équation de Boltzmann-Fermi-Dirac : c'est en fait la même, **mais en changeant ε en $-\varepsilon$** . Les propriétés des solutions, dans le cas Bose-Einstein, sont cependant bien différentes que dans le cas Fermi-Dirac ; là où dans ce dernier, elles sont *bornées a priori*, il survient dans le cas Bose-Einstein des phénomènes de *condensation*, concentrant certaines (parties de) solutions en un Dirac. Ainsi, des inégalités impliquant des bornes L^∞ semblent bien moins pertinentes dans le cas bosonique que dans le cas fermionique.

On peut toutefois aussi obtenir une comparaison entre l'entropie classique relative à l'équilibre et l'entropie bosonique relative à l'équilibre – voir annexe 6.A.

Inégalités de Csiszár-Kullback-Pinsker Nous avons présenté ces inégalités en première partie de cette introduction et en avons proposé une généralisation à une large famille d'entropies et faisant intervenir des normes L^p , $1 \leq p \leq 2$, à poids. Nous donnons ci-dessous la forme de ces inégalités dans le cas de l'entropie de Fermi-Dirac relative à l'équilibre – simplifiée non optimale, voir proposition 6.10 au chapitre 6 pour une version optimisée.

Soit $\varpi : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ mesurable et $p \in [1, 2]$. Pour tout $\varepsilon > 0$ et $0 \leq f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ tel que $1 - \varepsilon f \geq 0$ et f n'est pas l'état saturé (voir (1.93)), supposant que toutes les normes ci-dessous sont finies, on a

$$\|f - \mathcal{M}_\varepsilon^f\|_{L^p_\varpi}^2 \leq 2 \max\left(\|\mathcal{M}_\varepsilon^f\|_{L^{\frac{p}{2-p}}_\varpi}, \|f\|_{L^{\frac{p}{2-p}}_\varpi}\right) H_\varepsilon[f | \mathcal{M}_\varepsilon^f], \quad (1.105)$$

où $\mathcal{M}_\varepsilon^f$ est la statistique de Fermi-Dirac associée à ε et f . Pour $p = 2$, on interprète $L^{\frac{p}{2-p}}$ comme L^∞ , et on a défini les espaces L^p_ϖ en (1.36).

Les inégalités de CKP nous permettront dans la suite de passer d'une convergence *au sens de l'entropie relative à l'équilibre* (qui n'est pas une norme), à une réelle convergence en norme – typiquement, une norme L^1 , L^1_2 ou L^2 à poids.

1.4.3 Relaxation vers l'équilibre avec un taux algébrique explicite

Dans le chapitre 7, qui est une reproduction de [39], en collaboration avec B. Lods, nous utilisons les résultats du chapitre 6 pour obtenir, pour les solutions de l'équation de Boltzmann-Fermi-Dirac avec *cut-off et potentiels durs* (voir plus bas les hypothèses du théorème 1.14) un **taux de convergence vers l'équilibre algébrique, explicite** et, pour un certain $\varepsilon^{\text{in}} > 0$ fixé dépendant uniquement de la condition initiale f_{in} et du noyau de collision considéré, **uniforme en** $\varepsilon \leq \varepsilon^{\text{in}}$.

1.4.3.1 Résultats principaux

Donnons directement le théorème central de ce chapitre, avec ses hypothèses précises. L'existence et unicité des solutions de (1.89) sous les hypothèses considérées ont été prouvées dans [123].

Théorème 1.14

Un taux explicite de relaxation vers l'équilibre. Soit B un noyau de collision de la forme *potentiels durs avec cut-off*, c'est-à-dire, pour $v, v_* \in \mathbb{R}^3$, $\sigma \in \mathbb{S}^2$ et avec $\sigma' = \frac{v-v_*}{|v-v_*|}$,

$$B(v, v_*, \sigma) = b(\sigma \cdot \sigma') |v - v_*|^\gamma,$$

où $\gamma \in (0, 1]$, et b est appelé *noyau angulaire*, satisfaisant l'hypothèse de cut-off $b \in L^1((-1, 1))$, et tel que $b \geq b_0$ pour un certain $b_0 > 0$. Soit $0 \leq f_{\text{in}} \in L^1_3(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. Alors il existe des constantes explicites $C_H > 0$ et $\varepsilon^{\text{in}} > 0$, dépendant uniquement de $\gamma, b, \rho_{\text{in}}, u_{\text{in}}, T_{\text{in}}, \|f_{\text{in}}\|_{L^1_3}$ et $\|f_{\text{in}}\|_\infty$, telles que pour tout $\varepsilon \in (0, \varepsilon^{\text{in}}]$, la solution unique f^ε de (1.89) associée à ε et la donnée initiale f_{in} satisfait, pour tout temps $t \geq 0$,

$$H_\varepsilon[f^\varepsilon(t) | \mathcal{M}_\varepsilon^{f_{\text{in}}}] \leq C_H (1+t)^{-\frac{1}{\gamma}}. \quad (1.106)$$

De plus, pour tout $p \geq 1$ et $k \geq 0$, il existe $C_{H,p,k} > 0$, avec les mêmes propriétés que C_H , telles que pour tout temps $t \geq 0$,

$$\left\| f^\varepsilon(t) - \mathcal{M}_\varepsilon^{f_{\text{in}}} \right\|_{L^p_k} \leq C_{H,p,k} (1+t)^{-\frac{1}{2p\gamma}}. \quad (1.107)$$

Le résultat que nous proposons donne, via (1.107), un **taux de convergence à l'équilibre explicite dans tout** L^p_k , avec $1 \leq p < \infty$ et $k \geq 0$. Rappelons que la norme L^p_k a été définie en (1.35).

Pour obtenir le théorème 1.14, nous avons montré le résultat suivant, qui présente un intérêt en soi :

Théorème 1.15

Une borne supérieure uniforme en $\varepsilon > 0$. Sous les mêmes hypothèses et notations que le théorème 1.14, il existe une constante $C_\infty > 0$, dépendant uniquement de $\gamma, b, \rho_{\text{in}}, u_{\text{in}}, T_{\text{in}}, \|f_{\text{in}}\|_{L^1_3}$ et $\|f_{\text{in}}\|_\infty$, telle que pour tout $\varepsilon > 0$, la solution unique f^ε de (1.89) associée à ε et la donnée initiale f_{in} satisfait

$$\sup_{t \geq 0} \|f^\varepsilon(t)\|_\infty \leq C_\infty. \quad (1.108)$$

Remarque 1.10. En réalité, les hypothèses du théorème 1.15 sont un peu moins restrictives que celles du théorème 1.14, et ne requièrent pas de borne inférieure uniforme sur b (la condition $b \geq b_0$).

Le théorème précédent 1.15 donne pour les solutions une *borne* L^∞ *uniforme* en $\varepsilon > 0$. Cette uniformité est cruciale, car elle permet alors de déduire, avec les mêmes notations que dans le théorème, que pour tout $\kappa_0 \in (0, 1)$ et $\varepsilon \in (0, (1 - \kappa_0)\mathbf{C}_\infty^{-1}]$, on a

$$1 - \varepsilon f^\varepsilon \geq \kappa_0.$$

Ainsi, nous pouvons reconnecter avec les résultats obtenus au chapitre 6.

1.4.3.2 Stratégies de preuve

Nous donnons ici de manière succincte les stratégies employées dans les preuves des deux théorèmes énoncés plus haut.

Stratégie de preuve du théorème 1.14 L'idée est d'obtenir *en premier lieu la décroissance de l'entropie relative à l'équilibre* (1.106), puis d'en déduire (1.107) grâce aux *inégalités de Csiszár-Kullback-Pinsker* (1.105).

On obtient (1.106) grâce à la *méthode entropique* :

1. on part d'une inégalité fonctionnelle reliant l'entropie à la dissipation d'entropie obtenue dans le cas Fermi-Dirac depuis une inégalité connue du cas classique, grâce à la méthode de transfert présentée au chapitre 6, donnant pour une fonction f adaptée, *et sous l'hypothèse* $1 - \varepsilon f \geq \kappa_0$,

$$\mathcal{D}_\varepsilon(f) \geq C(\varepsilon, f, \kappa_0) H_\varepsilon[f | \mathcal{M}_\varepsilon^f]^{1+\delta},$$

où $\delta > 0$ et $C(\varepsilon, f, \kappa_0) > 0$ est une quantité dépendant de ε, f à travers certaines normes, et κ_0 ,

2. ayant fixé une donnée initiale f_{in} , on utilise le théorème 1.15 pour assurer, uniformément en $\varepsilon \in (0, (1 - \kappa)\mathbf{C}_\infty^{-1}]$, et pour f^ε solution de (1.89), la validité de l'hypothèse $1 - \varepsilon f^\varepsilon \geq \kappa_0$ et *une borne inférieure* $\mathbf{c} > 0$ à $C(\varepsilon, f^\varepsilon(t), \kappa_0)$, *uniforme en temps* $t \geq 0$ et en $\varepsilon \in (0, (1 - \kappa)\mathbf{C}_\infty^{-1}]$,
3. alors on a pour tout temps t

$$\frac{d}{dt} H_\varepsilon[f^\varepsilon(t) | \mathcal{M}_\varepsilon^{f_{\text{in}}}] \leq -\mathbf{c} H_\varepsilon[f^\varepsilon(t) | \mathcal{M}_\varepsilon^{f_{\text{in}}}]^{1+\delta},$$

et on obtient le résultat en appliquant un argument de type Grönwall à l'équation ci-dessus.

Les deux points clés de cette preuve résident donc en 1. une inégalité entropique, obtenue grâce au chapitre 6, et 2. la borne L^∞ donnée par le théorème 1.15.

Stratégie de preuve du théorème 1.15 La preuve de la borne L^∞ uniforme en $\varepsilon > 0$ donnée par le théorème 1.15 représente la majeure partie du travail effectué au chapitre 7. Nous obtiendrons ce théorème en *nous ramenant* encore une fois *au cas classique déjà étudié*, puis en *adaptant* la méthode de [8] :

1. pour tout $\varepsilon > 0$, on remarque que si f^ε est solution de l'équation de Boltzmann-Fermi-Dirac (homogène) avec cut-off, alors on a pour tout temps t que

$$\partial_t f^\varepsilon(t) \leq Q_0^+(f^\varepsilon(t), f^\varepsilon(t)) + \tilde{Q}_0^+(f^\varepsilon(t), f^\varepsilon(t)) - Q_0^-(f^\varepsilon(t), f^\varepsilon(t)),$$

où Q_0^+ et Q_0^- sont les opérateurs de gain et de perte de l'équation de *Boltzmann classique*, et \tilde{Q}_0^+ est un opérateur satisfaisant une propriété d'*adjonction* à Q_0^+ ; en particulier, le terme de droite *ne dépend pas du paramètre quantique* ε et *ressemble fortement à l'opérateur de Boltzmann classique*,

2. on adapte la preuve de [8], prouvant un résultat de borne L^∞ pour les solutions de Boltzmann classique ; cela est rendu possible grâce à l'équation précédente et le fait que *par adjonction, on récupère pour \tilde{Q}_0^+ des propriétés similaires à celles de Q_0^+* :
 - on obtiendra d'abord une borne L_γ^2 grâce notamment à une propriété connue de *gain de régularité* pour Q_0^+ (donc aussi pour \tilde{Q}_0^+),
 - on en déduira la borne L^∞ annoncée, qui est en particulier *indépendante du paramètre ε* .

Cela conclut la preuve de la convergence avec taux explicite annoncée. Ayant adapté une preuve du cas classique, nous aurons néanmoins considéré des noyaux de collision *du cas classique*. Les noyaux quantiques présentant une forme différente, on discute alors en annexe 7.A la possible extension des résultats énoncés aux cas des noyaux de collisions plus raisonnables d'un point de vue physique (voir [105]).

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Part I

A general framework for Boltzmann models for polyatomic gases

Overview

In this part, composed of Chapters 2 and 3, we provide a general framework for the modelling of polyatomic gases, in the Boltzmann context. This work was conducted in collaboration with M. Bisi and M. Groppi. Chapter 2 is the reproduction of [37], and Chapter 3 of [24]. In this part, the notation ε stands for the internal energy function.

This work is concerned with **modelling**.

ABSTRACT OF CHAPTER 2. A general framework for the kinetic modelling of non-relativistic polyatomic gases is proposed, where each particle is characterized by both its velocity and its internal state, and the Boltzmann collision operator involves suitably weighted integrals over the space of internal energies. The description of the internal structure of a molecule is kept highly general, and this allows classical and semi-classical models, such as the monoatomic gas description, the continuous internal energy structure, and the description with discrete internal energy levels, to fit our framework. We prove the H -Theorem for the proposed kinetic equation of Boltzmann type in this general setting, and characterize the equilibrium Maxwellian distribution and the thermodynamic number of degrees of freedom. Euler equations are derived, as zeroth-order approximation in a suitable asymptotic expansion. In addition, within this general framework, it is possible to build up new models, highly desirable for physical applications, where rotation and vibration are precisely described. Examples of models for the Hydrogen Fluoride gas are presented.

ABSTRACT OF CHAPTER 3. We propose a general kinetic framework for the description of a mixture of non-relativistic mono- or polyatomic gases undergoing any number of bimolecular reactions. The description of the internal structure of the molecules is kept general, in order to model it according to the physical properties of the considered species. The possibility of keeping separate rotational and vibrational energies of polyatomic particles is thus included in the present framework. Moreover, activation energy for chemical reactions is taken into account, allowing us to accurately describe the kinetics of the chemical process. We prove the validity of the H -Theorem, we recover the expected Maxwellian equilibrium distributions jointly with the mass-action laws of chemical reactions, and we obtain an explicit formula for the rate constant of a given chemical reaction. The system of Euler equations in the case of moderately slow chemical reactions is also derived.

Articles reproduced in this chapter

- [24] M. Bisi, T. Borsoni, and M. Groppi. « An internal state kinetic model for chemically reacting mixtures of monatomic and polyatomic gases ». In: *Kinet. Rel. Models* 17.2 (2024), pp. 276–311. DOI: 10.3934/krm.2023023.
- [37] T. Borsoni, M. Bisi, and M. Groppi. « A general framework for the kinetic modelling of polyatomic gases ». In: *Commun. Math. Phys.* (2022), pp. 1–52. DOI: 10.1007/s00220-022-04367-0.

A general framework for the kinetic modelling of polyatomic cases

Outline of the current chapter

2.1 Introduction	68
2.2 General setting and collision rules	70
2.3 Boltzmann model	73
2.3.1 Boltzmann collision operator	74
2.3.2 Note about degeneracy	76
2.3.3 Weak formulation	78
2.3.4 Collision invariants	80
2.4 H Theorem and collision equilibria	82
2.5 Euler limit	90
2.6 Equipartition Theorem	91
2.7 Models within the framework	93
2.7.1 Existing models	93
2.7.2 Combination of the continuous and discrete models	98
2.7.3 Building a model within the framework	99
2.8 Reduction to one real variable and comparison with Borgnakke-Larsen	103
2.9 Conclusions	108
Acknowledgements	111

2.1 Introduction

The purpose of this paper is to propose a consistent general Boltzmann-type model for a polyatomic gas, able to include the kinetic models already exploited in the pertinent literature, but also to give rise to more accurate descriptions of internal energies of polyatomic molecules. The construction of a reliable mathematical model for polyatomic gaseous particles is highly desirable in view of physical applications, since the main constituents of the atmosphere are polyatomic. A review of possible problems involving monoatomic and polyatomic species, possibly undergoing also chemical reactions, may be found in [136, 164]. For this reason, in last decades the investigation of polyatomic particles has gained interest not only in the frame of kinetic theory, but also in Extended Thermodynamics [145] and in the derivation of accurate schemes for fluid-dynamics equations [163, 151].

In kinetic theory, non-translational degrees of freedom of polyatomic particles are usually described by means of an internal energy variable, that may be assumed discrete or continuous. The basic features of the model with a finite set of discrete energy levels may be found in [100, 89]; the gas is considered as a sort of mixture of monatomic components, each one characterized by its energy level, and particles interact by binary collisions preserving total energy, but with possible exchange of energy between its kinetic and internal (excitation) forms, allowing thus particle transitions from one energy component to another. The kinetic model based on a continuous internal energy parameter I has been proposed by Borgnakke and Larsen in [35] and then extensively investigated in [75, 76]; the gas distribution function turns out to depend also on this energy variable, and macroscopic fields and Boltzmann operators involve integrations in dI with an associated integration weight $\varphi(I)$. This measure $\varphi(I) dI$ is a parameter of the model, and different options for it allow to reproduce any desired number of internal degrees of freedom. With the commonly adopted choice $\varphi(I) = I^\alpha$, this number of internal degrees of freedom is independent of the temperature of the gas (describing thus polytropic gases). On the other hand, the set of discrete internal energy levels proposed in [161, 100] allows to obtain a temperature-dependent number of degrees of freedom [29], with a specific heat at constant volume which resembles the physical laws of statistical mechanics [117]. Both formulations with discrete and continuous energy turn out to be well suited also in presence of simple chemical reactions (see for instance [100, 76]) and discrete energy levels are also well adapted to problems involving complex chemistry since real molecules actually have discrete energy levels [89].

Since Boltzmann equations are quite complicated to deal with, simpler kinetic models have been proposed, mainly of BGK or ES-BGK type, both for gases or mixtures with discrete energies [99, 26, 30] and for the continuous energy description [148, 12, 51, 27]. Hydrodynamic limits of kinetic equations have been performed, at Euler or Navier-Stokes accuracy, in order to build up consistent fluid-dynamic equations for the main macroscopic fields, focusing the attention on the transport coefficients, especially on the bulk viscosity or, equivalently, on the so-called dynamical pressure, a correction to the classical scalar pressure due to the polyatomic structure of molecules [141, 15, 28]. Such kinetic or hydrodynamic equations have been applied to simple physical problems, as the existence of shock-wave profiles [113, 114, 149, 140], the Poiseuille and thermal creep flows [85, 162], and suitable boundary conditions have been derived in order to allow the investigation of flow problems with solid boundaries [103].

The main drawback of these kinetic models is the fact that they wish to describe all internal features of polyatomic molecules by means of a single internal energy parameter (discrete or continuous). In order to improve the applicability of Boltzmann equations to real problems, more accurate models would be needed, able to separate the vibrational degrees of freedom from the rotational ones. More precisely, since the gap between two subsequent discrete levels is much lower for rotational energy than for vibrational energy [108], a reasonable way of modeling could approximate the rotational part by means of a continuous variable, keeping the vibrational part discrete. This is the main motivation for the present work; indeed, we would like to merge the existing discrete and continuous energy models in a general (abstract) framework, in order to combine their strength and obtain a full description of both rotation and vibra-

tion. Models with discrete vibrational degrees of freedom and continuous rotational states have long been used in the literature in order to analyse vibrational state-to-state non-equilibrium phenomena [136, 116]. Some attempts to distinguish vibrational from rotational energy have been performed also at kinetic level: in the discrete energy formulation, this aim could be achieved by choosing discrete energies depending on several discrete indices [89], but also other models have been proposed, of BGK or Fokker-Planck-type [126, 69] or in the frame of Extended Thermodynamics [16] (involving two continuous energy variables). The idea of introducing two different temperatures (translational and internal) in the kinetic model for a polyatomic gas, investigating then their influence on volume viscosity and other transport coefficients, has been developed in [136, 53, 14]. Moreover, a proper rovibrational collision model has been built up in order to study the internal energy excitation and dissociation processes behind a strong shockwave in a nitrogen flow [139].

We propose here a general kinetic framework for the description of a single polyatomic gas, in which each particle is characterized, in addition to its position and velocity, also by a suitable internal state ζ . The space of all admissible internal states \mathcal{E} is endowed with a measure μ . In other words, instead of considering a continuous or a discrete variable to describe the internal state of a given molecule, we use a single parameter ζ , and integration over the continuous variable or summation over the discrete one are replaced by a single integration over ζ against the given proper measure μ . Moreover, we clearly distinguish the state of a molecule ζ and the energy function $\varepsilon(\zeta)$, which associates to each state a suitable energy value.

The continuous and the discrete energy models may be included into this framework by choosing $\mathcal{E} = \mathbb{R}_+$ and $\mathcal{E} = \mathbb{N}$, respectively. We prove that, even keeping the space \mathcal{E} , the measure μ and the energy function $\varepsilon(\zeta)$ generic (not explicit), the collision rule determining post-collision velocities may be defined, and the corresponding Boltzmann equation fulfills the expected consistency properties. More precisely, the Boltzmann H theorem holds in the generic framework, and collision equilibria turn out to be provided by Maxwellian distributions depending on the internal energy function $\varepsilon(\zeta)$. The technical steps of the proofs rely essentially on the conservation of momentum and of total energy, therefore there is no need of fixing from the beginning the microscopic energy structure of particles. We remark that our framework describes isotropic gases, where polarization effects due to external fields acting on (non ionized) polyatomic gases may be neglected [129].

In more detail, the content of the paper is organized as follows. In section 2.2, we introduce the framework and its assumptions, and we make the collision rules explicit. Our method is inspired by [75, 76, 25], with some necessary modifications, since the procedure in such references is specifically designed for a continuous or discrete internal variable. Section 2.3 focuses then on the Boltzmann collision operator and on some of its main properties, as the weak formulation and the characterisation of collision invariants. In section 2.4 we prove the validity of the Boltzmann H-theorem, and we investigate the equilibrium Maxwellian distribution and the thermodynamic number of internal degrees of freedom. In section 2.5, the hydrodynamic Euler equations corresponding to our general model are derived. Sections 2.6 and 2.7 are devoted to modelling: we explain how to recover the monoatomic, continuous and discrete formulations, and we give insights on how to build consistent new models within our framework, including a description able to separate rotation and vibrations of polyatomic particles; examples of possible models are provided and commented on, with reference to the pertinent gas-dynamics literature. In Section 8, we show how is possible to reduce models fitting the general setting to a one-real-variable description with a suitable measure, similar to the continuous model with integration weight. We address the problem of computing this measure from the general setting, and show that the combination of a continuous model with weight and a discrete model reduces to a continuous model with a different weight that can be made explicit, allowing an easier treatment for numerical applications. Finally, section 2.9 contains some concluding remarks and perspectives.

2.2 General setting and collision rules

We consider a gas composed of one species of molecules, which mass we denote by $m \in \mathbb{R}_+^*$. Each molecule is microscopically described by its velocity, denoted by v , and its internal state, denoted by ζ . The latter is usually related to rotation or vibration that occurs inside the molecule. We assume that there exists a set of all possible internal states \mathcal{E} , and that this set is a measure space. All molecules, being of the same species, are related to the same space \mathcal{E} . Secondly, we assume that to each internal state $\zeta \in \mathcal{E}$ corresponds an energy, that is, there exists an internal energy function $\varepsilon : \mathcal{E} \rightarrow \mathbb{R}$. The energy of a molecule with velocity v and internal state ζ is then equal to $\frac{m}{2}|v|^2 + \varepsilon(\zeta)$, the sum of its kinetic and internal parts.

Definition 2.1. We call space of internal states a non-empty measure space $(\mathcal{E}, \mathcal{A}, \mu)$, with $\mu(\mathcal{E}) \neq 0$.

To clarify here, \mathcal{E} is the space of internal states, \mathcal{A} is a σ -algebra on \mathcal{E} , and μ is a (non-negative) measure on $(\mathcal{E}, \mathcal{A})$. In the following definition, $\text{Bor}(\mathbb{R})$ is the set of Borelians of \mathbb{R} .

Definition 2.2. We call internal energy function a $(\mathcal{A}, \text{Bor}(\mathbb{R}))$ -measurable function $\varepsilon : \mathcal{E} \rightarrow \mathbb{R}$.

In our framework, we only require two assumptions on $(\mathcal{E}, \mathcal{A}, \mu)$ and ε , which both physically make sense. The first is to assume that ε admits an infimum.

Definition and assumption 2.1. We denote by ε^0 the essential infimum of ε in $\bar{\mathbb{R}}$ on \mathcal{E} under the measure μ , that is

$$\varepsilon^0 := \inf \text{ess}_\mu \{\varepsilon\} = \sup \left\{ R \in \mathbb{R}, \text{ s.t. } \mu(\varepsilon < R) = 0 \right\}, \quad (2.1)$$

and assume that $\varepsilon^0 \in \mathbb{R}$.

Definition 2.3. We define the grounded internal energy function $\bar{\varepsilon}$ by

$$\bar{\varepsilon} := \varepsilon - \varepsilon^0. \quad (2.2)$$

Note that by definition of ε^0 , $\inf \text{ess}_\mu \{\bar{\varepsilon}\} = 0$.

Remark 2.1. The reader shall remark that in this paper, the value of ε^0 has no importance. Indeed, ε^0 represents the fundamental energy of configuration of the molecule, and it plays a role only when chemical reactions are involved.

The second assumption is the well-definedness of the partition function.

Definition and assumption 2.2. We define the partition function Z , for all $\beta > 0$, as

$$Z(\beta) := \int_{\mathcal{E}} e^{-\beta \bar{\varepsilon}(\zeta)} d\mu(\zeta), \quad (2.3)$$

and assume that for all $\beta > 0$, $Z(\beta) < \infty$.

The choice of $\bar{\varepsilon}$ instead of simply ε in the definition of Z is explained in Remark 2.4. Assumptions 2.1 and 2.2 imply that $\forall R \in \mathbb{R}$, $\mu(\varepsilon < R) < \infty$, which itself implies that μ is σ -finite.

Proposition 2.1. Z is \mathcal{C}^∞ on \mathbb{R}_+^* and for all $k \in \mathbb{N}$ and $\beta > 0$ and, denoting its derivatives by $Z^{(k)}(\beta) = \frac{d^k Z}{d\beta^k}$, we have

$$Z^{(k)}(\beta) = \int_{\mathcal{E}} (-\bar{\varepsilon}(\zeta))^k e^{-\beta \bar{\varepsilon}(\zeta)} d\mu(\zeta). \quad (2.4)$$

Proof. Remarking that for all $x \in \mathbb{R}_+$ and $k \in \mathbb{N}$, $e^{\frac{x}{2}} \geq \frac{(\frac{x}{2})^k}{k!}$, we get the inequality $x^k e^{-x} \leq 2^k k! e^{-\frac{x}{2}}$. Since $\bar{\varepsilon} \geq 0$ μ -a.e., we get for all $k \in \mathbb{N}$ and $\beta > 0$, $\int_{\mathcal{E}} \bar{\varepsilon}(\zeta)^k e^{-\beta \bar{\varepsilon}(\zeta)} d\mu(\zeta) < +\infty$ and the result comes by dominated convergence. \square

We consider a binary collision and define the collision rule. The states (velocity and internal state) of the pre-collision molecules are denoted by (v, ζ) and (v_*, ζ_*) , and the states of the post-collision molecules are denoted by (v', ζ') and (v'_*, ζ'_*) . In each collision momentum and total energy are conserved

$$\begin{cases} mv + mv_* = mv' + mv'_* \\ \frac{m}{2}|v|^2 + \varepsilon(\zeta) + \frac{m}{2}|v_*|^2 + \varepsilon(\zeta_*) = \frac{m}{2}|v'|^2 + \varepsilon(\zeta') + \frac{m}{2}|v'_*|^2 + \varepsilon(\zeta'_*). \end{cases} \quad (2.5)$$

The parallelogram identity yields

$$\begin{aligned} |v - v_*|^2 &= 2(|v|^2 + |v_*|^2) - |v + v_*|^2 \\ &= |v' - v'_*|^2 + \frac{4}{m}(\varepsilon(\zeta') + \varepsilon(\zeta'_*) - \varepsilon(\zeta) - \varepsilon(\zeta_*)). \end{aligned}$$

We set

$$\Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*) := \frac{1}{4}|v - v_*|^2 + \frac{1}{m}(\varepsilon(\zeta) + \varepsilon(\zeta_*) - \varepsilon(\zeta') - \varepsilon(\zeta'_*)), \quad (2.6)$$

we then have

$$\frac{1}{4}|v' - v'_*|^2 = \Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*). \quad (2.7)$$

We deduce that the collision can occur only when Δ is non-negative, and in this case, by a classical argument, there exists $\omega \in \mathbb{S}^2$ (two-dimensional unit sphere) such that

$$\begin{cases} v' &= \frac{v + v_*}{2} + \sqrt{\Delta} T_\omega \begin{bmatrix} v - v_* \\ |v - v_*| \end{bmatrix} \\ v'_* &= \frac{v + v_*}{2} - \sqrt{\Delta} T_\omega \begin{bmatrix} v - v_* \\ |v - v_*| \end{bmatrix} \end{cases} \quad (2.8)$$

where T_ω is the symmetry with respect to $(\mathbb{R}\omega)^\perp$,

$$\forall V \in \mathbb{S}^2, \quad T_\omega[V] := V - 2(\omega \cdot V)\omega \in \mathbb{S}^2.$$

It is not required to extend formula (2.8) to the set $\{(v, v) \text{ s.t. } v \in \mathbb{R}^3\}$, since it is negligible.

From the previous computation, it is clear that not any collision is possible. If, before collision, two molecules are in low energy internal states with close velocities, they cannot reach too much high energy internal states after collision. For this reason, we fix at first the pre- and post-collision internal states, and then we consider the space of pre-collision velocity pairs that make the collision possible. In the following definition, $E[\zeta, \zeta_*, \zeta', \zeta'_*]$ is the set of pre-collision velocity pairs (v, v_*) so that a collision $(v, \zeta), (v_*, \zeta_*) \rightarrow (\cdot, \zeta'), (\cdot, \zeta'_*)$ is allowed.

Definition 2.4. For all $\zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}$, we define

$$E[\zeta, \zeta_*, \zeta', \zeta'_*] := \left\{ (v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3 \text{ s.t. } \Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*) \geq 0 \right\}, \quad (2.9)$$

where Δ is defined by (2.6).

It can be proved that for all $\zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}$, the interior of $E[\zeta, \zeta_*, \zeta', \zeta'_*]$ is non-empty, unbounded and arcwise connected.

Now we can define the transformation linking the pre and post-collision velocities.

Definition 2.5. We define for all $\zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}$ and $\omega \in \mathbb{S}^2$,

$$S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*] : \begin{cases} E[\zeta, \zeta_*, \zeta', \zeta'_*] & \rightarrow \\ (v, v_*) & \mapsto \left(\frac{v + v_*}{2} + \sqrt{\Delta} T_\omega \left[\frac{v - v_*}{|v - v_*|} \right], \frac{v + v_*}{2} - \sqrt{\Delta} T_\omega \left[\frac{v - v_*}{|v - v_*|} \right] \right). \end{cases} \quad (2.10)$$

Lemma 2.2. $S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*]$ is well-defined and a bijection, with

$$(S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*])^{-1} = S_\omega[\zeta', \zeta'_*, \zeta, \zeta_*].$$

Proof. Let $\zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}$, $\omega \in \mathbb{S}^2$. First, we show that the transformation is well-defined. We fix $(v, v_*) \in E[\zeta, \zeta_*, \zeta', \zeta'_*]$. We have that $\Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*) \geq 0$. We define $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$. Then

$$\begin{aligned} \Delta(v', v'_*, \zeta', \zeta'_*, \zeta, \zeta_*) &= \frac{1}{4}|v' - v'_*|^2 + \frac{1}{m}(\varepsilon(\zeta') + \varepsilon(\zeta'_*) - \varepsilon(\zeta) - \varepsilon(\zeta_*)) \\ &= \frac{1}{4} \left(2\sqrt{\Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*)} \right)^2 + \frac{1}{m}(\varepsilon(\zeta) + \varepsilon(\zeta_*) - \varepsilon(\zeta) - \varepsilon(\zeta_*)) \\ &= \Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*) + \frac{1}{m}(\varepsilon(\zeta') + \varepsilon(\zeta'_*) - \varepsilon(\zeta) - \varepsilon(\zeta_*)) \\ &= \frac{1}{4}|v - v_*|^2 \geq 0. \end{aligned}$$

Thus $(v', v'_*) \in E[\zeta', \zeta'_*, \zeta, \zeta_*]$. The application is well-defined.

Let us now prove that the transformation $S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*]$ is a bijection. We fix $(v', v'_*) \in E[\zeta', \zeta'_*, \zeta, \zeta_*]$ and define $(v, v_*) = S_\omega[\zeta', \zeta'_*, \zeta, \zeta_*](v', v'_*)$. First, we just proved (with inverted notations) that $(v, v_*) \in E[\zeta, \zeta_*, \zeta', \zeta'_*]$ and $\Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*) = \frac{1}{4}|v' - v'_*|^2$. Now we also remark that

$$v + v_* = v' + v'_*,$$

and

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

because T_ω is a symmetry. Since $\Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*) = \frac{1}{4}|v' - v'_*|^2$, we deduce that

$$\frac{v + v_*}{2} + \sqrt{\Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*)} T_\omega \left[\frac{v - v_*}{|v - v_*|} \right] = \frac{v' + v'_*}{2} + \frac{1}{2}|v' - v'_*| \frac{v' - v'_*}{|v' - v'_*|} = v'.$$

Analogously,

$$\frac{v + v_*}{2} - \sqrt{\Delta(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*)} T_\omega \left[\frac{v - v_*}{|v - v_*|} \right] = \frac{v' + v'_*}{2} - \frac{1}{2}|v' - v'_*| \frac{v' - v'_*}{|v' - v'_*|} = v'_*.$$

so that $S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*) = (v', v'_*)$, which ends the proof. \square

Lemma 2.3. *The Jacobian of the transformation $S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*]$ is given by the formula*

$$J[S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*]](v, v_*) = \frac{|v' - v'_*|}{|v - v_*|}, \quad (2.11)$$

where $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$.

Proof. This proof is based on that one of Lemma 1 in [76]. We decompose the transformation in a chain of elementary changes of variable. For the sake of clarity, we fix $\zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}$ and $\omega \in \mathbb{S}^2$, and denote the transformation $S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*]$ by simply writing

$$(v, v_*) \mapsto (v', v'_*).$$

First, we pass to the center-of-mass reference frame. The transformations $A_1 : (v, v_*) \mapsto (g, G)$ where $g = v - v_*$, $G = (v + v_*)/2$, and $B_1 : (g', G') \mapsto (v', v'_*)$ have both Jacobian equal to 1. Since $G = G'$, we are led to study the transformation $C_1 : g \mapsto g'$. Now, we pass to spherical coordinates for g and g' . We perform the transformations $A_2 : g \mapsto (|g|, g/|g|)$ and $B_2 : (|g'|, g'/|g'|) \mapsto g'$, and finally we study the transformation $C_2 : (|g|, g/|g|) \mapsto (|g'|, g'/|g'|)$ taking into account the determinant $|g'|^2/|g|^2$ of the Jacobian coming from A_2 and B_2 . Since T_ω is a symmetry, we have

$$\begin{aligned} & J \left[\left(|g|, \frac{g}{|g|} \right) \mapsto \left(2\sqrt{\frac{1}{4}|g|^2 + \frac{1}{m}(\varepsilon(\zeta) + \varepsilon(\zeta_*) - \varepsilon(\zeta') - \varepsilon(\zeta'_*))}, T_\omega \left[\frac{g}{|g|} \right] \right) \right] \\ &= J \left[|g| \mapsto 2\sqrt{\frac{1}{4}|g|^2 + \frac{1}{m}(\varepsilon(\zeta) + \varepsilon(\zeta_*) - \varepsilon(\zeta') - \varepsilon(\zeta'_*))} \right] \\ &= \frac{\frac{1}{2}|g|}{\sqrt{\frac{1}{4}|g|^2 + \frac{1}{m}(\varepsilon(\zeta) + \varepsilon(\zeta_*) - \varepsilon(\zeta') - \varepsilon(\zeta'_*))}} = \frac{|g|}{|g'|}. \end{aligned}$$

Multiplying by $|g'|^2/|g|^2$, we finally obtain

$$J[S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*]](v, v_*) = \frac{|g'|}{|g|} = \frac{|v' - v'_*|}{|v - v_*|},$$

where $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$. \square

2.3 Boltzmann model

We consider a distribution function f that represents the density of molecules of the studied gas. This density depends on 4 parameters:

- 2 macroscopic parameters: the time $t \in \mathbb{R}_+$ and the position in space x , typically $x \in \mathbb{R}^3$ or \mathbb{T}^3
- 2 microscopic parameters: the velocity $v \in \mathbb{R}^3$ and the internal state $\zeta \in \mathcal{E}$

As a distribution function, f is non-negative, so that we study $f(t, x, v, \zeta) \in \mathbb{R}_+$. Moreover, we assume that for all (t, x) , $f(t, x, \cdot, \cdot) \in L^1(\mathbb{R}^3 \times \mathcal{E}, d\nu d\mu(\zeta))$. The evolution of this distribution function is governed by the Boltzmann equation

$$\partial_t f(t, x, v, \zeta) + v \cdot \nabla_x f(t, x, v, \zeta) = \mathcal{B}(f, f)(t, x, v, \zeta), \quad (2.12)$$

where \mathcal{B} is the Boltzmann collision operator we define in a following subsection.

If ϕ defined on $\mathbb{R}^3 \times \mathcal{E}$ is a microscopic extensive quantity (test function, often called molecular property), then the associated macroscopic quantity is

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \phi(v, \zeta) f(t, x, v, \zeta) \, dv \, d\mu(\zeta).$$

Typical choice for the molecular properties are $\phi = m$, $\phi = mv$ and $\phi = \frac{m}{2}|v|^2 + \varepsilon(\zeta)$, giving the mass density ρ , velocity u and total energy density e , respectively, namely

$$\begin{aligned} \rho(t, x) &:= \int_{\mathcal{E}} \int_{\mathbb{R}^3} m f(t, x, v, \zeta) \, dv \, d\mu(\zeta) \\ u(t, x) &:= \frac{1}{\rho(t, x)} \int_{\mathcal{E}} \int_{\mathbb{R}^3} m v f(t, x, v, \zeta) \, dv \, d\mu(\zeta) \\ e(t, x) &:= \frac{1}{\rho(t, x)} \int_{\mathcal{E}} \int_{\mathbb{R}^3} \left(\frac{m}{2} |v|^2 + \varepsilon(\zeta) \right) f(t, x, v, \zeta) \, dv \, d\mu(\zeta). \end{aligned}$$

We can also define the temperature by

$$T(t, x) := \Theta^{-1} \left(\frac{1}{\rho(t, x)} \int_{\mathcal{E}} \int_{\mathbb{R}^3} \left(\frac{m}{2} |v - u|^2 + \bar{\varepsilon}(\zeta) \right) f(t, x, v, \zeta) \, dv \, d\mu(\zeta) \right), \quad (2.13)$$

where we recall that by definition (equation (2.2)) $\bar{\varepsilon} = \varepsilon - \varepsilon^0$, while $\Theta : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is a suitable function related to the integral of the specific heat at constant volume (the precise definition will be given later, in equation (2.31) in Section 2.4).

2.3.1 Boltzmann collision operator

The Boltzmann operator, representing the effect of collisions on the change of velocities and internal states of each molecule, is composed by a loss and a gain term

$$\mathcal{B} = \mathcal{B}_+ - \mathcal{B}_-.$$

We focus on the microscopic aspect and put temporarily aside the variables t and x . When two molecules collide, not all possible post-collision states are equiprobable. This idea is translated in the concept of the collision (or scattering) kernel B , which encapsulates the information on the interaction potential (for example a hard sphere or Lennard-Jones one). As well known, the collision kernel is related to the differential cross section Σ through the formula $B = |v - v_*| \Sigma$.

In this paper, for a purpose of generality, following the line of [97] we make as few assumptions as possible on the collision kernel B .

Definition 2.6. *The collision kernel B is a measurable function*

$$B : \begin{cases} \mathbb{R}^3 \times \mathbb{R}^3 \times \mathcal{E} \times \mathcal{E} \times \mathcal{E} \times \mathcal{E} \times \mathbb{S}^2 \rightarrow \mathbb{R}_+ \\ (v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) \mapsto B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega). \end{cases} \quad (2.14)$$

Assumption 2.1. Symmetry. For a.e. $v, v_* \in \mathbb{R}^3$, for μ -a.e. $\zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}$ and a.e. $\omega \in \mathbb{S}^2$,

$$B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) = B(v_*, v, \zeta_*, \zeta, \zeta', \zeta'_*, \omega). \quad (2.15)$$

Assumption 2.2. Micro-reversibility. For a.e. $v, v_* \in \mathbb{R}^3$, for μ -a.e. $\zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}$ and a.e. $\omega \in \mathbb{S}^2$,

$$|v - v_*| B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) = |v' - v'_*| B(v', v'_*, \zeta', \zeta'_*, \zeta, \zeta_*, \omega). \quad (2.16)$$

where $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$.

Definition and assumption 2.3. We denote by $\mathbb{S}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*]$ the subset of \mathbb{S}^2 such that for all $\omega \in \mathbb{S}^2$,

$$\omega \in \mathbb{S}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*] \iff B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) > 0.$$

We assume that for a.e. $v, v_* \in \mathbb{R}^3$ and μ -a.e. $\zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}$,

$$\begin{aligned} (v, v_*) \in E[\zeta, \zeta_*, \zeta', \zeta'_*] &\iff \mathbb{S}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*] \text{ has positive measure,} \\ \mathbb{S}^2 \setminus \mathbb{S}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*] &\text{ has zero measure.} \end{aligned} \quad (2.17)$$

This assumption 2.3 has the following meaning: if a collision is possible, then there exists a non-negligible set of angles ω for which the kernel is positive; if, on the other hand, a collision is not allowed, then the corresponding kernel is zero. Finally, if the collision is elastic, then the set of angles ω for which the kernel is positive is the whole sphere \mathbb{S}^2 (minus a negligible set). We thus allow, for inelastic collisions, the kernel to be zero for a non-negligible set of angles. This is an important feature, already present for example in [97] for the case of reacting spheres.

Note that the symmetry and micro-reversibility assumptions are not in contradiction with the positivity assumption, due to the fact the the function $\mathbf{1}_{\Delta \geq 0}$ also has symmetry and reversibility properties. Moreover, setting $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$, the symmetry and micro-reversibility assumptions imply

$$\mathbb{S}^2[v_*, v, \zeta_*, \zeta, \zeta'_*, \zeta'] = \mathbb{S}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*] = \mathbb{S}^2[v', v'_*, \zeta', \zeta'_*, \zeta, \zeta_*].$$

We are now ready to define the Boltzmann collision operator. The loss term of the collision operator expresses the fact that a collision involving a molecule with state (v, ζ) causes a change of the state. Thus for all states $(v, \zeta) \in \mathbb{R}^3 \times \mathcal{E}$, and recalling that B is null for not admissible collisions, the loss term reads as

$$\mathcal{B}_-(f, f)(v, \zeta) := \iiint_{\mathcal{E}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f(v, \zeta) f(v_*, \zeta_*) B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) d\omega dv_* d\mu^{\otimes 3}(\zeta_*, \zeta', \zeta'_*). \quad (2.18)$$

The gain term of the collision operator expresses the production of the state (v, ζ) by collisions. Thus the gain term is obtained by considering *all collisions* for which (v, ζ) is a post-collision state. We have already proved in Lemma 2.2 that if $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$ then $(v, v_*) = S_\omega[\zeta', \zeta'_*, \zeta, \zeta_*](v', v'_*)$, therefore the gain term will be symmetric to the loss one as expected. In more detail, denoting by χ the Dirac mass on \mathbb{R}^3 , the gain term is defined by

$$\begin{aligned} \mathcal{B}_+(f, f)(v, \zeta) := &\iiint_{\mathcal{E}^3} \iint_{E[\zeta', \zeta'_*, \zeta, \zeta_*]} \int_{\mathbb{S}^2} \chi(\tilde{v} = v) f(v', \zeta') f(v'_*, \zeta'_*) B(v', v'_*, \zeta', \zeta'_*, \zeta, \zeta_*, \omega) \\ &d\omega dv' dv'_* d\mu^{\otimes 3}(\zeta', \zeta'_*, \zeta_*, \zeta_*), \end{aligned}$$

where just for convenience we define $(\tilde{v}, \tilde{v}_*) = S_\omega[\zeta', \zeta'_*, \zeta, \zeta_*](v', v'_*)$, in order to be able to perform the

change of variables $(\tilde{v}, \tilde{v}_*) = S_\omega[\zeta', \zeta'_*, \zeta, \zeta_*](v', v'_*)$ (recalling that $S_\omega[\zeta', \zeta'_*, \zeta, \zeta_*]$ is a \mathcal{C}^1 -diffeomorphism on $E[\zeta', \zeta'_*, \zeta, \zeta_*]$, except on a negligible set) leading to

$$\mathcal{B}_+(f, f)(v, \zeta) = \iiint_{\mathcal{E}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f(v', \zeta') f(v'_*, \zeta'_*) J[(S_\omega[\zeta', \zeta'_*, \zeta, \zeta_*])^{-1}] \\ B(v', v'_*, \zeta', \zeta'_*, \zeta, \zeta_*, \omega) d\omega dv_* d\mu^{\otimes 3}(\zeta', \zeta'_*, \zeta_*),$$

where we went back to the original notation, changing \tilde{v}_* to v_* . The Jacobian of

$$(S_\omega[\zeta', \zeta'_*, \zeta, \zeta_*])^{-1} = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*]$$

is given by equation (2.11), and it provides

$$\mathcal{B}_+(f, f)(v, \zeta) = \iiint_{\mathcal{E}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f(v', \zeta') f(v'_*, \zeta'_*) \frac{|v' - v'_*|}{|v - v_*|} B(v', v'_*, \zeta', \zeta'_*, \zeta, \zeta_*, \omega) \\ \times d\omega dv_* d\mu^{\otimes 3}(\zeta', \zeta'_*, \zeta_*).$$

Using now the micro-reversibility condition on B , Assumption 2.2, we finally get

$$\mathcal{B}_+(f, f)(v, \zeta) = \iiint_{\mathcal{E}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f(v', \zeta') f(v'_*, \zeta'_*) B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) d\omega dv_* d\mu^{\otimes 3}(\zeta_*, \zeta'_*, \zeta_*), \quad (2.19)$$

where we recall that $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$. Since f and B are non-negative measurable functions, the gain and loss terms are always defined. In order to define the full collision term, we impose the following assumption on f .

Assumption 2.3. For a.e. $v \in \mathbb{R}^3$ and for μ -a.e. $\zeta \in \mathcal{E}$,

$$\mathcal{B}_-(f, f)(v, \zeta) + \mathcal{B}_+(f, f)(v, \zeta) < \infty.$$

Writing $B(\cdot) \equiv B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega)$ to lighten the notations, the full Boltzmann collision operator writes, for all $v \in \mathbb{R}^3$ and $\zeta \in \mathcal{E}$,

$$\mathcal{B}(f, f)(v, \zeta) = \iiint_{\mathcal{E}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left(f(v', \zeta') f(v'_*, \zeta'_*) - f(v, \zeta) f(v_*, \zeta_*) \right) B(\cdot) d\omega dv_* d\mu^{\otimes 3}(\zeta_*, \zeta'_*, \zeta_*), \quad (2.20)$$

where $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$.

Remark 2.2. Alternatively, one can define the Boltzmann collision operator using transition probabilities instead of B , see [89].

2.3.2 Note about degeneracy

The concept of degeneracy appears when the internal description is done through the direct consideration of energy levels. For instance, in a quantum description, different proper states can sometimes have the same energy. The number of proper states sharing the same energy level is called the *degeneracy* of this energy level. When degeneracy is considered in kinetic theory, it usually appears in the micro-reversibility condition of the collision kernel (see for example Section 4.2.4 in Giovangigli [90], equations (4.2.7) and (4.2.8)), and ultimately in the formulation of the Boltzmann integral. We show in this subsection that, without loss of generality, it is possible to assume no degeneracy in the micro-reversibility condition and take this into account through the measure μ . Note also that if the internal

description is done through the proper states instead of directly through the energy levels, there is no degeneracy to consider.

The degeneracy is a measurable positive function on the space of internal states

$$a : \mathcal{E} \rightarrow \mathbb{R}_+^*.$$

The micro-reversibility condition taking degeneracy into account writes (see Section 4.2.4 in Giovangigli [90], equation (4.2.8))

$$|v - v_*| B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) a(\zeta) a(\zeta_*) = |v' - v'_*| B(v', v'_*, \zeta', \zeta'_*, \zeta, \zeta_*, \omega) a(\zeta') a(\zeta'_*). \quad (2.21)$$

Classical symmetry condition for cross-sections should be valid only if the molecular states are non-degenerate [84]. However, Waldmann [159] has shown that semi-classical Boltzmann modelling is indeed admissible for all molecules, even with degeneracy properties, provided the quantum mechanical cross-sections are replaced by suitably degeneracy averaged cross-sections [159, 81]. Symmetry property (2.21) may be obtained owing to the invariance of the Hamiltonian under the combined operation of space inversion and time reversal [159, 128]. We remark that in the classical model with a continuous internal energy variable I [35, 75, 76], the weight function $\varphi(I)$ in the Boltzmann kernel plays the role of the degeneracy function $a(\cdot)$.

With the same reasoning as in the previous subsection 2.3.1, the collision term writes in this case

$$\begin{aligned} \mathcal{B}(f, f)(v, \zeta) = & \iiint_{\mathcal{E}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left(\frac{a(\zeta) a(\zeta_*)}{a(\zeta') a(\zeta'_*)} f(v', \zeta') f(v'_*, \zeta'_*) - f(v, \zeta) f(v_*, \zeta_*) \right) \\ & \times B(\cdot) d\omega dv_* d\mu^{\otimes 3}(\zeta_*, \zeta', \zeta'_*). \end{aligned}$$

Let us now define

$$\tilde{B}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) = \frac{B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega)}{a(\zeta') a(\zeta'_*)}, \quad d\tilde{\mu}(\zeta) = a(\zeta) d\mu(\zeta), \quad \tilde{f}(v, \zeta) = \frac{f(v, \zeta)}{a(\zeta)}.$$

Then \tilde{B} verifies the assumptions of our framework. Now let us set

$$\tilde{\mathcal{B}}(\tilde{f}, \tilde{f})(v, \zeta) = \iiint_{\mathcal{E}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left(\tilde{f}(v', \zeta') \tilde{f}(v'_*, \zeta'_*) - \tilde{f}(v, \zeta) \tilde{f}(v_*, \zeta_*) \right) \tilde{B}(\cdot) d\omega dv_* d\tilde{\mu}^{\otimes 3}(\zeta_*, \zeta', \zeta'_*).$$

Then

$$\begin{aligned} \tilde{\mathcal{B}}(\tilde{f}, \tilde{f})(v, \zeta) = & \frac{1}{a(\zeta)} \iiint_{\mathcal{E}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left(\frac{a(\zeta) a(\zeta_*)}{a(\zeta') a(\zeta'_*)} f(v', \zeta') f(v'_*, \zeta'_*) - f(v, \zeta) f(v_*, \zeta_*) \right) \\ & B(\cdot) d\omega dv_* d\mu^{\otimes 3}(\zeta_*, \zeta', \zeta'_*), \end{aligned}$$

hence $\tilde{\mathcal{B}}(\tilde{f}, \tilde{f})(v, \zeta) = \frac{1}{a(\zeta)} \mathcal{B}(f, f)(v, \zeta)$. It follows that

$$\tilde{\mathcal{B}}(\tilde{f}, \tilde{f})(v, \zeta) d\tilde{\mu}(\zeta) = \frac{1}{a(\zeta)} \mathcal{B}(f, f)(v, \zeta) a(\zeta) d\mu(\zeta) = \mathcal{B}(f, f)(v, \zeta) d\mu(\zeta)$$

and

$$\tilde{f}(v, \zeta) d\tilde{\mu}(\zeta) = \frac{1}{a(\zeta)} f(v, \zeta) a(\zeta) d\mu(\zeta) = f(v, \zeta) d\mu(\zeta).$$

Thus it is equivalent to study the model $(\mathcal{E}, \mathcal{A}, \mu)$ with the kernel B and degeneracy a , and the model

$(\mathcal{E}, \mathcal{A}, \tilde{\mu})$ with the kernel \tilde{B} and no degeneracy. In our framework, degeneracy can be simply included in the measure on the space of internal states, and does not appear in the micro-reversibility condition.

2.3.3 Weak formulation

In this section, we study the weak formulation of the collision integral that will later enable us to deduce the conservation laws and collision invariants.

Proposition 2.4. *Let $\psi : \mathbb{R}^3 \times \mathcal{E} \rightarrow \mathbb{R}$ be a measurable function such that*

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_-(f, f)(v, \zeta) |\psi(v, \zeta)| \, dv \, d\mu(\zeta) + \int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_+(f, f)(v, \zeta) |\psi(v, \zeta)| \, dv \, d\mu(\zeta) < \infty.$$

Then

$$\begin{aligned} \int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}(f, f)(v, \zeta) \psi(v, \zeta) \, dv \, d\mu(\zeta) &= -\frac{1}{4} \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} \left(f(v', \zeta') f(v'_*, \zeta'_*) - f(v, \zeta) f(v_*, \zeta_*) \right) \\ &\quad \times \left[\psi(v', \zeta') + \psi(v'_*, \zeta'_*) - \psi(v, \zeta) - \psi(v_*, \zeta_*) \right] B(\cdot) \, d\omega \, dv \, dv_* \, d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*) \end{aligned}$$

where $(v', v'_*) = S_{\omega}[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$.

Proof. First we have, thanks to the symmetry conditions on B and Fubini's Theorem,

$$\begin{aligned} &\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_-(f, f)(v, \zeta) \psi(v, \zeta) \, dv \, d\mu(\zeta) \\ &= \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} f(v, \zeta) f(v_*, \zeta_*) \psi(v, \zeta) B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) \, d\omega \, dv \, dv_* \, d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*) \\ &= \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} f(v_*, \zeta_*) f(v, \zeta) \psi(v_*, \zeta_*) B(v_*, v, \zeta_*, \zeta, \zeta', \zeta'_*, \omega) \, d\omega \, dv_* \, dv \, d\mu^{\otimes 4}(\zeta_*, \zeta, \zeta', \zeta'_*) \\ &= \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} f(v, \zeta) f(v_*, \zeta_*) \psi(v_*, \zeta_*) B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) \, d\omega \, dv \, dv_* \, d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*), \end{aligned}$$

thus

$$\begin{aligned} &\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_-(f, f)(v, \zeta) \psi(v, \zeta) \, dv \, d\mu(\zeta) \\ &= \frac{1}{2} \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} f(v, \zeta) f(v_*, \zeta_*) [\psi(v, \zeta) + \psi(v_*, \zeta_*)] B(\cdot) \, d\omega \, dv \, dv_* \, d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*). \end{aligned}$$

Now by renaming all the variables, we get

$$\begin{aligned} \int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_-(f, f)(v, \zeta) \psi(v, \zeta) \, dv \, d\mu(\zeta) &= \frac{1}{2} \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} f(v', \zeta') f(v'_*, \zeta'_*) [\psi(v', \zeta') + \psi(v'_*, \zeta'_*)] \\ &\quad \times B(v', v'_*, \zeta', \zeta'_*, \zeta, \zeta_*, \omega) \, d\omega \, dv' \, dv'_* \, d\mu^{\otimes 4}(\zeta', \zeta'_*, \zeta, \zeta_*). \end{aligned}$$

We now perform the change of variables $(v, v_*) = S_{\omega}[\zeta', \zeta'_*, \zeta, \zeta_*](v', v'_*)$, use the formula for the Jacobian (2.11) and the micro-reversibility condition and obtain

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_-(f, f)(v, \zeta) \psi(v, \zeta) \, dv \, d\mu(\zeta) = \frac{1}{2} \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} f(v', \zeta') f(v'_*, \zeta'_*) [\psi(v', \zeta') + \psi(v'_*, \zeta'_*)] \\ \times B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) \, d\omega \, dv \, dv_* \, d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*).$$

where $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$. We deduce that

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_-(f, f)(v, \zeta) \psi(v, \zeta) \, dv \, d\mu(\zeta) \\ = \frac{1}{4} \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} \left(f(v', \zeta') f(v'_*, \zeta'_*) [\psi(v', \zeta') + \psi(v'_*, \zeta'_*)] + f(v, \zeta) f(v_*, \zeta_*) [\psi(v, \zeta) + \psi(v_*, \zeta_*)] \right) \\ B(\cdot) \, d\omega \, dv \, dv_* \, d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*).$$

where $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$.

On the other hand, since

$$\mathcal{B}_+(f, f)(v, \zeta) = \iiint_{\mathcal{E}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f(v', \zeta') f(v'_*, \zeta'_*) B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) \, d\omega \, dv_* \, d\mu^{\otimes 3}(\zeta_*, \zeta'_*, \zeta'_*),$$

where $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$, we have

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_+(f, f)(v, \zeta) \psi(v, \zeta) \, dv \, d\mu(\zeta) \\ = \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} f(v', \zeta') f(v'_*, \zeta'_*) \psi(v, \zeta) B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) \, d\omega \, dv \, dv_* \, d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*).$$

Applying the change of variables $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$ using the formula for the Jacobian, equation (2.11), together with the micro-reversibility condition on B , Assumption 2.2, we obtain

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_+(f, f)(v, \zeta) \psi(v, \zeta) \, dv \, d\mu(\zeta) \\ = \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} f(v', \zeta') f(v'_*, \zeta'_*) \psi(v, \zeta) B(v', v'_*, \zeta', \zeta'_*, \zeta, \zeta_*, \omega) \, d\omega \, dv' \, dv'_* \, d\mu^{\otimes 4}(\zeta', \zeta'_*, \zeta, \zeta_*)$$

where v in the last integral is defined by $(v, v_*) = S_\omega[\zeta', \zeta'_*, \zeta, \zeta_*](v', v'_*)$. By simply renaming the variables (exchange of prime and non-prime), we get

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_+(f, f)(v, \zeta) \psi(v, \zeta) \, dv \, d\mu(\zeta) \\ = \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} f(v, \zeta) f(v_*, \zeta_*) \psi(v', \zeta') B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) \, d\omega \, dv \, dv_* \, d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*)$$

where v' is defined by $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$. By using the same arguments as previously, we get

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_+(f, f)(v, \zeta) \psi(v, \zeta) \, dv \, d\mu(\zeta) \\ = \frac{1}{4} \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} \left(f(v', \zeta') f(v'_*, \zeta'_*) [\psi(v, \zeta) + \psi(v_*, \zeta_*)] + f(v, \zeta) f(v_*, \zeta_*) [\psi(v', \zeta') + \psi(v'_*, \zeta'_*)] \right)$$

$$B(\cdot) d\omega dv dv_* d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*).$$

where $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$. Putting the previous results together yields

$$\begin{aligned} \int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}(f, f)(v, \zeta) \psi(v, \zeta) dv d\mu(\zeta) &= -\frac{1}{4} \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} \left(f(v', \zeta') f(v'_*, \zeta'_*) - f(v, \zeta) f(v_*, \zeta_*) \right) \\ &\times \left[\psi(v', \zeta') + \psi(v'_*, \zeta'_*) - \psi(v, \zeta) - \psi(v_*, \zeta_*) \right] B(\cdot) d\omega dv dv_* d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*). \end{aligned}$$

□

2.3.4 Collision invariants

Definition 2.7. ψ is a collision invariant if and only if for μ -a.e. $\zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}$, a.e. $(v, v_*) \in E[\zeta, \zeta_*, \zeta', \zeta'_*]$ and a.e. $\omega \in \mathbb{S}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*]$,

$$\psi(v', \zeta') + \psi(v'_*, \zeta'_*) = \psi(v, \zeta) + \psi(v_*, \zeta_*), \quad (2.22)$$

where $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$.

First, we immediately deduce from the conservation laws (2.5) that if there exists $\alpha \in \mathbb{R}$, $\beta \in \mathbb{R}^3$ and $\gamma \in \mathbb{R}$ such that for a.e. $v \in \mathbb{R}^3$ and μ -a.e. $\zeta \in \mathcal{E}$,

$$\psi(v, \zeta) = \alpha + \beta \cdot v + \gamma \left(\frac{m}{2} |v|^2 + \varepsilon(\zeta) \right),$$

then ψ is a collision invariant. In this subsection, we prove that all collision invariants verifying a certain integrability assumption have this form.

Lemma 2.5. For all $\zeta \in \mathcal{E}$ and $\omega \in \mathbb{S}^2$,

$$S_\omega[\zeta, \zeta, \zeta, \zeta] \equiv \bar{S}_\omega : \begin{cases} \mathbb{R}^3 \times \mathbb{R}^3 & \longrightarrow & \mathbb{R}^3 \times \mathbb{R}^3 \\ (v, v_*) & \mapsto & \left(\frac{v+v_*}{2} + \frac{|v-v_*|}{2} T_\omega \left[\frac{v-v_*}{|v-v_*|} \right], \frac{v+v_*}{2} - \frac{|v-v_*|}{2} T_\omega \left[\frac{v-v_*}{|v-v_*|} \right] \right) \end{cases}$$

Proof. For any $v, v_* \in \mathbb{R}^3$,

$$\Delta(v, v_*, \zeta, \zeta, \zeta, \zeta) = \frac{1}{4} |v - v_*|^2 + \frac{1}{m} (\varepsilon(\zeta) + \varepsilon(\zeta) - \varepsilon(\zeta) - \varepsilon(\zeta)) = \frac{1}{4} |v - v_*|^2 \geq 0$$

so that

$$E[\zeta, \zeta, \zeta, \zeta] = \left\{ (v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3 \text{ s.t. } \Delta(v, v_*, \zeta, \zeta, \zeta, \zeta) \geq 0 \right\} = \mathbb{R}^3 \times \mathbb{R}^3.$$

Now let $(v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3$. We set $(v', v'_*) = S_\omega[\zeta, \zeta, \zeta, \zeta](v, v_*)$. Then

$$\begin{aligned} v' &= \frac{v+v_*}{2} + \sqrt{\Delta(\cdot)} T_\omega \left[\frac{v-v_*}{|v-v_*|} \right] \\ &= \frac{v+v_*}{2} + \frac{|v-v_*|}{2} T_\omega \left[\frac{v-v_*}{|v-v_*|} \right], \end{aligned}$$

and analogously

$$v'_* = \frac{v+v_*}{2} - \frac{|v-v_*|}{2} T_\omega \left[\frac{v-v_*}{|v-v_*|} \right].$$

Thus we indeed have

$$S_\omega[\zeta, \zeta, \zeta, \zeta] : \begin{cases} \mathbb{R}^3 \times \mathbb{R}^3 & \longrightarrow & \mathbb{R}^3 \times \mathbb{R}^3 \\ (v, v_*) & \mapsto & \left(\frac{v+v_*}{2} + \frac{|v-v_*|}{2} T_\omega \left[\frac{v-v_*}{|v-v_*|} \right], \frac{v+v_*}{2} - \frac{|v-v_*|}{2} T_\omega \left[\frac{v-v_*}{|v-v_*|} \right] \right). \end{cases}$$

□

The following Theorem 2.1 is the well-known characterization of collision invariants in the elastic case.

Theorem 2.1. *Let $r_0 > 0$ and $\phi \in L^1(\mathbb{R}^3, e^{-|v|^2/r_0} dv)$ such that for a.e. $(v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3$ and $\omega \in \mathbb{S}^2$,*

$$\phi(v'(v, v_*, \omega)) + \phi(v'_*(v, v_*, \omega)) = \phi(v) + \phi(v_*).$$

with $(v'(v, v_, \omega), v'_*(v, v_*, \omega)) = \bar{S}_\omega(v, v_*)$. Then there exists $(\alpha, \beta, \gamma) \in \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}$ such that for a.e. $v \in \mathbb{R}^3$,*

$$\phi(v) = \alpha + \beta \cdot v + \frac{\gamma}{2}|v|^2.$$

Proof. For the proof, we refer the reader to Bouchut and Golse [43], Chapter 2.

□

The following Theorem 2.2 characterises collision invariants in the general setting.

Theorem 2.2. *Let ψ be a collision invariant, such that for μ -a.e. $\zeta \in \mathcal{E}$ there exists $r_\zeta > 0$ such that $\psi(\cdot, \zeta) \in L^1(\mathbb{R}^3, e^{-|v|^2/r_\zeta} dv)$. Then there exists $(\alpha, \beta, \gamma) \in \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}$ such that for μ -a.e. $\zeta \in \mathcal{E}$ and a.e. $v \in \mathbb{R}^3$,*

$$\psi(v, \zeta) = \alpha + \beta \cdot v + \gamma \left(\frac{m}{2} |v|^2 + \varepsilon(\zeta) \right).$$

Proof. Let us denote by $\tilde{\mathcal{E}}$ the set such that $\mu(\mathcal{E} \setminus \tilde{\mathcal{E}}) = 0$, and for all $\zeta \in \tilde{\mathcal{E}}$, there exists $r_\zeta > 0$ such that $\psi(\cdot, \zeta) \in L^1(\mathbb{R}^3, e^{-|v|^2/r_\zeta} dv)$ and for all $\zeta_*, \zeta', \zeta'_* \in \tilde{\mathcal{E}}$, a.e. $(v, v_*) \in E[\zeta, \zeta_*, \zeta', \zeta'_*]$ and a.e. $\omega \in \mathbb{S}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*]$,

$$\psi(v', \zeta') + \psi(v'_*, \zeta'_*) = \psi(v, \zeta) + \psi(v_*, \zeta_*),$$

where (v', v'_*) are defined by $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$.

First, we consider the equality for $\zeta = \zeta_* = \zeta' = \zeta'_* \in \tilde{\mathcal{E}}$. From Lemma 2.5, Assumption 2.3 (in our framework, all angles are allowed in elastic collisions) and Theorem 2.1, there exists $(\alpha_\zeta, \beta_\zeta, \gamma_\zeta) \in \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}$ such that for a.e. $v \in \mathbb{R}^3$,

$$\psi(v, \zeta) = \alpha_\zeta + \beta_\zeta \cdot v + \gamma_\zeta \left(\frac{1}{2} |v|^2 \right). \quad (2.23)$$

Let us now consider again the equation (2.22), using formula (2.23), $\zeta = \zeta_* \in \tilde{\mathcal{E}}$ and $\zeta' = \zeta'_* \in \tilde{\mathcal{E}}$. It writes, for a.e. $(v, v_*) \in E[\zeta, \zeta, \zeta', \zeta']$ and a.e. $\omega \in \mathbb{S}^2[v, v_*, \zeta, \zeta, \zeta', \zeta']$,

$$2\alpha_\zeta + \beta_\zeta \cdot (v + v_*) + \gamma_\zeta \left(\frac{1}{2} |v|^2 + \frac{1}{2} |v_*|^2 \right) = 2\alpha_{\zeta'} + \beta_{\zeta'} \cdot (v' + v'_*) + \gamma_{\zeta'} \left(\frac{1}{2} |v'|^2 + \frac{1}{2} |v'_*|^2 \right)$$

where $(v', v'_*) = S_\omega[\zeta, \zeta, \zeta', \zeta'](v, v_*)$. By assumption 2.3, at fixed v, v_*, ζ, ζ' , the set of angles ω for which the above equation holds, $\mathbb{S}^2[v, v_*, \zeta, \zeta, \zeta', \zeta']$, is not negligible. Using the conservation equations

(2.5), we thus get for a.e. v, v_* such that $\frac{1}{4}|v - v_*|^2 \geq \frac{2}{m}(\varepsilon(\zeta') - \varepsilon(\zeta))$,

$$2\left(\alpha_\zeta - \alpha_{\zeta'} - \frac{\gamma_{\zeta'}}{m}(\varepsilon(\zeta') - \varepsilon(\zeta))\right) + (\beta_\zeta - \beta_{\zeta'}) \cdot (v + v_*) + (\gamma_\zeta - \gamma_{\zeta'})\left(\frac{1}{2}|v|^2 + \frac{1}{2}|v_*|^2\right) = 0.$$

The above is a polynomial in (v, v_*) vanishing on a non-empty open set of \mathbb{R}^6 , hence

$$\begin{aligned}\gamma_\zeta &= \gamma_{\zeta'} \\ \beta_\zeta &= \beta_{\zeta'} \\ \alpha_\zeta - \gamma_{\zeta'} \frac{\varepsilon(\zeta)}{m} &= \alpha_{\zeta'} - \gamma_{\zeta'} \frac{\varepsilon(\zeta')}{m}.\end{aligned}$$

We conclude that there exists $(\alpha, \beta, \gamma) \in \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}$ such that for a.e. $v \in \mathbb{R}^3$ and for all $\zeta \in \tilde{\mathcal{E}}$ (thus μ -a.e. $\zeta \in \mathcal{E}$),

$$\psi(v, \zeta) = \alpha + \beta \cdot v + \gamma \left(\frac{m}{2}|v|^2 + \varepsilon(\zeta)\right).$$

□

2.4 H Theorem and collision equilibria

Theorem 2.3. H Theorem. *Let $f : \mathbb{R}^3 \times \mathcal{E} \rightarrow \mathbb{R}_+$ be a measurable function such that for a.e. $v \in \mathbb{R}^3$ and μ -a.e. $\zeta \in \mathcal{E}$, $f(v, \zeta) > 0$. We assume that*

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_-(f, f)(v, \zeta) |\ln(f)(v, \zeta)| \, dv \, d\mu(\zeta) + \int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}_+(f, f)(v, \zeta) |\ln(f)(v, \zeta)| \, dv \, d\mu(\zeta) < \infty.$$

Then

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}(f, f)(v, \zeta) \ln(f)(v, \zeta) \, dv \, d\mu(\zeta) \leq 0, \quad (2.24)$$

and

$$\begin{aligned}\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}(f, f)(v, \zeta) \ln(f)(v, \zeta) \, dv \, d\mu(\zeta) &= 0 \\ \Downarrow \\ \mathcal{B}(f, f)(v, \zeta) &= 0 \text{ for a.e. } v \in \mathbb{R}^3 \text{ and } \mu\text{-a.e. } \zeta \in \mathcal{E} \\ \Downarrow \\ \ln(f) &\text{ is a collision invariant.}\end{aligned}$$

Proof. This proof is highly inspired by a proof which can be found in [43], Chapter 2. First we define, for μ -a.e. $\zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}$, a.e. $(v, v_*) \in E[\zeta, \zeta_*, \zeta', \zeta'_*]$ and a.e. $\omega \in \mathbb{S}^2$,

$$\mathcal{P}[f](v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) := \frac{1}{4}(f(v', \zeta')f(v'_*, \zeta'_*) - f(v, \zeta)f(v_*, \zeta_*)) \ln\left(\frac{f(v', \zeta')f(v'_*, \zeta'_*)}{f(v, \zeta)f(v_*, \zeta_*)}\right),$$

where $(v', v'_*) = S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$. Now by remarking that

$$\forall x > 0, \quad (x - 1)\ln(x) \geq 0,$$

we have, since $f > 0$ and considering $x = \frac{f(v', \zeta') f(v_*, \zeta'_*)}{f(v, \zeta) f(v_*, \zeta_*)} > 0$,

$$\mathcal{P}[f](v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) = \frac{1}{4} f(v, \zeta) f(v_*, \zeta_*) (x - 1) \ln(x) \geq 0.$$

Using Proposition 2.4 with $\psi = \ln(f)$,

$$\begin{aligned} & \int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}(f, f)(v, \zeta) \ln(f)(v, \zeta) \, dv \, d\mu(\zeta) \\ &= - \iiint_{\mathcal{E}^4} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} \mathcal{P}[f](v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) B(\cdot) \, d\omega \, dv \, dv_* \, d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*). \end{aligned}$$

Now from $b \geq 0$ and $\mathcal{P}[f] \geq 0$,

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}(f, f)(v, \zeta) \ln(f)(v, \zeta) \, dv \, d\mu(\zeta) \leq 0.$$

Let us now focus on the case of equality. Since the integrand $\mathcal{P}[f]b$ is non-negative, it must be equal to zero.

$$\begin{aligned} & \int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}(f, f)(v, \zeta) \ln(f)(v, \zeta) \, dv \, d\mu(\zeta) = 0 \\ \implies & \iiint_{\mathcal{E}^4} \iint_{E[\zeta, \zeta_*, \zeta', \zeta'_*]} \int_{\mathbb{S}^2} \mathcal{P}[f](v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) B(\cdot) \, d\omega \, dv \, dv_* \, d\mu^{\otimes 4}(\zeta, \zeta_*, \zeta', \zeta'_*) = 0 \\ \implies & \mathcal{P}[f](v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) = 0 \quad \text{for a.e. } v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega \\ \implies & \mathcal{P}[f](v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) = 0 \quad \text{for } \mu\text{-a.e. } \zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}, \text{ a.e. } (v, v_*) \in E[\zeta, \zeta_*, \zeta', \zeta'_*] \\ & \text{and a.e. } \omega \in \mathbb{S}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*], \end{aligned}$$

where we recall that the set $\mathbb{S}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*]$ is defined by Definition 2.3. Now since $f > 0$ and

$$\forall x > 0, \quad (x - 1) \ln(x) = 0 \implies x = 1,$$

we finally obtain, writing \cdot in place of $v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*$ to lighten the notations,

$$\begin{aligned} & \mathcal{P}[f](\cdot, \omega) = 0 \quad \text{for } \mu\text{-a.e. } \zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}, \text{ a.e. } (v, v_*) \in E[\zeta, \zeta_*, \zeta', \zeta'_*] \text{ and a.e. } \omega \in \mathbb{S}^2[\cdot] \\ \implies & f' f'_* = f f_* \quad \text{for } \mu\text{-a.e. } \zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}, \text{ a.e. } (v, v_*) \in E[\zeta, \zeta_*, \zeta', \zeta'_*], \text{ a.e. } \omega \in \mathbb{S}^2[\cdot] \\ \implies & \ln(f) \text{ is a collision invariant.} \end{aligned}$$

Note also that

$$\begin{aligned} & \ln(f) \text{ is a collision invariant} \\ \implies & f' f'_* = f f_* \quad \text{for } \mu\text{-a.e. } \zeta, \zeta_*, \zeta', \zeta'_* \in \mathcal{E}, \text{ a.e. } (v, v_*) \in E[\zeta, \zeta_*, \zeta', \zeta'_*], \text{ a.e. } \omega \in \mathbb{S}^2[\cdot] \\ \implies & \mathcal{B}(f, f)(v, \zeta) = 0 \quad \text{for a.e. } v \in \mathbb{R}^3 \text{ and } \mu\text{-a.e. } \zeta \in \mathcal{E} \\ \implies & \int_{\mathcal{E}} \int_{\mathbb{R}^3} \mathcal{B}(f, f)(v, \zeta) \ln(f)(v, \zeta) \, dv \, d\mu(\zeta) = 0, \end{aligned}$$

which ends the proof. □

Let us assume that there exists $f \in L^1(\mathbb{R}^3 \times \mathcal{E}, dv d\mu(\zeta))$ such that f verifies assumptions of Theorem 2.3 and $\ln(f)$ verifies the hypotheses of Theorem 2.2. From Theorem 2.2, $\exists(\alpha, \beta, \gamma) \in \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}$ such that for a.e. $v \in \mathbb{R}^3$ and μ -a.e. $\zeta \in \mathcal{E}$,

$$\ln(f)(v, \zeta) = \alpha + \beta \cdot v + \gamma \left(\frac{m}{2} |v|^2 + \varepsilon(\zeta) \right).$$

Since $f \in L^1(\mathbb{R}^3 \times \mathcal{E}, dv d\mu(\zeta))$, we have $\gamma < 0$. Let us now set

$$T = -\frac{1}{k_B \gamma}, \quad u = -\frac{\beta}{m \gamma}, \quad A = \exp \left(\alpha - \frac{|\beta|^2}{2m\gamma} \right),$$

where k_B is the Boltzmann constant. Then

$$f(v, \zeta) = A \exp \left(-\frac{m|v - u|^2}{2k_B T} - \frac{\varepsilon(\zeta)}{k_B T} \right).$$

and it can be easily checked that u is the average velocity of f , while T will provide its temperature (see below). Note that indeed $f \in L^1(\mathbb{R}^3 \times \mathcal{E}, dv d\mu(\zeta))$ thanks to Assumption 2.2. We define the density ρ

$$\rho := \int_{\mathcal{E}} \int_{\mathbb{R}^3} m f(v, \zeta) dv d\mu(\zeta).$$

Then, almost everywhere,

$$f = \mathcal{M}[\rho, u, T],$$

where, for all $(v, \zeta) \in \mathbb{R}^3 \times \mathcal{E}$,

$$\mathcal{M}[\rho, u, T](v, \zeta) := \frac{\rho}{m} \frac{\exp \left(-\frac{m|v - u|^2}{2k_B T} - \frac{\varepsilon(\zeta)}{k_B T} \right)}{\left(\frac{2\pi k_B T}{m} \right)^{3/2} \int_{\mathcal{E}} \exp \left(-\frac{\varepsilon(\zeta_*)}{k_B T} \right) d\mu(\zeta_*)},$$

which we can rewrite

$$\mathcal{M}[\rho, u, T](v, \zeta) = \rho m^{1/2} (2\pi k_B T)^{-3/2} Z \left(\frac{1}{k_B T} \right)^{-1} \exp \left(-\frac{m|v - u|^2}{2k_B T} - \frac{\bar{\varepsilon}(\zeta)}{k_B T} \right), \quad (2.25)$$

where $\bar{\varepsilon}$ and Z are defined by equations (2.2) and (2.3).

First, note that by definition of ρ ,

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} m \mathcal{M}[\rho, u, T](v, \zeta) dv d\mu(\zeta) = \rho > 0.$$

Also,

$$\frac{1}{\rho} \int_{\mathcal{E}} \int_{\mathbb{R}^3} m v \mathcal{M}[\rho, u, T](v, \zeta) dv d\mu(\zeta) = m^{3/2} (2\pi k_B T)^{-3/2} \int_{\mathbb{R}^3} v \exp \left(-\frac{m|v - u|^2}{2k_B T} \right) dv = u.$$

The total energy density at collision equilibrium writes

$$\begin{aligned} e^{eq}[u, T] &:= \frac{m}{\rho} \int_{\mathcal{E}} \int_{\mathbb{R}^3} \left(\frac{m}{2} |v|^2 + \varepsilon(\zeta) \right) \mathcal{M}[\rho, u, T](v, \zeta) \, \mathrm{d}v \, \mathrm{d}\mu(\zeta) \\ &= m^{3/2} (2\pi k_B T)^{-3/2} \int_{\mathbb{R}^3} \frac{m}{2} |v|^2 \exp\left(-\frac{m|v-u|^2}{2k_B T}\right) \, \mathrm{d}v + \frac{\int_{\mathcal{E}} \varepsilon(\zeta) \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) \, \mathrm{d}\mu(\zeta)}{\int_{\mathcal{E}} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) \, \mathrm{d}\mu(\zeta)}, \end{aligned}$$

and is finite thanks to Assumption 2.2 and Proposition 2.1. The term associated with the velocity is well-known, and a classical computation gives

$$m^{3/2} (2\pi k_B T)^{-3/2} \int_{\mathbb{R}^3} \frac{m}{2} |v|^2 \exp\left(-\frac{m|v-u|^2}{2k_B T}\right) \, \mathrm{d}v = \frac{m}{2} |u|^2 + \frac{3}{2} k_B T.$$

Remark that

$$\frac{\int_{\mathcal{E}} \varepsilon(\zeta) \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) \, \mathrm{d}\mu(\zeta)}{\int_{\mathcal{E}} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) \, \mathrm{d}\mu(\zeta)} = \varepsilon^0 + \frac{\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) \, \mathrm{d}\mu(\zeta)}{\int_{\mathcal{E}} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) \, \mathrm{d}\mu(\zeta)},$$

where we recall that $\varepsilon^0 = \inf \operatorname{ess}_{\mu} \{\varepsilon\}$ and $\bar{\varepsilon} = \varepsilon - \varepsilon^0$, see equation (2.2).

Definition 2.8. We define the (thermodynamic) number of internal degrees of freedom δ by

$$\delta(T) := \frac{2}{k_B T} \left(\frac{\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) \, \mathrm{d}\mu(\zeta)}{\int_{\mathcal{E}} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) \, \mathrm{d}\mu(\zeta)} \right). \quad (2.26)$$

We notice that, since $\bar{\varepsilon} \geq 0$ μ -a.e., $\delta \geq 0$.

The total energy density at collision equilibrium finally writes

$$e^{eq}[u, T] = \varepsilon^0 + \frac{m}{2} |u|^2 + \frac{3 + \delta(T)}{2} k_B T.$$

$3 + \delta(T)$ is the *total* (thermodynamic) number of degrees of freedom at temperature T , provided by the sum of the 3 translational degrees of freedom and of the number of internal ones $\delta(T)$.

Definition 2.9. We define the specific heat at constant volume c_V , for all $T > 0$,

$$c_V(T) := \frac{3 + D(T)}{2}, \quad (2.27)$$

where

$$D(T) := \frac{\mathrm{d}(T\delta(T))}{\mathrm{d}T}.$$

Remark 2.3. We recall that, from Proposition 2.1, the partition function Z defined by equation (2.3) is \mathcal{C}^∞ . Remarking that

$$T\delta(T) = -\frac{2}{k_B} (\ln(Z))' \left(\frac{1}{k_B T} \right),$$

then the function $T \mapsto T\delta(T)$ is C^∞ on \mathbb{R}_+^* and D is thus well-defined.

In the following propositions we show various mathematical properties of the function $\delta(T)$.

Proposition 2.6. *If $\mu(\varepsilon = \varepsilon^0) > 0$, then*

$$\delta(T) \xrightarrow{T \rightarrow 0^+} 0 \quad \text{and} \quad D(T) \xrightarrow{T \rightarrow 0^+} 0.$$

Proof. First, note that $\mu(\varepsilon = \varepsilon^0) > 0 \implies \mu(\bar{\varepsilon} = 0) > 0$. Since μ -a.e., $\bar{\varepsilon} \geq 0$, we then have for $k \in \mathbb{N}$

$$\int_{\mathcal{E}} \left(\frac{\bar{\varepsilon}}{k_B T} \right)^k \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) d\mu(\zeta) = \mathbf{1}_{k=0} \times \mu(\bar{\varepsilon} = 0) + \int_{\bar{\varepsilon} > 0} \left(\frac{\bar{\varepsilon}}{k_B T} \right)^k \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) d\mu(\zeta).$$

Now remark that for all $y > 0$, $e^{y/2} \geq 1 + \frac{y}{2} + \frac{y^2}{8}$. Thus

$$ye^{-y} \leq 2e^{-y/2} \quad \text{and} \quad y^2 e^{-y} \leq 8e^{-y/2}.$$

Thus it comes

$$\begin{aligned} \delta(T) &= 2 \frac{\int_{\mathcal{E}} \frac{\bar{\varepsilon}}{k_B T} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) d\mu(\zeta)}{\int_{\mathcal{E}} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) d\mu(\zeta)} \leq 2 \frac{\int_{\bar{\varepsilon} > 0} \frac{\bar{\varepsilon}}{k_B T} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) d\mu(\zeta)}{\mu(\bar{\varepsilon} = 0)} \\ &\leq \frac{4}{\mu(\bar{\varepsilon} = 0)} \int_{\bar{\varepsilon} > 0} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{2k_B T}\right) d\mu(\zeta). \end{aligned}$$

We can prove that (see proof of Proposition 2.8) $0 \leq D(T) \leq 2 \frac{\int_{\mathcal{E}} \left(\frac{\bar{\varepsilon}}{k_B T}\right)^2 \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) d\mu(\zeta)}{\int_{\mathcal{E}} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) d\mu(\zeta)}$, which

implies

$$0 \leq D(T) \leq 2 \frac{\int_{\bar{\varepsilon} > 0} \left(\frac{\bar{\varepsilon}}{k_B T}\right)^2 \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) d\mu(\zeta)}{\mu(\bar{\varepsilon} = 0)} \leq \frac{16}{\mu(\bar{\varepsilon} = 0)} \int_{\bar{\varepsilon} > 0} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{2k_B T}\right) d\mu(\zeta).$$

Now for all $\zeta \in \{\bar{\varepsilon} > 0\}$, $e^{-x\bar{\varepsilon}(\zeta)} \xrightarrow{x \rightarrow \infty} 0$. Since $(\zeta \mapsto e^{-x\bar{\varepsilon}(\zeta)})_{x>0}$ is a non-decreasing family of positive functions, we get by monotone convergence

$$\int_{\bar{\varepsilon} > 0} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \xrightarrow{x \rightarrow \infty} 0.$$

It follows that $\int_{\bar{\varepsilon} > 0} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{2k_B T}\right) d\mu(\zeta) \xrightarrow{T \rightarrow 0^+} 0$, and thus, since $\mu(\bar{\varepsilon} = 0) > 0$,

$$0 \leq \delta(T) \leq \frac{4}{\mu(\bar{\varepsilon} = 0)} \int_{\bar{\varepsilon} > 0} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{2k_B T}\right) d\mu(\zeta) \xrightarrow{T \rightarrow 0^+} 0$$

and

$$0 \leq D(T) \leq \frac{16}{\mu(\bar{\varepsilon} = 0)} \int_{\bar{\varepsilon} > 0} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{2k_B T}\right) d\mu(\zeta) \xrightarrow{T \rightarrow 0^+} 0,$$

so that finally

$$\delta(T) \xrightarrow{T \rightarrow 0^+} 0 \quad \text{and} \quad D(T) \xrightarrow{T \rightarrow 0^+} 0.$$

□

Proposition 2.7. *For all $T > 0$,*

$$\delta(T) = \frac{1}{T} \int_0^T D(T') dT'.$$

Proof. We have for $T_1, T_2 > 0$, $\int_{T_1}^{T_2} D(T') dT' = T_2 \delta(T_2) - T_1 \delta(T_1)$. We thus want to prove that $T \delta(T) \xrightarrow{T \rightarrow 0^+} 0$. We proceed by disjunction of case. First, if $\mu(\varepsilon = \varepsilon^0) > 0$, then from Proposition 2.6, $\delta(T) \xrightarrow{T \rightarrow 0^+} 0$, so we also have $T \delta(T) \xrightarrow{T \rightarrow 0^+} 0$. If on the other hand $\mu(\varepsilon = \varepsilon^0) = 0$, then since $\varepsilon^0 = \inf \text{ess}_\mu \{\varepsilon\}$, we have $\mu(0 < \bar{\varepsilon} \leq r) = \mu(\varepsilon^0 < \varepsilon \leq \varepsilon^0 + r) > 0$ for all $r > 0$. Then from Lemma 2.19 in Appendix, for all $r > 0$,

$$\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \underset{x \rightarrow \infty}{\sim} \int_{\bar{\varepsilon} \leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) + o\left(\int_{\bar{\varepsilon} \leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)\right),$$

and

$$\int_{\mathcal{E}} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \underset{x \rightarrow \infty}{\sim} \int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) + o\left(\int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)\right).$$

Since $\mu(\{0 < \bar{\varepsilon} \leq r\}) > 0$ and $\bar{\varepsilon} \geq 0$ μ -a.e., $\int_{\bar{\varepsilon} \leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) > 0$, so that

$$\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \underset{x \rightarrow \infty}{\sim} \int_{\bar{\varepsilon} \leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta).$$

Also, $\mu(\{\bar{\varepsilon} \leq r\}) > 0$ implies $\int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) > 0$, so that

$$\int_{\mathcal{E}} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \underset{x \rightarrow \infty}{\sim} \int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta).$$

Hence

$$\frac{\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)}{\int_{\mathcal{E}} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)} \underset{x \rightarrow \infty}{\sim} \frac{\int_{\bar{\varepsilon} \leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)}{\int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)}.$$

Thus there exists $x_r > 0$ such that for all $x \geq x_r$,

$$0 \leq \frac{\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)}{\int_{\mathcal{E}} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)} \leq 2 \frac{\int_{\bar{\varepsilon} \leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)}{\int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)} \leq 2r.$$

Since it is true for all $r > 0$, we finally get

$$\frac{\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)}{\int_{\mathcal{E}} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)} \xrightarrow{x \rightarrow \infty} 0.$$

It follows that in any case

$$T\delta(T) = \frac{2}{k_B} \frac{\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) e^{-\frac{\bar{\varepsilon}(\zeta)}{k_B T}} d\mu(\zeta)}{\int_{\mathcal{E}} e^{-\frac{\bar{\varepsilon}(\zeta)}{k_B T}} d\mu(\zeta)} \xrightarrow{T \rightarrow 0^+} 0.$$

□

Remark 2.4. This Proposition 2.7 along with Remark 2.3 justify our choice to define the partition function by $\int_{\mathcal{E}} e^{-\beta \bar{\varepsilon}(\zeta)} d\mu(\zeta)$ (with $\bar{\varepsilon}$) instead of simply $\int_{\mathcal{E}} e^{-\beta \varepsilon(\zeta)} d\mu(\zeta)$ (with ε). Indeed, if the second definition were taken, and δ were still defined by $-\frac{2}{k_B T} (\ln(Z))' \left(\frac{1}{k_B T}\right)$, then $\varepsilon^0 \neq 0$ would imply $\delta(T) \underset{T \rightarrow 0}{\sim} \frac{2\varepsilon^0}{k_B T}$, which is non-physical. On the other hand, choosing $\bar{\varepsilon}$ in the definition always yields $T\delta(T) \xrightarrow{T \rightarrow 0} 0$, and thus the formula $\delta(T) = \frac{1}{T} \int_0^T D(T') dT'$, which is physically coherent.

As a consequence of Proposition 2.7, the total energy at the equilibrium may be cast as

$$e^{eq}[u, T] = \varepsilon^0 + \frac{m}{2} |u|^2 + \int_0^T c_V(T') k_B dT'.$$

A probabilistic interpretation may also be provided for the functions $\delta(T)$ and $D(T)$. Indeed, for $T > 0$, we define the Gibbs (probability) measure ν_T on $(\mathcal{E}, \mathcal{A})$ by

$$\frac{d\nu_T}{d\mu}(\zeta) = Z \left(\frac{1}{k_B T} \right)^{-1} \exp \left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T} \right), \quad (2.28)$$

where Z is the partition function defined by equation (2.3); then for all $T > 0$, $(\mathcal{E}, \mathcal{A}, \nu_T)$ is a probability space. Since $\bar{\varepsilon} : \mathcal{E} \rightarrow \mathbb{R}$ is $(\mathcal{A}, \text{Bor}(\mathbb{R}))$ -measurable, it is a real random variable on $(\mathcal{E}, \mathcal{A}, \nu_T)$.

Proposition 2.8. For all $T > 0$,

$$\delta(T) = 2 \mathbb{E}_{\nu_T} \left[\frac{\bar{\varepsilon}}{k_B T} \right], \quad (2.29)$$

and

$$D(T) = 2 \text{Var}_{\nu_T} \left[\frac{\bar{\varepsilon}}{k_B T} \right], \quad (2.30)$$

where \mathbb{E}_{ν_T} and Var_{ν_T} are respectively the expectation and the variance under the probability ν_T .

Proof. The following computations are possible thanks to Assumption 2.2. The first part of the proposition comes from

$$\frac{\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) \exp \left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T} \right) d\mu(\zeta)}{\int_{\mathcal{E}} \exp \left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T} \right) d\mu(\zeta)} = \int_{\mathcal{E}} \bar{\varepsilon}(\zeta) Z \left(\frac{1}{k_B T} \right)^{-1} \exp \left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T} \right) d\mu(\zeta) = \int_{\mathcal{E}} \bar{\varepsilon}(\zeta) d\nu_T(\zeta) = \mathbb{E}_{\nu_T}[\bar{\varepsilon}].$$

For equation (2.30), we remark that from Proposition 2.1,

$$\mathbb{E}_{\nu_T}[\bar{\varepsilon}] = \frac{\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) \exp \left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T} \right) d\mu(\zeta)}{\int_{\mathcal{E}} \exp \left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T} \right) d\mu(\zeta)} = \frac{-Z' \left(\frac{1}{k_B T} \right)}{Z \left(\frac{1}{k_B T} \right)},$$

$$\mathbb{E}_{\nu_T} [\bar{\varepsilon}^2] = \frac{\int_{\mathcal{E}} \bar{\varepsilon}(\zeta)^2 \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) d\mu(\zeta)}{\int_{\mathcal{E}} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) d\mu(\zeta)} = \frac{Z''\left(\frac{1}{k_B T}\right)}{Z\left(\frac{1}{k_B T}\right)}.$$

It follows that

$$\begin{aligned} D(T) &= 2 \frac{d}{k_B dT} \left(\frac{-Z'\left(\frac{1}{k_B T}\right)}{Z\left(\frac{1}{k_B T}\right)} \right) = \frac{2}{(k_B T)^2} \left(\frac{Z''\left(\frac{1}{k_B T}\right)}{Z\left(\frac{1}{k_B T}\right)} - \left(\frac{-Z'\left(\frac{1}{k_B T}\right)}{Z\left(\frac{1}{k_B T}\right)} \right)^2 \right) \\ &= \frac{2}{(k_B T)^2} (\mathbb{E}_{\nu_T} [\bar{\varepsilon}^2] - (\mathbb{E}_{\nu_T} [\bar{\varepsilon}])^2) = \frac{2}{(k_B T)^2} \text{Var}_{\nu_T} [\bar{\varepsilon}] = 2 \text{Var}_{\nu_T} \left[\frac{\bar{\varepsilon}}{k_B T} \right]. \end{aligned}$$

□

Corollary 2.9. For all $T > 0$, $D(T) \geq 0$.

Proof. It is an immediate consequence of Proposition 2.8.

□

Corollary 2.10. If there exists $R \in \mathbb{R}$ such that $\varepsilon \leq R$ μ -a.e., then

$$\delta(T) \xrightarrow{T \rightarrow \infty} 0, \quad \text{and} \quad D(T) \xrightarrow{T \rightarrow \infty} 0.$$

Proof. Necessarily $R \geq \varepsilon^0$, and from Proposition 2.8

$$0 \leq \delta(T) = 2 \mathbb{E}_{\nu_T} \left[\frac{\bar{\varepsilon}}{k_B T} \right] \leq \frac{2(R - \varepsilon^0)}{k_B T} \xrightarrow{T \rightarrow \infty} 0,$$

and

$$0 \leq D(T) = 2 \text{Var}_{\nu_T} \left[\frac{\bar{\varepsilon}}{k_B T} \right] \leq 2 \mathbb{E}_{\nu_T} \left[\left(\frac{\bar{\varepsilon}}{k_B T} \right)^2 \right] \leq \frac{2(R - \varepsilon^0)^2}{(k_B T)^2} \xrightarrow{T \rightarrow \infty} 0.$$

□

We define now the function Θ , for all $T \in \mathbb{R}_+^*$, as

$$\Theta(T) := \int_0^T c_V(T') k_B dT', \quad (2.31)$$

such that

$$e^{eq}[u, T] = \varepsilon^0 + \frac{m}{2} |u|^2 + \Theta(T).$$

Proposition 2.11. Θ is continuous on \mathbb{R}_+^* , can be extended by continuity to \mathbb{R}_+ , setting $\Theta(0) = 0$, increasing on \mathbb{R}_+ , with $\Theta(T) \xrightarrow{T \rightarrow \infty} \infty$, and thus a bijection from \mathbb{R}_+ to \mathbb{R}_+ .

Proof. The result is immediate, since from Corollary 2.9 we have $c_V \geq \frac{3}{2}$.

□

We then have

$$T = \Theta^{-1} \left(\frac{m}{\rho} \int_{\mathcal{E}} \int_{\mathbb{R}^3} \left(\frac{m}{2} |v - u|^2 + \bar{\varepsilon}(\zeta) \right) f(v, \zeta) \, dv \, d\mu(\zeta) \right),$$

which explains and rigorously justifies the definition of temperature stated in equation (2.13).

2.5 Euler limit

Let us assume that there exists f solution to the Boltzmann equation (2.12) such that for all t, x , $f(t, x, \cdot, \cdot)$ is a Maxwellian, that is

$$f(t, x, v, \zeta) = \mathcal{M}[\rho(t, x), u(t, x), T(t, x)](v, \zeta).$$

Since

$$\partial_t f(t, x, v, \zeta) + v \cdot \nabla_x f(t, x, v, \zeta) = \mathcal{B}(f, f)(t, x, v, \zeta)$$

and

$$\int_{\mathcal{E}} \int_{\mathbb{R}^3} \begin{pmatrix} m \\ mv \\ \frac{m}{2} |v|^2 + \varepsilon(\zeta) \end{pmatrix} \mathcal{B}(f, f)(t, x, v, \zeta) \, dv \, d\mu(\zeta) = 0,$$

we have

$$\begin{aligned} \partial_t \left(\int_{\mathcal{E}} \int_{\mathbb{R}^3} m f(t, x, v, \zeta) \, dv \, d\mu(\zeta) \right) + \operatorname{div}_x \left(\int_{\mathcal{E}} \int_{\mathbb{R}^3} m v f(t, x, v, \zeta) \, dv \, d\mu(\zeta) \right) &= 0 \\ \partial_t \left(\int_{\mathcal{E}} \int_{\mathbb{R}^3} m v f(t, x, v, \zeta) \, dv \, d\mu(\zeta) \right) + \operatorname{div}_x \left(\int_{\mathcal{E}} \int_{\mathbb{R}^3} m v \otimes v f(t, x, v, \zeta) \, dv \, d\mu(\zeta) \right) &= 0 \\ \partial_t \left(\int_{\mathcal{E}} \int_{\mathbb{R}^3} \left(\frac{m}{2} |v|^2 + \varepsilon(\zeta) \right) f(t, x, v, \zeta) \, dv \, d\mu(\zeta) \right) + \operatorname{div}_x \left(\int_{\mathcal{E}} \int_{\mathbb{R}^3} v \left(\frac{m}{2} |v|^2 + \varepsilon(\zeta) \right) f(t, x, v, \zeta) \, dv \, d\mu(\zeta) \right) &= 0. \end{aligned}$$

Since $f(t, x, v, \zeta) = \mathcal{M}[\rho(t, x), u(t, x), T(t, x)](v, \zeta)$, we have from the definitions of mass, momentum, and total energy

$$\begin{aligned} \partial_t \rho + \operatorname{div}_x (\rho u) &= 0 \\ \partial_t (\rho u) + \operatorname{div}_x \left(\int_{\mathcal{E}} \int_{\mathbb{R}^3} m v \otimes v \mathcal{M}[\rho, u, T](v, \zeta) \, dv \, d\mu(\zeta) \right) &= 0 \\ \partial_t \left(\rho \varepsilon^0 + \frac{1}{2} \rho |u|^2 + \frac{\rho}{m} \frac{3 + \delta(T)}{2} k_B T \right) + \operatorname{div}_x \left(\int_{\mathcal{E}} \int_{\mathbb{R}^3} v \left(\frac{m}{2} |v|^2 + \varepsilon(\zeta) \right) \mathcal{M}[\rho, u, T](v, \zeta) \, dv \, d\mu(\zeta) \right) &= 0. \end{aligned}$$

We are left with two terms to compute. First, by a classical argument (see [43], Chapter 2),

$$\begin{aligned} \int_{\mathcal{E}} \int_{\mathbb{R}^3} m v \otimes v \mathcal{M}[\rho, u, T](v, \zeta) \, dv \, d\mu(\zeta) &= \rho m^{1/2} (2\pi k_B T)^{-3/2} \int_{\mathbb{R}^3} m v \otimes v \exp \left(-\frac{m |v - u|^2}{2k_B T} \right) \, dv \\ &= \rho u \otimes u + \frac{\rho}{m} k_B T \mathbf{I}_d, \end{aligned}$$

where \mathbf{I}_d is the identity matrix. Also by a classical argument,

$$\begin{aligned}
& \int_{\mathcal{E}} \int_{\mathbb{R}^3} v \left(\frac{m}{2} |v|^2 + \varepsilon(\zeta) \right) \mathcal{M}[\rho, u, T](v, \zeta) \, dv \, d\mu(\zeta) \\
&= \rho m^{1/2} (2\pi k_B T)^{-3/2} \int_{\mathbb{R}^3} v \frac{m}{2} |v|^2 \exp\left(-\frac{m|v-u|^2}{2k_B T}\right) \, dv + \int_{\mathcal{E}} \int_{\mathbb{R}^3} v \varepsilon(\zeta) \mathcal{M}[\rho, u, T](v, \zeta) \, dv \, d\mu(\zeta) \\
&= \frac{1}{2} \rho |u|^2 u + \frac{\rho}{m} k_B T u + \frac{\rho}{m} \frac{3}{2} k_B T u + \frac{\rho}{m} \left(\frac{\int_{\mathcal{E}} \varepsilon(\zeta) \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) \, d\mu(\zeta)}{\int_{\mathcal{E}} \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) \, d\mu(\zeta)} \right) u \\
&= \frac{1}{2} \rho |u|^2 u + \frac{\rho}{m} k_B T u + \frac{\rho}{m} \frac{3 + \delta(T)}{2} k_B T u + \frac{\rho}{m} \varepsilon^0 u.
\end{aligned}$$

We set

$$p(t, x) := \frac{\rho}{m} k_B T(t, x) \quad \text{and} \quad \theta(t, x) := \frac{3 + \delta(T(t, x))}{2} k_B T(t, x).$$

Remarking that $\partial_t(\rho \varepsilon^0) + \operatorname{div}_x(\rho \varepsilon^0 u) = \varepsilon^0(\partial_t \rho + \operatorname{div}_x(\rho u)) = 0$, we obtain the compressible Euler set of equations, with ρ the density, u the velocity, p the pressure and θ the specific internal energy density.

$$\left\{ \begin{array}{l} \partial_t \rho + \operatorname{div}_x(\rho u) = 0 \\ \partial_t(\rho u) + \operatorname{div}_x(\rho u \otimes u) + \nabla_x p = 0 \\ \partial_t \left(\frac{1}{2} \rho |u|^2 + \frac{\rho}{m} \theta \right) + \operatorname{div}_x \left(\frac{1}{2} \rho |u|^2 u + \frac{\rho}{m} \theta u + p u \right) = 0. \end{array} \right. \quad (2.32)$$

2.6 Equipartition Theorem

In this section we show how is possible to combine different measure spaces of internal states into a unique kinetic model for the considered polyatomic gas.

Theorem 2.4. Equipartition Theorem. *Let $L \in \mathbb{N}^*$. Consider $(\mathcal{E}_l, \mathcal{A}_l, \mu_l)_{1 \leq l \leq L}$, and for all $1 \leq l \leq L$, $\varepsilon_l : (\mathcal{E}_l, \mathcal{A}_l) \rightarrow (\mathbb{R}, \operatorname{Bor}(\mathbb{R}))$ measurable such that Assumptions 2.1 and 2.2 hold for all (μ_l, ε_l) . Let us define*

$$\mathcal{E} = \mathcal{E}_1 \times \cdots \times \mathcal{E}_L, \quad \mathcal{A} = \mathcal{A}_1 \otimes \cdots \otimes \mathcal{A}_L, \quad \mu = \mu_1 \otimes \cdots \otimes \mu_L$$

and

$$\forall \zeta = (\zeta_1, \dots, \zeta_L) \in \mathcal{E}, \quad \varepsilon(\zeta) = \sum_{l=1}^L \varepsilon_l(\zeta_l).$$

Then Assumptions 2.1 and 2.2 hold for (μ, ε) , and for all $T > 0$, the Gibbs measure defined in (2.28) turns out to be

$$\nu_T = \nu_T^1 \otimes \cdots \otimes \nu_T^L$$

and moreover one has

$$\delta(T) = \sum_{l=1}^L \delta_l(T), \quad D(T) = \sum_{l=1}^L D_l(T).$$

Proof. Let $T > 0$. Let us first prove that $\nu_T = \nu_T^1 \otimes \cdots \otimes \nu_T^L$. We first remark that $\bar{\varepsilon}(\zeta) = \sum_{l=1}^L \bar{\varepsilon}_l(\zeta_l)$.

Let $A = (A_1, \dots, A_L) \in \mathcal{A}_1 \times \dots \times \mathcal{A}_L$. Then

$$\begin{aligned} \int_A \exp\left(-\frac{\bar{\varepsilon}(\zeta)}{k_B T}\right) d\mu(\zeta) &= \int_{A_1} \dots \int_{A_L} \left(\exp\left(-\frac{\sum_{l=1}^L \bar{\varepsilon}_l(\zeta_l)}{k_B T}\right) \right) d\mu_1(\zeta_1) \dots d\mu_L(\zeta_L) \\ &= \int_{A_1} \dots \int_{A_L} \left(\prod_{l=1}^L \exp\left(-\frac{\bar{\varepsilon}_l(\zeta_l)}{k_B T}\right) \right) d\mu_1(\zeta_1) \dots d\mu_L(\zeta_L) \\ &= \prod_{l=1}^L \int_{A_l} \exp\left(-\frac{\bar{\varepsilon}_l(\zeta_l)}{k_B T}\right) d\mu_l(\zeta_l). \end{aligned}$$

Since this also holds for $A = \mathcal{E} = \mathcal{E}_1 \times \dots \times \mathcal{E}_L$, we then have

$$\nu_T(A) = \prod_{l=1}^L \frac{\int_{A_l} \exp\left(-\frac{\bar{\varepsilon}_l(\zeta_l)}{k_B T}\right) d\mu_l(\zeta_l)}{\int_{\mathcal{E}_l} \exp\left(-\frac{\bar{\varepsilon}_l(\zeta_l)}{k_B T}\right) d\mu_l(\zeta_l)} = \prod_{l=1}^L \nu_T^l(A_l),$$

that is $\nu_T = \nu_T^1 \otimes \dots \otimes \nu_T^L$.

Each ε_l (thus also $\bar{\varepsilon}_l$) can also be seen as a real random variable on $(\mathcal{E}, \mathcal{A}, \nu_T)$, by setting $\varepsilon_l(\zeta) \equiv \varepsilon_l(\zeta_l)$. It follows that

$$\delta(T) = 2 \mathbb{E}_{\nu_T} \left[\frac{\bar{\varepsilon}}{k_B T} \right] = 2 \mathbb{E}_{\nu_T} \left[\sum_{l=1}^L \frac{\bar{\varepsilon}_l}{k_B T} \right] = 2 \sum_{l=1}^L \mathbb{E}_{\nu_T} \left[\frac{\bar{\varepsilon}_l}{k_B T} \right] = \sum_{l=1}^L \delta_l(T).$$

Finally, since $\varepsilon_1, \dots, \varepsilon_L$ are independent under ν_T (ν_T is tensorized and they each depend on a different variable),

$$D(T) = 2 \text{Var}_{\nu_T} \left[\frac{\bar{\varepsilon}}{k_B T} \right] = 2 \text{Var}_{\nu_T} \left[\sum_{l=1}^L \frac{\bar{\varepsilon}_l}{k_B T} \right] = 2 \sum_{l=1}^L \text{Var}_{\nu_T} \left[\frac{\bar{\varepsilon}_l}{k_B T} \right] = \sum_{l=1}^L D_l(T).$$

□

We show now the results relevant to some particular options.

Proposition 2.12. *Let $C_1, C_2 > 0$, $\beta > 0$ and $\alpha > -1$. Denoting by $\text{Bor}(\mathbb{R})$ the set Borelians of \mathbb{R} , we consider*

$$(\mathcal{E}, \mathcal{A}, d\mu(\zeta)) = (\mathbb{R}, \text{Bor}(\mathbb{R}), C_1 |z|^\alpha dz), \quad \varepsilon(z) = C_2 |z|^\beta.$$

Then for all $T > 0$,

$$\delta(T) = D(T) = \frac{2(\alpha+1)}{\beta}.$$

Proof. Set $T > 0$ and $\alpha > -1$. Performing the change of variables $x = C_2 |z|^\beta$, and then $y = x/(k_B T)$, we get

$$\begin{aligned} \int_{\mathbb{R}} C_2 |z|^\beta \exp\left(-\frac{C_2 |z|^\beta}{k_B T}\right) C_1 |z|^\alpha dz &= \frac{2C_1 C_2^{\frac{\alpha-1}{\beta}}}{\beta} \int_0^\infty x \exp\left(-\frac{x}{k_B T}\right) x^{\frac{\alpha}{\beta}} x^{\frac{1-\beta}{\beta}} dx \\ &= \frac{2C_1 C_2^{\frac{\alpha-1}{\beta}}}{\beta} \int_0^\infty x^{\frac{\alpha+1}{\beta}} \exp\left(-\frac{x}{k_B T}\right) dx \end{aligned}$$

$$\begin{aligned}
&= \frac{2C_1 C_2^{\frac{\alpha-1}{\beta}}}{\beta} (k_B T)^{\frac{\alpha+1}{\beta}+1} \int_0^\infty y^{\frac{\alpha+1}{\beta}} e^{-y} dy \\
&= \frac{2C_1 C_2^{\frac{\alpha-1}{\beta}}}{\beta} (k_B T)^{\frac{\alpha+1}{\beta}+1} \left(\frac{\alpha+1}{\beta}\right) \int_0^\infty y^{\frac{\alpha+1}{\beta}-1} e^{-y} dy.
\end{aligned}$$

Analogously, performing the same changes of variables

$$\begin{aligned}
\int_{\mathbb{R}} \exp\left(-\frac{C_2|z|^\beta}{k_B T}\right) C_1|z|^\alpha dz &= \frac{2C_1 C_2^{\frac{\alpha-1}{\beta}}}{\beta} \int_0^\infty \exp\left(-\frac{x}{k_B T}\right) x^{\frac{\alpha}{\beta}} x^{\frac{1-\beta}{\beta}} dx \\
&= \frac{2C_1 C_2^{\frac{\alpha-1}{\beta}}}{\beta} \int_0^\infty x^{\frac{\alpha+1}{\beta}-1} \exp\left(-\frac{x}{k_B T}\right) dx \\
&= \frac{2C_1 C_2^{\frac{\alpha-1}{\beta}}}{\beta} (k_B T)^{\frac{\alpha+1}{\beta}} \int_0^\infty y^{\frac{\alpha+1}{\beta}-1} e^{-y} dy.
\end{aligned}$$

We deduce that

$$\delta(T) = \frac{2}{k_B T} \frac{\int_{\mathbb{R}} C_2|z|^\beta \exp\left(-\frac{C_2|z|^\beta}{k_B T}\right) C_1|z|^\alpha dz}{\int_{\mathbb{R}} \exp\left(-\frac{C_2|z|^\beta}{k_B T}\right) C_1|z|^\alpha dz} = \frac{2(\alpha+1)}{\beta}.$$

Since δ does not depend on T , we have $D(T) = \delta(T) = \frac{2(\alpha+1)}{\beta}$. □

Corollary 2.13. *We consider $a_1, \dots, a_d > 0$ and*

$$(\mathcal{E}, \mathcal{A}, d\mu(\zeta)) = (\mathbb{R}^d, \text{Bor}(\mathbb{R}^d), dz), \quad \varepsilon(z) = \sum_{l=1}^d a_l z_l^2.$$

Then for all $T > 0$,

$$\delta(T) = D(T) = d.$$

Proof. This Corollary is a consequence of Proposition 2.12 with $\alpha = 0$, $\beta = 2$, and Proposition 2.4 with $(\mathcal{E}_l, \mathcal{A}_l, d\mu_l) = (\mathbb{R}, \text{Bor}(\mathbb{R}), dz)$ and $\varepsilon_l(z) = a_l z^2$ for $1 \leq l \leq d$. □

2.7 Models within the framework

2.7.1 Existing models

In this subsection, we show that our framework encapsulates various existing models. The parameters to choose in order to build the model are $(\mathcal{E}, \mathcal{A}, \mu)$ and ε .

The monoatomic gas

The model for the monoatomic gas is the classical Boltzmann model, which considers elastic collisions only. We refer the reader to [43]. To recover this model in our framework, simply set $\mathcal{E} = \{0\}$,

$\mathcal{A} = \mathcal{P}(\mathcal{E})$, $\mu(\{0\}) = 1$ and $\varepsilon(0) = \varepsilon^0 \in \mathbb{R}$. Then the state of a molecule is described by $(v, \zeta) \in \mathbb{R}^3 \times \{0\}$, thus simply by $v \in \mathbb{R}^3$. The conservation laws become

$$\begin{cases} mv + mv_* = mv' + mv'_* \\ \frac{m}{2}|v|^2 + \varepsilon^0 + \frac{m}{2}|v_*|^2 + \varepsilon^0 = \frac{m}{2}|v'|^2 + \varepsilon^0 + \frac{m}{2}|v'_*|^2 + \varepsilon^0, \end{cases}$$

which simplify into the conservation laws of an elastic collision

$$\begin{cases} v + v_* = v' + v'_* \\ |v|^2 + |v_*|^2 = |v'|^2 + |v'_*|^2. \end{cases}$$

From there, the classical post-collision velocities

$$\begin{cases} v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2} T_\omega \begin{bmatrix} v - v_* \\ |v - v_*| \end{bmatrix} \\ v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2} T_\omega \begin{bmatrix} v - v_* \\ |v - v_*| \end{bmatrix} \end{cases}$$

are recovered. The number of internal degrees of freedom and heat capacity at constant volume associated with this model are, as expected,

$$\delta = 0 \quad \text{and} \quad c_V = \frac{3}{2},$$

reproducing that fact that an atom has only the three translational degrees of freedom.

The weighted model with one continuous variable

This model was originally proposed by Borgnakke et al. in [35] and completed with the introduction of a weight φ of integration by Desvilletes et al. in [75, 76] in order to accurately describe polyatomic gases with the introduction of a single parameter I related to the internal energy of the molecule. The state of a molecule is described by $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$, and the associated internal energy is $\frac{m}{2}|v|^2 + I$.

To recover this model in our framework, set $\mathcal{E} = \mathbb{R}_+$, \mathcal{A} the set of Borelians of \mathbb{R}_+ , $d\mu(I) = \varphi(I)dI$, and for $I \in \mathbb{R}_+$, $\varepsilon(I) = I$. The conservation laws of a collision write, when the collision is possible, as

$$\begin{cases} mv + mv_* = mv' + mv'_* \\ \frac{m}{2}|v|^2 + I + \frac{m}{2}|v_*|^2 + I_* = \frac{m}{2}|v'|^2 + I' + \frac{m}{2}|v'_*|^2 + I'_*. \end{cases}$$

Since I is a continuous parameter, in [76], Desvilletes et al. introduce $e = \frac{m}{4}|v - v_*|^2 + I + I_*$,

$r = \frac{I'}{I' + I'_*}$ and $R = \frac{\frac{m}{4}|v' - v'_*|^2}{e}$. Using these parameters, the post-collision velocities write in their formulation

$$\begin{cases} v' = \frac{v + v_*}{2} + \sqrt{Re} T_\omega \begin{bmatrix} v - v_* \\ |v - v_*| \end{bmatrix} \\ v'_* = \frac{v + v_*}{2} - \sqrt{Re} T_\omega \begin{bmatrix} v - v_* \\ |v - v_*| \end{bmatrix} \end{cases}$$

Our formula for post-collision velocities is equivalent and writes, for allowed collisions,

$$\begin{cases} v' &= \frac{v+v_*}{2} + \sqrt{\frac{1}{4}|v-v_*|^2 + \frac{1}{m}(I+I_*-I'-I'_*)} T_\omega \left[\frac{v-v_*}{|v-v_*|} \right] \\ v'_* &= \frac{v+v_*}{2} - \sqrt{\frac{1}{4}|v-v_*|^2 + \frac{1}{m}(I+I_*-I'-I'_*)} T_\omega \left[\frac{v-v_*}{|v-v_*|} \right] \end{cases}$$

The main technical difference between the two approaches is that the authors in [76] fix all the pre-collision parameters (velocities, internal energies, r and R) and study then the transformation

$$\tilde{S}_\omega : (v, v_*, I, I_*, r, R) \mapsto (v', v'_*, I', I'_*, r', R')$$

defined on $\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}_+ \times [0, 1] \times [0, 1]$, while, in our framework, we fix pre-collision velocities and all pre- and post-interaction internal energies and we study the transformation

$$S_\omega[I, I_*, I', I'_*] : (v, v_*) \mapsto (v', v'_*)$$

defined on $E[I, I_*, I', I'_*]$.

We are able to prove that the two methods are equivalent. Indeed, we denote by Φ the bijection

$$\Phi : \begin{cases} \tilde{\Omega} \rightarrow \Omega \\ (v, v_*, I, I_*, r, R) \mapsto (v, v_*, I, I_*, I', I'_*), \end{cases}$$

where $\tilde{\Omega} = (\mathbb{R}^3)^2 \times (\mathbb{R}_+)^2 \times [0, 1]^2$ and $\Omega = \{(v, v_*, I, I_*, I', I'_*) \in (\mathbb{R}^3)^2 \times (\mathbb{R}_+)^4, (v, v_*) \in E[I, I_*, I', I'_*]\}$. Its Jacobian can be computed and is equal to

$$J[\Phi](v, v_*, I, I_*, r, R) = (1-R)e^2,$$

where we recall that $e = \frac{m}{4}|v-v_*|^2 + I + I_* = \frac{m}{4}|v'-v'_*|^2 + I' + I'_* = e'$. Then

$$\begin{aligned} S_\omega[I, I_*, I', I'_*](v, v_*) &= (v', v'_*) \\ \Phi \circ \tilde{S}_\omega \circ \Phi^{-1}(v, v_*, I, I_*, I', I'_*) &= (v', v'_*, I', I'_*, I, I_*), \end{aligned}$$

and we remark that (see Lemma 1. in [76] and equation (2.11))

$$\begin{aligned} J[\Phi \circ \tilde{S}_\omega \circ \Phi^{-1}](v, v_*, I, I_*, I', I'_*) &= (1-R')(e')^2 \frac{(1-R)|v'-v'_*|}{(1-R')|v-v_*|} \frac{1}{(1-R)e^2} \\ &= \frac{|v'-v'_*|}{|v-v_*|} = J[S_\omega[I, I_*, I', I'_*]](v, v_*). \end{aligned}$$

The authors in [76] consider a kernel $\tilde{B} : \tilde{\Omega} \times \mathbb{S}^2 \rightarrow \mathbb{R}_+$ with the micro-reversibility conditions

$$\begin{aligned} \tilde{B}(v, v_*, I, I_*, R, r, \omega) &= \tilde{B}(v_*, v, I_*, I, R, 1-r, \omega) \\ \tilde{B}(v, v_*, I, I_*, R, r, \omega) &= \tilde{B}(v', v'_*, I', I'_*, R', r', \omega). \end{aligned}$$

We define on $\Omega \times \mathbb{S}^2$

$$B(v, v_*, I, I_*, I', I'_*, \omega) = \frac{1}{e^2} |v-v_*|^{-1} \frac{\tilde{B}(\cdot, \omega) \circ \Phi^{-1}(v, v_*, I, I_*, I', I'_*)}{\varphi(I)\varphi(I_*)\varphi(I')\varphi(I'_*)},$$

and set B to zero elsewhere. Then, since $e = e'$,

$$\begin{aligned} B(v, v_*, I, I_*, I', I'_*, \omega) &= B(v_*, v, I_*, I, I'_*, I', \omega) \\ |v - v_*| B(v, v_*, I, I_*, I', I'_*, \omega) &= |v' - v'_*| B(v', v'_*, I', I'_*, I, I_*, \omega), \end{aligned}$$

which are the symmetry and micro-reversibility conditions in our framework. It follows that the difference of approach is purely technical, and does not lead to theoretical discrepancies. The same distribution f and macroscopic quantities are recovered. Indeed, in this case, with $\zeta = I$,

$$\begin{aligned} \mathcal{B}(f, f)(v, \zeta) &= \iiint_{\mathcal{E}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left(f(v', \zeta') f(v'_*, \zeta'_*) - f(v, \zeta) f(v_*, \zeta_*) \right) B(\cdot) \, d\omega \, dv_* \, d\mu^{\otimes 3}(\zeta_*, \zeta', \zeta'_*) \\ &= \iiint_{(\mathbb{R}_+)^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left(f(v', I') f(v'_*, I'_*) - f(v, I) f(v_*, I_*) \right) B(\cdot) \, d\omega \, dv_* \, \varphi(I_*) \varphi(I') \varphi(I'_*) \, dI_* \, dI' \, dI'_* \\ &= \int_{\mathbb{S}^2} \int_{\Omega[v, I]} \left(f(v', I') f(v'_*, I'_*) - f(v, I) f(v_*, I_*) \right) \tilde{B}(\cdot, \omega) \circ \Phi^{-1}(\cdot) \frac{dv_* \, dI_* \, dI' \, dI'_* \, d\omega}{e^2 |v - v_*| \varphi(I)} \\ &= \int_{\mathbb{S}^2} \int_{\tilde{\Omega}[v, I]} \left(f(v', I') f(v'_*, I'_*) - f(v, I) f(v_*, I_*) \right) |v - v_*|^{-1} \tilde{B}(\cdot, \omega) \frac{J[\Phi](\cdot)}{e^2} \times \frac{dv_* \, dI_* \, dR \, dr \, d\omega}{\varphi(I)} \\ &= \iint_{[0,1]^2} \int_{\mathbb{R}_+} \int_{\mathbb{S}^2} \left(f(v', I') f(v'_*, I'_*) - f(v, I) f(v_*, I_*) \right) |v - v_*|^{-1} (1 - R) \tilde{B}(\cdot, \omega) \frac{d\omega \, dv_* \, dI_* \, dR \, dr}{\varphi(I)}, \end{aligned}$$

where we recall that $J[\Phi](v, v_*, I, I_*, r, R) = (1 - R)e^2$ is the Jacobian of Φ . We denoted by $\Omega[v, I]$ the set of (v_*, I_*, I', I'_*) such that $(v, v_*, I, I_*, I', I'_*) \in \Omega$ and the same for $\tilde{\Omega}$. We recover the same macroscopic quantities as well, for example the density

$$\rho(t, x) = \int_{\mathcal{E}} \int_{\mathbb{R}^3} m f(t, x, v, \zeta) \, dv \, d\mu(\zeta) = \int_{\mathbb{R}_+} \int_{\mathbb{R}^3} m f(t, x, v, I) \, dv \, \varphi(I) \, dI.$$

Remark 2.5. *The approach in [35, 76] consists in distributing the energy of the incoming molecules simultaneously to the post-collision relative kinetic energy and to the internal states, whereas, in our framework, we fix the pre and post-collision internal states and consider afterwards the set of pre-collision velocity pairs for which this collision is possible.*

This model is generally used with $\varphi(I) = I^\alpha$, with $\alpha > -1$. From Proposition 2.12, we recover that in this case ($\beta = 1$ in the proposition), the number of internal degrees of freedom and heat capacity at constant volume are

$$\delta = 2(\alpha + 1) \quad \text{and} \quad c_V = \frac{5}{2} + \alpha.$$

The model with discrete energy levels

In order to accurately describe the vibration inside molecules, a model with a discrete-energy levels description is proposed by Groppi and Spiga in [100]. The authors consider a finite set of internal energy levels $(\varepsilon_n)_{n \in \llbracket 0, N \rrbracket} \in \mathbb{R}^{N+1}$. The state of a molecule is then $(v, n) \in \mathbb{R}^3 \times \llbracket 0, N \rrbracket$, and the associated withal energy is $\frac{m}{2}|v|^2 + \varepsilon_n$. The authors define $\delta_{ij}^{kl} = \frac{4}{m}(\varepsilon_k + \varepsilon_l - \varepsilon_i - \varepsilon_j)$, $g = |v - v_*|$ and $g' = |v' - v'_*|$.

A collision is allowed when $g^2 - \delta_{ij}^{kl} \geq 0$, with then $g' = \sqrt{g^2 - \delta_{ij}^{kl}}$.

To recover this model in our framework, we set $\mathcal{E} = \llbracket 0, N \rrbracket$, $\mathcal{A} = \mathcal{P}(\llbracket 0, N \rrbracket)$, μ the counting measure on

$\llbracket 0, N \rrbracket$ and for $n \in \llbracket 0, N \rrbracket$, $\varepsilon(n) = \varepsilon_n$. Indeed, note that

$$g^2 - \delta_{ij}^{kl} \geq 0 \iff \frac{1}{4}|v - v_*|^2 + \frac{1}{m}(\varepsilon_i + \varepsilon_j - \varepsilon_k - \varepsilon_l) \geq 0 \iff \Delta(v, v_*, i, j, k, l) \geq 0,$$

where Δ is defined in equation (2.6). Moreover, the authors give (formula 2.6 in [100])

$$dv' dv'_* d\Omega' = \mathbf{1}_{g^2 \geq \delta_{ij}^{kl}} \frac{g'}{g} dv dv_* d\Omega,$$

which corresponds in our framework to the Jacobian of the transformation $(v, v_*) \mapsto (v', v'_*)$, see formula (2.11). The authors in [100] give the following post-collision velocities

$$\begin{aligned} v' &= \frac{v + v_*}{2} + \frac{1}{2} \sqrt{g^2 - \delta_{ij}^{kl}} \Omega \\ v'_* &= \frac{v + v_*}{2} - \frac{1}{2} \sqrt{g^2 - \delta_{ij}^{kl}} \Omega, \end{aligned}$$

where $\Omega \in \mathbb{S}^2$. Now remark that $\frac{1}{2} \sqrt{g^2 - \delta_{ij}^{kl}} = \sqrt{\Delta(v, v_*, i, j, k, l)}$ and there exists (assuming $v \neq v_*$) $\omega \in \mathbb{S}^2$ such that $\Omega = T_\omega \left[\frac{v - v_*}{|v - v_*|} \right]$. We then have, like in our framework,

$$\begin{aligned} v' &= \frac{v + v_*}{2} + \sqrt{\Delta(v, v_*, i, j, k, l)} T_\omega \left[\frac{v - v_*}{|v - v_*|} \right] \\ v'_* &= \frac{v + v_*}{2} - \sqrt{\Delta(v, v_*, i, j, k, l)} T_\omega \left[\frac{v - v_*}{|v - v_*|} \right]. \end{aligned}$$

The authors in [100] define the cross-section σ_{ij}^{kl} , with the symmetry and micro-reversibility conditions

$$\begin{aligned} \sigma_{ij}^{kl}(v, v_*, \omega) &= \sigma_{ji}^{lk}(v_*, v, \omega) \\ |v - v_*|^2 \sigma_{ij}^{kl}(v, v_*, \omega) &= |v' - v'_*|^2 \sigma_{ij}^{kl}(v', v'_*, \omega). \end{aligned}$$

By defining the collision kernel

$$B(v, v_*, i, j, k, l, \omega) = \mathbf{1}_{g^2 \geq \delta_{ij}^{kl}} |v - v_*| \sigma_{ij}^{kl}(v, v_*, \omega),$$

B verifies the positivity assumption (if σ_{ij}^{kl} is properly defined) and from the properties assumed for σ_{ij}^{kl} we recover

$$\begin{aligned} B(v, v_*, i, j, k, l, \omega) &= B(v_*, v, j, i, l, k, \omega) \\ |v - v_*| B(v, v_*, i, j, k, l, \omega) &= |v' - v'_*| B(v', v'_*, k, l, i, j, \omega). \end{aligned}$$

Finally, with $(\zeta, \zeta_*, \zeta', \zeta'_*) = (i, j, k, l)$,

$$\begin{aligned} \mathcal{B}(f, f)(v, \zeta) &= \iiint_{\mathcal{E}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left(f(v', \zeta') f(v'_*, \zeta'_*) - f(v, \zeta) f(v_*, \zeta_*) \right) B(\cdot) d\omega dv_* d\mu^{\otimes 3}(\zeta_*, \zeta', \zeta'_*) \\ &= \sum_{j, k, l \in \llbracket 0, N \rrbracket} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left(f(v', k) f(v'_*, l) - f(v, i) f(v_*, j) \right) B(v, v_*, i, j, k, l, \omega) d\omega dv_* \end{aligned}$$

$$= \sum_{j,k,l \in \llbracket 0, N \rrbracket} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \mathbf{1}_{g^2 \geq \delta_{ij}^{kl}} |v - v_*| \sigma_{ij}^{kl}(v, v_*, \omega) \left(f_k(v') f_l(v'_*) - f_i(v) f_j(v_*) \right) d\omega dv_*,$$

with the notation $f_i(v) = f(v, i)$. The same macroscopic quantities are recovered as well, for instance the density

$$\rho(t, x) = \int_{\mathcal{E}} \int_{\mathbb{R}^3} m f(t, x, v, \zeta) dv d\mu(\zeta) = \sum_{i=0}^N \int_{\mathbb{R}^3} m f_i(t, x, v) dv.$$

2.7.2 Combination of the continuous and discrete models

The continuous and discrete models can be combined in our framework. Let us consider a finite set of internal energy levels $(\epsilon_n)_{n \in \llbracket 0, N \rrbracket} \in \mathbb{R}^{N+1}$ and a weight function φ on \mathbb{R}_+ . We can build the following model

$$(\mathcal{E}, \mathcal{A}, d\mu(\zeta)) = (\mathbb{R}_+ \times \llbracket 0, N \rrbracket, \text{Bor}(\mathbb{R}_+) \otimes \mathcal{P}(\llbracket 0, N \rrbracket), \varphi(I) dI \times 1), \quad \varepsilon(I, n) = I + \epsilon_n, \quad (2.33)$$

where 1 stands for the counting measure. The Boltzmann operator writes

$$\begin{aligned} \mathcal{B}(f, f)(v, I, i) = & \sum_{j,k,l \in \llbracket 0, N \rrbracket} \iiint_{(\mathbb{R}_+)^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left(f_k(v', I') f_l(v'_*, I'_*) - f_i(v, I) f_j(v_*, I_*) \right) \\ & \times B(\cdot) d\omega dv_* \varphi(I_*) dI_* \varphi(I') dI' \varphi(I'_*) dI'_*. \end{aligned}$$

Let us set $\epsilon^0 = \min_{0 \leq n \leq N} \{\epsilon_n\}$. From Theorem 2.4, the Maxwellian writes

$$\begin{aligned} \mathcal{M}[\rho, u, T](v, I, i) = \\ \rho m^{1/2} (2\pi k_B T)^{-3/2} Z_c \left(\frac{1}{k_B T} \right)^{-1} Z_d \left(\frac{1}{k_B T} \right)^{-1} \exp \left(-\frac{m|v - u|^2}{2k_B T} - \frac{I}{k_B T} - \frac{\epsilon_i - \epsilon^0}{k_B T} \right), \end{aligned}$$

where Z_c and Z_d are the partition functions respectively associated with the continuous and discrete parts, for all $\beta > 0$

$$Z_c(\beta) = \int_{\mathbb{R}_+} e^{-\beta I} \varphi(I) dI, \quad Z_d(\beta) = \sum_{n=0}^N e^{-\beta(\epsilon_n - \epsilon^0)}.$$

Finally, again from Theorem 2.4, the number of internal degrees of freedom writes

$$\delta(T) = \delta_c(T) + \delta_d(T) = \frac{2}{k_B T} \frac{\int_{\mathbb{R}_+} I \exp \left(-\frac{I}{k_B T} \right) \varphi(I) dI}{\int_{\mathbb{R}_+} \exp \left(-\frac{I}{k_B T} \right) \varphi(I) dI} + \frac{2}{k_B T} \frac{\sum_{n=0}^N (\epsilon_n - \epsilon^0) \exp \left(-\frac{(\epsilon_n - \epsilon^0)}{k_B T} \right)}{\sum_{n=0}^N \exp \left(-\frac{(\epsilon_n - \epsilon^0)}{k_B T} \right)}.$$

As seen previously, if $\varphi(I) = I^\alpha$ with $\alpha > -1$, then $\delta_c = 2(\alpha + 1)$. This model with internal energy described by two different variables, a continuous and a discrete one, may be used to separate the vibrational energy of a molecule from the rotational part. As suggested in [108], the rotational energy may be modelled by means of a continuous variable, while for the vibrational energy a discrete approximation is more suitable. Note that the number of internal degrees of freedom turns out to be, as expected, the sum of the vibrational and the rotational ones.

2.7.3 Building a model within the framework

In this subsection, we explain how to build a model for a polyatomic gas within our framework, with an example. Building an accurate model corresponds to giving an accurate description of the internal states of a given molecule. On this subject, the main field to rely on is Molecular Mechanics/Quantum Chemistry, see for example [107]. There are various phenomena to be taken into account, typically rotation, vibration, electronic excitation and nuclei spin, that could also be correlated. For the sake of simplicity of the mathematical model, it could be enough to take only rotation and vibration into account, and assume them to be uncorrelated, but there are physical problems where this kind of description is too simplistic. The most appropriate model in a given situation typically depends on the considered regime and the desired degree of complexity and accuracy. This is the reason why we wish not to propose one model, but to give examples and insights on how to build realistic models inside our framework.

Quantum description of the internal structure

To our knowledge, the currently best internal description of a molecule is given by quantum mechanics. Suppose to have a Hamiltonian operator \hat{H} . Let $\{\lambda_q\}_{q \in Q}$ be the set of its (real) eigenvalues, where Q is a discrete set (e.g. $\mathbb{N}, \mathbb{N}^2, \dots$). We denote by r_q the dimension of the eigenvector space associated with the eigenvalue λ_q . The values λ_q are the possible measurable energy levels associated with the operator \hat{H} , and r_q is the so-called degeneracy of the q^{th} energy level. We then consider a subset $\tilde{Q} \subset Q$, the set of energy levels of the *bound states* (the physically admissible energy levels), and build the following model

$$(\mathcal{E}, \mathcal{A}, \mu) = (\tilde{Q}, \mathcal{P}(\tilde{Q}), (r_q)_q), \quad \varepsilon(q) = \lambda_q,$$

where the notation $\mu = (r_q)_q$ means that $\mu(\{q\}) = r_q$. As we explained in subsection 2.3.2, degeneracy is indeed included in the model via the measure μ .

We remark that if the set of bound states $\tilde{Q} = Q$ and $\inf\{\lambda_q\}_{q \in Q} = 0$, then we recover the formula of statistical mechanics for the partition function (see [110], Chapter 9)

$$Z(\beta) = \sum_{q \in Q} e^{-\beta \lambda_q} r_q = \text{Tr}(e^{-\beta \hat{H}}),$$

where $\text{Tr}(e^{-\beta \hat{H}})$ is the trace of the operator $e^{-\beta \hat{H}}$.

Remark 2.6. *The framework we present in this paper, with the Boltzmann equation 2.12 is "at most" semi-classical, in the sense that the velocity part is described by classical mechanics. A full quantum mechanical Boltzmann equation was derived by Waldmann [158] and Snider [147]. In our framework, we assume that the gas is isotropic (no polarization effects), and other quantum considerations would only appear in the internal structure $(\mathcal{E}, \mathcal{A}, \mu)$, ε of the molecule.*

Semi-classical description of the internal structure

A possible approach is to consider only rotation and vibration, describing independently rotation with classical mechanics and vibration with quantum mechanics. The description of vibration is thus exactly the model of the previous paragraph, with a Hamiltonian describing only vibration,

$$(\mathcal{E}_{vib}, \mathcal{A}_{vib}, \mu_{vib}) = (\tilde{Q}, \mathcal{P}(\tilde{Q}), (r_q)_q), \quad \varepsilon_{vib}(q) = \lambda_q.$$

We assume the molecule to be a rigid rotor, that is, in the description of rotation we assume that no deformation is induced in the molecule. The rotation-related internal state we consider is thus the angular

velocity of the molecule in a coordinate system attached to the molecule. In general, this angular velocity lives in \mathbb{R}^3 , however when the molecule is linear, being symmetric by rotation around its own axis, the contribution of the angular momentum's coordinate along this axis can be assumed to be 0 (this approximation can be found for example in [155], section 7). Thus, in the case of a linear molecule, the angular momentum, in a coordinate system attached to the molecule with one axis being the molecule's axis, would live in \mathbb{R}^2 . Moreover, in the linear case, the moment of inertia is the same in both directions. This way of modelling leads to the following framework for the description of rotation

$$(\mathcal{E}_{rot}, \mathcal{A}_{rot}, \mathbf{d}\mu_{rot}(z)) = \left(\mathbb{R}^d, \text{Bor}(\mathbb{R}^d), \mathbf{d}z \right), \quad \varepsilon_{rot}(z) = \frac{1}{2} \sum_{i=1}^d \mathcal{I}_i z_i^2,$$

where \mathcal{I}_i is the moment of inertia along the i -th axis, z is the angular velocity in a coordinate system attached to the molecule, $d = 2$ and $\mathcal{I}_1 = \mathcal{I}_2 = \mathcal{I}$ if the molecule is linear, $d = 3$ if the molecule is non-linear. The model taking rotation and vibration into account then writes

$$(\mathcal{E}, \mathcal{A}, \mathbf{d}\mu(\zeta)) = \left(\mathbb{R}^d \times \tilde{Q}, \text{Bor}(\mathbb{R}^d) \otimes \mathcal{P}(\tilde{Q}), \mathbf{d}z r_q \right), \quad \varepsilon(z, q) = \frac{1}{2} \sum_{i=1}^d \mathcal{I}_i z_i^2 + \lambda_q,$$

From Theorem 2.4, for all $T > 0$,

$$\mathbf{d}\nu_T(z, q) = \mathbf{d}\nu_T^{rot}(z) \mathbf{d}\nu_T^{vib}(q) = \prod_{i=1}^d \frac{\exp\left(-\frac{\mathcal{I}_i z_i^2}{2k_B T}\right)}{\left(\frac{2\pi k_B T}{\mathcal{I}_i}\right)^{1/2}} \mathbf{d}z \frac{\exp\left(-\frac{(\lambda_q - \lambda^0)}{k_B T}\right)}{\sum_{q' \in \tilde{Q}} \exp\left(-\frac{(\lambda_{q'} - \lambda^0)}{k_B T}\right)} r_q.$$

Moreover, setting $\lambda^0 = \inf_{q \in \tilde{Q}} \{\lambda_q\}$ ($\in \mathbb{R}$ by assumption) and using Theorem 2.4 and Proposition 2.12, the number of internal degrees of freedom turns out to be

$$\delta(T) = \delta_{rot}(T) + \delta_{vib}(T) = d + 2 \frac{\sum_{q \in \tilde{Q}} \frac{(\lambda_q - \lambda^0)}{k_B T} \exp\left(-\frac{(\lambda_q - \lambda^0)}{k_B T}\right) r_q}{\sum_{q \in \tilde{Q}} \exp\left(-\frac{(\lambda_q - \lambda^0)}{k_B T}\right) r_q}.$$

Example: the $^1\text{H}^{19}\text{F}$ gas

As an example, we propose four models within our framework for the Hydrogen Fluoride ($^1\text{H}^{19}\text{F}$) gas. We focus only on rotation and vibration. We propose two semi-classical models and two quantum models. For the formulas of eigenvalues presented hereafter, we refer to the Chapter *Spectroscopy Constants of Diatomic Molecules* in [104].

1. **Harmonic semi-classical model.** We describe the internal states of $^1\text{H}^{19}\text{F}$ with a semi-classical approach. Since this molecule is diatomic, it is linear, so that $d = 2$ and $\mathcal{I}_1 = \mathcal{I}_2$ in the description of rotation, and has only one mode of vibration. In this simplified model, the Hamiltonian is assumed to include the harmonic potential (model of the quantum harmonic oscillator). This leads to the model

$$(\mathcal{E}, \mathcal{A}, \mathbf{d}\mu(\zeta)) = \left(\mathbb{R}^2 \times \mathbb{N}, \text{Bor}(\mathbb{R}^2) \otimes \mathcal{P}(\mathbb{N}), \mathbf{d}z \times 1 \right), \quad \varepsilon(z, n) = \underbrace{\frac{1}{2} \mathcal{I} |z|^2}_{\text{rotation}} + \underbrace{h c \nu_e \left(n + \frac{1}{2} \right)}_{\text{vibration}},$$

where \mathcal{I} is the moment of inertia associated with $^1\text{H}^{19}\text{F}$, h is the Planck constant (expressed in SI units),

c the speed of light (expressed in $\text{cm}\cdot\text{s}^{-1}$) and ν_e the wavenumber (expressed in cm^{-1}). Defining $T_{vib} = hc\nu_e/k_B$, the number of internal degrees of freedom writes

$$\delta_1(T) = \delta_1^{rot}(T) + \delta_1^{vib}(T) = 2 + 2 \frac{T_{vib}/T}{\exp(T_{vib}/T) - 1}.$$

2. Anharmonic semi-classical model. Instead of using the harmonic potential, the Morse potential is a useful approximation of the actual internuclear potential, since it allows anharmonicity and an explicit computation of the eigenvalues of the Hamiltonian. The family of eigenvalues is, up to a constant (see Morse [133]),

$$\left(hc\nu_e \left(n + \frac{1}{2} \right) - hc\nu_e x_e \left(n + \frac{1}{2} \right)^2 \right)_{n \in \mathbb{N}}$$

where x_e represents anharmonicity. Not all eigenvalues correspond to bound states. We thus restrict the family to the set $\llbracket 0, N_{max} \rrbracket$, where $N_{max} = \left\lfloor \frac{1}{2x_e} \right\rfloor - 1$. With this potential, the model becomes

$$\begin{aligned} (\mathcal{E}, \mathcal{A}, d\mu(\zeta)) &= (\mathbb{R}^2 \times \llbracket 0, N_{max} \rrbracket, \text{Bor}(\mathbb{R}^2) \otimes \mathcal{P}(\llbracket 0, N_{max} \rrbracket), dz \times 1), \\ \varepsilon(z, n) &= \frac{1}{2} \mathcal{I} |z|^2 + hc\nu_e \left(n + \frac{1}{2} \right) - \underbrace{hc\nu_e x_e \left(n + \frac{1}{2} \right)^2}_{\text{anharmonicity}}. \end{aligned}$$

The number of internal degrees of freedom writes

$$\delta_2(T) = \delta_2^{rot}(T) + \delta_2^{vib}(T) = 2 + \delta_2^{vib}(T).$$

3. Simplified quantum model. Here we use a quantum description for both rotation and vibration. To simplify, we describe independently rotation and vibration, using the rigid-rotor assumption for rotation and the harmonic potential for vibration. Since $^1\text{H}^{19}\text{F}$ is a diatomic molecule, there is only one mode of vibration. This leads to the model

$$(\mathcal{E}, \mathcal{A}, \mu) = \left(\mathbb{N} \times \mathbb{N}, \mathcal{P}(\mathbb{N}) \otimes \mathcal{P}(\mathbb{N}), (2J+1)_{(J,n) \in \mathbb{N}^2} \right), \quad \varepsilon(J, n) = \underbrace{B_r J(J+1)}_{\text{rotation}} + \underbrace{hc\nu_e \left(n + \frac{1}{2} \right)}_{\text{vibration}},$$

where B_r is the rotational constant associated with $^1\text{H}^{19}\text{F}$. Defining $T_{vib} = hc\nu_e/k_B$, the number of internal degrees of freedom writes

$$\delta_3(T) = \delta_3^{rot}(T) + \delta_3^{vib}(T) = \delta_3^{rot}(T) + 2 \frac{T_{vib}/T}{\exp(T_{vib}/T) - 1}.$$

4. Improved quantum model. For a better description, we can also take into account the correlation of rotation and vibration, considering non-rigid rotation, and using the Morse potential for vibration to allow for anharmonicity. This would lead to the model

$$(\mathcal{E}, \mathcal{A}, \mu) = \left(\tilde{Q}, \mathcal{P}(\tilde{Q}), (2J+1)_{(J,n) \in \tilde{Q}} \right),$$

$$\varepsilon(J, n) = \underbrace{\left(B_r - \alpha \left(n + \frac{1}{2} \right) \right)}_{\text{rot-vib coupling}} J(J+1) - \underbrace{\frac{D[J(J+1)]^2}{hc}}_{\text{centrifugal distortion}} + \underbrace{hc\nu_e \left(n + \frac{1}{2} \right) - hc\nu_e x_e \left(n + \frac{1}{2} \right)^2}_{\text{anharmonicity}},$$

where \tilde{Q} is the set of bound states, defined by

$$\tilde{Q} = \left\{ (J, n) \in \mathbb{N}^2, \varepsilon(J, n) \geq \varepsilon(J-1, n) \text{ and } \varepsilon(J, n-1) \geq \varepsilon(J, n) \right\} \subset \llbracket 0, J_{max} \rrbracket \times \llbracket 0, N_{max} \rrbracket.$$

We denote by δ_4 the number of internal degrees of freedom in this improved case, which cannot be written as the sum of rotational and vibrational parts due to the coupling.

From [104] we know that reasonable data for ${}^1\text{H}^{19}\text{F}$ are $\nu_e = 4138.39\text{cm}^{-1}$, $\nu_e x_e = 89.94\text{cm}^{-1}$, $B_r/hc = 20.95\text{cm}^{-1}$, $\alpha/hc = 0.793\text{cm}^{-1}$ and $D/hc = 0.00215\text{cm}^{-1}$. The value of \mathcal{I} does not matter in the computation of the number of internal degrees of freedom. Just for the sake of comparison of our proposed models, we plot on Fig. 2.1 the various numbers of internal degrees of freedom δ_1 , δ_2 , δ_3 and δ_4 corresponding to these data, as functions of the temperature (in log-scale), expressed in Kelvin (K). The temperature ranges from 10 to 10 000 K. We see that in this example vibration is negligible for $T \lesssim 1000\text{K}$, and becomes important around $2000 \sim 3000\text{K}$. The direct computation of δ from the choice of the model can be useful to quickly check the validity of an approximation in a given regime.

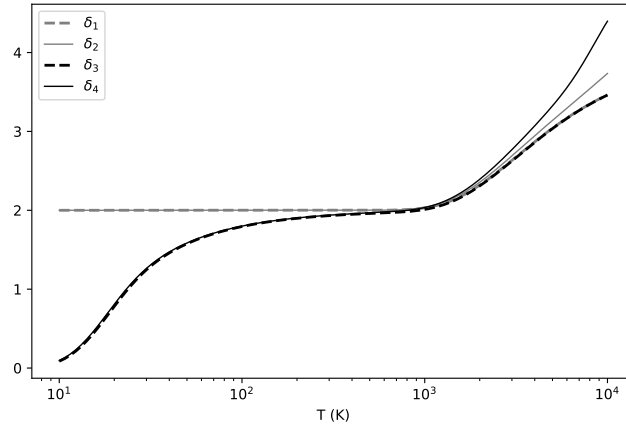


Figure 2.1 – Number of internal degrees of freedom in the various models as functions of temperature, with log-scale x -axis.

We plot on Fig. 2.2 the same numbers of internal degrees of freedom as on Fig. 2.1, for temperature ranging from 10^3 to 10^6K . The decrease of δ_2 and δ_4 after $T \sim 10^4\text{K}$ corresponds to the result of Corollary 2.10. While the number of internal degrees of freedom is expected to increase with temperature, this plot is an illustration of possible limits of validity of the framework. Indeed, high-temperatures considerations such as bond-breaking are not taken into account in our setting.

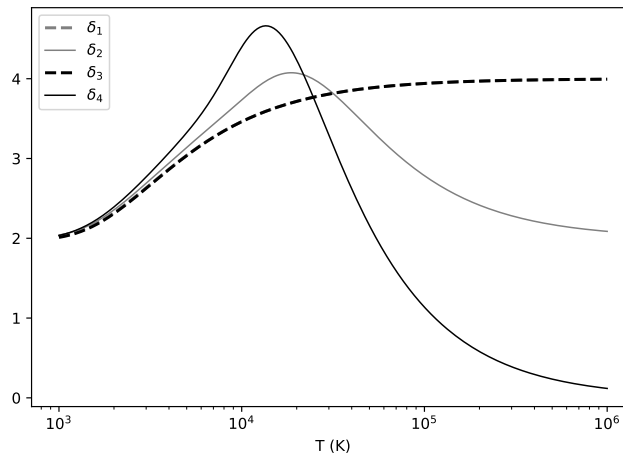


Figure 2.2 – Number of internal degrees of freedom in the various models at high temperatures.

2.8 Reduction to one real variable and comparison with Borgnakke-Larsen

In the previous section, we saw that our general framework allows to build a whole range of models that can be of great complexity. This possibility can be a strength in regards of the precision it allows in the description of the internal structure. However, too much complexity can be a weakness in regards of numerical aspects. Notably, the strength of the model proposed by Borgnakke and Larsen [35] is that the internal structure is described by a single real parameter $I \in \mathbb{R}_+$, which is highly desirable for numerical simulations. In this section, we show that any model fitting our framework can, under a condition on the collision kernel, be reduced to a one-real-parameter model. This means that all the complexity can be concentrated in a suitable measure on \mathbb{R}_+ . If this measure has a density, then it can be written as $\varphi(I) dI$ and we recover the model with one continuous variable proposed by Desvilletes et al. [75, 76], which is suited for numerical applications. While this weight φ in the original approach in [75, 76] is a parameter chosen a posteriori in order to recover desired macroscopic properties (e.g. the number of internal degrees of freedom), in our case it is computed from the physical structure of the molecule, through the reduction process that we present in this section.

Definition 2.10. We define $\mu^{\bar{\varepsilon}}$ as the image measure of μ by $\bar{\varepsilon}$ on \mathbb{R}_+ , for all $A \in \text{Bor}(\mathbb{R}_+)$,

$$\mu^{\bar{\varepsilon}}(A) := \mu(\bar{\varepsilon}^{-1}(A)).$$

Theorem 2.5. If the collision kernel B depends on the internal states only through their associated energy (see Remark 2.7 below), then the general model

$$(\mathcal{E}, \mathcal{A}, \mu), \quad \varepsilon$$

can be reduced to the model with one non-negative variable

$$(\mathbb{R}_+, \text{Bor}(\mathbb{R}_+), \mu^{\bar{\varepsilon}}), \quad I \mapsto I + \varepsilon^0.$$

Proof. First, remark that the set $E[\zeta, \zeta_*, \zeta', \zeta'_*]$ and the transformation $S_\omega[\zeta, \zeta_*, \zeta', \zeta'_*]$ depend on the internal states $\zeta, \zeta_*, \zeta', \zeta'_*$ only through their energy, cf. equations (2.9) and (2.10). It follows that if B and f depend on the internal states only through their energy, the same holds for $\mathcal{B}(f, f)$. Thus, in the deep structure of our framework, all dependence on ζ is in fact a dependence on $\varepsilon(\zeta)$ when it is the case for B . From the change of variable formula, for any measurable function $\phi : \mathbb{R} \rightarrow \mathbb{R}$ such that one of the following integrals makes sense,

$$\int_{\mathcal{E}} \phi(\varepsilon(\zeta)) \, d\mu(\zeta) = \int_{\mathcal{E}} (\phi(\cdot + \varepsilon^0) \circ \bar{\varepsilon})(\zeta) \, d\mu(\zeta) = \int_{\mathbb{R}_+} \phi(I + \varepsilon^0) \, d\mu^{\bar{\varepsilon}}(I).$$

Applying this change of variable to all integrals in this paper ends the proof. \square

Remark 2.7. We say that B depends on the internal states only through their energy if

$$B(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) \equiv \tilde{B}(v, v_*, \varepsilon(\zeta), \varepsilon(\zeta_*), \varepsilon(\zeta'), \varepsilon(\zeta'_*), \omega).$$

This trivially holds true for all existing kernels constructed within the existing models presented in Subsection 2.7.1, since for the discrete model there is a bijection between the set of indexes and the set of energy levels, and for the continuous model with weight, the internal state is the energy: in this case $\zeta = I = \varepsilon(\zeta)$. To the knowledge of the authors, all existing kernel for polyatomic gases considered up to now have this property.

Theorem 2.5 establishes a link between two points of view. The first, the one of the present paper, is *state-based*, considering a space of internal (physical) states \mathcal{E} . The second, the one of the reduced model, which is an extension of the model with continuous energy I and weight φ proposed by Desvilletes et al. [75, 76] (when $\mu^{\bar{\varepsilon}}$ is absolutely continuous with respect to the Lebesgue measure, there exists $\varphi \in L^1(\mathbb{R}_+)$ such that $d\mu^{\bar{\varepsilon}}(I) = \varphi(I) \, dI$), is *energy-based*, since the variable of interest is directly the internal energy of the molecule. Theorem 2.5 shows that to any states-based model corresponds an energy-based one (that is, a model with one continuous variable I and measure $\mu^{\bar{\varepsilon}}$ weight φ). Since the measure $\mu^{\bar{\varepsilon}}$ weight φ corresponds to the image measure of μ by $\bar{\varepsilon}$, it can easily be computed from the state-based model of the molecule, which is a major difference of approach of that can be found in [75, 76] where φ is computed with *a posteriori* knowledge of the number of degrees of freedom of the gas, moreover usually assuming it to be temperature-independent. In the following propositions we show some examples of this reduction for some physically meaningful models presented in the previous section, the link with existing models known to be accurate at describing rotation, and the computation of a weight φ describing rotation and vibration, which is, as expected, *not* of the form I^α .

Proposition 2.14. Let $d \in \mathbb{N}^*$. The model

$$(\mathbb{R}^d, \text{Bor}(\mathbb{R}^d), \mathbf{d}z), \quad \varepsilon(z) = \frac{1}{2} \mathcal{I} |z|^2$$

can be reduced to

$$(\mathbb{R}_+, \text{Bor}(\mathbb{R}_+), C_d(\mathcal{I}) I^{\frac{d}{2}-1} \, dI), \quad I \mapsto I,$$

with $C_d(\mathcal{I}) = 2^{\frac{d}{2}-1} \mathcal{I}^{-\frac{d}{2}} \text{Leb}_{d-1}(\mathbb{S}^{d-1})$, where Leb_{d-1} is the Lebesgue measure of dimension $d-1$.

Proof. We compute $\mu^{\bar{\varepsilon}}$. Let $A \in \text{Bor}(\mathbb{R}_+)$.

$$\mu^{\bar{\varepsilon}}(A) = \int_{\mathbb{R}^d} \mathbf{1}_{\frac{1}{2} \mathcal{I} |z|^2 \in A} \, \mathbf{d}z = \text{Leb}_{d-1}(\mathbb{S}^{d-1}) \int_{\mathbb{R}_+} \mathbf{1}_{\frac{1}{2} \mathcal{I} r^2 \in A} r^{d-1} \, dr = \int_{\mathbb{R}_+} \mathbf{1}_{I \in A} C_d(\mathcal{I}) I^{\frac{d}{2}-1} \, dI,$$

with $C_d(\mathcal{I}) = 2^{\frac{d}{2}-1} \mathcal{I}^{-\frac{d}{2}} \text{Leb}_{d-1}(\mathbb{S}^{d-1})$. It follows that

$$d\mu^{\bar{\varepsilon}}(I) = C_d(\mathcal{I}) I^{\frac{d}{2}-1} dI.$$

□

Remark 2.8. We saw in subsection 2.7.3 that the value of the moment of inertia of the molecule \mathcal{I} has no importance at equilibrium, however Proposition 2.14 shows that it should be taken into account outside equilibrium.

We also remark that the reduced version of classical model for the rotation of a linear molecule presented in subsection 2.7.3 is, with $C_2(\mathcal{I}) = \frac{2\pi}{\mathcal{I}}$,

$$(\mathbb{R}_+, \text{Bor}(\mathbb{R}_+), C_2(\mathcal{I}) dI), \quad I \mapsto I.$$

This model, being the the model with continuous variable I and weight $\varphi(I) = C_2(\mathcal{I})$, that is the one of Borgnakke-Larsen [35], is indeed well-known to be accurate in describing rotation for diatomic molecules. On the other hand, the reduction of the classical model for the rotation of a non-linear molecule presented in subsection 2.7.3 can be harder in general, because the computation of the measure relies on the computation of the surface of a triaxial ellipsoid. Nevertheless in this case, assuming $\mathcal{I}_i = \mathcal{I}_j = \mathcal{I}$ and with $C_3(\mathcal{I}) = \frac{4\sqrt{2}\pi}{\mathcal{I}^{3/2}}$, the model reduces to

$$(\mathbb{R}_+, \text{Bor}(\mathbb{R}_+), C_3(\mathcal{I}) \sqrt{I} dI), \quad I \mapsto I,$$

which is the model with continuous variable I and weight $\varphi(I) = C_3(\mathcal{I}) \sqrt{I}$, well-known for the description of rotation for non-linear molecules.

Proposition 2.15. Let Q be a discrete set, $(\epsilon_q)_{q \in Q} \in \mathbb{R}^Q$ and $(r_q)_{q \in Q} \in (\mathbb{R}_+^*)^Q$. We denote by $\epsilon^0 = \inf\{\epsilon_q\}_{q \in Q}$ and we assume $\epsilon^0 \in \mathbb{R}$ and that for all $\beta > 0$ one has $\sum_{q \in Q} e^{-\beta(\epsilon_q - \epsilon^0)} r_q < \infty$. Then the model

$$(Q, \mathcal{P}(Q), (r_q)_{q \in Q}), \quad \varepsilon(q) = \epsilon_q$$

can be reduced to

$$\left(\mathbb{R}_+, \text{Bor}(\mathbb{R}_+), \sum_{q \in Q} r_q \chi_{\epsilon_q - \epsilon^0} \right), \quad I \mapsto I + \epsilon^0,$$

where $\chi_{\epsilon_q - \epsilon^0}$ is the Dirac mass at $\epsilon_q - \epsilon^0$.

Proof. For $A \in \text{Bor}(\mathbb{R}_+)$, we have

$$\mu^{\bar{\varepsilon}}(A) = \mu(\bar{\varepsilon}^{-1}(A)) = \sum_{q \in Q} r_q \mathbf{1}_{\bar{\varepsilon}(q) \in A} = \sum_{q \in Q} r_q \mathbf{1}_{\epsilon_q - \epsilon^0 \in A} = \sum_{q \in Q} r_q \chi_{\epsilon_q - \epsilon^0}(A).$$

□

Proposition 2.16. Reduction of a combination. Let $(\mathcal{E}_1, \mathcal{A}_1, \mu_1)$, ε_1 and $(\mathcal{E}_2, \mathcal{A}_2, \mu_2)$, ε_2 be two general models. Then the combined model

$$(\mathcal{E}, \mathcal{A}, \mu) = (\mathcal{E}_1 \times \mathcal{E}_2, \mathcal{A}_1 \otimes \mathcal{A}_2, \mu_1 \otimes \mu_2), \quad \varepsilon(\zeta_1, \zeta_2) = \varepsilon_1(\zeta_1) + \varepsilon_2(\zeta_2)$$

can be reduced to

$$\left(\mathbb{R}_+, \text{Bor}(\mathbb{R}_+), \mu_1^{\bar{\varepsilon}_1} * \mu_2^{\bar{\varepsilon}_2} \right), \quad I \mapsto I + \varepsilon_1^0 + \varepsilon_2^0,$$

where $*$ stands for the convolution of measures and we recall that $\mu_i^{\bar{\varepsilon}_i}$, $i = 1, 2$ is the image measure of μ_i by $\bar{\varepsilon}_i$.

Proof. First of all, note that $\bar{\varepsilon}(\zeta_1, \zeta_2) = \bar{\varepsilon}_1(\zeta_1) + \bar{\varepsilon}_2(\zeta_2)$. Thus, denoting by $\mu^{\bar{\varepsilon}}$ the image measure of μ by $\bar{\varepsilon}$, we have for $A \in \text{Bor}(\mathbb{R}_+)$

$$\begin{aligned} \mu^{\bar{\varepsilon}}(A) &= \int_{\mathcal{E}_1} \int_{\mathcal{E}_2} \mathbf{1}_{\bar{\varepsilon}_1(\zeta_1) + \bar{\varepsilon}_2(\zeta_2) \in A} \, d\mu_1(\zeta_1) \, d\mu_2(\zeta_2) \\ &= \int_{\mathbb{R}_+} \int_{\mathbb{R}_+} \mathbf{1}_{I_1 + I_2 \in A} \, d\mu_1^{\bar{\varepsilon}_1}(I_1) \, d\mu_2^{\bar{\varepsilon}_2}(I_2) = \mu_1^{\bar{\varepsilon}_1} * \mu_2^{\bar{\varepsilon}_2}(A). \end{aligned}$$

□

Corollary 2.17. *The Harmonic semi-classical model for the ${}^1\text{H}^{19}\text{F}$ gas presented in Subsection 2.7.3,*

$$(\mathcal{E}, \mathcal{A}, d\mu(\zeta)) = (\mathbb{R}^2 \times \mathbb{N}, \text{Bor}(\mathbb{R}^2) \otimes \mathcal{P}(\mathbb{N}), dz \times 1), \quad \varepsilon(z, n) = \frac{1}{2}\mathcal{I}|z|^2 + hc\nu_e \left(n + \frac{1}{2} \right),$$

can be reduced to

$$(\mathbb{R}_+, \text{Bor}(\mathbb{R}_+), \varphi_{HF}(I) \, dI), \quad I \mapsto I + \frac{1}{2}hc\nu_e,$$

with

$$\varphi_{HF}(I) = C_2(\mathcal{I}) \left[\frac{I}{hc\nu_e} \right]. \quad (2.34)$$

Proof. This is a consequence of Proposition 2.14 with $d = 2$, Proposition 2.15 with $Q = \mathbb{N}$, $r_n = 1$ and $\varepsilon_n = hc\nu_e \left(n + \frac{1}{2} \right)$, and Proposition 2.16 with $(\mathcal{E}_1, \mathcal{A}_1, d\mu_1(\zeta_1)) = (\mathbb{R}^2, \text{Bor}(\mathbb{R}^2), dz)$, $\varepsilon_1(z) = \frac{1}{2}\mathcal{I}|z|^2$ and $(\mathcal{E}_2, \mathcal{A}_2, d\mu_2(\zeta_2)) = (\mathbb{N}, \mathcal{P}(\mathbb{N}), 1)$, $\varepsilon_2(n) = hc\nu_e \left(n + \frac{1}{2} \right)$.

□

This Corollary 2.17 illustrates the use of the reduction process: the model with continuous variable I and weight φ_{HF} corresponds to the model (classical for rotation, Harmonic quantum for vibration) for the ${}^1\text{H}^{19}\text{F}$ gas. The reader shall note that φ_{HF} is *not of the form* $I \mapsto I^\alpha$. As a matter of illustration, we plot on Fig. 2.3 the function φ_{HF} .

Corollary 2.18. Reduction of the combination of the continuous and discrete models. *More generally, let $\varphi_0 \in L_{loc}^1(\mathbb{R}_+, dI)$ be non-negative and non identically zero, Q a discrete set and $(r_q)_{q \in Q} \in (\mathbb{R}_+^*)^Q$. We denote by $\varepsilon^0 = \inf\{\varepsilon_q\}_{q \in Q}$ and we assume $\varepsilon^0 \in \mathbb{R}$ and that for all $\beta > 0$ one has $\sum_{q \in Q} e^{-\beta(\varepsilon_q - \varepsilon^0)} r_q < \infty$. Then the model*

$$(\mathbb{R}_+ \times Q, \text{Bor}(\mathbb{R}_+) \otimes \mathcal{P}(Q), \varphi_0(I) \, dI \, r_q), \quad \varepsilon(I, q) = I + \varepsilon_q$$

can be reduced to

$$(\mathbb{R}_+, \text{Bor}(\mathbb{R}_+), \varphi(I) \, dI), \quad I \mapsto I + \varepsilon^0,$$

with

$$\varphi(I) = \sum_{q \in Q} \mathbf{1}_{\varepsilon_q \leq I + \varepsilon^0} r_q \varphi_0(I + \varepsilon^0 - \varepsilon_q). \quad (2.35)$$

Proof. Again, this result directly follows from Propositions 2.15 and 2.16. □

Remark 2.9. *Still from Proposition 2.16, the model with two continuous variables with weights*

$$(\mathbb{R}_+ \times \mathbb{R}_+, \text{Bor}(\mathbb{R}_+) \otimes \text{Bor}(\mathbb{R}_+), \varphi_1(I_1) \, dI_1 \, \varphi_2(I_2) \, dI_2), \quad \varepsilon(I_1, I_2) = I_1 + I_2,$$

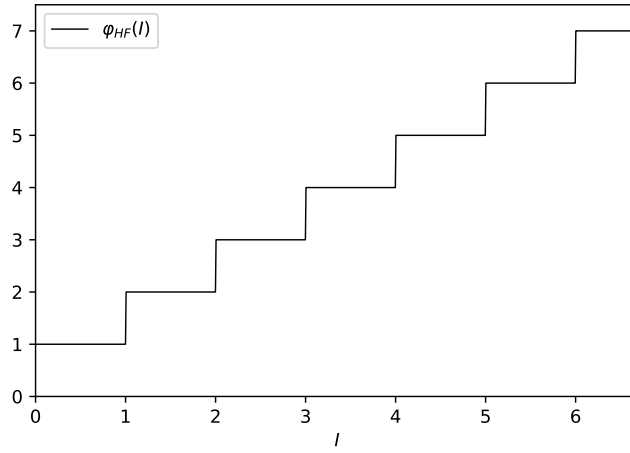


Figure 2.3 – Plot of φ_{HF} , re-scaled with $C_2(\mathcal{I}) \equiv 1$ and $hc\nu_e \equiv 1$.

can be reduced to the continuous model with weight $\varphi_1 * \varphi_2$, where $\varphi_1 * \varphi_2(I) = \int_0^I \varphi_1(I') \varphi_2(I - I') dI'$.

Remark 2.10. If we denote by $\delta_{\mu^{\bar{\varepsilon}}}$ the number of internal degrees of freedom associated with the general model $(\mathcal{E}, \mathcal{A}, \mu)$, ε , we get $\delta_{\mu_1^{\bar{\varepsilon}_1} * \mu_2^{\bar{\varepsilon}_2}} = \delta_{\mu_1^{\bar{\varepsilon}_1}} + \delta_{\mu_2^{\bar{\varepsilon}_2}}$ from the Equipartition Theorem 2.4. Thus $\mu^{\bar{\varepsilon}} \mapsto \delta_{\mu^{\bar{\varepsilon}}}$ is a morphism.

A comment on numerical aspects

Not only the process of model reduction links the *state*-based and *energy*-based points of view, it is also useful for numerical considerations. For instance, the space of internal states of the semi-classical model for $^1\text{H}^{19}\text{F}$ is $\mathbb{R}^2 \times \mathbb{N}$, whereas it is \mathbb{R}_+ for any reduced model, which is far more efficient to be used for numerical simulations. In order to construct an approximate model suited and efficient for simulation, one wishes to approximate the measure $\mu^{\bar{\varepsilon}}$ by a discrete measure, a finite sum of Diracs, of the form

$\sum_{k=1}^N r_k \chi_{\bar{\varepsilon}_k}$. Then the numerically-suited approximation of the general model

$$(\mathcal{E}, \mathcal{A}, \mu), \quad \varepsilon$$

is thus the discrete model

$$([1, N], \mathcal{P}([1, N]), (r_k)_{1 \leq k \leq N}), \quad (\bar{\varepsilon}_k + \varepsilon^0)_{1 \leq k \leq N},$$

At fixed N , we suggest to choose the $(r_k, \bar{\varepsilon}_k)_{1 \leq k \leq N}$ that minimizes a distance (for instance the 1 or 2-Wassertein distance, explicit in 1D) between the Gibbs probability measures associated with the measures

$\mu^{\bar{\varepsilon}}$ and $\sum_{k=1}^N r_k \chi_{\bar{\varepsilon}_k}$ at a temperature coherent with the considered problem. In [125], Magin et al. propose

to simplify a discrete model for dinitrogen (N_2) composed of 9390 rotation-vibration energy-levels by

creating energy bins, and replace the first model with an approximate discrete one composed of only 500 energy levels, which corresponds to approximating a sum a 9390 Diracs by a sum of 500 Diracs. This binning method can be extended to the general case. Like in section 2.3. of [125], consider a family of disjoint compact intervals of \mathbb{R}_+ , $(R_k)_{1 \leq k \leq N}$, and define the average energy of the k -th bin by

$$\epsilon_k := \varepsilon^0 + \frac{1}{r_k} \int_{R_k} I d\mu^{\bar{\varepsilon}}(I), \quad (2.36)$$

where $r_k := \mu^{\bar{\varepsilon}}(R_k)$ is the degeneracy associated with this energy level, with R_k such that r_k is not equal to zero. The choice of $(R_k)_{1 \leq k \leq N}$ can be arbitrary, or made by minimizing a distance, like we suggested earlier.

2.9 Conclusions

In this paper we have built up a general framework for the kinetic modelling of non-relativistic mono and polyatomic gases. It is based on a set of allowed internal states \mathcal{E} endowed with a suitable measure μ . Each particle is characterized by a proper state $\zeta \in \mathcal{E}$ with associated energy $\varepsilon(\zeta)$. Owing only to conservation of momentum and total energy, we are able to define the collision rule and the corresponding Boltzmann operator leaving \mathcal{E} , μ and $\varepsilon(\zeta)$ generic (not explicit). The Boltzmann H-Theorem has been proved in this general setting, and Maxwellian equilibria (depending also on internal energy) have been explicitly recovered. Also the number of internal degrees of freedom has been investigated, and the fluid–dynamic Euler equations have been derived. We have shown that usual models such as the monoatomic gas, the continuous internal energy description with weights [76], and the discrete energy levels description [100, 89] fit into our framework. Moreover, several different models may be built within the present general framework, as semi-classical models and quantum description (as main example, we have proposed four models for the hydrogen fluoride).

The main advantage of this general setting is to be able to construct a model from direct physical considerations, since we consider *internal states* and no longer directly *energy*. For instance, instead of considering from the beginning the rotational energy of a molecule, we may start from the angular velocity and construct the energy by the laws of classical mechanics (owing to inertia tensor). Moreover, thanks to the Equipartition Theorem, we are allowed to combine any pair of different internal states spaces $\mathcal{E}_1 \times \mathcal{E}_2$ and the corresponding measures as $\mu_1 \otimes \mu_2$ thus, as an important consequence, we have the possibility to keep separate the vibrational and the rotational parts of the internal energy of polyatomic molecules. Indeed, setting the space of internal states as $\mathcal{E} = \mathbb{R}_+ \times \mathbb{N}$ and $\varepsilon(I, n) = I + e_n$, we are able to describe the rotational energy by means of a continuous variable, and the vibrational one by a discrete energy variable, as suggested in [108]. Analogously, also the options of keeping both kinds of internal energies continuous (as in Extended Thermodynamics) or discrete are admissible.

Finally we have also shown that, generically, all models that fit our framework can be reduced to a one-real-parameter model, similar to the continuous internal energy model with weights, at the price of suitably changing, in a rigorous way, the integration measure. In this reduction procedure the considerations on states turn out to be summed up into the energy (the reduced model considers the internal energy directly). From theory to simulation, given a molecule to study, we suggest to first construct the *state-based* (general) model of the molecule from its physical description, then compute the associated energy law $\mu^{\bar{\varepsilon}}$ by performing the reduction process and finally define the numerically-suited approximate discrete model as detailed in Section 2.8. Also for the investigation of other interesting mathematical properties of the Boltzmann operator in this general frame, as the validity of the Fredholm alternative for the linearized operator, and the corresponding rigorous Chapman-Enskog asymptotic expansion up to Navier-Stokes equations, the original internal states formulation could be more intuitive to use. We finally remark that even the combination of the continuous and the discrete energy model finally turns out

to be, after the reduction, a continuous model with a weight explicitly computed in the paper, and this is a quite surprising result.

Of course it would be desirable to include in the kinetic model even more physical features of polyatomic particles. For instance, the quantum mechanical Boltzmann equation derived by Waldmann [158] and Snider [147] is able to describe also the polarization resulting from the effect of external fields on polyatomic gases [129]. Such model admits two vectorial collision invariants, corresponding to momentum and angular momentum, bearing in mind that polyatomic particles are generally non spherical, and also the corresponding macroscopic equations include a proper angular momentum conservation equation [128, 84, 129]. It is well known [128] that in absence of polarization effects, namely for isotropic gases, the quantum mechanical theory yields the same formal results as classical or semi-classical approaches considered in this paper, but a general kinetic framework able to include also possible polarization (and therefore additional collision invariants) could be an interesting further step in kinetic investigation of polyatomic gases.

We aim also at extending our general way of modelling to mixtures of polyatomic gases, possibly undergoing chemical reactions. Of course collision rules, and consequently some technical parts of the proofs, would be much more complicated due to the presence of mass ratios and of the amount of energy produced or consumed by chemical reactions. The investigation of a suitable general framework for gas mixtures will be the subject of a future work.

Lemma 2.19. *Let $r > 0$, assume that $\mu(\{0 < \bar{\varepsilon} \leq r\}) > 0$. Then*

$$\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \underset{x \rightarrow \infty}{=} \int_{\bar{\varepsilon} \leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) + o\left(\int_{\bar{\varepsilon} \leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)\right)$$

and
$$\int_{\mathcal{E}} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \underset{x \rightarrow \infty}{=} \int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) + o\left(\int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)\right).$$

Proof. First, we have that

$$\int_{\mathcal{E}} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) = \int_{\bar{\varepsilon} \leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) + \int_{\bar{\varepsilon} > r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta),$$

and
$$\int_{\mathcal{E}} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) = \int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) + \int_{\bar{\varepsilon} > r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta).$$

Thus we must prove

$$\int_{\bar{\varepsilon} > r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \underset{x \rightarrow \infty}{=} o\left(\int_{\bar{\varepsilon} \leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)\right),$$

$$\int_{\bar{\varepsilon} > r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \underset{x \rightarrow \infty}{=} o\left(\int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)\right).$$

First, note that

$$\int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \geq \mu(\{\bar{\varepsilon} \leq r\}) e^{-xr}.$$

Since $\mu(\{\bar{\varepsilon} \leq r\}) > 0$, we deduce that $\int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) > 0$ and

$$0 \leq \frac{\int_{\bar{\varepsilon} > r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)}{\int_{\bar{\varepsilon} \leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)} \leq \frac{e^{xr}}{\mu(\{\bar{\varepsilon} \leq r\})} \int_{\bar{\varepsilon} > r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) = \frac{1}{\mu(\{\bar{\varepsilon} \leq r\})} \int_{\bar{\varepsilon} > r} e^{-x(\bar{\varepsilon}(\zeta)-r)} d\mu(\zeta).$$

Now note that, on the set $\{\bar{\varepsilon} > r\}$,

$$e^{-x(\bar{\varepsilon}(\zeta)-r)} \xrightarrow{x \rightarrow \infty} 0.$$

Also, $(\zeta \mapsto e^{-x(\bar{\varepsilon}(\zeta)-r)})_{x>0}$ is a non-increasing family of non-negative functions on the set $\{\bar{\varepsilon} > r\}$. By monotone convergence theorem,

$$\int_{\bar{\varepsilon}>r} e^{-x(\bar{\varepsilon}(\zeta)-r)} d\mu(\zeta) \xrightarrow{x \rightarrow \infty} 0.$$

We deduce that

$$\frac{\int_{\bar{\varepsilon}>r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)}{\int_{\bar{\varepsilon}\leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)} \xrightarrow{x \rightarrow \infty} 0,$$

that is our goal

$$\int_{\bar{\varepsilon}>r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \underset{x \rightarrow \infty}{=} o\left(\int_{\bar{\varepsilon}\leq r} e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)\right).$$

Concerning the other goal, it obviously holds

$$\int_{\bar{\varepsilon}\leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \geq e^{-xr} \int_{\bar{\varepsilon}\leq r} \bar{\varepsilon}(\zeta) d\mu(\zeta),$$

and, since $\mu(\{0 < \bar{\varepsilon} \leq r\}) > 0$, we deduce that $\int_{\bar{\varepsilon}\leq r} \bar{\varepsilon}(\zeta) d\mu(\zeta) > 0$. Moreover,

$$\int_{\bar{\varepsilon}\leq r} \bar{\varepsilon}(\zeta) d\mu(\zeta) \leq r\mu(\{\bar{\varepsilon} \leq r\}) < \infty$$

(last inequality has been shown in Section 2.2). It follows that

$$0 \leq \frac{\int_{\bar{\varepsilon}>r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)}{\int_{\bar{\varepsilon}\leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)} \leq \frac{e^{xr}}{\int_{\bar{\varepsilon}\leq r} \bar{\varepsilon}(\zeta) d\mu(\zeta)} \int_{\bar{\varepsilon}>r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) = \frac{\int_{\bar{\varepsilon}>r} \bar{\varepsilon}(\zeta) e^{-x(\bar{\varepsilon}(\zeta)-r)} d\mu(\zeta)}{\int_{\bar{\varepsilon}\leq r} \bar{\varepsilon}(\zeta) d\mu(\zeta)}.$$

Now note that, on the set $\{\bar{\varepsilon} > r\}$,

$$\bar{\varepsilon}(\zeta) e^{-x(\bar{\varepsilon}(\zeta)-r)} \xrightarrow{x \rightarrow \infty} 0.$$

Also, $(\zeta \mapsto \bar{\varepsilon}(\zeta) e^{-x(\bar{\varepsilon}(\zeta)-r)})_{x>0}$ is a non-increasing family of nonnegative functions on the set $\{\bar{\varepsilon} > r\}$. By dominated convergence theorem,

$$\int_{\bar{\varepsilon}>r} \bar{\varepsilon}(\zeta) e^{-x(\bar{\varepsilon}(\zeta)-r)} d\mu(\zeta) \xrightarrow{x \rightarrow \infty} 0.$$

We deduce that

$$\frac{\int_{\bar{\varepsilon}>r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)}{\int_{\bar{\varepsilon}\leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)} \xrightarrow{x \rightarrow \infty} 0,$$

that is

$$\int_{\bar{\varepsilon}>r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta) \underset{x \rightarrow \infty}{=} o\left(\int_{\bar{\varepsilon}\leq r} \bar{\varepsilon}(\zeta) e^{-x\bar{\varepsilon}(\zeta)} d\mu(\zeta)\right).$$

□

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Chapter 3

An internal state kinetic model for chemically reacting mixtures of monatomic and polyatomic gases

Outline of the current chapter

3.1	Introduction	117
3.2	Setting	118
3.3	Collision model	120
	Collision rules and transformation	121
3.4	The Boltzmann model	123
	Distribution function and kinetic equation	123
	Macroscopic quantities	123
	3.4.1 Boltzmann operator	124
	Mechanical and chemical collision operators	126
	3.4.2 Mechanical and global collision invariants	127
	3.4.3 H-Theorem	130
3.5	Equilibrium	131
	3.5.1 Mechanical equilibrium	132
	3.5.2 Mechanical and chemical equilibrium	134
	3.5.3 Rate of reaction	136
3.6	Euler limit	140
3.7	Example of a computation of the rate of reaction	143
3.8	Reduced models and energy of reaction	144
3.9	Example of a three species gas mixture undergoing one chemical reaction	145
	State-based model	146
	Corresponding energy-based model	146
	Quantities of interest	147
3.10	Conclusion	148

3.A Auxiliary lemma	149
3.B Physical and chemical quantities reminder	151

3.1 Introduction

The kinetic approach to the description of gas mixtures has a long tradition, and in the literature integro-differential models of Boltzmann type [112, 61], or suitable simpler BGK approximations [11, 32] have been proposed and investigated. Many of the models for inert mixtures have been generalized to gas species undergoing chemical reactions; however, the major part of existing kinetic descriptions of reactive frames assumes the presence of only one bimolecular and reversible reaction, involving monatomic gases [144, 99, 97, 132, 50]. These models are thus too simplistic, since it is well known that each real bimolecular reaction involves at least a polyatomic species; even in simpler transitions of dissociation or recombination type, one needs to model polyatomic molecules. For this reason, the kinetic approach has been extended also to polyatomic gases, modelling the non-translational degrees of freedom by means of an internal energy variable, that could be assumed discrete or continuous. The Boltzmann model with discrete energy levels may be found for instance in [89, 100], while the model with a continuous internal energy has been proposed and investigated in [75, 76]. In case of continuous internal energy, the Boltzmann collision operator involves an integral over the energy variable, with a suitable weight function related to the number of degrees of freedom of the considered species, that diverges in case of a monatomic gas; consequently, the kinetic description of mixtures of monatomic and polyatomic species needs to model collisions involving atoms separately, by means of classical Boltzmann operators [76]. A Chapman–Enskog closure and a BGK approximation of this model have been recently investigated [19, 49]. On the other hand, in the discrete energy frame a monatomic gas could be easily recovered as a species having only one energy level, but even in this simpler case a BGK model allowing to involve mixtures of monatomic and polyatomic species (namely, with each gas characterized by its own number of energy levels) has been only recently built up [30].

As concerns reacting mixtures, it is well known that a collision may change the nature of the molecules only if the total energy of the impinging particles exceeds the activation energy which characterizes the considered chemical reaction [18], but this threshold is taken into account only in some of the existing kinetic models [96, 115, 142]. Moreover, the generalization of the kinetic approach to mixtures involving chains of chemical reactions is not straightforward, even if the possible presence of several reacting species is already taken into account in some classical references [146, 89]. In this respect, some specific problems have been faced at Boltzmann level for monatomic gases in [68, 70] and macroscopic equations have been constructed owing to suitable entropy principles [41]; moreover, as concerns polyatomic species, dissociation and recombination processes affecting a diatomic gas have been investigated [130, 98], and a general kinetic model for an arbitrary number of reactions on crystal surfaces involving monatomic or polyatomic species has been dealt with in [13].

In order to improve the generality of the kinetic description of polyatomic gases, we have recently proposed [37] a kinetic Boltzmann model where the internal structure of a molecule is described by a single internal state parameter, belonging to a suitable space. Proper options for such a space of internal states and for the measure defined on it allow to reproduce some models commonly used in kinetic theory for polyatomic particles: the description based on a set of discrete internal energy levels [100, 89], and the one involving a continuous internal energy variable [76]. Moreover, it has been shown that within this general framework it is possible to build up new models desirable in physical applications, including the possibility to separate the internal energy into two different components, the rotational and the vibrational ones. We are able to recover the existing attempts of separating these two internal energies using different discrete indices [89] or two continuous energy variables [69, 16], and also to approximate rotational energy by means of a continuous variable keeping the vibrational one discrete; this way of modelling turns out to be physically reasonable, since the gap between two subsequent discrete levels is much lower for rotational than for vibrational energy [108]. The consistency of our kinetic Boltzmann model for polyatomic gases has been proved, together with the validity of the H–theorem for each choice of the space of internal states and of its measure. We have also shown that, under suitable assumptions on

the Boltzmann cross sections, it is possible to reduce the models fitting our general internal state setting to a one-real-variable description with a suitable measure, similar to the classical continuous model with integration weight.

The aim of this work is to extend the Boltzmann model proposed in [37] to a mixture of monatomic and polyatomic gases, possibly undergoing bimolecular and reversible chemical reactions. Each gas is characterized by its own space of internal states, endowed with a suitable measure; in this way we could manage simultaneously monatomic species (with a fixed internal energy) and polyatomic constituents with discrete or continuous internal energy structure (or even both, if rotational and vibrational energies are kept separate). Unlike many existing kinetic models described above, in our general framework an arbitrary number of bimolecular reactions could be taken into account, and each species could be involved in more than one reaction; even the activation energy of each chemical reaction is included in the relevant Boltzmann cross section. Of course collision rules are more complicated than for a single polyatomic gas investigated in [37], due to the presence of mass ratios and of the amount of energy produced or consumed by chemical reactions. After the presentation of our setting and of the Boltzmann operators for elastic and chemical interactions, the collision invariants of mechanical scattering and of global (mechanical plus chemical) Boltzmann operators are determined and the Boltzmann H-theorem is proved, leading to the expected Maxwellian equilibria depending also on the internal energy, with suitable mass action laws relating number densities of gases involved in the admissible chemical reactions with temperature of the mixture. Euler equations in case of moderately slow chemical reactions (namely, in an elastic dominated regime) are also derived.

In more detail, the article is organized as follows. In Section 2, the general setting considered in this paper is described, as well as the admissible collisions. Section 3 is devoted to the collision rules and to their properties, while Section 4 deals with the Boltzmann equations; specifically, after introducing main macroscopic fields and elastic and chemical Boltzmann operators together with the assumptions on the cross sections, mechanical and global collision invariants are determined and the H-theorem is proved. In Section 5, the equilibrium configurations are discussed, focusing the attention at first on the mechanical equilibria and on the corresponding thermodynamic properties (internal degrees of freedom, specific heat at constant volume, and macroscopic fields of each species), and then on the global collision equilibria, involving the mass action laws relevant to the admissible chemical reactions. The Euler limit in a mechanical dominated regime is then investigated in Section 6. The following short sections are devoted to possible applications of our framework: Section 7 shows an example of a computation of a rate of reaction, in Section 8 we discuss the possibility of reducing our general description to a model with only one continuous variable (at the price of complicating the measure space), and in Section 9 we provide an explicit realistic example involving three gas species undergoing a bimolecular reversible reaction. Section 10 contains some concluding remarks and perspectives. We have collected in two appendices a technical result (in Appendix A) and, for readers' convenience, some tables summarizing all physical and chemical quantities used in this paper (in Appendix B).

3.2 Setting

We describe our non-relativistic kinetic framework for the study of mixture of gases (mono- or polyatomic), with or without chemical reactions. We consider a gas mixture composed of N species. Each molecule of the gas is described by its species label i and its state, namely its velocity v and internal state ζ , representing for instance rotation and vibration. The species or state of a molecule is assumed to possibly change only because of a binary interaction, which can be a mechanical collision or a chemical reaction.

While it is common to consider from the beginning the energy of reaction in the study of chemical reactions, we decide not to adopt this point of view in this paper. Indeed, our approach consists in con-

sidering that the reacting molecules form an isolated system, with no exchange of matter or energy with the environment, in contrast with the option that the reacting molecules form a closed system, possibly exchanging energy with its environment. This choice is motivated by a wish of simplicity and generality of the formulation. As can be seen in [107, Chapter 1], the energy of reaction is the difference between the fundamental potential energy of the products and of the reactants, that is of the two local minima in Fig. 3.1, and this is how the energy of reaction appears in our framework. Figure 3.1 is borrowed from [107, Chapter 1] and illustrates the evolution of the potential energy during an exothermic chemical reaction. Here, some of the potential energy of the reactants is converted into kinetic, or rotational, vibrational, etc., energy for the products, so that the chemical reaction induces an overall growth of temperature. In our framework, the potential energy of configuration is taken into account in the internal description, so that there is no need to a priori introduce any energy of reaction. The equivalence of our formulation with others used in kinetic theory regarding this consideration will be investigated in Section 3.8.

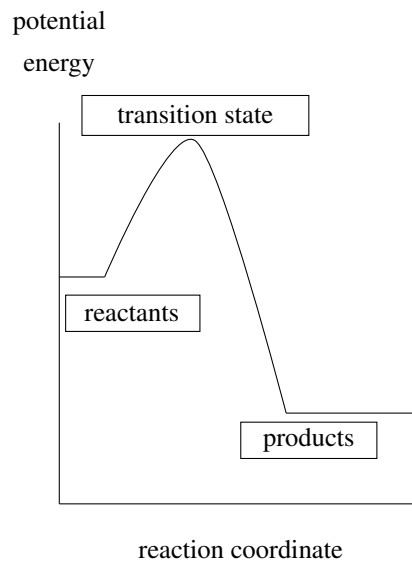


Figure 3.1 – Reaction coordinate diagram

Another feature appearing in Figure 3.1 is the existence of a transition state. It is a state of maximum potential energy, and the chemical reaction may occur only if the reactants have enough energy to get to this state [107, Chapter 1]. In the Boltzmann framework, collisions are considered instantaneous, so that species transition state does not have to be studied and does not appear in the conservation laws. This feature is taken into account here as a potential barrier, linked to the activation energy, to overcome for a chemical reaction to be possible, as it will be explained in Section 3.3.

Following [37], we associate to each species of the gas, labelled by $i \in \llbracket 1, N \rrbracket$ (the set of integer numbers such that $1 \leq i \leq N$), a measured space of internal states $(\mathcal{E}_i, \mathcal{A}_i, \mu_i)$, with \mathcal{E}_i the set of internal states, \mathcal{A}_i a σ -algebra on \mathcal{E}_i and μ_i a measure on \mathcal{E}_i adapted to \mathcal{A}_i , an \mathcal{A}_i -measurable internal energy function $\varepsilon_i : \mathcal{E}_i \rightarrow \mathbb{R}$, and we denote by m_i the mass of a molecule of this species. Hence each species can be described with its own adapted model. For instance, we may study a mixture of three gases, the first one described by the monatomic model, the second by the weighted continuous internal energy model [35, 75, 76] and the third by a discrete internal energy model [100, 25].

Following [37], we assume that ε_i admits a finite essential infimum under μ_i denoted by ε_i^0 , and define the grounded internal energy function

$$\bar{\varepsilon}_i = \varepsilon_i - \varepsilon_i^0. \quad (3.1)$$

We define Z_i , the partition function of the species i , by

$$Z_i(\beta) = \int_{\mathcal{E}_i} e^{-\beta \bar{\varepsilon}_i(\zeta)} \mathbf{d}\mu_i(\zeta), \quad (3.2)$$

and assume that $Z_i(\beta) < \infty$ for any $\beta > 0$. The choice of $\bar{\varepsilon}_i$ in the definition of the partition function Z_i is motivated by physical considerations, as explained in [37, Remark 4.2].

The quantity ε_i^0 corresponds to the fundamental energy of the molecule, hence to its potential energy of configuration. It plays a role in chemical reactions.

The way we handle an arbitrary number of chemical reactions is the following. We consider a space of allowed collisions, denoted by Ω . When the collision of particles of species i and j transforming them into particles k and l is possible, we write $\{(i, j) \rightarrow (k, l)\} \in \Omega$. We assume that

- mechanical collisions are allowed collisions, that is, for any $1 \leq i, j \leq N$,

$$\{(i, j) \rightarrow (i, j)\} \in \Omega; \quad (3.3)$$

- collisions are symmetric and can happen in both directions, that is

$$\{(i, j) \rightarrow (k, l)\} \in \Omega \iff \{(j, i) \rightarrow (l, k)\} \in \Omega \iff \{(k, l) \rightarrow (i, j)\} \in \Omega; \quad (3.4)$$

- a redundant symmetry property, implying that every collision is accounting for exactly once when $k = l$ and twice when $k \neq l$

$$\{(i, j) \rightarrow (k, l)\} \in \Omega \iff \{(i, j) \rightarrow (l, k)\} \in \Omega; \quad (3.5)$$

- collisions are mass conserving, that is for any $\{(i, j) \rightarrow (k, l)\} \in \Omega$,

$$m_i + m_j = m_k + m_l. \quad (3.6)$$

For any allowed collision $\{(i, j) \rightarrow (k, l)\} \in \Omega$, we denote by $\kappa_{ij}^{kl} \in \mathbb{R}$ the energy of the transition state of the collision. We make the following assumptions on κ_{ij}^{kl} .

- For any $\{(i, j) \rightarrow (k, l)\} \in \Omega$,

$$\kappa_{ij}^{kl} \geq \max(\varepsilon_i^0 + \varepsilon_j^0, \varepsilon_k^0 + \varepsilon_l^0). \quad (3.7)$$

- For any $\{(i, j) \rightarrow (k, l)\} \in \Omega$,

$$\kappa_{ij}^{kl} = \kappa_{ji}^{lk} = \kappa_{ij}^{lk} = \kappa_{kl}^{ij}. \quad (3.8)$$

- We assume no transition states for mechanical collisions, that is, for any $(i, j) \in \llbracket 1, N \rrbracket^2$,

$$\kappa_{ij}^{ij} = \varepsilon_i^0 + \varepsilon_j^0. \quad (3.9)$$

We illustrate in Figure 3.2 the role of the quantities $\varepsilon_i^0, \varepsilon_j^0, \varepsilon_k^0, \varepsilon_l^0$ and κ_{ij}^{kl} in the case of a chemical reaction; we highlight in particular that the potential energy of configuration of the system of the two molecules labelled by i and j is $\varepsilon_i^0 + \varepsilon_j^0$.

3.3 Collision model

We consider a collision $\{(i, j) \rightarrow (k, l)\} \in \Omega$. The states of the pre-collision molecules are denoted by $(v, \zeta) \in \mathbb{R}^3 \times \mathcal{E}_i$ and $(v_*, \zeta_*) \in \mathbb{R}^3 \times \mathcal{E}_j$, and the states of the post-collision molecules are denoted

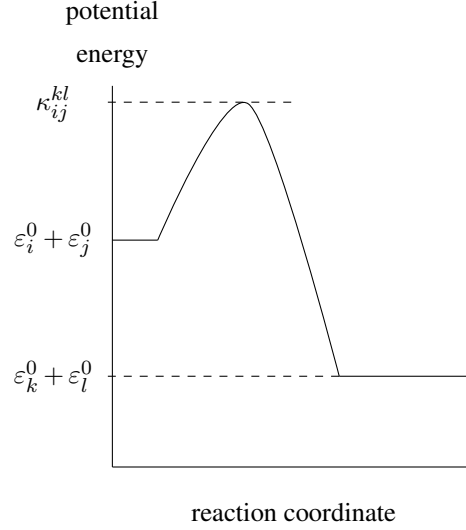


Figure 3.2 – Reaction coordinate diagram with reference energy thresholds

by $(v', \zeta') \in \mathbb{R}^3 \times \mathcal{E}_k$ and $(v_*, \zeta_*) \in \mathbb{R}^3 \times \mathcal{E}_l$. Writing the conservation of momentum and energy of the isolated system yields

$$\begin{cases} m_i v + m_j v_* = m_k v' + m_l v_*' \\ \frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) + \frac{1}{2} m_j |v_*|^2 + \varepsilon_j(\zeta_*) = \frac{1}{2} m_k |v'|^2 + \varepsilon_k(\zeta') + \frac{1}{2} m_l |v_*'|^2 + \varepsilon_l(\zeta_*'). \end{cases} \quad (3.10)$$

Notice that in this state-based formulation no energy of chemical reaction appears in (3.10). An explanation and link with the usual Borgnakke–Larsen formulation of the energy conservation law for chemical reactions [76] is provided in Section 3.8.

Collision rules and transformation

We set $m_{ij}^* = \frac{m_i m_j}{m_i + m_j}$ and $M_{ij} = m_i + m_j$. Notice that

$$\frac{1}{2} m_i |v|^2 + \frac{1}{2} m_j |v_*|^2 = \frac{m_{ij}^*}{2} |v - v_*|^2 + \frac{M_{ij}}{2} \left| \frac{m_i v + m_j v_*}{m_i + m_j} \right|^2.$$

Using the conservation laws (3.6) and (3.10), we have

$$\frac{M_{ij}}{2} \left| \frac{m_i v + m_j v_*}{m_i + m_j} \right|^2 = \frac{M_{kl}}{2} \left| \frac{m_k v' + m_l v_*'}{m_k + m_l} \right|^2$$

from which we deduce that

$$\frac{m_{ij}^*}{2} |v - v_*|^2 + \varepsilon_i(\zeta) + \varepsilon_j(\zeta_*) = \frac{m_{kl}^*}{2} |v' - v_*'|^2 + \varepsilon_k(\zeta') + \varepsilon_l(\zeta_*').$$

Let us set

$$\Delta_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*) = \frac{m_{ij}^*}{m_{kl}^*} |v - v_*|^2 + \frac{2}{m_{kl}^*} (\varepsilon_i(\zeta) + \varepsilon_j(\zeta_*) - \varepsilon_k(\zeta') - \varepsilon_l(\zeta'_*)), \quad (3.11)$$

which satisfies the symmetry property

$$\Delta_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*) = \Delta_{ji}^{lk}(v_*, v, \zeta_*, \zeta, \zeta'_*, \zeta'). \quad (3.12)$$

We then have

$$|v' - v_*'|^2 = \Delta_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*), \quad (3.13)$$

and by a classical argument we conclude that there exists $\omega \in \mathbb{S}^2$ such that

$$\begin{cases} v' = \frac{m_i v + m_j v_*}{M_{ij}} + \frac{m_l}{M_{kl}} \sqrt{\Delta_{ij}^{kl}} T_\omega \left[\frac{v - v_*}{|v - v_*|} \right] \\ v_*' = \frac{m_i v + m_j v_*}{M_{ij}} - \frac{m_k}{M_{kl}} \sqrt{\Delta_{ij}^{kl}} T_\omega \left[\frac{v - v_*}{|v - v_*|} \right], \end{cases} \quad (3.14)$$

where T_ω is the symmetry with respect to $(\mathbb{R}\omega)^\perp$,

$$\forall V \in \mathbb{S}^2, \quad T_\omega[V] := V - 2(\omega \cdot V)\omega \in \mathbb{S}^2. \quad (3.15)$$

Note that (3.14) makes sense if and only if $\Delta_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*) \geq 0$.

For any allowed collision $\{(i, j) \rightarrow (k, l)\} \in \Omega$ and $(\zeta, \zeta_*, \zeta', \zeta'_*) \in \mathcal{E}_i \times \mathcal{E}_j \times \mathcal{E}_k \times \mathcal{E}_l$, we define the set of pre-collision velocities (v, v_*) such that the collision

$$(v, \zeta) \in \mathbb{R}^3 \times \mathcal{E}_i, (v_*, \zeta_*) \in \mathbb{R}^3 \times \mathcal{E}_j \quad \longrightarrow \quad (\cdot, \zeta') \in \mathbb{R}^3 \times \mathcal{E}_k, (\cdot, \zeta'_*) \in \mathbb{R}^3 \times \mathcal{E}_l$$

is possible, namely

$$\begin{aligned} & E_{ij}^{kl}[\zeta, \zeta_*, \zeta', \zeta'_*] \\ &= \left\{ (v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3 \left| \frac{m_{ij}^*}{2} |v - v_*|^2 + \varepsilon_i(\zeta) + \varepsilon_j(\zeta_*) \geq \max(\varepsilon_k(\zeta') + \varepsilon_l(\zeta'_*), \kappa_{ij}^{kl}) \right. \right\}. \end{aligned} \quad (3.16)$$

Notice that κ_{ij}^{kl} appears in the definition of $E_{ij}^{kl}[\zeta, \zeta_*, \zeta', \zeta'_*]$ as a potential barrier.

Definition 3.1. For any allowed collision $\{(i, j) \rightarrow (k, l)\} \in \Omega$, $(\zeta, \zeta_*, \zeta', \zeta'_*) \in \mathcal{E}_i \times \mathcal{E}_j \times \mathcal{E}_k \times \mathcal{E}_l$ and $\omega \in \mathbb{S}^2$, we define the transformation

$$\begin{aligned} & S_\omega^{ijkl}[\zeta, \zeta_*, \zeta', \zeta'_*] : \\ & \begin{cases} E_{ij}^{kl}[\zeta, \zeta_*, \zeta', \zeta'_*] & \longrightarrow & E_{kl}^{ij}[\zeta', \zeta'_*, \zeta, \zeta_*] \\ (v, v_*) \mapsto & \left(\frac{m_i v + m_j v_*}{M_{ij}} + \frac{m_l}{M_{kl}} \sqrt{\Delta_{ij}^{kl}} T_\omega \left[\frac{v - v_*}{|v - v_*|} \right], \right. \\ & \left. \frac{m_i v + m_j v_*}{M_{ij}} - \frac{m_k}{M_{kl}} \sqrt{\Delta_{ij}^{kl}} T_\omega \left[\frac{v - v_*}{|v - v_*|} \right] \right), \end{cases} \end{aligned} \quad (3.17)$$

where Δ_{ij}^{kl} and T_ω are defined in (3.11) and (3.15), respectively.

The transformation $S_\omega^{ijkl}[\zeta, \zeta_*, \zeta', \zeta'_*]$ links, at fixed angle ω and internal states $\zeta, \zeta_*, \zeta', \zeta'_*$, the pre- and post-collision velocities.

Lemma 3.1. *For any allowed collision $\{(i, j) \rightarrow (k, l)\} \in \Omega$, $(\zeta, \zeta_*, \zeta', \zeta'_*) \in \mathcal{E}_i \times \mathcal{E}_j \times \mathcal{E}_k \times \mathcal{E}_l$ and $\omega \in \mathbb{S}^2$, $S_\omega^{ijkl}[\zeta, \zeta_*, \zeta', \zeta'_*]$ is well-defined and is a bijection, with*

$$\left(S_\omega^{ijkl}[\zeta, \zeta_*, \zeta', \zeta'_*]\right)^{-1} = S_\omega^{klij}[\zeta', \zeta'_*, \zeta, \zeta_*].$$

Lemma 3.2. *The Jacobian of the transformation $S_\omega^{ijkl}[\zeta, \zeta_*, \zeta', \zeta'_*]$ is given by the formula*

$$J \left[S_\omega^{ijkl}[\zeta, \zeta_*, \zeta', \zeta'_*] \right] = \frac{m_i m_j}{m_k m_l} \times \frac{|v' - v'_*|}{|v - v_*|}. \quad (3.18)$$

The proofs are similar to those of [37, Lemmas 2.1 and 2.2].

3.4 The Boltzmann model

Distribution function and kinetic equation

We study the function F describing the density of molecules of every species. For $i \in \llbracket 1, N \rrbracket$, the density associated with the species i is denoted by F_i . It depends on four variables:

- 2 macroscopic variables: the time $t \in \mathbb{R}$ or \mathbb{R}_+ and the position in space $x \in \mathbb{R}^3$ or \mathbb{T}^3 ;
- 2 kinetic variables: the velocity $v \in \mathbb{R}^3$ and the internal state $\zeta \in \mathcal{E}_i$.

As a distribution function, F_i is non-negative, so that we study $F_i(t, x, v, \zeta) \in \mathbb{R}_+$. Moreover, we assume that for any (t, x) , $F_i(t, x, \cdot, \cdot) \in L^1(\mathbb{R}^3 \times \mathcal{E}_i, dv d\mu_i(\zeta))$. The evolution of this distribution function is governed by the Boltzmann equation

$$\partial_t F_i(t, x, v, \zeta) + v \cdot \nabla_x F_i(t, x, v, \zeta) = \mathcal{B}(F, F)_i(t, x, v, \zeta), \quad (3.19)$$

where \mathcal{B} is the Boltzmann collision operator we define in the following subsection.

Macroscopic quantities

From the density function we can compute the macroscopic quantities. Let $i \in \llbracket 1, N \rrbracket$. If ϕ defined on $\mathbb{R}^3 \times \mathcal{E}_i$ is a molecular property, then the associated macroscopic quantity for the species i is

$$\int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \phi(v, \zeta) F_i(t, x, v, \zeta) dv d\mu_i(\zeta).$$

Typically, $\phi = m_i$, $\phi = m_i v$ and $\phi = \frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta)$ give the macroscopic mass density ρ_i (and macroscopic number density n_i), velocity u_i and specific energy density e_i of the species i , respectively, as

$$\begin{aligned} \rho_i(t, x) &= \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} m_i F_i(t, x, v, \zeta) dv d\mu_i(\zeta) \quad \text{and} \quad n_i(t, x) = \frac{\rho_i(t, x)}{m_i} \\ u_i(t, x) &= \frac{1}{\rho_i(t, x)} \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} m_i v F_i(t, x, v, \zeta) dv d\mu_i(\zeta) \\ e_i(t, x) &= \frac{1}{n_i(t, x)} \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \left(\frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) \right) F_i(t, x, v, \zeta) dv d\mu_i(\zeta). \end{aligned}$$

The total (number and mass) density, average velocity and specific energy density are given by

$$\bar{n} = \sum_{i=1}^N n_i, \quad \bar{\rho} = \sum_{i=1}^N \rho_i, \quad \underline{u} = \sum_{i=1}^N \frac{n_i}{\bar{n}} u_i, \quad \bar{e} = \sum_{i=1}^N \frac{n_i}{\bar{n}} e_i.$$

Finally, one can define the temperature of the species i by

$$T_i = \Theta_i^{-1} \left(\frac{1}{n_i} \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \left(\frac{1}{2} m_i |v - u_i|^2 + \bar{e}_i(\zeta) \right) F_i(v, \zeta) \, dv \, d\mu_i(\zeta) \right), \quad (3.20)$$

where $\Theta_i(T) = \frac{3}{2} k_B T - \log(Z_i)' \left(\frac{1}{k_B T} \right)$, as well as the temperature of the whole gas

$$T = \bar{\Theta} \left[\left(\frac{n_i}{\bar{n}} \right) \right]^{-1} \left(\frac{1}{\bar{n}} \sum_{i=1}^N \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \left(\frac{1}{2} m_i |v - u_i|^2 + \bar{e}_i(\zeta) \right) F_i(v, \zeta) \, dv \, d\mu_i(\zeta) \right), \quad (3.21)$$

where $\bar{\Theta} \left[\left(\frac{n_i}{\bar{n}} \right) \right] (T) = \sum_{i=1}^N \frac{n_i}{\bar{n}} \Theta_i(T)$. Justifications for the definitions (3.20) and (3.21) and a proof that they coincide with the species and global temperatures defined in classical kinetic models will be provided in Section 3.5.

3.4.1 Boltzmann operator

The Boltzmann operator acts as a source term in Equation (3.19) and represents the fact that collisions between molecules change their velocities and internal states.

Collision kernel

When two molecules collide, not all possible post-collision states are equiprobable. This idea is translated in the concept of the collision kernel, linked with the cross-section. This kernel encapsulates the information on the interaction potential, for example a hard sphere or Lennard-Jones one [61]. The collision kernel B is a family of measurable functions

$$B_{ij}^{kl} : \begin{cases} \mathbb{R}^3 \times \mathbb{R}^3 \times \mathcal{E}_i \times \mathcal{E}_j \times \mathcal{E}_k \times \mathcal{E}_l \times \mathbb{S}^2 \rightarrow \mathbb{R}_+ \\ (v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) \mapsto B_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega), \end{cases} \quad (3.22)$$

for any $i, j, k, l \in \llbracket 1, N \rrbracket$.

Assumption 3.1. Symmetry. The kernel B is symmetric in the following sense: if $\{(i, j) \rightarrow (k, l)\} \in \Omega$, then for a.e. $v, v_* \in \mathbb{R}^3$, for $\mu_i \otimes \mu_j \otimes \mu_k \otimes \mu_l$ -a.e. $(\zeta, \zeta_*, \zeta', \zeta'_*) \in \mathcal{E}_i \times \mathcal{E}_j \times \mathcal{E}_k \times \mathcal{E}_l$ and a.e. $\omega \in \mathbb{S}^2$,

$$B_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) = B_{ji}^{lk}(v_*, v, \zeta_*, \zeta, \zeta'_*, \zeta', \omega) = B_{ij}^{lk}(v, v_*, \zeta, \zeta_*, \zeta'_*, \zeta', \omega). \quad (3.23)$$

When $k \neq l$, due to the redundancy (3.5), one should think of B_{ij}^{kl} as half the physical collision kernel.

Assumption 3.2. Micro-reversibility. For $\{(i, j) \rightarrow (k, l)\} \in \Omega$, for a.e. $v, v_* \in \mathbb{R}^3$, for $\mu_i \otimes \mu_j \otimes \mu_k \otimes \mu_l$ -a.e. $(\zeta, \zeta_*, \zeta', \zeta'_*) \in \mathcal{E}_i \times \mathcal{E}_j \times \mathcal{E}_k \times \mathcal{E}_l$ and a.e. $\omega \in \mathbb{S}^2$,

$$m_i^2 m_j^2 |v - v_*| B_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) = m_k^2 m_l^2 |v' - v'_*| B_{kl}^{ij}(v', v'_*, \zeta', \zeta'_*, \zeta, \zeta_*, \omega), \quad (3.24)$$

where $(v', v'_*) = S_\omega^{ijkl}[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$.

The kernel B is positive when a collision is possible, and equal to zero when it is not admissible. The following positivity requirement, namely Assumption 3.3, also links our way of dealing with transition states with the approach used in [95, 96, 115], where the energy of the transition state is taken into account in the kernel through the introduction of a step function relative to the activation energy.

Definition 3.2. For $\{(i, j) \rightarrow (k, l)\} \in \Omega$, for a.e. $v, v_* \in \mathbb{R}^3$, for $\mu_i \otimes \mu_j \otimes \mu_k \otimes \mu_l$ -a.e. $(\zeta, \zeta_*, \zeta', \zeta'_*) \in \mathcal{E}_i \times \mathcal{E}_j \times \mathcal{E}_k \times \mathcal{E}_l$, we define $\mathbb{S}_{ijkl}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*]$ as the subset of \mathbb{S}^2 such that for any $\omega \in \mathbb{S}^2$,

$$\omega \in \mathbb{S}_{ijkl}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*] \iff B_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) > 0.$$

Assumption 3.3. We assume that

$$(v, v_*) \in E_{ij}^{kl}[\zeta, \zeta_*, \zeta', \zeta'_*] \iff \mathbb{S}_{ijkl}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*] \text{ contains a neighbourhood of } \frac{v - v_*}{|v - v_*|}, \text{ and } \mathbb{S}^2 \setminus \mathbb{S}_{iii}^2[v, v_*, \zeta, \zeta, \zeta, \zeta] \text{ has zero measure.}$$

Modified density and kernel

The density F_i and kernel B are physically meaningful, however, in order to lighten the calculations later on, it is useful to define the following modified density f_i and modified kernel b .

Definition 3.3. For $i \in \llbracket 1, N \rrbracket$, let $c_i = \frac{1}{m_i^3}$. We define

$$f_i = c_i F_i, \quad b_{ij}^{kl} = \frac{B_{ij}^{kl}}{c_i c_j}. \quad (3.25)$$

We notice that b satisfies the same positivity and symmetry conditions as B , Assumptions 3.3 and 3.1. Moreover, b satisfies the following micro-reversibility condition: for $\{(i, j) \rightarrow (k, l)\} \in \Omega$, for a.e. $v, v_* \in \mathbb{R}^3$, for $\mu_i \otimes \mu_j \otimes \mu_k \otimes \mu_l$ -a.e. $(\zeta, \zeta_*, \zeta', \zeta'_*) \in \mathcal{E}_i \times \mathcal{E}_j \times \mathcal{E}_k \times \mathcal{E}_l$ and a.e. $\omega \in \mathbb{S}^2$,

$$\frac{|v - v_*|}{m_i m_j} b_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) = \frac{|v' - v'_*|}{m_k m_l} b_{kl}^{ij}(v', v'_*, \zeta', \zeta'_*, \zeta, \zeta_*, \omega), \quad (3.26)$$

where $(v', v'_*) = S_\omega^{ijkl}[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$.

Boltzmann collision operator

Writing $B_{ij}^{kl} \equiv B_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega)$ for brevity, we define the Boltzmann collision operator for the species i by, for any $v \in \mathbb{R}^3$ and $\zeta \in \mathcal{E}_i$,

$$\begin{aligned} & B(F, F)_i(v, \zeta) \\ &= \sum_{j, k, l=1}^N \int_{\mathcal{E}_l} \int_{\mathcal{E}_k} \int_{\mathcal{E}_j} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left(\left(\frac{m_i m_j}{m_k m_l} \right)^3 F_k(v', \zeta') F_l(v'_*, \zeta'_*) - F_i(v, \zeta) F_j(v_*, \zeta_*) \right) \\ & \quad \times B_{ij}^{kl} d\omega dv_* d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_l(\zeta'_*). \end{aligned} \quad (3.27)$$

Recall that collisions with $k \neq l$ are redundantly accounted for twice here, see (3.5), but in this case the kernel B_{ij}^{kl} equals half the physical collision kernel. In terms of f_i and b_{ij}^{kl} , (3.27) writes more symmetrically

$$\begin{aligned} \mathcal{B}(F, F)_i(v, \zeta) &= \sum_{j,k,l=1}^N \int_{\mathcal{E}_l} \int_{\mathcal{E}_k} \int_{\mathcal{E}_j} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} (f_k(v', \zeta') f_l(v'_*, \zeta'_*) - f_i(v, \zeta) f_j(v_*, \zeta_*)) \\ &\quad \times b_{ij}^{kl} d\omega dv_* d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_l(\zeta'_*), \end{aligned}$$

where we write $b_{ij}^{kl} \equiv b_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega)$ for brevity. We finally denote

$$\begin{aligned} \mathcal{B}_+(F, F)_i(v, \zeta) &= \sum_{j,k,l=1}^N \int_{\mathcal{E}_l} \int_{\mathcal{E}_k} \int_{\mathcal{E}_j} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_k(v', \zeta') f_l(v'_*, \zeta'_*) b_{ij}^{kl} d\omega dv_* d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_l(\zeta'_*) \end{aligned}$$

and

$$\begin{aligned} \mathcal{B}_-(F, F)_i(v, \zeta) &= \sum_{j,k,l=1}^N \int_{\mathcal{E}_l} \int_{\mathcal{E}_k} \int_{\mathcal{E}_j} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(v, \zeta) f_j(v_*, \zeta_*) b_{ij}^{kl} d\omega dv_* d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_l(\zeta'_*) \end{aligned}$$

the gain and loss parts of the operator, respectively, so that formally,

$$\mathcal{B} = \mathcal{B}_+ - \mathcal{B}_-.$$

Mechanical and chemical collision operators

In our framework, there is no need to clearly distinguish chemical reactions from mechanical collisions. However, it can be useful to make this distinction, notably for the derivation of the Euler equations and the study of *moderately slow chemical reactions*, for which mechanical equilibrium is reached way before chemical equilibrium.

We define the set of mechanical collisions Ω_{mech} and the set of chemical collisions Ω_{chem} by

$$\Omega_{mech} = \left\{ \{(i, j) \rightarrow (i, j)\}, \{(i, j) \rightarrow (j, i)\}, (i, j) \in \llbracket 1, N \rrbracket^2 \right\}, \Omega_{chem} = \Omega \setminus \Omega_{mech}. \quad (3.28)$$

Definition 3.4. We define the mechanical collision Boltzmann operator $\mathcal{B}_{mech}(F, F)$, for any $i \in \llbracket 1, N \rrbracket$, $v \in \mathbb{R}^3$ and $\zeta \in \mathcal{E}_i$, by

$$\begin{aligned} \mathcal{B}_{mech}(F, F)_i(v, \zeta) &= \sum_{j=1}^N \int_{\mathcal{E}_j^2} \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} (f_i(v', \zeta') f_j(v'_*, \zeta'_*) - f_i(v, \zeta) f_j(v_*, \zeta_*)) \\ &\quad \times b_{ij}^{ij} d\omega dv_* d\mu_j(\zeta_*) d\mu_i(\zeta') d\mu_j(\zeta'_*) \\ &= \sum_{j,k,l} \int_{\mathcal{E}_l} \int_{\mathcal{E}_k} \int_{\mathcal{E}_j} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} (f_k(v', \zeta') f_l(v'_*, \zeta'_*) - f_i(v, \zeta) f_j(v_*, \zeta_*)) \\ &\quad \left\{ (i, j) \rightarrow (k, l) \right\} \in \Omega_{mech} \\ &\quad \times b_{ij}^{kl} d\omega dv_* d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_l(\zeta'_*), \end{aligned}$$

and the chemical collision Boltzmann operator $\mathcal{B}_{chem}(F, F)$, for any $i \in \llbracket 1, N \rrbracket$, $v \in \mathbb{R}^3$ and $\zeta \in \mathcal{E}_i$, by

$$\begin{aligned} & \mathcal{B}_{chem}(F, F)_i(v, \zeta) \\ &= \sum_{j,k,l} \int_{\mathcal{E}_l} \int_{\mathcal{E}_k} \int_{\mathcal{E}_j} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} (f_k(v', \zeta') f_l(v'_*, \zeta'_*) - f_i(v, \zeta) f_j(v_*, \zeta_*)) \\ & \quad \left\{ (i,j) \rightarrow (k,l) \right\} \in \Omega_{chem} \\ & \quad \times b_{ij}^{kl} d\omega dv d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_l(\zeta'_*). \end{aligned}$$

Since $\{\Omega_{mech}, \Omega_{chem}\}$ is a partition of Ω ,

$$\mathcal{B}(F, F)_i(v, \zeta) = \mathcal{B}_{mech}(F, F)_i(v, \zeta) + \mathcal{B}_{chem}(F, F)_i(v, \zeta).$$

A weak formulation of the collision operator holds with the following proposition.

Proposition 3.3. For all $i \in \llbracket 1, N \rrbracket$, let $\psi_i : \mathbb{R}^3 \times \mathcal{E}_i \rightarrow \mathbb{R}$ be a measurable function such that

$$\int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \left[\mathcal{B}_-(F, F)_i(v, \zeta) + \mathcal{B}_+(F, F)_i(v, \zeta) \right] |\psi_i(v, \zeta)| dv d\mu_i(\zeta) < \infty,$$

then

$$\begin{aligned} & \sum_{i=1}^N \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{B}(F, F)_i(v, \zeta) \psi_i(v, \zeta) dv d\mu_i(\zeta) \\ &= -\frac{1}{4} \sum_{i,j,k,l=1}^N \int_{\mathcal{E}_i} \int_{\mathcal{E}_j} \int_{\mathcal{E}_k} \int_{\mathcal{E}_l} \iint_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} (f_k(v', \zeta') f_l(v'_*, \zeta'_*) - f_i(v, \zeta) f_j(v_*, \zeta_*)) \\ & \quad \times \left[\psi_k(v', \zeta') + \psi_l(v'_*, \zeta'_*) - \psi_i(v, \zeta) - \psi_j(v_*, \zeta_*) \right] \\ & \quad \times b_{ij}^{kl} d\omega dv dv_* d\mu_i(\zeta) d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_l(\zeta'_*). \end{aligned} \quad (3.29)$$

The proof, relying on the symmetry and micro-reversibility of the kernel b , is analogous to the one in [37, Proposition 3.1].

3.4.2 Mechanical and global collision invariants

In this subsection, we study the *mechanical* and *collision* invariants. Mechanical invariants are related to the equilibrium of mechanical collisions only, whereas global collision invariants are related to the equilibrium of both mechanical collisions and chemical reactions.

Definition 3.5. We say that $\psi = (\psi_i)$, where $\psi_i : \mathbb{R}^3 \times \mathcal{E}_i \rightarrow \mathbb{R}$, is a *mechanical invariant* if for any $i, j \in \llbracket 1, N \rrbracket$, for $\mu_i \otimes \mu_j \otimes \mu_i \otimes \mu_j$ -a.e. $(\zeta, \zeta_*, \zeta', \zeta'_*) \in \mathcal{E}_i \times \mathcal{E}_j \times \mathcal{E}_i \times \mathcal{E}_j$, a.e. $(v, v_*) \in E_{ij}^{ij}[\zeta, \zeta_*, \zeta', \zeta'_*]$ and a.e. $\omega \in \mathbb{S}_{ijij}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*]$,

$$\psi_i(v', \zeta') + \psi_j(v'_*, \zeta'_*) = \psi_i(v, \zeta) + \psi_j(v_*, \zeta_*), \quad (3.30)$$

where (v', v'_*) are defined by $(v', v'_*) = S_{\omega}^{ijij}[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$.

Definition 3.6. We say that $\psi = (\psi_i)$, where $\psi_i : \mathbb{R}^3 \times \mathcal{E}_i \rightarrow \mathbb{R}$, is a *global collision invariant* if for any allowed collision $\{(i, j) \rightarrow (k, l)\} \in \Omega$, for $\mu_i \otimes \mu_j \otimes \mu_k \otimes \mu_l$ -a.e. $(\zeta, \zeta_*, \zeta', \zeta'_*) \in \mathcal{E}_i \times \mathcal{E}_j \times \mathcal{E}_k \times \mathcal{E}_l$, a.e.

$(v, v_*) \in E_{ij}^{kl}[\zeta, \zeta_*, \zeta', \zeta'_*]$ and a.e. $\omega \in \mathbb{S}_{ijkl}^2[v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*]$,

$$\psi_k(v', \zeta') + \psi_l(v'_*, \zeta'_*) = \psi_i(v, \zeta) + \psi_j(v_*, \zeta_*), \quad (3.31)$$

where (v', v'_*) are defined by $(v', v'_*) = S_{\omega}^{ijkl}[\zeta, \zeta_*, \zeta', \zeta'_*](v, v_*)$.

Since Ω contains all collisions, a collision invariant is also a mechanical invariant.

Let $(\alpha_i) \in \mathbb{R}^N$ and $(\beta, \gamma) \in \mathbb{R}^3 \times \mathbb{R}$. Let us define ψ such that for any $\zeta \in \mathcal{E}_i$ and $v \in \mathbb{R}^3$

$$\psi_i(v, \zeta) = \alpha_i + \beta \cdot m_i v + \gamma \left(\frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) \right).$$

Then the conservation laws (3.10) straightforwardly imply that ψ is a mechanical invariant. If moreover, for any $\{(i, j) \rightarrow (k, l)\} \in \Omega_{chem}$, $\alpha_i + \alpha_j = \alpha_k + \alpha_l$, then ψ is a collision invariant.

Proposition 3.4. *Let ψ be a mechanical invariant, such that for any $i \in \llbracket 1, N \rrbracket$ and μ_i -a.e. $\zeta \in \mathcal{E}_i$ there exists $r_\zeta > 0$ such that $\psi_i(\cdot, \zeta) \in L^1(\mathbb{R}^3, e^{-|v|^2/r_\zeta} dv)$. Then there exists $(\alpha_i) \in \mathbb{R}^N$ and $(\beta, \gamma) \in \mathbb{R}^3 \times \mathbb{R}$ such that for any $i \in \llbracket 1, N \rrbracket$, for μ_i -a.e. $\zeta \in \mathcal{E}_i$ and a.e. $v \in \mathbb{R}^3$,*

$$\psi_i(v, \zeta) = \alpha_i + \beta \cdot m_i v + \gamma \left(\frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) \right). \quad (3.32)$$

Proof. First, we consider Equation (3.30) for $i = j = k = l$ (since by hypothesis $\{(i, i) \rightarrow (i, i)\} \in \Omega$). The assumption on the potential barrier for mechanical collisions (3.9) yields $\kappa_{ii}^{ii} = \varepsilon_i^0 + \varepsilon_i^0$, hence we obtain from [37, Theorem 3.2] that there exists $(\alpha_i, \beta_i, \gamma_i) \in \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}$ such that for any $i \in \llbracket 1, N \rrbracket$ and μ_i -a.e. $\zeta \in \mathcal{E}_i$ and a.e. $v \in \mathbb{R}^3$,

$$\psi_i(v, \zeta) = \alpha_i + \beta_i \cdot v + \gamma_i \left(\frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) \right). \quad (3.33)$$

Let us now consider again Equation (3.30), using formula (3.33), with $i = k$, $j = l$ (since by hypothesis $\{(i, j) \rightarrow (i, j)\} \in \Omega$), $\zeta = \zeta' \in \mathcal{E}_i$, $\zeta_* = \zeta'_* \in \mathcal{E}_j$, with ζ and ζ_* such that equality (3.33) holds. By definition, the set of allowed pre-collision velocities writes in this case

$$E_{ij}^{ij}[\zeta, \zeta_*, \zeta, \zeta_*] = \left\{ (v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3 \text{ s.t. } \frac{m_{ij}^*}{2} |v - v_*|^2 \geq \kappa_{ij}^{ij} - \varepsilon_i(\zeta) - \varepsilon_j(\zeta_*) \right\}.$$

Using the assumption on the potential barrier for mechanical collisions (3.9) thus yields

$$E_{ij}^{ij}[\zeta, \zeta_*, \zeta, \zeta_*] = \mathbb{R}^3 \times \mathbb{R}^3. \quad (3.34)$$

Moreover, we have

$$\sqrt{\Delta_{ij}^{ij}(v, v_*, \zeta, \zeta_*, \zeta, \zeta_*)} = |v - v_*|,$$

so that

$$v' = \frac{m_i v + m_j v_*}{M_{ij}} + \frac{m_j}{M_{ij}} T_\omega [v - v_*],$$

hence v' is a continuous function of v, v_*, ω . The same applies for v'_* .

Now combining (3.33) with (3.30), we get

$$\alpha_i + \alpha_j + \beta_i \cdot v + \beta_j \cdot v_* + \gamma_i \left(\frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) \right) + \gamma_j \left(\frac{1}{2} m_j |v_*|^2 + \varepsilon_j(\zeta_*) \right)$$

$$= \alpha_i + \alpha_j + \beta_i \cdot v' + \beta_j \cdot v'_* + \gamma_i \left(\frac{1}{2} m_i |v'|^2 + \varepsilon_i(\zeta) \right) + \gamma_j \left(\frac{1}{2} m_j |v'_*|^2 + \varepsilon_j(\zeta_*) \right),$$

simplifying into

$$\begin{aligned} & \beta_i \cdot v - \beta_i \cdot v' + \beta_j \cdot v_* - \beta_j \cdot v'_* + \gamma_i \left(\frac{1}{2} m_i |v|^2 \right) \\ & - \gamma_i \left(\frac{1}{2} m_i |v'|^2 \right) + \gamma_j \left(\frac{1}{2} m_j |v_*|^2 \right) - \gamma_j \left(\frac{1}{2} m_j |v'_*|^2 \right) = 0. \end{aligned} \quad (3.35)$$

By hypothesis and from Equation (3.34), the above expression holds for a.e. $(v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3$ and a.e. $\omega \in \mathbb{S}_{ijij}^2[v, v_*, \zeta, \zeta_*, \zeta, \zeta_*]$. Since it is continuous in v, v_*, ω , and Assumption 3.3 ensures that $\mathbb{S}_{ijij}^2[v, v_*, \zeta, \zeta_*, \zeta, \zeta_*]$ contains a neighbourhood of $\frac{v-v_*}{|v-v_*|}$, Equation (3.35) actually holds for all $(v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3$ and ω in some neighbourhood of $\frac{v-v_*}{|v-v_*|}$. We can thus consider $\omega = \frac{v-v_*}{|v-v_*|}$ in the equation, so that

$$T_\omega \left[\frac{v-v_*}{|v-v_*|} \right] = -\frac{v-v_*}{|v-v_*|},$$

implying

$$v' = \frac{m_i v + m_j v_*}{M_{ij}} - \frac{m_j}{M_{ij}} (v - v_*) = \frac{m_i - m_j}{M_{ij}} v + \frac{2m_j}{M_{ij}} v_*$$

and

$$v'_* = \frac{m_i v + m_j v_*}{M_{ij}} + \frac{m_i}{M_{ij}} (v - v_*) = \frac{2m_i}{M_{ij}} v + \frac{m_j - m_i}{M_{ij}} v_*.$$

Equation (3.35) becomes

$$\begin{aligned} & \beta_i \cdot v + \beta_j \cdot v_* - \beta_i \cdot \left(\frac{m_i - m_j}{M_{ij}} v + \frac{2m_j}{M_{ij}} v_* \right) \\ & - \beta_j \cdot \left(\frac{2m_i}{M_{ij}} v + \frac{m_j - m_i}{M_{ij}} v_* \right) + \gamma_i \left(\frac{1}{2} m_i |v|^2 \right) \\ & + \gamma_j \left(\frac{1}{2} m_j |v_*|^2 \right) - \gamma_i \left(\frac{1}{2} m_i \left| \frac{m_i - m_j}{M_{ij}} v + \frac{2m_j}{M_{ij}} v_* \right|^2 \right) \\ & - \gamma_j \left(\frac{1}{2} m_j \left| \frac{2m_i}{M_{ij}} v + \frac{m_j - m_i}{M_{ij}} v_* \right|^2 \right) = 0. \end{aligned}$$

The above equality holds for all $(v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3$. Since it is a polynomial in v and v_* , all coefficients must be equal to 0. Focusing on the coefficient in front of v yields

$$\begin{aligned} \beta_i - \left(\frac{m_i - m_j}{M_{ij}} \right) \beta_i - \frac{2m_i}{M_{ij}} \beta_j &= 0 \iff (m_i + m_j - (m_i - m_j)) \beta_i = 2m_i \beta_j \\ &\iff \frac{\beta_i}{m_i} = \frac{\beta_j}{m_j}. \end{aligned}$$

We deduce that there exists $\beta \in \mathbb{R}^3$ such that for any $1 \leq i \leq N$, $\beta_i = m_i \beta$. Now focusing on the

coefficient in front of $|v|^2$ yields

$$\begin{aligned} \frac{m_i}{2}\gamma_i - \frac{m_i}{2}\gamma_i \left(\frac{m_i - m_j}{M_{ij}}\right)^2 - \frac{m_j}{2}\gamma_j \left(\frac{2m_i}{M_{ij}}\right)^2 &= 0 \\ \iff ((m_i + m_j)^2 - (m_i - m_j)^2)\gamma_i &= 4m_i m_j \gamma_j \\ \iff \gamma_i &= \gamma_j. \end{aligned}$$

We conclude that there exists $\gamma \in \mathbb{R}$ such that for any $1 \leq i \leq N$, $\gamma_i = \gamma$, ending the proof. \square

Corollary 3.5. *Let ψ be a collision invariant, such that for any $i \in \llbracket 1, N \rrbracket$ and μ_i -a.e. $\zeta \in \mathcal{E}_i$ there exists $r_\zeta > 0$ such that $\psi_i(\cdot, \zeta) \in L^1(\mathbb{R}^3, e^{-|v|^2/r_\zeta} dv)$. Then there exists $(\alpha_i) \in \mathbb{R}^N$ such that $\alpha_i + \alpha_j = \alpha_k + \alpha_l$ for any $\{(i, j) \rightarrow (k, l)\} \in \Omega_{chem}$ and $(\beta, \gamma) \in \mathbb{R}^3 \times \mathbb{R}$, such that for any $i \in \llbracket 1, N \rrbracket$, μ_i -a.e. $\zeta \in \mathcal{E}_i$ and a.e. $v \in \mathbb{R}^3$,*

$$\psi_i(v, \zeta) = \alpha_i + \beta \cdot m_i v + \gamma \left(\frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) \right). \quad (3.36)$$

Proof. Since ψ is a collision invariant, it is also a mechanical invariant. From Proposition 3.4, there exists $(\alpha_i) \in \mathbb{R}^N$ and $(\beta, \gamma) \in \mathbb{R}^3 \times \mathbb{R}$ such that for any $i \in \llbracket 1, N \rrbracket$, for μ_i -a.e. $\zeta \in \mathcal{E}_i$ and a.e. $v \in \mathbb{R}^3$,

$$\psi_i(v, \zeta) = \alpha_i + \beta \cdot m_i v + \gamma \left(\frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) \right).$$

We have to prove that functions of this form are collision invariants also of the non-mechanical collisions if and only if, for any $\{(i, j) \rightarrow (k, l)\} \in \Omega_{chem}$, we have

$$\alpha_i + \alpha_j = \alpha_k + \alpha_l.$$

Let $\{(i, j) \rightarrow (k, l)\} \in \Omega_{chem}$. There exists $(\zeta, \zeta_*, \zeta', \zeta'_*) \in \mathcal{E}_i \times \mathcal{E}_j \times \mathcal{E}_k \times \mathcal{E}_l$ and $(v, v_*) \in E_{ij}^{kl}[\zeta, \zeta_*, \zeta', \zeta'_*]$ such that Equation (3.31) holds, because for any ξ, ξ_*, ξ', ξ'_* , $E_{ij}^{kl}[\xi, \xi_*, \xi', \xi'_*]$ has non-zero Lebesgue measure. Equation (3.31) now writes

$$\begin{aligned} \alpha_i + \alpha_j + \beta \cdot (m_i v + m_j v_*) + \gamma \left(\frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) + \frac{1}{2} m_j |v_*|^2 + \varepsilon_j(\zeta_*) \right) \\ = \alpha_k + \alpha_l + \beta \cdot (m_k v' + m_l v'_*) + \gamma \left(\frac{1}{2} m_k |v'|^2 + \varepsilon_k(\zeta') + \frac{1}{2} m_l |v'_*|^2 + \varepsilon_l(\zeta'_*) \right), \end{aligned}$$

and from the conservation laws (3.10), we get $\alpha_i + \alpha_j = \alpha_k + \alpha_l$. \square

3.4.3 H-Theorem

The collision equilibrium can be characterized with the following theorem.

Theorem 3.1. *Let $F \in \prod_{i=1}^N L^1(\mathbb{R}^3 \times \mathcal{E}_i, dv d\mu_i(\zeta))$ such that for any $i \in \llbracket 1, N \rrbracket$, a.e. $v \in \mathbb{R}^3$ and μ_i -a.e. $\zeta \in \mathcal{E}_i$, $F_i(v, \zeta) > 0$. We assume that for any $i \in \llbracket 1, N \rrbracket$,*

$$\int_{\mathcal{E}_i} \int_{\mathbb{R}^3} [\mathcal{B}_-(F, F)_i(v, \zeta) + \mathcal{B}_+(F, F)_i(v, \zeta)] |\log(F_i)(v, \zeta)| dv d\mu_i(\zeta) < \infty.$$

We have, recalling that $c_i = \frac{1}{m_i^3}$,

$$\sum_{i=1}^N \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{B}(F, F)_i(v, \zeta) \log(c_i F_i)(v, \zeta) \, dv \, d\mu_i(\zeta) \leq 0. \quad (3.37)$$

Moreover, the following statements are equivalent

- (i) $\sum_{i=1}^N \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{B}(F, F)_i(v, \zeta) \log(c_i F_i)(v, \zeta) \, dv \, d\mu_i(\zeta) = 0$
- (ii) $\mathcal{B}(F, F)_i(v, \zeta) = 0$ for any $i \in \llbracket 1, N \rrbracket$, for a.e. $v \in \mathbb{R}^3$ and μ_i -a.e. $\zeta \in \mathcal{E}_i$
- (iii) $(\log(c_i F_i))_{1 \leq i \leq N}$ is a collision invariant.

The proof is similar to the one of [37, Theorem 4.1].

Moreover, the mechanical equilibrium can be characterized with the following theorem.

Corollary 3.6. *Let $F \in \prod_{i=1}^N L^1(\mathbb{R}^3 \times \mathcal{E}_i, dv \, d\mu_i(\zeta))$ such that for any $i \in \llbracket 1, N \rrbracket$, a.e. $v \in \mathbb{R}^3$ and μ_i -a.e. $\zeta \in \mathcal{E}_i$, $F_i(v, \zeta) > 0$. We assume that for any $i \in \llbracket 1, N \rrbracket$,*

$$\int_{\mathcal{E}_i} \int_{\mathbb{R}^3} [\mathcal{B}_{mech,-}(F, F)_i(v, \zeta) + \mathcal{B}_{mech,+}(F, F)_i(v, \zeta)] |\log(F_i)(v, \zeta)| \, dv \, d\mu_i(\zeta) < \infty.$$

We have, recalling that $c_i = \frac{1}{m_i^3}$,

$$\sum_{i=1}^N \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{B}_{mech}(F, F)_i(v, \zeta) \log(c_i F_i)(v, \zeta) \, dv \, d\mu_i(\zeta) \leq 0. \quad (3.38)$$

Moreover, the following statements are equivalent

- (i) $\sum_{i=1}^N \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{B}_{mech}(F, F)_i(v, \zeta) \log(c_i F_i)(v, \zeta) \, dv \, d\mu_i(\zeta) = 0$
- (ii) $\mathcal{B}_{mech}(F, F)_i(v, \zeta) = 0$ for any $i \in \llbracket 1, N \rrbracket$, for a.e. $v \in \mathbb{R}^3$ and μ_i -a.e. $\zeta \in \mathcal{E}_i$
- (iii) $(\log(c_i F_i))_{1 \leq i \leq N}$ is a mechanical invariant.

Since Ω_{mech} satisfies the assumptions of our framework, Theorem 3.1 is still valid when Ω is replaced by Ω_{mech} . In this case, the invariants involved are the mechanical invariants.

3.5 Equilibrium

The H-theorem along with the characterization of invariants allow to obtain the form of the equilibrium distribution, and to compute usual thermodynamic quantities, such as the number of degrees of freedom or the specific heat at constant volume.

Definition 3.7. *We define the extended Maxwellian family of distributions $(\mathcal{M}_i)_{1 \leq i \leq N}$ associated with densities $(n_i)_{1 \leq i \leq N} \in \mathbb{R}_+^{*N}$ (where $\mathbb{R}_+^* = \mathbb{R}_+ - \{0\}$), velocity $\underline{u} \in \mathbb{R}^3$*

and temperature $T > 0$ by, for any $1 \leq i \leq N$, $v \in \mathbb{R}^3$ and $\zeta \in \mathcal{E}_i$,

$$\mathcal{M}_i[n_i, \underline{u}, T](v, \zeta) = n_i \left(\frac{m_i}{2\pi k_B T} \right)^{3/2} Z_i^{-1} \left(\frac{1}{k_B T} \right) \exp \left(-\frac{m_i |v - \underline{u}|^2}{2k_B T} - \frac{\bar{\varepsilon}_i(\zeta)}{k_B T} \right), \quad (3.39)$$

where k_B stands for the Boltzmann constant and Z_i is the partition function of the species i defined in (3.2).

3.5.1 Mechanical equilibrium

We consider at first mechanical equilibrium configurations, namely suitable sets of distributions F such that $\mathcal{B}_{mech}(F, F) = 0$. We have the following proposition.

Proposition 3.7. *When mechanical equilibrium is reached, that is when $\mathcal{B}_{mech}(F, F) = 0$, there exists $(n_i)_{1 \leq i \leq N} \in \mathbb{R}_+^{*N}$, $\underline{u} \in \mathbb{R}^3$ and $T > 0$ such that, for any $1 \leq i \leq N$, a.e. $v \in \mathbb{R}^3$ and μ_i -a.e. $\zeta \in \mathcal{E}_i$,*

$$F_i(v, \zeta) = \mathcal{M}_i[n_i, \underline{u}, T](v, \zeta).$$

This result is quite classical and the proof is similar to the one shown in [37, Section 4].

Definition 3.8. *We define δ_i , the thermodynamic number of internal degrees of freedom of the species i , and c_V^i , the specific heat at constant volume of the species i , for any $T > 0$, by*

$$\delta_i(T) = \frac{2}{k_B T} \left(\frac{\int_{\mathcal{E}_i} \bar{\varepsilon}_i(\zeta) \exp \left(-\frac{\bar{\varepsilon}_i(\zeta)}{k_B T} \right) d\mu_i(\zeta)}{\int_{\mathcal{E}_i} \exp \left(-\frac{\bar{\varepsilon}_i(\zeta)}{k_B T} \right) d\mu_i(\zeta)} \right), \quad (3.40)$$

and

$$c_V^i(T) = \frac{3 + D_i(T)}{2}, \quad (3.41)$$

with

$$D_i(T) = \frac{d(T\delta_i(T))}{dT}. \quad (3.42)$$

Recall that the partition function Z_i defined by Equation (3.2) is C^∞ . Remarking that, from (3.40),

$$T\delta_i(T) = -\frac{2}{k_B} (\log(Z_i))' \left(\frac{1}{k_B T} \right),$$

the function $T \mapsto T\delta_i(T)$ is C^∞ on \mathbb{R}_+^* and D_i is indeed well-defined.

We recall in the following propositions and corollaries various mathematical properties of δ_i and D_i studied in [37].

Proposition 3.8. *If $\mu_i(\varepsilon_i = \varepsilon_i^0) > 0$, then*

$$\delta_i(T) \xrightarrow{T \rightarrow 0^+} 0 \quad \text{and} \quad D_i(T) \xrightarrow{T \rightarrow 0^+} 0.$$

Proposition 3.9. *For any $T > 0$,*

$$\delta_i(T) = \frac{1}{T} \int_0^T D_i(T') dT'.$$

A probabilistic interpretation may also be provided for the functions $\delta_i(T)$ and $D_i(T)$. For $T > 0$, define the Gibbs probability measure ν_T^i on $(\mathcal{E}_i, \mathcal{A}_i)$ by

$$\frac{d\nu_T^i}{d\mu_i}(\zeta) = Z_i \left(\frac{1}{k_B T} \right)^{-1} \exp \left(-\frac{\bar{\varepsilon}_i(\zeta)}{k_B T} \right), \quad (3.43)$$

where Z_i is the partition function defined by Equation (3.2). Then for any $T > 0$, $(\mathcal{E}_i, \mathcal{A}_i, \nu_T^i)$ is a probability space. Since $\bar{\varepsilon}_i : \mathcal{E}_i \rightarrow \mathbb{R}_+$ is $(\mathcal{A}_i, \text{Bor}(\mathbb{R}))$ -measurable, it is a real random variable on $(\mathcal{E}_i, \mathcal{A}_i, \nu_T^i)$.

Proposition 3.10. *For any $T > 0$,*

$$\delta_i(T) = 2 \mathbb{E}_{\nu_T^i} \left[\frac{\bar{\varepsilon}_i}{k_B T} \right], \quad (3.44)$$

and

$$D_i(T) = 2 \text{Var}_{\nu_T^i} \left[\frac{\bar{\varepsilon}_i}{k_B T} \right], \quad (3.45)$$

where $\mathbb{E}_{\nu_T^i}$ and $\text{Var}_{\nu_T^i}$ are the expectation and the variance under the probability ν_T^i , respectively.

Corollary 3.11. *For any $T > 0$, we have $\delta_i(T) \geq 0$ and $D_i(T) \geq 0$.*

Corollary 3.12. *If there exists $R \in \mathbb{R}$ such that $\varepsilon_i \leq R \mu_i$ -a.e., then*

$$\delta_i(T) \xrightarrow{T \rightarrow \infty} 0, \quad \text{and} \quad D_i(T) \xrightarrow{T \rightarrow \infty} 0.$$

We set $\rho_i = m_i n_i$. We easily verify that

$$\int_{\mathcal{E}_i} \int_{\mathbb{R}^3} m_i \mathcal{M}_i[n_i, \underline{u}, T](v, \zeta) dv d\mu_i(\zeta) = \rho_i,$$

and

$$\int_{\mathcal{E}_i} \int_{\mathbb{R}^3} m_i v \mathcal{M}_i[n_i, \underline{u}, T](v, \zeta) dv d\mu_i(\zeta) = \rho_i \underline{u}.$$

Definition 3.9. *We define Θ_i , the microscopic energy function of the species i , for any $T > 0$, by*

$$\Theta_i(T) = \frac{3}{2} k_B T - \log(Z_i) \left(\frac{1}{k_B T} \right). \quad (3.46)$$

By definition (3.40), we also have $\Theta_i(T) = \frac{3 + \delta_i(T)}{2} k_B T$, and from (3.41)-(3.42),

$$\Theta_i(T) = \int_0^T c_V^i(T') k_B dT'.$$

We now define the specific energy density associated with the species i at equilibrium as

$$e_i^{eq}[\underline{u}, T] = \frac{1}{n_i} \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \left(\frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) \right) \mathcal{M}_i[n_i, \underline{u}, T](v, \zeta) dv d\mu_i(\zeta). \quad (3.47)$$

A straightforward computation leads to

$$e_i^{eq}[\underline{u}, T] = \varepsilon_i^0 + \frac{1}{2} m_i |\underline{u}|^2 + \Theta_i(T). \quad (3.48)$$

Notice that Θ_i is continuous on \mathbb{R}_+^* , can be extended by continuity to \mathbb{R}_+ setting $\Theta_i(0) = 0$, is increasing on \mathbb{R}_+ , with $\Theta_i(T) \xrightarrow{T \rightarrow \infty} \infty$, and thus is a bijection from \mathbb{R}_+ to \mathbb{R}_+ .

We then have for any i ,

$$T_i = \Theta_i^{-1} \left(\frac{1}{n_i} \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \left(\frac{1}{2} m_i |v - \underline{u}|^2 + \bar{\varepsilon}_i(\zeta) \right) F_i(v, \zeta) \, dv \, d\mu_i(\zeta) \right),$$

justifying (3.20), the definition of temperature of the species i , noticing that here, at mechanical equilibrium, $F_i = \mathcal{M}_i$ and $(u_i, T_i) = (\underline{u}, T)$.

Letting $a_i = \frac{n_i}{\bar{n}}$ be the density fraction of the species i , we define the average specific energy at equilibrium by

$$\bar{e}^{eq}[(a_i), \underline{u}, T] = \sum_{i=1}^N a_i e_i^{eq}[\underline{u}, T]. \quad (3.49)$$

We have

$$\bar{e}^{eq}[(a_i), \underline{u}, T] = \underbrace{\sum_{i=1}^N a_i \varepsilon_i^0}_{\text{potential}} + \underbrace{\sum_{i=1}^N a_i \frac{1}{2} m_i |\underline{u}|^2}_{\text{bulk}} + \underbrace{\sum_{i=1}^N a_i \Theta_i(T)}_{\text{micro}},$$

where we notice the separation of the potential energy, bulk kinetic energy and “microscopic” energy (coming from the contribution of both kinetic and internal contributions at microscopic level). We define

$$\bar{\Theta}[(a_i)](T) = \sum_{i=1}^N a_i \Theta_i(T). \quad (3.50)$$

The function $\bar{\Theta}[(a_i)]$ is continuous on \mathbb{R}_+^* , can be extended by continuity to \mathbb{R}_+ , setting $\bar{\Theta}[(a_i)](0) = 0$, is increasing on \mathbb{R}_+ , with $\bar{\Theta}[(a_i)](T) \xrightarrow{T \rightarrow \infty} \infty$, and thus it is a bijection from \mathbb{R}_+ to \mathbb{R}_+ .

We then have

$$T = \bar{\Theta} \left[\left(\frac{n_i}{\bar{n}} \right) \right]^{-1} \left(\frac{1}{\bar{n}} \sum_{i=1}^N \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \left(\frac{1}{2} m_i |v - \underline{u}|^2 + \bar{\varepsilon}_i(\zeta) \right) F_i(v, \zeta) \, dv \, d\mu_i(\zeta) \right),$$

justifying the definition of the mean temperature in (3.21) when noticing that here, at mechanical equilibrium, $F_i = \mathcal{M}_i$ and $u_i = \underline{u}$.

3.5.2 Mechanical and chemical equilibrium

We now consider global steady states, namely mechanical and chemical equilibria. Obviously, every proposition of the previous subsection still holds. We now obtain in addition the mass-action law for each admissible reaction.

Definition 3.10. We define C_i^0 , the chemical constant of the species i , for any $T > 0$, by

$$C_i^0(T) = (2\pi m_i k_B T)^{3/2} Z_i \left(\frac{1}{k_B T} \right) e^{-\frac{\varepsilon_i^0}{k_B T}}. \quad (3.51)$$

We also define, for any chemical reaction $\{(i, j) \rightarrow (k, l)\} \in \Omega_{chem}$, the equilibrium constant

$$\begin{aligned} \mathcal{K}_{ij}^{kl}(T) &= \frac{C_k^0(T) C_l^0(T)}{C_i^0(T) C_j^0(T)} = \prod_{p \in \{i, j, k, l\}} \left\{ (2\pi m_p k_B T)^{3\sigma_p/2} Z_p \left(\frac{1}{k_B T} \right)^{\sigma_p} \right\} \exp \left(-\frac{(\Delta \varepsilon^0)_{ij}^{kl}}{k_B T} \right), \end{aligned} \quad (3.52)$$

with stoichiometric coefficients $\sigma_k = \sigma_l = -\sigma_i = -\sigma_j = 1$ and we recall that $(\Delta \varepsilon^0)_{ij}^{kl} = \varepsilon_k^0 + \varepsilon_l^0 - \varepsilon_i^0 - \varepsilon_j^0$ is interpreted as the energy consumed by the chemical reaction.

We now state the mass-action law of chemistry.

Theorem 3.2. Mass-action law. *When collision equilibrium is reached, that is when $\mathcal{B}(F, F) = 0$, there exists $(n_i^{eq})_{1 \leq i \leq N} \in \mathbb{R}_+^{*N}$, $\underline{u} \in \mathbb{R}^3$ and $T > 0$ such that, for any $1 \leq i \leq N$, a.e. $v \in \mathbb{R}^3$ and μ_i -a.e. $\zeta \in \mathcal{E}_i$,*

$$F_i(v, \zeta) = \mathcal{M}_i[n_i^{eq}, \underline{u}, T](v, \zeta),$$

with \mathcal{M}_i given in (3.39), and for any chemical reaction $\{(i, j) \rightarrow (k, l)\} \in \Omega_{chem}$, the following mass-action law holds

$$\frac{n_k^{eq} n_l^{eq}}{n_i^{eq} n_j^{eq}} = \mathcal{K}_{ij}^{kl}(T). \quad (3.53)$$

Proof. Theorem 3.1 ensures that $(\log(c_i F_i))_{1 \leq i \leq N}$ is a collision invariant and Corollary 3.5 yields the existence of $(\alpha_i) \in \mathbb{R}^N$, $\beta \in \mathbb{R}^3$ and $\gamma \in \mathbb{R}$ such that $\alpha_k + \alpha_l = \alpha_i + \alpha_j$ for any $\{(i, j) \rightarrow (k, l)\} \in \Omega_{chem}$, and for any $i \in \llbracket 1, N \rrbracket$, for a.e. $v \in \mathbb{R}^3$ and μ_i -a.e. $\zeta \in \mathcal{E}_i$,

$$\log(c_i F_i)(v, \zeta) = \alpha_i + \beta \cdot m_i v + \gamma \left(\frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta) \right).$$

Setting $T = -\frac{1}{k_B \gamma}$, $\underline{u} = -\frac{1}{\gamma} \beta$ and $A_i = \exp \left(\alpha_i + m_i \frac{|\beta|^2}{2\gamma} \right)$ for any i , we get

$$F_i(v, \zeta) = \frac{1}{c_i} A_i \exp \left(-\frac{m_i |v - \underline{u}|^2}{2k_B T} - \frac{\varepsilon_i(\zeta)}{k_B T} \right).$$

We set $n_i^{eq} = \frac{C_i^0(T)}{A_i}$, and recover, recalling that $c_i = \frac{1}{m_i^3}$, $F_i = \mathcal{M}_i[n_i^{eq}, \underline{u}, T]$, where \mathcal{M}_i is given in (3.39).

We consider a chemical reaction $\{(i, j) \rightarrow (k, l)\} \in \Omega_{chem}$. Since $\alpha_k + \alpha_l = \alpha_i + \alpha_j$ and $m_k + m_l = m_i + m_j$, we obtain $A_i A_j = A_k A_l$, leading to

$$\frac{n_k^{eq} n_l^{eq}}{n_i^{eq} n_j^{eq}} = \frac{C_k^0(T) C_l^0(T)}{C_i^0(T) C_j^0(T)},$$

which ends the proof. \square

3.5.3 Rate of reaction

Assumption 3.4. From now on, we assume that the dependence on (v, v_*) in the kernel is through $v - v_*$, i.e. there exists \tilde{B}_{ij}^{kl} such that

$$\tilde{B}_{ij}^{kl}(v - v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) = B_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega). \quad (3.54)$$

We assume the chemical reaction to be *moderately slow* compared to the effect of mechanical collisions, which leads us to investigate the case where mechanical equilibrium has already been reached, implying $F_i = \mathcal{M}_i[n_i, u, T]$ for any i , but not chemical equilibrium. Since in this case $\mathcal{B}_{mech}(F, F) = 0$, the Boltzmann equation for the species i writes, for $(t, x, v, \zeta) \in \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathcal{E}_i$,

$$\partial_t F_i(t, x, v, \zeta) + v \cdot \nabla_x F_i(t, x, v, \zeta) = \mathcal{B}_{chem}(F(t, x, \cdot, \cdot), F(t, x, \cdot, \cdot))_i(v, \zeta).$$

For brevity, we do not write the variables t, x in the following. Recall that, using the notation $f_i = c_i F_i$ and $b_{ij}^{kl} = \frac{B_{ij}^{kl}}{c_i c_j}$,

$$\begin{aligned} & \mathcal{B}_{chem}(F, F)_i(v, \zeta) \\ &= \sum_{j,k,l} \int_{\mathcal{E}_l} \int_{\mathcal{E}_k} \int_{\mathcal{E}_j} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} (f_k(v', \zeta') f_l(v'_*, \zeta'_*) - f_i(v, \zeta) f_j(v_*, \zeta_*)) \\ & \quad \{ (i,j) \rightarrow (k,l) \} \in \Omega_{chem} \\ & \quad \times b_{ij}^{kl} d\omega dv_* d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_l(\zeta'_*). \end{aligned}$$

Definition 3.11. We define r_{ij}^{kl} , the rate of the reaction $\{(i, j) \rightarrow (k, l)\}$, by

$$\begin{aligned} r_{ij}^{kl} &= \int_{\mathcal{E}_l} \int_{\mathcal{E}_k} \int_{\mathcal{E}_j} \int_{\mathcal{E}_i} \int_{(\mathbb{R}^3)^2} \int_{\mathbb{S}^2} (f_k(v', \zeta') f_l(v'_*, \zeta'_*) - f_i(v, \zeta) f_j(v_*, \zeta_*)) \\ & \quad \times b_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) d\omega dv dv_* d\mu_i(\zeta) d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_l(\zeta'_*). \end{aligned} \quad (3.55)$$

We also define r_i , the reaction rate of the species i by

$$r_i = \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{B}_{chem}(F, F)_i(v, \zeta) dv d\mu_i(\zeta) = \sum_{j,k,l} r_{ij}^{kl}. \quad (3.56)$$

$$\{ (i,j) \rightarrow (k,l) \} \in \Omega_{chem}$$

Lemma 3.13. For any $\{(i, j) \rightarrow (k, l)\} \in \Omega_{chem}$,

$$r_{ij}^{kl} = r_{ij}^{lk} = r_{ji}^{lk} = -r_{kl}^{ij}. \quad (3.57)$$

Proof. The symmetry assumption (3.23) on B , and thus on b , straightforwardly implies $r_{ij}^{kl} = r_{ij}^{lk} = r_{ji}^{lk}$, while the Jacobian formula of $S_{\omega}^{ijkl}[\zeta, \zeta_*, \zeta', \zeta'_*]$ along with the micro-reversibility condition (3.26) on b also straightforwardly implies $r_{ij}^{kl} = -r_{kl}^{ij}$. \square

We define \bar{B}_{ij}^{kl} , the average kernel relevant to the reaction $\{(i, j) \rightarrow (k, l)\}$, for any $g \in \mathbb{R}^3$ and

$(\zeta, \zeta_*) \in \mathcal{E}_i \times \mathcal{E}_j$,

$$\bar{B}_{ij}^{kl}(g, \zeta, \zeta_*) = \int_{\mathcal{E}_i} \int_{\mathcal{E}_k} \int_{\mathbb{S}^2} \tilde{B}_{ij}^{kl}(g, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) d\omega d\mu_k(\zeta') d\mu_l(\zeta'_*), \quad (3.58)$$

with \tilde{B}_{ij}^{kl} defined in (3.54).

Define the relative kinetic Gibbs probability of the species i and j at temperature $T > 0$ on \mathbb{R}^3 by

$$d\lambda_T^{ij}(g) = \left(\frac{m_{ij}^*}{2\pi k_B T} \right)^{3/2} \exp\left(-\frac{m_{ij}^* |g|^2}{2k_B T} \right) dg, \quad (3.59)$$

where m_{ij}^* is the reduced mass. Then, for any $T > 0$, \bar{B}_{ij}^{kl} is a real random variable on the space $\mathbb{R}^3 \times \mathcal{E}_i \times \mathcal{E}_j$ endowed with the probability $\lambda_T^{ij} \otimes \nu_T^i \otimes \nu_T^j$.

Definition 3.12. We define \mathcal{K}_{ij}^{kl} , the rate constant of the chemical reaction $\{(i, j) \rightarrow (k, l)\}$, for any $T > 0$, by

$$\mathcal{K}_{ij}^{kl}(T) = \mathbb{E}_{\lambda_T^{ij} \otimes \nu_T^i \otimes \nu_T^j} \left[\bar{B}_{ij}^{kl} \right], \quad (3.60)$$

where $\mathbb{E}_{\lambda_T^{ij} \otimes \nu_T^i \otimes \nu_T^j}$ stands for the expectation under the probability $\lambda_T^{ij} \otimes \nu_T^i \otimes \nu_T^j$.

The rate constant only depends on the considered species, the collision kernel and the temperature.

Definition 3.13. We say that \bar{B}_{ij}^{kl} is energy-non-decreasing (resp. energy-non-increasing) if for a.e. $g, g' \in \mathbb{R}^3$, μ_i -a.e. $\zeta, \zeta' \in \mathcal{E}_i$ and μ_j -a.e. $\zeta_*, \zeta'_* \in \mathcal{E}_j$,

$$\begin{aligned} \frac{m_{ij}^*}{2} |g|^2 + \varepsilon_i(\zeta) + \varepsilon_j(\zeta_*) &\leq \frac{m_{ij}^*}{2} |g'|^2 + \varepsilon_i(\zeta') + \varepsilon_j(\zeta'_*) \\ \implies \bar{B}_{ij}^{kl}(g, \zeta, \zeta_*) &\leq \bar{B}_{ij}^{kl}(g', \zeta', \zeta'_*) \\ (\text{resp. } \implies \bar{B}_{ij}^{kl}(g, \zeta, \zeta_*) &\geq \bar{B}_{ij}^{kl}(g', \zeta', \zeta'_*)). \end{aligned}$$

Proposition 3.14. If \bar{B}_{ij}^{kl} is energy-non-decreasing and $\text{Leb}_{\mathbb{R}^3} \otimes \mu_i \otimes \mu_j$ -non-constant, then \mathcal{K}_{ij}^{kl} is an increasing function of temperature. If \bar{B}_{ij}^{kl} is $\text{Leb}_{\mathbb{R}^3} \otimes \mu_i \otimes \mu_j$ -constant, then \mathcal{K}_{ij}^{kl} is a constant function of temperature. If \bar{B}_{ij}^{kl} is energy-non-increasing and $\text{Leb}_{\mathbb{R}^3} \otimes \mu_i \otimes \mu_j$ -non-constant, then \mathcal{K}_{ij}^{kl} is a decreasing function of temperature.

This is a straightforward consequence of Lemma 3.18 in Appendix A, with $\mathcal{X} = \mathbb{R}^3 \times \mathcal{E}_i \times \mathcal{E}_j$, $\eta = \text{Leb}_{\mathbb{R}^3} \otimes \mu_i \otimes \mu_j$, $\varphi = \bar{B}_{ij}^{kl}$ and

$$\psi(g, \zeta, \zeta_*) = \frac{1}{k_B} \left(\frac{m_{ij}^*}{2} |g|^2 + \bar{\varepsilon}_i(\zeta) + \bar{\varepsilon}_j(\zeta_*) \right).$$

Proposition 3.15. The rate of reaction writes

$$r_{ij}^{kl} = \mathcal{K}_{kl}^{ij}(T) n_k n_l - \mathcal{K}_{ij}^{kl}(T) n_i n_j, \quad (3.61)$$

and the following relation holds

$$\mathcal{K}_{kl}^{ij}(T) = \frac{\mathcal{K}_{ij}^{kl}(T)}{\mathcal{K}_{ij}^{kl}(T)}, \quad (3.62)$$

where \mathcal{K}_{ij}^{kl} has been defined in (3.52).

Proof. Let us fix j, k, l such that $\{(i, j) \rightarrow (k, l)\} \in \Omega_{chem}$. We denote

$$\begin{aligned} \mathcal{I}_{ij}^{kl}(v, \zeta) &= \int_{\mathcal{E}_l} \int_{\mathcal{E}_k} \int_{\mathcal{E}_j} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} (f_k(v', \zeta') f_l(v'_*, \zeta'_*) - f_i(v, \zeta) f_j(v_*, \zeta_*)) \\ &\quad \times b_{ij}^{kl} d\omega dv_* d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_l(\zeta'_*). \end{aligned}$$

Since we assumed mechanical equilibrium, F has a Maxwellian form, and we deduce from the conservation laws (3.10) that

$$f_k(v', \zeta') f_l(v'_*, \zeta'_*) = \frac{n_k n_l}{n_i n_j} \frac{1}{\mathcal{K}_{ij}^{kl}(T)} f_i(v, \zeta) f_j(v_*, \zeta_*).$$

We set

$$R_{ij}^{kl}(T) = \frac{n_k n_l}{\mathcal{K}_{ij}^{kl}(T)} - n_i n_j.$$

Then, recalling that $f_i f_j b_{ij}^{kl} = F_i F_j B_{ij}^{kl}$ and the assumption (3.54) on B , we have

$$\begin{aligned} \mathcal{I}_{ij}^{kl}(v, \zeta) &= \frac{R_{ij}^{kl}(T)}{n_i n_j} \int_{\mathcal{E}_l} \int_{\mathcal{E}_k} \int_{\mathcal{E}_j} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} F_i(v, \zeta) F_j(v_*, \zeta_*) \\ &\quad \times \tilde{B}_{ij}^{kl}(v - v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) d\omega dv_* d\mu_j(\zeta_*) d\mu_k(\zeta') d\mu_l(\zeta'_*), \end{aligned}$$

simplifying into

$$\mathcal{I}_{ij}^{kl}(v, \zeta) = \frac{R_{ij}^{kl}(T)}{n_i n_j} \int_{\mathcal{E}_j} \int_{\mathbb{R}^3} F_i(v, \zeta) F_j(v_*, \zeta_*) \bar{B}_{ij}^{kl}(v - v_*, \zeta, \zeta_*) dv_* d\mu_j(\zeta_*).$$

The rate of the reaction $\{(i, j) \rightarrow (k, l)\}$ then writes

$$\begin{aligned} r_{ij}^{kl} &= \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{I}_{ij}^{kl}(v, \zeta) dv d\mu_i(\zeta) \\ &= \frac{R_{ij}^{kl}(T)}{n_i n_j} \int_{\mathcal{E}_i} \int_{\mathcal{E}_j} \iint_{(\mathbb{R}^3)^2} \mathcal{M}_i[n_i, \underline{u}, T] \mathcal{M}_j[n_j, \underline{u}, T] \bar{B}_{ij}^{kl}(v - v_*, \zeta, \zeta_*) \\ &\quad dv dv_* d\mu_j(\zeta_*) d\mu_i(\zeta). \end{aligned}$$

Applying the change of variables $(v, v_*) \mapsto (v + \underline{u}, v_* + \underline{u})$ yields

$$\begin{aligned} r_{ij}^{kl} &= \frac{R_{ij}^{kl}(T)}{n_i n_j} \int_{\mathcal{E}_i} \int_{\mathcal{E}_j} \iint_{(\mathbb{R}^3)^2} \mathcal{M}_i[n_i, 0, T] \mathcal{M}_j[n_j, 0, T] \bar{B}_{ij}^{kl}(v - v_*, \zeta, \zeta_*) \\ &\quad dv dv_* d\mu_j(\zeta_*) d\mu_i(\zeta) \\ &= R_{ij}^{kl}(T) \left(\frac{m_i}{2\pi k_B T} \right)^{3/2} \left(\frac{m_j}{2\pi k_B T} \right)^{3/2} Z_i^{-1} \left(\frac{1}{k_B T} \right) Z_j^{-1} \left(\frac{1}{k_B T} \right) \\ &\quad \times \int_{\mathcal{E}_i} \int_{\mathcal{E}_j} e^{-\frac{\varepsilon_i(\zeta) + \varepsilon_j(\zeta_*)}{k_B T}} \iint_{(\mathbb{R}^3)^2} e^{-\frac{m_i |v|^2 + m_j |v_*|^2}{2k_B T}} \bar{B}_{ij}^{kl}(v - v_*, \zeta, \zeta_*) \end{aligned}$$

$$dv dv_* d\mu_i(\zeta) d\mu_j(\zeta_*).$$

In the integral in (v, v_*) , we perform the change of variables

$$(v, v_*) \mapsto \left(v - v_*, \frac{m_i v + m_j v_*}{m_i + m_j} \right) = (g, G)$$

of unitary Jacobian. Recalling that $m_{ij}^* = \frac{m_i m_j}{m_i + m_j}$ and $M_{ij} = m_i + m_j$, we have

$$\frac{1}{2} m_{ij}^* |g|^2 + \frac{1}{2} M_{ij} |G|^2 = \frac{1}{2} m_i |v|^2 + \frac{1}{2} m_j |v_*|^2,$$

and we obtain that the previous integral in (v, v_*) rewrites as

$$\left(\frac{2\pi k_B T}{m_{ij}^*} \right)^{3/2} \int_{\mathbb{R}^3} e^{-\frac{m_{ij}^* |g|^2}{2k_B T}} \bar{B}_{ij}^{kl}(g, \zeta, \zeta_*) dg.$$

It follows that

$$\begin{aligned} r_{ij}^{kl} &= R_{ij}^{kl}(T) \left(\frac{m_{ij}^*}{2\pi k_B T} \right)^{3/2} Z_i \left(\frac{1}{k_B T} \right)^{-1} Z_j \left(\frac{1}{k_B T} \right)^{-1} \\ &\times \int_{\mathcal{E}_i} \int_{\mathcal{E}_j} \int_{\mathbb{R}^3} \exp \left(-\frac{m_{ij}^* |g|^2}{2k_B T} - \frac{\bar{\varepsilon}_i(\zeta) + \bar{\varepsilon}_j(\zeta_*)}{k_B T} \right) \bar{B}_{ij}^{kl}(g, \zeta, \zeta_*) dg d\mu_i(\zeta) d\mu_j(\zeta_*), \end{aligned}$$

which rewrites as

$$r_{ij}^{kl} = R_{ij}^{kl}(T) \mathbb{E}_{\lambda_T^{ij} \otimes \nu_T^i \otimes \nu_T^j} [\bar{B}_{ij}^{kl}] = \left(\frac{n_k n_l}{\mathcal{K}_{ij}^{kl}(T)} - n_i n_j \right) \mathcal{K}_{ij}^{kl}(T).$$

Finally, since $r_{ij}^{kl} = -r_{kl}^{ij}$ and the above expression is a polynomial in n_i, n_j, n_k, n_l , we obtain (3.62) by identification and (3.61) follows. \square

Corollary 3.16. *The reaction rate of the species i writes*

$$r_i = \sum_{j,k,l} \mathcal{K}_{kl}^{ij}(T) n_k n_l - \mathcal{K}_{ij}^{kl}(T) n_i n_j.$$

$$\{(i,j) \rightarrow (k,l)\} \in \Omega_{chem}$$

This corollary is a straightforward consequence of Proposition 3.15.

Redundancy-free quantities. Let us recall that since the reaction $\{(i,j) \rightarrow (k,l)\}$ is technically the same as $\{(i,j) \rightarrow (l,k)\}$, the physical rate of this reaction actually writes, when $k \neq l$,

$$\bar{r}_{ij}^{kl} = r_{ij}^{kl} + r_{ij}^{lk}. \quad (3.63)$$

Similarly, the physical rate constant of this reaction actually writes, when $k \neq l$,

$$\bar{\mathcal{K}}_{ij}^{kl} = \mathcal{K}_{ij}^{kl} + \mathcal{K}_{ij}^{lk}. \quad (3.64)$$

We highlight that this is coherent, as we already pointed out that in the case $k \neq l$ the kernel B_{ij}^{kl} may be

thought of as half the physical one, and both the rate of reaction and the rate constant linearly depend on it.

3.6 Euler limit

In this section we derive the system of Euler equations in the case of moderately slow chemical reactions, that is, when mechanical equilibrium is assumed. Then Corollary 3.6 ensures that $\mathcal{B}_{mech}(F, F) = 0$ a.e., and for any $i \in \llbracket 1, N \rrbracket$, all $t \in \mathbb{R}_+$, $x \in \mathbb{R}^3$, a.e. $v \in \mathbb{R}^3$ and μ_i -a.e. $\zeta \in \mathcal{E}_i$,

$$F_i(t, x, v, \zeta) = \mathcal{M}_i[n_i(t, x), \underline{u}(t, x), T(t, x)](v, \zeta).$$

We define $(\Delta\varepsilon^0)_{ij}^{kl}$, the energy consumed by the chemical reaction $\{(i, j) \rightarrow (k, l)\}$, by

$$(\Delta\varepsilon^0)_{ij}^{kl} = \varepsilon_k^0 + \varepsilon_l^0 - \varepsilon_i^0 - \varepsilon_j^0. \quad (3.65)$$

Now we define the set of families of chemical reactions

$$\bar{\Omega}_{chem} = \left\{ \left\{ \{i, j\} \rightleftharpoons \{k, l\} \right\} \text{ s.t. } \{(i, j) \rightarrow (k, l)\} \in \Omega_{chem} \right\}, \quad (3.66)$$

accounting exactly once for each different chemical reaction, in the sense that

$$\begin{aligned} \left\{ \{i, j\} \rightleftharpoons \{k, l\} \right\} &= \left\{ \{j, i\} \rightleftharpoons \{l, k\} \right\} = \left\{ \{k, l\} \rightleftharpoons \{i, j\} \right\} = \left\{ \{l, k\} \rightleftharpoons \{j, i\} \right\} \\ &= \left\{ \{i, j\} \rightleftharpoons \{l, k\} \right\} = \left\{ \{j, i\} \rightleftharpoons \{k, l\} \right\} = \left\{ \{k, l\} \rightleftharpoons \{j, i\} \right\} = \left\{ \{l, k\} \rightleftharpoons \{i, j\} \right\}. \end{aligned}$$

The symmetry properties of $(\Delta\varepsilon^0)_{ij}^{kl}$ and of r_{ij}^{kl} , (3.57), straightforwardly imply

$$\begin{aligned} (\Delta\varepsilon^0)_{ij}^{kl} r_{ij}^{kl} &= (\Delta\varepsilon^0)_{ji}^{lk} r_{ji}^{lk} = (\Delta\varepsilon^0)_{kl}^{ij} r_{kl}^{ij} = (\Delta\varepsilon^0)_{lk}^{ji} r_{lk}^{ji} \\ &= (\Delta\varepsilon^0)_{ij}^{lk} r_{ij}^{lk} = (\Delta\varepsilon^0)_{ji}^{kl} r_{ji}^{kl} = (\Delta\varepsilon^0)_{kl}^{ji} r_{kl}^{ji} = (\Delta\varepsilon^0)_{lk}^{ij} r_{lk}^{ij}, \end{aligned} \quad (3.67)$$

allowing the following (3.71) to make sense.

Theorem 3.3. *We set*

$$\bar{n} = \sum_{i=1}^N n_i, \quad \bar{\rho} = \sum_{i=1}^N m_i n_i, \quad \bar{\delta} = \frac{1}{\bar{n}} \sum_{i=1}^N n_i \delta_i(T), \quad p = \bar{n} k_B T. \quad (3.68)$$

The Euler system of equations at mechanical equilibrium is given by

$$\forall i \in \llbracket 1, N \rrbracket, \partial_t n_i + \operatorname{div}_x(n_i \underline{u}) = r_i, \quad (3.69)$$

$$\partial_t(\bar{\rho} \underline{u}) + \operatorname{div}_x(\bar{\rho} \underline{u} \otimes \underline{u}) + \nabla_x p = 0, \quad (3.70)$$

$$\begin{aligned} &\partial_t \left(\frac{1}{2} \bar{\rho} |\underline{u}|^2 + \bar{n} \frac{3 + \bar{\delta}}{2} k_B T \right) + \operatorname{div}_x \left(\frac{1}{2} \bar{\rho} |\underline{u}|^2 \underline{u} + \bar{n} \frac{3 + \bar{\delta}}{2} k_B T \underline{u} + p \underline{u} \right) \\ &= \sum_{\{i, j\} \rightleftharpoons \{k, l\} \in \bar{\Omega}_{chem}} (\Delta\varepsilon^0)_{ij}^{kl} \bar{r}_{ij}^{kl}, \end{aligned} \quad (3.71)$$

where, recalling that \bar{r}_{ij}^{kl} and \bar{K}_{ij}^{kl} are the redundancy-free quantities defined in (3.63)–(3.64),

$$\bar{r}_{ij}^{kl} = r_{ij}^{kl} + r_{ij}^{lk} = \bar{K}_{kl}^{ij}(T)n_k n_l - \bar{K}_{ij}^{kl}(T)n_i n_j, \quad \text{and} \quad r_i = \sum_{\substack{j,k,l \\ \{(i,j) \rightarrow (k,l)\} \in \Omega_{chem}}} r_{ij}^{kl}.$$

Proof. Since $\mathcal{B}_{mech}(F, F) = 0$, the Boltzmann equation now writes, for any $1 \leq i \leq N$,

$$\partial_t F_i(t, x, v, \zeta) + v \cdot \nabla_x F_i(t, x, v, \zeta) = \mathcal{B}_{chem}(F(t, x, \cdot, \cdot), F(t, x, \cdot, \cdot))_i(v, \zeta). \quad (3.72)$$

By definition of r_i , given in (3.56), integrating (3.72) in $v \in \mathbb{R}^3$ and $\zeta \in \mathcal{E}_i$ straightforwardly yields (3.69).

Now let ψ be such that for any $i \in \llbracket 1, N \rrbracket$, $v \in \mathbb{R}^3$ and $\zeta \in \mathcal{E}_i$, $\psi_i(v, \zeta) = m_i v$. Since ψ is a collision invariant, we have for any t and x

$$\sum_{i=1}^N \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{B}_{chem}(F(t, x, \cdot, \cdot), F(t, x, \cdot, \cdot))_i(v, \zeta) \psi_i(v, \zeta) \, dv \, d\mu_i(\zeta) = 0. \quad (3.73)$$

Combining (3.72) and (3.73) yields

$$\partial_t \left(\sum_{i=1}^N \rho_i \underline{u} \right) + \operatorname{div}_x \left(\sum_{i=1}^N \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{M}_i[n_i, \underline{u}, T](v, \zeta) m_i v \otimes v \, dv \, d\mu_i(\zeta) \right) = 0.$$

By a standard computation (see [43, Chapter 2]),

$$\begin{aligned} & \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{M}_i[n_i, \underline{u}, T](v, \zeta) m_i v \otimes v \, dv \, d\mu_i(\zeta) \\ &= m_i n_i \left(\frac{m_i}{2\pi k_B T} \right)^{3/2} \int_{\mathbb{R}^3} \exp\left(-\frac{m_i |v - \underline{u}|^2}{2k_B T}\right) v \otimes v \, dv \\ &= \rho_i \underline{u} \otimes \underline{u} + n_i k_B T \mathbf{I}_d, \end{aligned}$$

where \mathbf{I}_d stands for the identity matrix of dimension 3, which allows to conclude for (3.70).

Finally, let ψ be such that for any $i \in \llbracket 1, N \rrbracket$, $v \in \mathbb{R}^3$ and $\zeta \in \mathcal{E}_i$, $\psi_i(v, \zeta) = \frac{1}{2} m_i |v|^2 + \varepsilon_i(\zeta)$. Again, ψ is a collision invariant, so that

$$\sum_{i=1}^N \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{B}_{chem}(F(t, x, \cdot, \cdot), F(t, x, \cdot, \cdot))_i(v, \zeta) \psi_i(v, \zeta) \, dv \, d\mu_i(\zeta) = 0. \quad (3.74)$$

We recall (3.48), for any $i \in \llbracket 1, N \rrbracket$,

$$\int_{\mathcal{E}_i} \int_{\mathbb{R}^3} \mathcal{M}_i[n_i, \underline{u}, T](v, \zeta) \psi_i(v, \zeta) \, dv \, d\mu_i(\zeta) = \frac{1}{2} \rho_i |\underline{u}|^2 + n_i \frac{3 + \delta_i(T)}{2} k_B T + n_i \varepsilon_i^0. \quad (3.75)$$

On the other hand, again by a standard computation for the velocity-related term (see [43, Chapter 2]), for any $i \in \llbracket 1, N \rrbracket$,

$$\int_{\mathcal{E}_i} \int_{\mathbb{R}^3} v \psi_i(v, \zeta) \mathcal{M}_i[n_i, \underline{u}, T](v, \zeta) \, dv \, d\mu_i(\zeta)$$

$$\begin{aligned}
&= \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} v \frac{1}{2} m_i |v|^2 \mathcal{M}_i[n_i, \underline{u}, T](v, \zeta) \, dv \, d\mu_i(\zeta) \\
&\quad + \int_{\mathcal{E}_i} \int_{\mathbb{R}^3} v \varepsilon_i(\zeta) \mathcal{M}_i[n_i, \underline{u}, T](v, \zeta) \, dv \, d\mu_i(\zeta) \\
&= n_i \left(\frac{m_i}{2\pi k_B T} \right)^{3/2} \int_{\mathbb{R}^3} v \frac{1}{2} m_i |v|^2 \exp\left(-\frac{m_i |v - \underline{u}|^2}{2k_B T}\right) \, dv \\
&\quad + n_i \left(\frac{\int_{\mathcal{E}_i} \varepsilon_i(\zeta) \exp\left(-\frac{\bar{\varepsilon}_i(\zeta)}{k_B T}\right) \, d\mu_i(\zeta)}{\int_{\mathcal{E}_i} \exp\left(-\frac{\bar{\varepsilon}_i(\zeta)}{k_B T}\right) \, d\mu_i(\zeta)} \right) \underline{u} \\
&= \frac{1}{2} \rho_i |\underline{u}|^2 \underline{u} + n_i k_B T \underline{u} + n_i \frac{3}{2} k_B T \underline{u} + n_i \left(\varepsilon_i^0 + \frac{\delta_i(T)}{2} k_B T \right) \underline{u}.
\end{aligned}$$

Therefore we get

$$\begin{aligned}
&\int_{\mathcal{E}_i} \int_{\mathbb{R}^3} v \psi_i(v, \zeta) \mathcal{M}_i[n_i, \underline{u}, T](v, \zeta) \, dv \, d\mu_i(\zeta) \\
&= \left(\frac{1}{2} \rho_i |\underline{u}|^2 + n_i k_B T + n_i \frac{3 + \delta_i(T)}{2} k_B T + n_i \varepsilon_i^0 \right) \underline{u}.
\end{aligned} \tag{3.76}$$

From the definition of $\bar{\delta}$ given in (3.68) we note that it depends on (n_i) and T . Now notice that, for any $i \in \llbracket 1, N \rrbracket$,

$$\partial_t (n_i \varepsilon_i^0) + \operatorname{div}_x (n_i \varepsilon_i^0 \underline{u}) = \varepsilon_i^0 (\partial_t n_i + \operatorname{div}_x (n_i \underline{u})) = \varepsilon_i^0 r_i. \tag{3.77}$$

Combining (3.72) and (3.74)–(3.77) while summing over $i \in \llbracket 1, N \rrbracket$ yields

$$\partial_t \left(\frac{1}{2} \bar{\rho} |\underline{u}|^2 + \bar{n} \frac{3 + \bar{\delta}}{2} k_B T \right) + \operatorname{div}_x \left(\frac{1}{2} \bar{\rho} |\underline{u}|^2 \underline{u} + p \underline{u} + \bar{n} \frac{3 + \bar{\delta}}{2} k_B T \underline{u} \right) = - \sum_{i=1}^N \varepsilon_i^0 r_i. \tag{3.78}$$

Using the symmetry property of the rate constant, Lemma 3.13, we notice that

$$\begin{aligned}
\sum_{i=1}^N \varepsilon_i^0 r_i &= \sum_{i=1}^N \varepsilon_i^0 \sum_{\substack{j,k,l \\ \{(i,j) \rightarrow (k,l)\} \in \Omega_{chem}}} r_{ij}^{kl} = \sum_{\{(i,j) \rightarrow (k,l)\} \in \Omega_{chem}} \varepsilon_i^0 r_{ij}^{kl} \\
&= \sum_{\{(j,i) \rightarrow (l,k)\} \in \Omega_{chem}} \varepsilon_j^0 r_{ji}^{lk} = \sum_{\{(i,j) \rightarrow (k,l)\} \in \Omega_{chem}} \varepsilon_j^0 r_{ij}^{kl}
\end{aligned}$$

and similarly

$$\sum_{i=1}^N \varepsilon_i^0 r_i = - \sum_{\{(i,j) \rightarrow (k,l)\} \in \Omega_{chem}} \varepsilon_k^0 r_{ij}^{kl} = - \sum_{\{(i,j) \rightarrow (k,l)\} \in \Omega_{chem}} \varepsilon_l^0 r_{ij}^{kl}.$$

It follows from these symmetry arguments that

$$- \sum_{i=1}^N \varepsilon_i^0 r_i = \sum_{\{\{i,j\} \rightleftharpoons \{k,l\}\} \in \bar{\Omega}_{chem}} (\Delta \varepsilon^0)_{ij}^{kl} \bar{r}_{ij}^{kl}, \tag{3.79}$$

where the sum is taken now over the set $\bar{\Omega}_{chem}$ defined in (3.66). Combining (3.78) with (3.79), we obtain (3.71). \square

Notice that, since $\bar{\kappa}_{ij}^{kl}$, δ_i and $(\Delta\varepsilon^0)_{ij}^{kl}$ are known, the system (3.69)–(3.71) is composed of $N + 3 + 1$ equations for $N + 3 + 1$ unknowns (namely $(n_i)_{1 \leq i \leq N}$, \underline{u} and T), hence it is a closed system.

3.7 Example of a computation of the rate of reaction

The purpose of this section is to show how to introduce the potential barriers κ_{ij}^{kl} (explained in Section 2) in the framework. Define $E_a = \kappa_{ij}^{kl} - \varepsilon_i^0 - \varepsilon_j^0$ the activation energy of the reaction $\{(i, j) \rightarrow (k, l)\}$, and assume $E_a > 0$. We assume that the species i and j are monatomic, implying $\mathcal{E}_i = \mathcal{E}_j = \{0\}$ and \bar{B}_{ij}^{kl} depends only on $g \in \mathbb{R}^3$. The quantities in this subsection are redundancy-free.

Proposition 3.17. *We consider the kernel used in [95, 96]. Let $\beta > 0$, define for any $g \in \mathbb{R}^3$,*

$$\bar{B}_{ij}^{kl}(g) = \beta \left(1 - \frac{E_a}{\frac{m_{ij}^*}{2}|g|^2} \right) \mathbf{1}_{\frac{m_{ij}^*}{2}|g|^2 \geq E_a}. \quad (3.80)$$

Then the rate constant is given, for any $T > 0$, by the formula

$$\kappa_{ij}^{kl}(T) = \frac{2\beta}{\sqrt{\pi}} \left[\Gamma\left(\frac{3}{2}, \frac{E_a}{k_B T}\right) - \frac{E_a}{k_B T} \Gamma\left(\frac{1}{2}, \frac{E_a}{k_B T}\right) \right], \quad (3.81)$$

where Γ stands for the upper incomplete Gamma function.

The kernel (3.80), that takes into account that a reaction can occur only if the in-going kinetic energy is greater than the activation energy, does satisfy the assumptions of our framework because of how we took the transition state energy κ_{ij}^{kl} into account in (3.16). If we had not, the kernel would not have satisfied the positivity requirement, namely Assumption 3.3, and could not have been considered.

Proof. We recall the definition (3.60) of the rate constant. Let $\alpha > -3$ and set, for $g \in \mathbb{R}^3$,

$$\chi_\alpha(g) = |g|^\alpha \mathbf{1}_{\frac{m_{ij}^*}{2}|g|^2 \geq E_a}.$$

Then, for any $T > 0$,

$$\begin{aligned} \mathbb{E}_{\chi_T^{ij}}[\chi_\alpha] &= \left(\frac{m_{ij}^*}{2\pi k_B T} \right)^{3/2} \int_{\mathbb{R}^3} |g|^\alpha \mathbf{1}_{\frac{m_{ij}^*}{2}|g|^2 \geq E_a} e^{-\frac{m_{ij}^*|g|^2}{2k_B T}} dg \\ &= 4\pi \left(\frac{m_{ij}^*}{2\pi k_B T} \right)^{3/2} \int_{\mathbb{R}_+} z^\alpha \mathbf{1}_{\frac{m_{ij}^*}{2}z^2 \geq E_a} e^{-\frac{m_{ij}^*z^2}{2k_B T}} z^2 dz \\ &= \frac{2}{\sqrt{\pi}} \left(\frac{2k_B T}{m_{ij}^*} \right)^{\frac{\alpha}{2}} \int_{\frac{E_a}{k_B T}}^{\infty} x^{\frac{\alpha+3}{2}-1} e^{-x} dx. \end{aligned}$$

Denoting by Γ the upper incomplete Gamma function, defined as

$$\Gamma(\alpha, y) = \int_y^{\infty} x^{\alpha-1} e^{-x} dx,$$

we deduce that

$$\mathbb{E}_{\lambda_T^{ij}}[\chi_0] = \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \frac{E_a}{k_B T}\right), \text{ and } \mathbb{E}_{\lambda_T^{ij}}[\chi_{-2}] = \frac{2}{\sqrt{\pi}} \left(\frac{m_{ij}^*}{2k_B T}\right) \Gamma\left(\frac{1}{2}, \frac{E_a}{k_B T}\right).$$

It comes that

$$\mathcal{K}_{ij}^{kl}(T) = \beta \mathbb{E}_{\lambda_T^{ij}} \left[\chi_0 - \left(\frac{2E_a}{m_{ij}^*}\right) \chi_{-2} \right] = \frac{2\beta}{\sqrt{\pi}} \left[\Gamma\left(\frac{3}{2}, \frac{E_a}{k_B T}\right) - \frac{E_a}{k_B T} \Gamma\left(\frac{1}{2}, \frac{E_a}{k_B T}\right) \right].$$

□

We plot \mathcal{K}_{ij}^{kl} given in (3.81) in Fig. 3.3, as well as the rate constant provided by Arrhenius' law $\mathcal{K}_{Arr}(T) = \beta e^{-\frac{E_a}{k_B T}}$ as a matter of comparison. We observe that both provide similar trends. Since Arrhenius' law is empirical, Fig. 3.3 shows a good agreement of our theoretical result with respect to experimental ones.

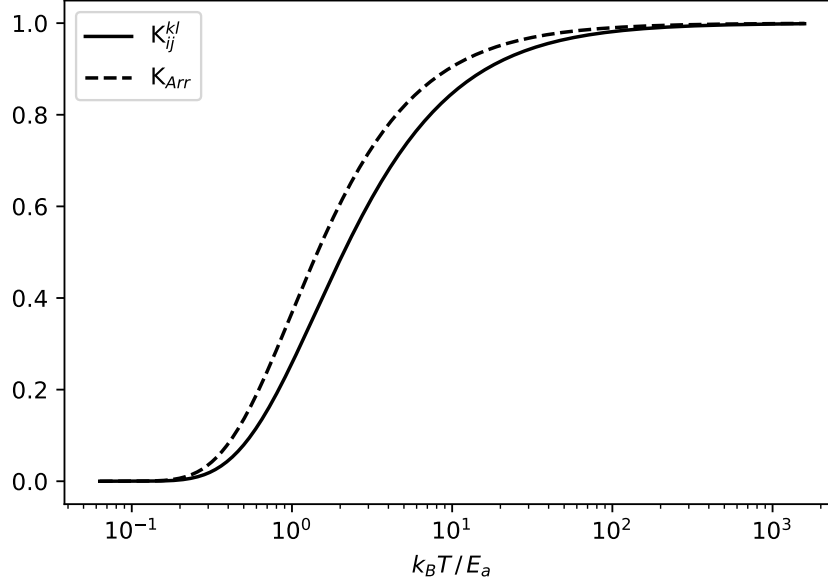


Figure 3.3 – Plot of \mathcal{K}_{ij}^{kl} given in (3.81) and \mathcal{K}_{Arr} as functions of $\frac{k_B T}{E_a}$, with $\beta = 1$.

Remark 3.1. The kernel (3.80) is energy-non-decreasing and non-constant. We verify in Fig. 3.3 that \mathcal{K}_{ij}^{kl} is indeed increasing with temperature, as stated in Proposition 3.14.

3.8 Reduced models and energy of reaction

As explained in [37, Section 8] for a single polyatomic gas, to any state-based model it can be associated an energy-based one, corresponding typically to the Borgnakke-Larsen description with integration

weight [35, 75, 76] when the initial description is not totally discrete [25, 100]. This kind of reduction may be extended also to inert or reactive gas mixtures. Let $1 \leq i \leq N$, and consider $\mu_i^{\bar{\varepsilon}_i}$ the image measure on \mathbb{R}_+ of μ_i by $\bar{\varepsilon}_i$. Using the change of variables formula, one then easily concludes that the two following descriptions are equivalent in the kinetic framework:

- *State-based.* The molecule of the species i is described by its velocity $v \in \mathbb{R}^3$ and internal state $\zeta \in \mathcal{E}_i$, where the space \mathcal{E}_i is endowed with the measure μ_i . The associated energy of the molecule is $\frac{1}{2}m_i|v|^2 + \varepsilon_i(\zeta)$.
- *Energy-based.* The molecule of the species i is described by its velocity $v \in \mathbb{R}^3$ and non-potential internal energy $I \in \mathbb{R}_+$, where the space \mathbb{R}_+ is endowed with the measure $\mu_i^{\bar{\varepsilon}_i}$. The associated energy of the molecule is $\frac{1}{2}m_i|v|^2 + I + \varepsilon_i^0$. The quantity ε_i^0 corresponds to the fundamental potential energy of configuration of the molecule.

Recall the law of conservation of energy (3.10) for a collision $\{(i, j) \rightarrow (k, l)\}$

$$\frac{1}{2}m_i|v|^2 + \varepsilon_i(\zeta) + \frac{1}{2}m_j|v_*|^2 + \varepsilon_j(\zeta_*) = \frac{1}{2}m_k|v'|^2 + \varepsilon_k(\zeta') + \frac{1}{2}m_l|v'_*|^2 + \varepsilon_l(\zeta'_*). \quad (3.82)$$

Rewriting this equation with the reduced models gives

$$\frac{1}{2}m_i|v|^2 + I + \varepsilon_i^0 + \frac{1}{2}m_j|v_*|^2 + I_* + \varepsilon_j^0 = \frac{1}{2}m_k|v'|^2 + I' + \varepsilon_k^0 + \frac{1}{2}m_l|v'_*|^2 + I'_* + \varepsilon_l^0,$$

that is

$$\frac{1}{2}m_i|v|^2 + I + \frac{1}{2}m_j|v_*|^2 + I_* = \frac{1}{2}m_k|v'|^2 + I' + \frac{1}{2}m_l|v'_*|^2 + I'_* + (\Delta\varepsilon^0)_{ij}^{kl}, \quad (3.83)$$

where $(\Delta\varepsilon^0)_{ij}^{kl} = \varepsilon_k^0 + \varepsilon_l^0 - \varepsilon_i^0 - \varepsilon_j^0$ is thus interpreted as the energy consumed by the chemical reaction ($(\Delta\varepsilon^0)_{ij}^{ij} = 0$ in the case of a mechanical collision). The formulation (3.83) coincides with the one considered in [76], and we highlight the fact that it is, from the reduction process, indeed equivalent to (3.82). Further details on the equivalence of these formulations for a single gas may be found in [37, Theorem 8.1].

However, the formulations (3.82) and (3.83) do differ in two aspects. First, (3.82) is completely microscopic, in the sense that it describes the system of the two colliding molecules as an isolated one, that is neither exchanging mass nor energy with its environment. On the other hand, in (3.83), some energy, namely $(\Delta\varepsilon^0)_{ij}^{kl}$, is exchanged with the environment. This means that the system of the two colliding molecules is not considered to be isolated, and this point of view is not completely microscopic. The second aspect is that (3.82) has the same form for both mechanical collisions and chemical reactions, which allows not to distinguish them for the main part of this work, while in the formulation (3.83), used in [76], one has to separate mechanical and reactive Boltzmann operators.

3.9 Example of a three species gas mixture undergoing one chemical reaction

This section has the purpose of explaining to the reader how a model may be built on a toy example in our general framework. We consider a gas composed of dihydrogen H_2 , diiodine I_2 , and hydrogen iodide HI , undergoing the reaction



State-based model

We choose, for this example, to describe those three molecules with a semi-classical model, with harmonic potential in the description of vibration. For the complete and detailed setting of this model, the authors refer the reader to [37, Subsection 7.3]. We report here, for completeness, some insights into its construction.

We assume the molecule to be a rigid rotor, that is, in the description of rotation we assume that no deformation is induced in the molecule. The rotation-related internal state we consider is thus the angular velocity of the molecule in a coordinate system attached to it. In general, this angular velocity is in \mathbb{R}^3 , however when the molecule is linear, being symmetric by rotation around its own axis, the contribution of the angular momentum's coordinate along this axis can be assumed to be 0. Since dihydrogen, diiodine and hydrogen iodine are diatomic (hence linear) molecules, we consider their angular velocities to be in \mathbb{R}^2 , and there exists, for each $A \in \{\text{H}_2, \text{I}_2, \text{HI}\}$, a moment of inertia \mathcal{I}_A such that the kinetic energy of rotation associated with the molecule A with angular velocity z writes

$$\frac{1}{2}\mathcal{I}_A|z|^2.$$

Due again to the diatomic nature of the involved molecules, there is for each of them only one type of vibration, which we describe with the model of the quantum harmonic oscillator. Letting h be the Planck constant, c the speed of light and ν_A the wavenumber associated with the molecule $A \in \{\text{H}_2, \text{I}_2, \text{HI}\}$, the energy associated with the mode of vibration $l \in \mathbb{N}$ (the l^{th} energy level) writes

$$hc\nu_A\left(l + \frac{1}{2}\right).$$

We hence consider the internal state to be $\zeta = (z, l)$, so that each model writes, for $A \in \{\text{H}_2, \text{I}_2, \text{HI}\}$, as

$$\begin{aligned} (\mathcal{E}_A, \mathcal{A}_A, d\mu_A(\zeta)) &= (\mathbb{R}^2 \times \mathbb{N}, \text{Bor}(\mathbb{R}^2) \otimes \mathcal{P}(\mathbb{N}), dz \times 1), \\ \varepsilon_A(z, l) &= \frac{1}{2}\mathcal{I}_A|z|^2 + hc\nu_A\left(l + \frac{1}{2}\right), \end{aligned} \quad (3.85)$$

with $dz \times 1$ denoting the tensor product of the Lebesgue measure on \mathbb{R}^2 and the counting measure on \mathbb{N} .

Corresponding energy-based model

Applying the process of reduction explained above, that is computing the image measure $\mu_A^{\bar{\varepsilon}_A}$, the energy-based model corresponding to (3.85) is the Borgnakke-Larsen model with weight φ_A and fundamental energy $\frac{1}{2}hc\nu_A$,

$$(\mathbb{R}_+, \text{Bor}(\mathbb{R}_+), \varphi_A(I) dI), \quad I \mapsto I + \frac{1}{2}hc\nu_A, \quad (3.86)$$

with, for $I \in \mathbb{R}_+$,

$$\varphi_A(I) = \frac{2\pi}{\mathcal{I}_A} \left\lceil \frac{I}{hc\nu_A} \right\rceil, \quad (3.87)$$

where $\lceil \cdot \rceil$ is the ceiling function (upper integer part).

Quantities of interest

We immediately deduce from the model (3.85) that

$$\varepsilon_A^0 = \frac{1}{2}hc\nu_A,$$

implying that the energy consumed by the reaction $\text{H}_2 + \text{I}_2 \rightarrow 2\text{HI}$ is

$$\Delta\varepsilon^0 = 2\varepsilon_{\text{HI}}^0 - \varepsilon_{\text{H}_2}^0 - \varepsilon_{\text{I}_2}^0 = hc \left(\nu_{\text{HI}} - \frac{\nu_{\text{H}_2} + \nu_{\text{I}_2}}{2} \right).$$

The partition function of the species $A \in \{\text{H}_2, \text{I}_2, \text{HI}\}$ writes, for any $\beta > 0$, as

$$\begin{aligned} Z_A(\beta) &= \left(\int_{\mathbb{R}^2} e^{-\beta \frac{\mathcal{I}_A |z|^2}{2}} \mathbf{d}z \right) \left(\sum_{l=0}^{\infty} e^{-\beta l hc \nu_A} \right) = \frac{2\pi}{\beta \mathcal{I}_A} \times \frac{1}{1 - e^{-\beta hc \nu_A}} \\ &= \frac{2\pi}{\mathcal{I}_A} \int_{\mathbb{R}_+} e^{-\beta I} \left[\frac{I}{hc \nu_A} \right] \mathbf{d}I. \end{aligned} \quad (3.88)$$

Also, one easily proves that, letting $T_A^0 = hc\nu_A/k_B$, the number of internal degrees of freedom writes, for any $T > 0$, as

$$\delta_A(T) = 2 + 2 \frac{T_A^0/T}{\exp(T_A^0/T) - 1}.$$

At mechanical equilibrium there exists $n_{\text{H}_2}, n_{\text{I}_2}, n_{\text{HI}}, \underline{u}, T$ such that the state-based equilibrium distribution writes, for $(v, z, l) \in \mathbb{R}^3 \times \mathbb{R}^2 \times \mathbb{N}$, as

$$\begin{aligned} \mathcal{M}_A^{\text{state}}[n_A, \underline{u}, T](v, z, l) \\ = n_A \left(\frac{m_A}{2\pi k_B T} \right)^{3/2} Z_A^{-1} \left(\frac{1}{k_B T} \right) \exp \left(-\frac{m_A |v - \underline{u}|^2}{2k_B T} - \frac{\frac{1}{2} \mathcal{I}_A |z|^2 + l hc \nu_A}{k_B T} \right), \end{aligned} \quad (3.89)$$

for which the integrations are performed in the space $(\mathbb{R}^3 \times \mathbb{R}^2 \times \mathbb{N}, \mathbf{d}v \mathbf{d}z \times 1)$. On the other hand, the energy-based equilibrium distribution writes, for $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$, as

$$\begin{aligned} \mathcal{M}_A^{\text{energy}}[n_A, \underline{u}, T](v, I) \\ = n_A \left(\frac{m_A}{2\pi k_B T} \right)^{3/2} Z_A^{-1} \left(\frac{1}{k_B T} \right) \exp \left(-\frac{m_A |v - \underline{u}|^2}{2k_B T} - \frac{I}{k_B T} \right), \end{aligned} \quad (3.90)$$

for which the integrations are performed in the space $(\mathbb{R}^3 \times \mathbb{R}_+, \mathbf{d}v \varphi_A(I) \mathbf{d}I)$. At chemical equilibrium, we obtain in this example the mass-action law

$$\frac{n_{\text{HI}}^2}{n_{\text{H}_2} n_{\text{I}_2}} = \underbrace{\frac{m_{\text{HI}}^3}{m_{\text{H}_2}^{3/2} m_{\text{I}_2}^{3/2}}}_{\text{translation}} \times \underbrace{\frac{\mathcal{I}_{\text{H}_2} \mathcal{I}_{\text{I}_2}}{\mathcal{I}_{\text{HI}}^2}}_{\text{rotation}} \times \underbrace{\frac{\left(1 - e^{-\frac{hc\nu_{\text{H}_2}}{k_B T}}\right) \left(1 - e^{-\frac{hc\nu_{\text{I}_2}}{k_B T}}\right)}{\left(1 - e^{-\frac{hc\nu_{\text{HI}}}{k_B T}}\right)^2}}_{\text{vibration}} \times \underbrace{e^{-\frac{hc \left(\nu_{\text{HI}} - \frac{\nu_{\text{H}_2} + \nu_{\text{I}_2}}{2} \right)}{k_B T}}}_{\text{chemical}}$$

$$= \frac{m_{\text{HI}}^3}{m_{\text{H}_2}^{3/2} m_{\text{I}_2}^{3/2}} \times \frac{\mathcal{I}_{\text{H}_2} \mathcal{I}_{\text{I}_2}}{\mathcal{I}_{\text{HI}}^2} \times \frac{\sinh\left(\frac{hc\nu_{\text{H}_2}}{2k_B T}\right) \sinh\left(\frac{hc\nu_{\text{I}_2}}{2k_B T}\right)}{\sinh\left(\frac{hc\nu_{\text{HI}}}{2k_B T}\right)^2}. \quad (3.91)$$

We notably remark that

$$\begin{aligned} \frac{n_{\text{HI}}^2}{n_{\text{H}_2} n_{\text{I}_2}} &\underset{T \rightarrow 0^+}{\sim} \frac{m_{\text{HI}}^3}{m_{\text{H}_2}^{3/2} m_{\text{I}_2}^{3/2}} \times \frac{\mathcal{I}_{\text{H}_2} \mathcal{I}_{\text{I}_2}}{\mathcal{I}_{\text{HI}}^2} \times e^{-\frac{hc\left(\nu_{\text{HI}} - \frac{\nu_{\text{H}_2} + \nu_{\text{I}_2}}{2}\right)}{k_B T}}, \\ \frac{n_{\text{HI}}^2}{n_{\text{H}_2} n_{\text{I}_2}} &\underset{T \rightarrow \infty}{\rightarrow} \frac{m_{\text{HI}}^3}{m_{\text{H}_2}^{3/2} m_{\text{I}_2}^{3/2}} \times \frac{\mathcal{I}_{\text{H}_2} \mathcal{I}_{\text{I}_2}}{\mathcal{I}_{\text{HI}}^2} \times \frac{\nu_{\text{H}_2} \nu_{\text{I}_2}}{\nu_{\text{HI}}^2}. \end{aligned} \quad (3.92)$$

As expected from the fact that vibration activates with increasing temperature, we observe that, at low temperatures, the effect of vibration vanishes, whereas it does appear in the high temperature limit.

3.10 Conclusion

In this paper we extended the internal states general framework for polyatomic gases [37] to a mixture of monatomic or polyatomic gases, undergoing an arbitrary number of bimolecular chemical reactions. The proposed setting is general and it allows to describe the internal structure of each species of the mixture with its own adapted model, that may be monatomic, semi-classical, or any other model for the microscopic structure of a given molecule. In this way one is able to manage simultaneously monatomic gases, polyatomic constituents with a set of discrete energy levels or with continuous internal energy, polyatomic gases with two different internal variables to keep separate vibrational and rotational energies, and so on. The approach is completely microscopic, even when dealing with chemical reactions, and has been shown to be in complete agreement with previously known formulations, see Section 3.8. An important feature of our model is the inclusion in the general formulation of the notion of activation energy, which is of importance when studying the kinetics of chemical reactions, and for which an example is provided in Section 3.7.

We have defined the collision rules, Equations (3.10) and (3.17), studied the related collision invariants (Proposition 3.4 and Corollary 3.5), proved the H-Theorem (Theorem 3.1 and Corollary 3.6) and obtained the Maxwellian form related to the (mechanical) equilibrium, Equation (3.39), as well as mass action laws of chemical reactions, Theorem 3.2. As a hydrodynamic limit, we have formally recovered the Euler system of equations in presence of moderately slow chemical reactions, namely in an elastic dominated regime, Equations (3.69)–(3.71). We have derived a general formula for the rate constant of a given reaction, depending only on the global temperature of the gas and on the cross-section, see Equation (3.60), and proved it to be increasing with temperature whenever the latter increases with energy (Proposition 3.14).

The investigation of further mathematical properties of our system of Boltzmann equations could be an interesting and challenging future research line. At first, the compactness properties of linearized Boltzmann operators have gained much interest in recent literature, both for polyatomic gases [38, 52, 21] and for gas mixtures [45, 20], and it could be interesting to look for general conditions (on the space of internal states and on its measure) guaranteeing such compactness results. An additional topic worth to be investigated, in view of applications to physical problems, is the consistent derivation from our kinetic system of hydrodynamic equations beyond the Euler level. Specifically, a suitable Chapman–Enskog asymptotic procedure should allow to establish the relationships between Boltzmann and Navier–Stokes equations, with transport coefficients depending also on suitable averages of the Boltzmann microscopic

cross sections. Such coefficients could be made explicit in some specific situations, including the case of Maxwell molecules. A survey on the mathematical techniques for fluid–dynamic limits of kinetic models, with both formal and rigorous proofs, may be found in [91], and the formal Chapman–Enskog asymptotics for an inert mixture of monatomic and polyatomic gases, the latter ones having continuous internal energy, has been investigated in [19]. Analogous achievements for our general internal states Boltzmann framework, even in presence of chemical reactions, will be matter of future research.

3.A Auxiliary lemma

We prove here a technical lemma, needed in Proposition 3.14.

Lemma 3.18. *Let $(\mathcal{X}, \mathcal{T}, \eta)$ be a measured space such that $\eta(X) > 0$. Let $\psi, \varphi : \mathcal{X} \rightarrow \mathbb{R}_+$ be measurable applications, in the sense of \mathcal{T} on \mathcal{X} and the Borelians on \mathbb{R}_+ , such that ψ is non-constant η -a.e. and φ is η -non-constant, in the sense that*

$$\begin{aligned} \eta \otimes \eta(\{(x, x') \in \mathcal{X} \times \mathcal{X} \text{ s.t. } \psi(x) = \psi(x')\}) &= 0, \\ \eta \otimes \eta(\{(x, x') \in \mathcal{X} \times \mathcal{X} \text{ s.t. } \varphi(x) \neq \varphi(x')\}) &> 0. \end{aligned} \quad (3.93)$$

We assume that for any $T > 0$, defining $\psi_T(x) = \frac{\psi(x)}{T}$,

$$\int_{\mathcal{X}} (1 + \varphi(x)) e^{-\psi_T(x)} \mathrm{d}\eta(x) < \infty, \quad (3.94)$$

and for η -a.e. $x, x' \in \mathcal{X}$,

$$\psi(x) \leq \psi(x') \implies \varphi(x) \leq \varphi(x'). \quad (3.95)$$

Then the function $K : \mathbb{R}_+^* \rightarrow \mathbb{R}_+$, defined by

$$K(T) = \frac{\int_{\mathcal{X}} \varphi(x) e^{-\psi_T(x)} \mathrm{d}\eta(x)}{\int_{\mathcal{X}} e^{-\psi_T(x)} \mathrm{d}\eta(x)}, \quad T > 0,$$

is increasing on \mathbb{R}_+ .

Proof. First, for η -a.e. $x \in \mathcal{X}$, we have

$$\frac{\mathrm{d}}{\mathrm{d}T} \left(e^{-\psi_T(x)} \right) = \frac{\psi(x)}{T^2} e^{-\psi_T(x)}.$$

From the integrability assumption (3.94), the bound $ye^{-y} \leq 2e^{-y/2}$ for any $y \geq 0$ and the Cauchy-Schwarz inequality, K is \mathcal{C}^1 on \mathbb{R}_+^* , with

$$\begin{aligned} K'(T) &= -\frac{1}{T^2} \frac{\left(\int_{\mathcal{X}} \psi(x) e^{-\psi_T(x)} \mathrm{d}\eta(x) \right) \left(\int_{\mathcal{X}} \varphi(x) e^{-\psi_T(x)} \mathrm{d}\eta(x) \right)}{\left(\int_{\mathcal{X}} e^{-\psi_T(x)} \mathrm{d}\eta(x) \right)^2} \\ &\quad + \frac{1}{T^2} \frac{\int_{\mathcal{X}} \varphi(x) \psi(x) e^{-\psi_T(x)} \mathrm{d}\eta(x)}{\int_{\mathcal{X}} e^{-\psi_T(x)} \mathrm{d}\eta(x)}. \end{aligned}$$

We deduce that, for any $T > 0$,

$$\begin{aligned} K'(T) > 0 &\iff \int_{\mathcal{X}} \int_{\mathcal{X}} \varphi(x) \psi(x) e^{-\psi_T(x)} e^{-\psi_T(x')} \mathbf{d}\eta(x) \mathbf{d}\eta(x') \\ &> \int_{\mathcal{X}} \int_{\mathcal{X}} \psi(x) e^{-\psi_T(x)} \varphi(x') e^{-\psi_T(x')} \mathbf{d}\eta(x) \mathbf{d}\eta(x') \\ &\iff \int_{\mathcal{X}} \int_{\mathcal{X}} (\varphi(x) - \varphi(x')) \psi(x) e^{-(\psi_T(x) + \psi_T(x'))} \mathbf{d}\eta(x) \mathbf{d}\eta(x') > 0. \end{aligned}$$

We set

$$\mathcal{I} = \int_{\mathcal{X}} \int_{\mathcal{X}} (\varphi(x) - \varphi(x')) \psi(x) e^{-(\psi_T(x) + \psi_T(x'))} \mathbf{d}\eta(x) \mathbf{d}\eta(x').$$

Simply exchanging the indices, we have

$$\mathcal{I} = - \int_{\mathcal{X}} \int_{\mathcal{X}} (\varphi(x) - \varphi(x')) \psi(x') e^{-(\psi_T(x) + \psi_T(x'))} \mathbf{d}\eta(x) \mathbf{d}\eta(x'),$$

so that

$$\mathcal{I} = \frac{1}{2} \int_{\mathcal{X}} \int_{\mathcal{X}} (\varphi(x) - \varphi(x')) (\psi(x) - \psi(x')) e^{-(\psi_T(x) + \psi_T(x'))} \mathbf{d}\eta(x) \mathbf{d}\eta(x').$$

Hence, for any $T > 0$,

$$K'(T) > 0$$

$$\iff \iint_{\mathcal{X}^2} (\varphi(x) - \varphi(x')) (\psi(x) - \psi(x')) e^{-(\psi_T(x) + \psi_T(x'))} \mathbf{d}(\eta \otimes \eta)(x, x') > 0.$$

Assumptions (3.93) and (3.95) imply that the right-hand side integral is indeed positive for any $T > 0$, ending the proof. \square

3.B Physical and chemical quantities reminder

The purpose of this appendix is to sum up all the useful quantities defined in this paper, which have been collected in the following Tables 1, 2, 3.

Fundamental energy of the species i	$\varepsilon_i^0 = \text{inf ess}_{\mu_i} \{\varepsilon_i\}$
Grounded internal energy function of the species i	$\bar{\varepsilon}_i = \varepsilon_i - \varepsilon_i^0 : \mathcal{E}_i \rightarrow \mathbb{R}_+$
Energy law of the species i	$\mu_i^{\bar{\varepsilon}_i}$ is the image measure of μ_i by $\bar{\varepsilon}_i$
Partition function of the species i	$Z_i(\beta) = \int_{\mathcal{E}_i} e^{-\beta \bar{\varepsilon}_i(\zeta)} d\mu_i(\zeta) = \int_{\mathbb{R}_+} e^{-\beta I} d\mu_i^{\bar{\varepsilon}_i}(I)$
Gibbs measure on the space of internal states of the species i at temperature $T > 0$	$d\nu_T^i(\zeta) = Z \left(\frac{1}{k_B T} \right)^{-1} \exp \left(-\frac{\bar{\varepsilon}_i(\zeta)}{k_B T} \right) d\mu_i(\zeta)$
Gibbs measure on the space of internal energies of the species i at temperature $T > 0$	$d\tilde{\nu}_T^i(I) = Z \left(\frac{1}{k_B T} \right)^{-1} \exp \left(-\frac{I}{k_B T} \right) d\mu_i^{\bar{\varepsilon}_i}(I)$
Number of internal degrees of freedom of the species i at temperature $T > 0$	$\delta_i(T) = -\frac{2}{k_B T} (\log(Z_i))' \left(\frac{1}{k_B T} \right) = 2 \mathbb{E}_{\nu_T^i} \left[\frac{\bar{\varepsilon}_i}{k_B T} \right]$
Heat capacity at constant volume of the species i at temperature $T > 0$	$c_V^i(T) = \frac{3 + D_i(T)}{2},$ $D_i(T) = \frac{d(T\delta_i(T))}{dT} = \frac{2}{(k_B T)^2} (\log(Z_i))'' \left(\frac{1}{k_B T} \right) = 2 \text{Var}_{\nu_T^i} \left[\frac{\bar{\varepsilon}_i}{k_B T} \right]$

Table 3.1 – Quantities related to internal energy modelling of a single species

Reduced and total mass of species i and j	$m_{ij}^* = \frac{m_i m_j}{m_i + m_j}, \quad M_{ij} = m_i + m_j$
Energy consumed by the chemical reaction $\{(i, j) \rightarrow (k, l)\}$	$(\Delta \varepsilon^0)_{ij}^{kl} = \varepsilon_k^0 + \varepsilon_l^0 - \varepsilon_i^0 - \varepsilon_j^0$
Activation energy of $\{(i, j) \rightarrow (k, l)\}$	$E_a = \varepsilon_{ij}^{kl} - \varepsilon_i^0 - \varepsilon_j^0$
Averaged collision kernel	$\bar{B}_{ij}^{kl}(g, \zeta, \zeta_*) = \iint_{\varepsilon_k \times \varepsilon_l} \int_{\mathbb{S}^2} \tilde{B}_{ij}^{kl}(g, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) d\omega d\mu_k(\zeta') d\mu_l(\zeta'_*),$ $\tilde{B}_{ij}^{kl}(v - v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega) = B_{ij}^{kl}(v, v_*, \zeta, \zeta_*, \zeta', \zeta'_*, \omega)$

Table 3.2 – Fundamental quantities involved in interactions between different species

Relative kinetic Gibbs probability measure on \mathbb{R}^3 , of the species i and j at temperature $T > 0$	$d\lambda_T^{ij}(g) = \left(\frac{m_{ij}^*}{2\pi k_B T} \right)^{3/2} \exp\left(-\frac{m_{ij}^* g ^2}{2k_B T} \right) dg$
Rate constant of the chemical reaction $\{(i, j) \rightarrow (k, l)\}$ at temperature $T > 0$	$\mathcal{K}_{ij}^{kl}(T) = \mathbb{E}_{\lambda_T^{ij} \otimes \nu_T^i \otimes \nu_T^j} [\bar{B}_{ij}^{kl}]$
Rate of the chemical reaction $\{(i, j) \rightarrow (k, l)\}$ at temperature $T > 0$ and with respective densities n_i, n_j, n_k and n_l	$r_{ij}^{kl} = \mathcal{K}_{kl}^{ij}(T) n_k n_l - \mathcal{K}_{ij}^{kl}(T) n_i n_j$
Reaction rate of the species i	$r_i = \sum_{\substack{j, k, l \\ \{(i, j) \rightarrow (k, l)\} \in \Omega_{chem}}} r_{ij}^{kl}$
Equilibrium constant of the chemical reaction $\{(i, j) \rightarrow (k, l)\}$ at temperature $T > 0$, with $\sigma_k = \sigma_l = -\sigma_i = -\sigma_j = 1$	$\mathcal{K}_{ij}^{kl}(T) = \prod_{p \in \{i, j, k, l\}} \left\{ (2\pi m_p k_B T)^{3\sigma_p/2} Z_p \left(\frac{1}{k_B T} \right)^{\sigma_p} \right\} \times \exp\left(-\frac{(\Delta \varepsilon^0)_{ij}^{kl}}{k_B T} \right)$

Table 3.3 – Quantities related to mechanical or global collision equilibrium

Bibliography of the current chapter

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Part II

**Around a singular polyatomic model:
resonant and quasi-resonant collisions**

Overview

In this part, composed of Chapters 4 and 5, we study polyatomic gases undergoing resonant or quasi-resonant collisions. Chapter 4 is an *improvement* of [38]: the result and main proof presented here thus differ from the ones of the publication. Chapter 5 is not based on a publication. In this part, the notation ε stands for the quasi-resonance parameter.

This work deals with **functional analysis, modelling** and **numerical simulations**.

ABSTRACT OF CHAPTER 4. In this paper, we investigate a compactness property of the linearized Boltzmann operator in the context of a polyatomic gas, the molecules of which undergo resonant collisions. The peculiar structure of resonant collision rules allows to tensorize the problem into a velocity-related one, neighbouring the monatomic case, and an internal energy-related one. Our analysis is based on a specific treatment of the contributions due to the internal energy of the molecules. We also propose a geometric variant of Grad's proof of the same compactness property in the monatomic case.

ABSTRACT OF CHAPTER 5. In this chapter, we provide a Boltzmann model for a single polyatomic gas, the molecules of which undergo quasi-resonant collisions. We propose a rigorous characterization of the notion of quasi-resonance, obtain the H -Theorem associated with the model and a resonant asymptotics. We discuss the expected behaviour of solutions to the homogeneous quasi-resonant Boltzmann equation and claim that the kinetic and internal temperatures of such a solution should approximately satisfy an ODE system, of Landau-Teller type, which we make explicit from the Boltzmann level for a wide family of collision kernels. We perform a numerical experiment on the matter to somehow validate our claim.

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A compactness property of the linearized Boltzmann operator for a polyatomic gas undergoing resonant collisions

Outline of the current chapter

4.1 Introduction	162
4.2 Resonant collision model	163
Molecule model	164
Microscopic dynamics	164
Assumptions on the cross section	165
Kinetic operator, H theorem	167
4.3 Main result	168
4.4 Proof of the main result	168
4.4.1 Compactness of K_1	169
4.4.2 Compactness of K_2	170
4.4.3 Conclusion to the proof of Theorem 4.1	180
4.A Grad's proof revisited	180
4.A.1 Alternative change of variables	181
4.A.2 Study of the kernel form of K_2^m	183
4.B A technical lemma	189

4.1 Introduction

The study of linearized collisional operators in kinetic theory has been addressed in the literature long after the introduction of the corresponding quadratic operators [60]. In fact, taking as an initial reference point Boltzmann's article [34], the first questions about the linearized Boltzmann operator were studied several years later by Hilbert in [109]. Hilbert wrote the linearized operator in an integral form, in the case of a hard-sphere cross section in three spatial dimensions, and proved its compactness. Subsequently, Hecke [106] and Carleman [56] extended Hilbert's results and proved that the linearized Boltzmann operator is of Hilbert-Schmidt type.

A substantial improvement in the understanding of those compactness properties was given in [93] by Grad who, using an ingenious geometrical argument, proved the compactness of the linearized operator for a wide range of cross sections satisfying the so-called angular cut-off condition, which he previously introduced in [92]. He adapted Hecke's proof by stating that the linearized Boltzmann operator was still of Hilbert-Schmidt type in a weighted L^2 space.

For a long time, no further significant steps related to the problem were proposed. However, many natural questions remained open, such as, for example, the extension of Grad's result to linearized Boltzmann operators without imposing the angular cut-off condition, or the study of compactness properties for gaseous mixtures, described by systems of coupled Boltzmann equations. Regarding the weakening of assumptions about the cross section, we highlight that an important result of compactness, which does not suppose any small deflection cut-off assumption on the cross sections, is due to Mouhot and Strain [135].

When dealing with gaseous mixtures, the Grad geometric argument may fail. Indeed, if the species involved in the mixture have different molar masses, the symmetry between pre- and post-collisional velocities is lost. This symmetry was crucial in Grad's strategy. A new argument to recover the compactness property for gaseous monatomic mixtures with different masses has been proposed in [46], where the mono- and multi-species cases are treated in two different ways: Grad's method still applies in the case of mono-species collisions or when the masses of the colliding particles are equal, whereas a pre/post-collisional velocity-crossing argument is used to deal with collisions between particles with different masses. Note that, however, it degenerates when the masses of the colliding particles are equal. We refer to [45] for a more complete state-of-the-art on the compactness of the linearized Boltzmann operator and on the linearized operator for mixtures of monatomic gases.

The internal structure of polyatomic molecules influences the energy transfer during collisions, so that variables describing the internal state of a given molecule, such as its angular velocity or vibration mode, must be taken into account in the model, and appear in the energy conservation law during a collision. The corresponding kinetic models are based on various approaches. The first one consists of introducing a set of discrete internal energy variables and considering a set of particle densities satisfying a system of coupled kinetic equations. The compactness of the linearized collision operator in that case has been studied very recently in [20].

Another approach is based on the introduction of a continuous internal energy variable $I \in \mathbb{R}_+$ and the model describes the evolution of the particle density in an extended phase space, the variables then being time, position, velocity and internal energy. A mechanistic procedure for binary encounters in polyatomic gases was provided by Borgnakke and Larsen [35], and the corresponding linearized collisional operator was recently studied in [21, 52].

In both approaches, one considers the molecule's internal energy as the variable encapsulating its internal structure. A generalization was proposed in [37], where the internal variable is rather the internal state of the molecule, for instance, its angular velocity and vibrational modes. It was proven that this consideration of the states is equivalent to a model considering directly a continuous internal energy variable I in the set \mathbb{R}_+ endowed with some measure μ , called energy law, computable from the model of the molecule and fully characterizing it in the kinetic context, as soon as the interaction kernel itself

depends only on the internal states only through their energy. The case when μ is a discrete measure corresponds to the model with discrete energy levels, and the case when μ has a density with respect to the Lebesgue measure corresponds to the Borgnakke-Larsen models [35, 47, 75, 76].

In this paper, we place ourselves in this latter setting, considering the internal energy I in \mathbb{R}_+ endowed with the measure μ . The underlying model on the molecule is assumed to be semi-classical, in the sense that rotation should be described using classical mechanics, and vibration using quantum mechanics. Recalling that μ is explicitly computable from the model of the molecule, the semi-classical setting allows us to ensure that μ has a density with respect to the Lebesgue measure, which can be upper- and lower-bounded by power laws around 0 and infinity, which is helpful in the proof of our main theorem.

The specific and singular case we study is when the molecules of the gas undergo resonant collisions. This means that the microscopic internal and kinetic energies are separately conserved and cannot be handled by using the Borgnakke-Larsen procedure. This behaviour has been observed in some physical situations, such as in the collisions between selectively excited CO_2 molecules [120].

A kinetic operator describing resonant collisions has recently been proposed in [44], but the study of the compactness of the corresponding linearized operator has not yet been carried out. The purpose of this article is hence to fill in this gap and therefore to study the compactness property of the associated linearized operator.

Although our approach to the problem is consistent with the traditional strategy and consists of the rewriting of the linearized operator in a kernel form, its practical realization required to face specific difficulties and allowed to introduce a new viewpoint, mainly in the treatment of the internal energy variables. In the process, we also propose a variant change of variables, alternative to the one proposed by Grad in [93], which may be of further interest, in the polyatomic mixture case.

Besides, it is clear that the properties of the cross section may heavily influence the proof strategies. However, the precise form of the cross section for resonant collisions cannot be completely deduced from purely mechanical arguments and the corresponding conservation laws. Several forms of cross-sections have been proposed in the literature for the Borgnakke-Larsen model, in both elastic and inelastic cases, see, for example, [63, 62]. Nevertheless, since, up to our knowledge, the cross sections for resonant collisions have not been explicitly derived yet, we therefore aim to be as general as possible, by assuming that the cross section can be upper-bounded by a product of terms depending, separately, on the velocity and the internal energy variables. It allows to deal on the one hand with the velocity terms, and on the other hand, with the internal energy ones.

The article is organized as follows. In Section 4.2, we describe the details of the model introduced in [44], the hypotheses on the measure μ characterizing the internal structure of the molecules, and the assumptions on the cross sections made for our analysis. Next, in Section 4.3, we state our main compactness result, which is proven in Section 4.4. The non-multiplicative part of the linearized operator is split into several contributions, whose compactness are proven separately. Eventually, in the appendix, we propose our alternative to Grad's change of variables and provide its related geometric interpretation.

4.2 Resonant collision model

We consider a gas composed of one species of polyatomic molecules with mass $m > 0$. These molecules evolve in the three-dimensional Euclidean space \mathbb{R}^3 , and are associated with a distribution function f , which depends on time $t \in \mathbb{R}_+$, position in space $x \in \mathbb{R}^3$, molecular velocity $v \in \mathbb{R}^3$ and internal energy $I \in \mathbb{R}_+$. Though, as this study only focuses on the Boltzmann collision operator, we discard the time and position variables t and x , and consider distribution functions depending only on v and I .

Molecule model

In regards with the general framework defined in [37], and where internal states are considered, any state-based model can be reduced into a simpler energy-based one, where the internal variable is simply the internal energy, through reduction process. To be more accurate, we work in a semi-classical setting: we choose to describe the rotation of the molecule by using the standard approach of classical mechanics and the vibration part within the quantum mechanics framework, and we adopt an energy-based view-point. Therefore, we consider a measure μ on the set of internal energies \mathbb{R}_+ , called the *energy law*, which encapsulates the internal structure of the molecule, and is absolutely continuous with respect to the Lebesgue measure. In the semi-classical case, the density of μ is typically a scale function, or a sum of pieces of square-roots, so that it behaves like a power law around 0, typically a constant or the square-root function, and behaves like another power law around infinity.

Hence, the previous considerations justify our choice about the following properties of μ , which will be supposed from now on.

Definition 4.1. *The measure μ is said admissible if it has a density φ against the Lebesgue measure on \mathbb{R}_+ ,*

$$\varphi(I) := \frac{d\mu(I)}{dI}, \quad I \in \mathbb{R}_+, \quad (4.1)$$

such that there exist $\beta_1, \beta_2 \geq 0$ and $C, C' > 0$ such that

$$C I^{\beta_1} \leq \varphi(I) \leq C' I^{\beta_1}, \quad \text{for a.e. } I \in [0, 1), \quad (4.2)$$

and

$$C I^{\beta_2} \leq \varphi(I) \leq C' I^{\beta_2}, \quad \text{for a.e. } I \geq 1. \quad (4.3)$$

Remark 4.1. *Assumption (4.3) could be relaxed into: for any $a > 0$, there exists $C_a > 0$ such that*

$$C_a I^{\beta_2 - a} \leq \varphi(I) \leq C' I^{\beta_2}, \quad \text{for a.e. } I \geq 1,$$

and the result of the present paper would still hold; though for a purpose of clarity we opted to rather consider assumption (4.3). An example of a function satisfying the above but not (4.3) is the application $I \mapsto \frac{I^{\beta_2}}{\log I}$.

Note that Definition 4.1 is coherent with the hypotheses of the continuous-energy model proposed by Borgnakke and Larsen [35], see also [76, 75]. Moreover, the standard assumption $d\mu(I) = C I^\alpha dI$ with $\alpha \geq 0$, which allows to recover a temperature-independent heat capacity at constant volume and number of internal degrees of freedom, is of course covered by (4.2)–(4.3).

We moreover define the internal partition function associated with the molecule model, for any temperature $T > 0$, by

$$Z(T) = \int_{\mathbb{R}_+} \exp\left(-\frac{I}{T}\right) d\mu(I). \quad (4.4)$$

Assumptions (4.2)–(4.3) on μ straightforwardly imply that q is well-defined and \mathcal{C}^∞ on \mathbb{R}_+^* .

In order to describe the model, we first consider the microscopic dynamics, then we introduce our hypotheses on the cross section and, finally, we write the kinetic model which governs the time evolution of the density f .

Microscopic dynamics

At fixed time and position, a given molecule is described by its velocity v and its internal energy I . The couple (v, I) is called the *state* of the molecule.

Let us consider the collision between two molecules. The pre-collision states are denoted by (v, I) and (v_*, I_*) , and the post-collision ones by (v', I') and (v'_*, I'_*) . The system of molecules being isolated, the total momentum and energy of the system are conserved during the collision, *i.e.*

$$v + v_* = v' + v'_*, \quad (4.5)$$

$$\frac{1}{2}m|v|^2 + I + \frac{1}{2}m|v_*|^2 + I_* = \frac{1}{2}m|v'|^2 + I' + \frac{1}{2}m|v'_*|^2 + I'_*. \quad (4.6)$$

Following [44], we suppose that the collisions are *resonant*, which means that (4.6) is a consequence of the two separate conservation laws

$$|v|^2 + |v_*|^2 = |v'|^2 + |v'_*|^2, \quad (4.7)$$

$$I + I_* = I' + I'_*, \quad (4.8)$$

ensuring that both kinetic and internal energy are separately conserved. In the resonant case, collision rules involving the velocities are the same as in the monatomic case. Consequently, Equations (4.5) and (4.7) imply the existence of $\sigma \in \mathbb{S}^2$ such that

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2}\sigma, \quad v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2}\sigma. \quad (4.9)$$

Besides, (4.8) straightforwardly implies that

$$I' \in [0, I + I_*], \quad I'_* = I + I_* - I'. \quad (4.10)$$

Assumptions on the cross section

We consider, in what follows, a cross section B depending on $(v, v_*, I, I_*, I', \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{S}^2$. Note that, because of (4.10), the dependence with respect to I'_* would be redundant. We emphasize that B is positive if and only if a collision is possible. Hence, (4.10) implies that, for almost every $(v, v_*, I, I_*, I', \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{S}^2$,

$$B(v, v_*, I, I_*, I', \sigma) > 0 \quad \iff \quad I' \leq I + I_*. \quad (4.11)$$

Moreover, B should satisfy the *symmetry* and *micro-reversibility* conditions: for almost every v, v_*, I, I_*, I' and σ ,

$$B(v_*, v, I_*, I, I + I_* - I', -\sigma) = B(v, v_*, I, I_*, I', \sigma), \quad (4.12)$$

$$B\left(\frac{v + v_*}{2} + \frac{|v - v_*|}{2}\sigma, \frac{v + v_*}{2} - \frac{|v - v_*|}{2}\sigma, I', I + I_* - I', I, \frac{v - v_*}{|v - v_*|}\right) = B(v, v_*, I, I_*, I', \sigma). \quad (4.13)$$

In the case of resonant collisions, something peculiar happens for the measure of integration associated with the post-collisional energy I' . Indeed, since $I_* = I + I_* - I'$, there is only one post-collisional energy variable, however it *must contain the information of both outgoing molecules*. In this event, the measure of integration associated with the variable I' is not simply μ but a measure related to *the convolution* of μ with itself. We define, for any $E_i \geq 0$, the measure $\mu_2[E_i]$ on $[0, E_i]$ by

$$d\mu_2[E_i](I') := \varphi(E_i - I')\varphi(I')dI', \quad I' \in [0, E_i]. \quad (4.14)$$

We claim that this family of measures is the correct one to consider for the variable I' in the definition of the Boltzmann operator (see Remark 4.2). This is pointed out in [40] where, defining the notion of *quasi-resonance*, the resonant model comes as a limit model and the latter measure naturally appears.

In order to obtain our main result, we moreover need B to satisfy several assumptions:

- there exist functions B_0 , b_k and b_i such that, for almost every v, v_*, I, I_*, I' and σ ,

$$\begin{aligned} B(v, v_*, I, I_*, I', \sigma) &= B_0 \left(|v - v_*|, \left| \cos \left(\widehat{v - v_*}, \sigma \right) \right|, I, I_*, I' \right) \\ &\leq b_k \left(|v - v_*|, \left| \cos \left(\widehat{v - v_*}, \sigma \right) \right| \right) b_i(I, I_*) \mathbf{1}_{I' \leq I + I_*}; \end{aligned} \quad (4.15)$$

- there exist $\delta_1 \in [0, 1)$, $\delta_2 \in [0, \frac{1}{2})$ and $C > 0$ such that, for almost every $\rho > 0$ and $\theta \in [0, 2\pi]$,

$$b_k(\rho, |\cos \theta|) \leq C \left(|\sin \theta| (\rho^2 + \rho^{-1}) + \rho + \rho^{-\delta_1} + |\sin \theta|^{-\delta_2} \right); \quad (4.16)$$

- there exist $\gamma \in (-2 - 2\beta_1, 2 + 2\beta_2)$ and $C > 0$ such that, for almost every $I, I_* > 0$,

$$b_i(I, I_*) \leq C \frac{(I + I_*)^{\gamma/2}}{\mu_2[I + I_*]([0, I + I_*])}, \quad (4.17)$$

where we recall that, by definition of μ_2 (see (4.14)), it holds for

$$\mu_2[E_i]([0, E_i]) = \int_0^{E_i} \varphi(E_i - J) \varphi(J) \, dJ. \quad (4.18)$$

We also define the averaged cross sections \bar{B} and \bar{B}_0 by

$$\begin{aligned} \bar{B}(v, v_*, I, I_*) &= \int_{\mathbb{S}^2} \int_{\mathbb{R}_+} B(v, v_*, I, I_*, I', \sigma) \, d\mu_2[I + I_*](I') \, d\sigma, \quad \text{for a.e. } (v, v_*, I, I_*), \\ \bar{B}_0(\rho, |\cos \theta|, I, I_*) &= \int_{\mathbb{R}_+} B_0(\rho, |\cos \theta|, I, I_*, I') \, d\mu_2[I + I_*](I'), \quad \text{for a.e. } (\rho, \theta, I, I_*). \end{aligned}$$

Assumptions (4.15)–(4.17) on B imply that, almost everywhere,

$$\bar{B}(v, v_*, I, I_*) \leq C (|v - v_*|^2 + |v - v_*|^{-1}) (I + I_*)^{\gamma/2}, \quad (4.19)$$

$$\bar{B}_0(\rho, |\cos \theta|, I, I_*) \leq C \left(|\sin \theta| (\rho^2 + \rho^{-1}) + \rho + \rho^{-\delta_1} + |\sin \theta|^{-\delta_2} \right) (I + I_*)^{\gamma/2}. \quad (4.20)$$

The reader may notice that, by linearity, the result proven in this paper also holds when the cross section B is a linear combination of cross sections satisfying assumptions (4.15)–(4.17). Since the case $\gamma = 0$ is covered by Assumption (4.17), it holds in particular when

$$b_i(I, I_*) \leq C \frac{1 + (I + I_*)^{\gamma/2}}{\mu_2[I + I_*]([0, I + I_*])}.$$

Possible cross sections in the polyatomic case have been discussed in [86] for the Borgnakke-Larsen collisions. Since, for all $\gamma \in (-1, 2) \subset (-2 - 2\beta_1, 2 + 2\beta_2)$,

$$|v - v_*|^\gamma + (I + I_*)^{\gamma/2} \leq C (|v - v_*|^2 + |v - v_*|^{-1}) \left[1 + (I + I_*)^{\gamma/2} \right],$$

we do cover here the general form of the cross section proposed in [86, Equation (3.1)], with the inclusion of negative powers, and the critical case $\gamma = 2$ whenever $\beta_2 > 0$. Finally, the reader shall notice that the renormalization by $\mu_2[I + I_*](\cdot)$ in (4.17) is a consequence of our choice of not parametrizing the internal energies. More precisely, in the case $\varphi(I) = I^\alpha$, if one chooses to parameterize the outgoing energy with $r \in [0, 1]$, such that $I' = r(I + I_*)$, then (4.17) would become $b_i(I, I_*) \leq C(I + I_*)^{\gamma/2}$, and the measure associated with the variable r would be, up to a multiplicative constant, $r^\alpha(1-r)^\alpha dr$. We choose in this work to adopt the viewpoint of the general framework defined in [37], and not to parametrize the internal energy part, as, if I' is kept as an integration variable, the forthcoming computations may be simplified. We highlight that, from a modeling point of view, this choice is equivalent to the one of parametrizing the allocation of the internal energy towards I' and I'_* , which is made in [44], due to the adaptation of the integration measure associated with I' . Hence, the results of the latter paper can be applied here.

Kinetic operator, H theorem

We can now define the Boltzmann collision operator associated with the resonant model, which writes, for any measurable function f such that the following makes sense, and almost every $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$,

$$Q(f, f)(v, I) = \int_{\mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{S}^2} (f(v', I')f(v'_*, I'_*) - f(v, I)f(v_*, I_*)) \times \\ \times B(v, v_*, I, I_*, I', \sigma) dv_* d\mu_2[I + I_*](I') d\mu(I_*) d\sigma, \quad (4.21)$$

where v', v'_* and I'_* in the integral are defined by (4.9)–(4.10).

Remark 4.2. We point out that choosing $\mu_2[I + I_*]$ as the integration measure associated with the variable I' in (4.21) is necessary (under the reversibility assumption (4.13) on B), as the measure

$$B(v, v_*, I, I_*, I', \sigma) d\sigma dv dv_* d\mu_2[I + I_*](I') d\mu(I) d\mu(I_*),$$

defined on

$$\{(v, v_*, I, I_*, I', \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{S}^2 \text{ such that } I' \leq I + I_*\},$$

is indeed reversible. This comes by noticing that the above rewrites as

$$B(v, v_*, I, I_*, I', \sigma) d\sigma dv dv_* \varphi(I) \varphi(I_*) \varphi(I') \varphi(I + I_* - I') dI dI_* dI'.$$

The H -theorem proved in [44] guarantees the existence of equilibrium states. In particular, the following result holds:

Proposition 4.1. For any positive function $g = g(v, I)$ such that the following quantity is defined, we have

$$\iint_{\mathbb{R}^3 \times \mathbb{R}_+} Q(g, g)(v, I) \log g(v, I) dv d\mu(I) \leq 0.$$

Moreover, the three following properties are equivalent:

- (i) $Q(\mathcal{M}, \mathcal{M}) = 0$,
- (ii) $\iint_{\mathbb{R}^3 \times \mathbb{R}_+} Q(\mathcal{M}, \mathcal{M})(v, I) \log(\mathcal{M})(v, I) dv d\mu(I) = 0$,

(iii) There exist $n \geq 0$, $u \in \mathbb{R}^3$, and $T_k, T_i > 0$ such that, for almost every $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$,

$$\mathcal{M}(v, I) = \frac{n}{Z(T_i)} \left(\frac{m}{2\pi T_k} \right)^{3/2} \exp \left(-\frac{m|v-u|^2}{2T_k} - \frac{I}{T_i} \right), \quad (4.22)$$

where we recall that Z is the partition function defined by (4.4).

The equilibrium state given by (4.22) writes as a product of two Gibbs distributions (which we also call Maxwellian functions by analogy to the monatomic case) with different temperatures T_k and T_i . This is a consequence of the specific conservation laws of resonant collisions, which allow no exchange between the kinetic and internal parts.

4.3 Main result

The standard perturbation setting for the Boltzmann equation combined with Proposition 4.1 allows us to consider, for some Maxwellian \mathcal{M} of the form (4.22), to define the linearized Boltzmann operator \mathcal{L} in the following way

$$\mathcal{L} = K - \bar{\nu} \text{Id}, \quad (4.23)$$

where the collision frequency $\bar{\nu}$, appearing in the multiplicative operator, is given by

$$\bar{\nu}(v, I) = \int_{\mathbb{R}^3 \times \mathbb{R}_+} \mathcal{M}(v_*, I_*) \bar{B}(v, v_*, I, I_*) \, dv_* \, d\mu(I_*),$$

and K reads

$$\begin{aligned} Kg(v, I) = \mathcal{M}(v, I)^{1/2} \int_{\mathbb{R}^3 \times (\mathbb{R}_+)^2 \times \mathbb{S}^2} & \left([\mathcal{M}^{-1/2}g](v', I') + [\mathcal{M}^{-1/2}g](v'_*, I'_*) - [\mathcal{M}^{-1/2}g](v_*, I_*) \right) \\ & \times \mathcal{M}(v_*, I_*) B(v, v_*, I, I_*, I', \sigma) \, dv_* \, d\mu_2[I + I_*](I') \, d\mu(I_*) \, d\sigma, \end{aligned}$$

where

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

Let us now state our main theorem.

Theorem 4.1. *The operator K is compact from $L^2(\mathbb{R}^3 \times \mathbb{R}_+, dv \, d\mu(I))$ to itself.*

The interest of the above theorem lies in its implications on the linearized Boltzmann operator \mathcal{L} . It proves, by (4.23), that \mathcal{L} writes as a sum of a compact and a multiplicative operator. This allows to use Fredholm's alternative, which itself may provide existence and uniqueness of a solution to the Boltzmann equation, in a close-to-equilibrium setting. Moreover, Theorem 4.1 along with (4.23) greatly simplifies the study of the spectrum of \mathcal{L} , as it reduces the study to one on $\bar{\nu}$.

4.4 Proof of the main result

Without loss of generality, we can assume that the Maxwellian \mathcal{M} has zero mean velocity, so that there exist $T_k, T_i > 0$ and $c > 0$ such that, for $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$,

$$\mathcal{M}(v, I) = c e^{-\frac{m|v|^2}{2T_k}} e^{-\frac{I}{T_i}}.$$

We define $M(v) = ce^{-\frac{m|v|^2}{2T_k}}$ the velocity part of \mathcal{M} , so that we can write $\mathcal{M}(v, I) = M(v)e^{-\frac{I}{T_i}}$. For the sake of simplicity, we assume $m = 1$ in the following, without loss of generality. Indeed, m only appears in M through the constant $\frac{m}{2T_k}$, so that proving our result with $m = 1$ for all $T_k > 0$ is equivalent with proving it for all $m, T_k > 0$.

The main idea in the proof of Theorem 4.1 is to use the specific structure of the resonant collision case in order to separate the variables v and I , and to be able to use the known results on the monatomic case. We decompose K as a sum of three operators, $K = K_1 + K_2 + K_3$, where

$$\begin{aligned} K_1 g(v, I) &= - \int_{\mathbb{R}^3 \times \mathbb{R}_+} g_* \mathcal{M}^{1/2} \mathcal{M}_*^{1/2} \bar{B}(v, v_*, I, I_*) \, dv_* \, d\mu(I_*), \\ K_2 g(v, I) &= \int_{\mathbb{R}^3 \times (\mathbb{R}_+)^2 \times \mathbb{S}^2} [\mathcal{M}^{-1/2} g]' \mathcal{M}^{1/2} \mathcal{M}_* B(v, v_*, I, I_*, I', \sigma) \, dv_* \, d\mu_2[I + I_*](I') \, d\mu(I_*) \, d\sigma, \\ K_3 g(v, I) &= \int_{\mathbb{R}^3 \times (\mathbb{R}_+)^2 \times \mathbb{S}^2} [\mathcal{M}^{-1/2} g]'_* \mathcal{M}^{1/2} \mathcal{M}_* B(v, v_*, I, I_*, I', \sigma) \, dv_* \, d\mu_2[I + I_*](I') \, d\mu(I_*) \, d\sigma, \end{aligned}$$

where we used the shorthands $f \equiv f(v, I)$, $f_* \equiv f(v_*, I_*)$, $f \equiv f(v', I')$ and $f \equiv f(v'_*, I'_*)$, and

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

Applying the change of variable $\sigma \mapsto -\sigma$ and $I' \mapsto I + I_* - I'$ in K_3 allows to recover the same form as K_2 , so that it is enough to prove that K_1 and K_2 are compact.

4.4.1 Compactness of K_1

In order to prove the compactness of K_1 , we observe that it is in fact a Hilbert-Schmidt operator. We define the kernel, for almost every v, I, v_*, I_* ,

$$\kappa_1(v, I, v_*, I_*) = -\mathcal{M}(v, I)^{1/2} \mathcal{M}(v_*, I_*)^{1/2} \bar{B}(v, v_*, I, I_*),$$

and write K_1 as a kernel operator as follows, for suitable functions g and $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$,

$$K_1 g(v, I) = \int_{\mathbb{R}^3 \times \mathbb{R}_+} g(v_*, I_*) \kappa_1(v, I, v_*, I_*) \, dv_* \, d\mu(I_*).$$

The following proposition ensures that K_1 is a well-defined and compact operator on $L^2(\mathbb{R}^3 \times \mathbb{R}_+, dv \, d\mu(I))$.

Proposition 4.2. *The kernel κ_1 belongs to $L^2\left((\mathbb{R}^3 \times \mathbb{R}_+)^2, dv \, d\mu(I) \, dv_* \, d\mu(I_*)\right)$.*

Proof. Applying the change of variables $(v, v_*) \mapsto (v - v_*, v + v_*) = (V_*, \xi)$ and recalling the bound (4.19) on \bar{B} , we have

$$\begin{aligned} & \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \kappa_1(v, I, v_*, I_*)^2 \, dv \, d\mu(I) \, dv_* \, d\mu(I_*) \\ &= c^2 \iiint_{(\mathbb{R}^3 \times \mathbb{R}_+)^2} e^{-\frac{|v|^2 + |v_*|^2}{2T_k}} e^{-\frac{I + I_*}{T_i}} \bar{B}(v, v_*, I, I_*)^2 \, dv \, d\mu(I) \, dv_* \, d\mu(I_*) \\ &\leq C \left(\iint_{(\mathbb{R}^3)^2} e^{-\frac{|V_*|^2 + |\xi|^2}{4T_k}} (|V_*|^2 + |V_*|^{-1})^2 \, dV_* \, d\xi \right) \left(\iint_{(\mathbb{R}_+)^2} e^{-\frac{I + I_*}{T_i}} (I + I_*)^\gamma \, d\mu^{\otimes 2}(I, I_*) \right), \end{aligned}$$

where both previous integrals in the parentheses are finite. We first focus on the case $\gamma \in [0, 2 + 2\beta_2)$. Assumptions (4.2)–(4.3) and the fact that $\beta_1 \geq 0$ imply in particular that $\varphi(I) \leq C(1 + I)^{\beta_2}$, leading to

$$\iint_{(\mathbb{R}_+)^2} e^{-\frac{I+I_*}{T_i}} (I + I_*)^\gamma d\mu^{\otimes 2}(I, I_*) \leq C \iint_{(\mathbb{R}_+)^2} e^{-\frac{I+I_*}{T_i}} (I + I_*)^\gamma (1 + I)^{\beta_2} (1 + I_*)^{\beta_2} dI dI_*,$$

which is clearly finite. On the other hand in the case $\gamma \in (-2 - 2\beta_1, 0)$, we split the integral into two parts as follows:

$$\int_{I+I_* \leq 1} e^{-\frac{I+I_*}{T_i}} (I + I_*)^\gamma d\mu^{\otimes 2}(I, I_*) + \int_{I+I_* \geq 1} e^{-\frac{I+I_*}{T_i}} (I + I_*)^\gamma d\mu^{\otimes 2}(I, I_*).$$

Again using $\varphi(I) \leq C(1 + I)^{\beta_2}$, the right-hand side is smaller than

$$C \iint_{(\mathbb{R}_+)^2} e^{-\frac{I+I_*}{T_i}} (1 + I)^{\beta_2} (1 + I_*)^{\beta_2} dI dI_*,$$

which is finite. For the left-hand side integral, we use the fact that both I and I_* are smaller than 1, so that assumption (4.3) implies $d\mu^{\otimes 2}(I, I_*) \leq CI^{\beta_1} I_*^{\beta_1} dI dI_*$, leading to this integral being smaller than

$$C \iint_{I+I_* \leq 1} (I + I_*)^\gamma I^{\beta_1} I_*^{\beta_1} dI dI_*.$$

Changing variables $I_* \mapsto X = I + I_*$,

$$\begin{aligned} & \iint_{I+I_* \leq 1} (I + I_*)^\gamma I^{\beta_1} I_*^{\beta_1} dI dI_* = \int_0^1 \left(\int_0^{1-I} (I + I_*)^\gamma I^{\beta_1} I_*^{\beta_1} dI_* \right) dI \\ &= \int_0^1 \left(\int_I^1 X^\gamma I^{\beta_1} (X - I)^{\beta_1} dX \right) dI = \int_0^1 X^\gamma \left(\int_0^X I^{\beta_1} (X - I)^{\beta_1} dI \right) dX \\ &= \left(\int_0^1 (1 - x)^{\beta_1} x^{\beta_1} dx \right) \int_0^1 X^{\gamma+2\beta_1+1} dX. \end{aligned}$$

Since $\beta_1 \geq 0$ and $\gamma + 2\beta_1 + 1 > -1$, we obtain the announced result. \square

The compactness of K_1 is then a straightforward consequence of Proposition 4.2, as it proves that K_1 , being a kernel operator with kernel κ_1 , is a Hilbert-Schmidt operator.

4.4.2 Compactness of K_2

With the same strategy as in [46], we prove the compactness of K_2 , using the fact that K_2 is compact if it satisfies

- a uniform decay at infinity, proven in Proposition 4.10,
- an equicontinuity property, proven in Proposition 4.11.

The consideration of resonant collision rules (4.7)–(4.8) along with the assumption (4.15) on the cross section allows us to deal separately with a term in v and another in I . While the term in the internal energy requires a specific treatment, the one in v corresponds to the well-known monatomic case, whose compactness has already been proved (see [93]). In our analysis though, we use an alternative change of variable, whose properties have been detailed in Appendix 4.A.

4.4.2.1 Writing K_2 in kernel form

The first step consists in writing K_2 as a kernel operator. For the sake of clarity, to emphasize that it is an integration variable, we change the notation $J \equiv I'$. Recall that, for suitable functions g and $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$,

$$K_2 g(v, I) = \int_{\mathbb{R}^3 \times (\mathbb{R}_+)^2 \times \mathbb{S}^2} g(v', J) \mathcal{M}(v', J)^{-1/2} \mathcal{M}^{1/2} \mathcal{M}_* B(v, v_*, I, I_*, J, \sigma) dv_* d\mu(I_*) d\mu_2[I + I_*](J) d\sigma.$$

We clearly have

$$\mathcal{M}(v', J)^{-1/2} \mathcal{M}(v, I)^{1/2} \mathcal{M}(v_*, I_*) = M(v')^{-1/2} M(v)^{1/2} M(v_*) e^{\frac{J-I-2I_*}{2T_i}}.$$

Thus $K_2 g(v, I)$ reads

$$K_2 g(v, I) = \int_{\mathbb{R}^3 \times (\mathbb{R}_+)^2 \times \mathbb{S}^2} g(v', J) M(v')^{-1/2} M(v)^{1/2} M(v_*) e^{\frac{J-I-2I_*}{2T_i}} B(v, v_*, I, I_*, J, \sigma) dv_* d\mu(I_*) d\mu_2[I + I_*](J) d\sigma.$$

We then perform several changes of variable in order to write K_2 as a kernel operator. With that purpose in mind, we recall the definition of the *modified Bessel function of first kind of order 0*, which we denote \mathbb{I}_0 throughout this paper,

$$\mathbb{I}_0(X) = \frac{1}{2\pi} \int_0^{2\pi} e^{X \cos \theta} d\theta, \quad X \in \mathbb{R}. \quad (4.24)$$

We have the following proposition.

Proposition 4.3. *We define, for $v, p \in \mathbb{R}^3$ and $I, I_*, J \in \mathbb{R}_+$,*

$$\begin{aligned} \psi(v, p, I, I_*, J) &= 8\pi c \int_{\mathbb{R}_+} \exp\left(-\frac{r^2 + |v|^2 |\sin(\widehat{v}, \widehat{p})|^2}{2T_k}\right) \mathbb{I}_0\left(\frac{r|v| |\sin(\widehat{v}, \widehat{p})|}{T_k}\right) \\ &\quad \times B_0\left(\sqrt{r^2 + |p|^2}, \frac{|r^2 - |p|^2|}{r^2 + |p|^2}, I, I_*, J\right) \frac{r}{\sqrt{r^2 + |p|^2}} dr, \end{aligned}$$

as well as, for $v, \eta \in \mathbb{R}^3$ and $I, I_*, J \in \mathbb{R}_+$,

$$\begin{aligned} \kappa_2(v, I, \eta, J) &= \int_{\mathbb{R}_+} e^{\frac{J-I-2I_*}{2T_i}} e^{-\frac{|\eta-v|^2}{8T_k}} e^{-\frac{1}{8T_k} \frac{(|\eta|^2 - |v|^2)^2}{|\eta-v|^2}} |\eta-v|^{-1} \psi(v, \eta-v, I, I_*, J) \varphi(I + I_* - J) d\mu(I_*). \end{aligned} \quad (4.25)$$

Then we have, for almost every $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$,

$$K_2(g)(v, I) = \iint_{\mathbb{R}^3 \times \mathbb{R}_+} g(\eta, J) \kappa_2(v, I, \eta, J) d\eta d\mu(J).$$

Proof. The proof is completely similar to the one presented in Appendix 4.A, with I, I_* and J treated as

parameters. Indeed, noticing that for any $E_i \geq 0$,

$$d\mu_2[E_i](J) = \varphi(E_i - J) d\mu(J), \quad J \in [0, E_i],$$

we get

$$K_2 g(v, I) = \iint_{(\mathbb{R}^+)^2} e^{\frac{J-I-2I_*}{2T_i}} \left[\iint_{\mathbb{R}^3 \times \mathbb{S}^2} g(v', J) M(v')^{-1/2} M(v)^{1/2} M(v_*) \right. \\ \left. B_0 \left(|v - v_*|, \left| \cos \left(\widehat{v - v_*}, \sigma \right) \right|, I, I_*, J \right) dv_* d\sigma \right] \varphi(I + I_* - J) d\mu^{\otimes 2}(I_*, J).$$

In the integral in v_* and σ , the variables I, I_* and J are fixed parameters, hence it can be written as

$$\iint_{\mathbb{R}^3 \times \mathbb{S}^2} h(v') M(v')^{-1/2} M(v)^{1/2} M(v_*) B^m \left(|v - v_*|, \left| \cos \left(\widehat{v - v_*}, \sigma \right) \right| \right) dv_* d\sigma,$$

which corresponds to the monatomic operator K_2^m defined in (4.40), with

$$h = g(\cdot, J), \quad B^m = B_0(\cdot, \cdot, I, I_*, J).$$

Applying Proposition 4.13 yields the required result. \square

4.4.2.2 Separation of the study into a kinetic and an internal parts

The following lemma allows to upper-bound the kernel κ_2 by a tensorized product of two kernels, one dealing with the velocities, one with the internal energies.

Lemma 4.4. *Let us define for $v, p, \eta \in \mathbb{R}^3$*

$$\psi_k(v, p) = 8\pi c \int_{\mathbb{R}_+} \exp\left(-\frac{r^2 + |v|^2 \sin(\widehat{v, p})^2}{2T_k}\right) \mathbb{I}_0\left(\frac{r|v| |\sin(\widehat{v, p})|}{T_k}\right) \\ \times b_k\left(\sqrt{r^2 + |p|^2}, \frac{|r^2 - |p|^2|}{r^2 + |p|^2}\right) \frac{r}{\sqrt{r^2 + |p|^2}} dr, \quad (4.26)$$

$$\kappa_k(v, \eta) = e^{-\frac{|\eta-v|^2}{8T_k}} e^{-\frac{1}{8T_k} \frac{(|\eta|^2 - |v|^2)^2}{|\eta-v|^2}} |\eta - v|^{-1} \psi_k(v, \eta - v), \quad (4.27)$$

and, for $I, J \in \mathbb{R}_+$,

$$\kappa_i(I, J) = \int_{\mathbb{R}_+} \mathbf{1}_{J \leq I + I_*} e^{\frac{J-I-2I_*}{2T_i}} b_i(I, I_*) \varphi(I + I_* - J) d\mu(I_*). \quad (4.28)$$

Then

$$\kappa_2(v, I, \eta, J) \leq \kappa_k(v, \eta) \kappa_i(I, J). \quad (4.29)$$

Proof. From (4.15), we have

$$\psi(v, p, I, I_*, J) \leq 8\pi c \int_{\mathbb{R}_+} \exp\left(-\frac{r^2 + |v|^2 \sin(\widehat{v, p})^2}{2T_k}\right) \mathbb{I}_0\left(\frac{r|v| |\sin(\widehat{v, p})|}{T_k}\right) \\ b_k\left(\sqrt{r^2 + |p|^2}, \frac{|r^2 - |p|^2|}{r^2 + |p|^2}\right) \frac{r}{\sqrt{r^2 + |p|^2}} b_i(I, I_*) \mathbf{1}_{J \leq I + I_*} dr$$

$$\leq \psi_k(v, p) b_i(I, I_*) \mathbf{1}_{J \leq I + I_*}.$$

Then, applying Proposition 4.3, we recover (4.29). \square

As already stated, (4.29) allows to separate the velocity part from the internal energy one. While a specific focus on the velocity part, corresponding to the monatomic case, is performed in Appendix 4.A, we deal in the following with κ_i , the kernel dedicated to the internal energy part.

4.4.2.3 Study of the kernel related to the internal part

We provide in the following lemma a convenient upper-bound on κ_i .

Lemma 4.5. *For any $\gamma \in (-2 - 2\beta_1, 2 + 2\beta_2)$, we have, for any $I, J \geq 0$,*

$$\kappa_i(I, J) \leq C e^{-\frac{|J-I|}{4T_i}} (1 + \max(I, J))^{-\zeta - \beta_2}, \quad \max(I, J) \geq 1 \quad (4.30)$$

$$\kappa_i(I, J) \leq C \int_{\max(I, J)}^2 E_i^{\frac{\gamma}{2} - 1} dE_i, \quad \max(I, J) < 1, \quad (4.31)$$

where $\zeta = 1 + \beta_2 - \frac{\gamma}{2} > 0$.

Proof. Denoting $E_i = I + I_*$, we have, using (4.17),

$$\begin{aligned} \kappa_i(I, J) &= \int_{\mathbb{R}_+} \mathbf{1}_{J \leq I + I_*} e^{-\frac{J-I-2I_*}{2T_i}} b_i(I, I_*) \varphi(I + I_* - J) \varphi(I_*) dI_* \\ &\leq \int_{\mathbb{R}_+} \mathbf{1}_{J \leq E_i} e^{-\frac{J+I-2E_i}{2T_i}} \frac{E_i^{\gamma/2}}{\mu_2[E_i]([0, E_i])} \varphi(E_i - J) \varphi(I_*) dI_*. \end{aligned}$$

For convenience, we denote in the following, for any $E_i \geq 0$,

$$\overline{\mu_2}(E_i) := \mu_2[E_i]([0, E_i]).$$

We now make the change of variable $I_* \mapsto E_i = I + I_*$, leading to

$$\kappa_i(I, J) \leq \int_{\max(I, J)}^{\infty} e^{-\frac{J+I-2E_i}{2T_i}} \frac{E_i^{\gamma/2}}{\overline{\mu_2}(E_i)} \varphi(E_i - J) \varphi(E_i - I) dE_i. \quad (4.32)$$

We split the above integral into two terms R_1 and R_2 , as

$$\begin{aligned} R_1 &= \int_{\max(I, J) + 1}^{\infty} e^{-\frac{J+I-2E_i}{2T_i}} \frac{E_i^{\gamma/2}}{\overline{\mu_2}(E_i)} \varphi(E_i - J) \varphi(E_i - I) dE_i, \\ R_2 &= \int_{\max(I, J)}^{\max(I, J) + 1} e^{-\frac{J+I-2E_i}{2T_i}} \frac{E_i^{\gamma/2}}{\overline{\mu_2}(E_i)} \varphi(E_i - J) \varphi(E_i - I) dE_i. \end{aligned}$$

Study of R_1 . We first focus on R_1 . We deduce from (4.72) in Lemma 4.18 in the appendix that for any $E_i \geq \max(I, J) + 1 \geq 1$,

$$\frac{E_i^{\frac{\gamma}{2}}}{\overline{\mu_2}(E_i)} \leq C E_i^{\frac{\gamma}{2} - 2\beta_2 - 1},$$

leading to, letting $\zeta = 1 + \beta_2 - \frac{\gamma}{2} > 0$, for any $E_i \geq \max(I, J) + 1$,

$$\frac{E_i^{\gamma/2}}{\mu_2(E_i)} \leq C E_i^{-\zeta - \beta_2} \leq C (\max(I, J) + 1)^{-\zeta - \beta_2},$$

as $\zeta + \beta_2 \geq 0$. Also, it comes from the assumption (4.3) on φ that for any $E_i \geq \max(I, J) + 1$,

$$\varphi(E_i - I) \leq C (E_i - I)^{\beta_2}, \quad \varphi(E_i - J) \leq C (E_i - J)^{\beta_2},$$

which leads to, for all $E_i \geq \max(I, J) + 1$,

$$\begin{aligned} e^{\frac{J+I-2E_i}{2T_i}} \varphi(E_i - J) \varphi(E_i - I) &= \left(e^{-\frac{(E_i-I)}{2T_i}} \varphi(E_i - I) \right) \left(e^{-\frac{(E_i-J)}{2T_i}} \varphi(E_i - J) \right) \\ &\leq C \left(e^{-\frac{(E_i-I)}{2T_i}} (E_i - I)^{\beta_2} \right) \left(e^{-\frac{(E_i-J)}{2T_i}} (E_i - J)^{\beta_2} \right) \leq C' e^{-\frac{(E_i-I)}{4T_i}} e^{-\frac{(E_i-J)}{4T_i}} = C' e^{\frac{J+I-2E_i}{4T_i}}, \end{aligned}$$

where we used the fact that there exist a constant $C > 0$ such that $e^{-x} x^{\beta_2} \leq C e^{-\frac{x}{2}}$ for any $x \geq 0$. We conclude that

$$R_1 \leq C (\max(I, J) + 1)^{-\zeta - \beta_2} \int_{\max(I, J) + 1}^{\infty} e^{\frac{J+I-2E_i}{4T_i}} dE_i.$$

Changing variables $E_i \mapsto X = E_i - \max(I, J)$, we get

$$\int_{\max(I, J) + 1}^{\infty} e^{\frac{J+I-2E_i}{4T_i}} dE_i = e^{-\frac{|J-I|}{4T_i}} \int_1^{\infty} e^{-\frac{X}{2T_i}} dX \leq C e^{-\frac{|J-I|}{4T_i}}.$$

All in all, we have proven that

$$R_1 \leq C e^{-\frac{|J-I|}{4T_i}} (\max(I, J) + 1)^{-\zeta - \beta_2}.$$

Notice in particular that if $\max(I, J) < 1$, then

$$R_1 \leq C \leq C' \int_{\max(I, J)}^2 E_i^{\frac{\gamma}{2} - 1} dE_i.$$

Study of R_2 . We now focus on R_2 , for which we consider three cases. We first change variables $X = E_i - \max(I, J)$,

$$\begin{aligned} R_2 &= e^{-\frac{|J-I|}{2T_i}} \int_0^1 e^{-\frac{X}{T_i}} \frac{(X + \max(I, J))^{\gamma/2}}{\mu_2(X + \max(I, J))} \varphi(X + \max(I, J) - J) \varphi(X + \max(I, J) - I) dX \\ &\leq e^{-\frac{|J-I|}{2T_i}} \int_0^1 \frac{(X + \max(I, J))^{\gamma/2}}{\mu_2(X + \max(I, J))} \varphi(X) \varphi(X + |J - I|) dX, \end{aligned}$$

where the last inequality comes with the bound $e^{-\frac{X}{T_i}} \leq 1$ and the fact that

$$\varphi(X + \max(I, J) - J) \varphi(X + \max(I, J) - I) = \varphi(X) \varphi(X + |J - I|).$$

Case 1. If $\max(I, J) \geq 1$ and $|J - I| \geq 1$, then the property (4.72) in Lemma 4.18 on $\overline{\mu_2}$ and the assumptions (4.2)–(4.3) imply that for any $X \in (0, 1)$,

$$\begin{aligned} \frac{(X + \max(I, J))^{\gamma/2}}{\overline{\mu_2}(X + \max(I, J))} &\leq C (X + \max(I, J))^{\frac{\gamma}{2} - 2\beta_2 - 1}, \\ \varphi(X) &\leq CX^{\beta_1}, \quad \varphi(X + |J - I|) \leq C(X + |J - I|)^{\beta_2}. \end{aligned}$$

It thus comes that

$$\begin{aligned} &\int_0^1 \frac{(X + \max(I, J))^{\gamma/2}}{\overline{\mu_2}(X + \max(I, J))} \varphi(X) \varphi(X + |J - I|) dX \\ &\leq C \int_0^1 (X + \max(I, J))^{-\zeta - \beta_2} X^{\beta_1} (X + |J - I|)^{\beta_2} dX \\ &\leq C \max(I, J)^{-\zeta - \beta_2} (1 + |J - I|)^{\beta_2} \int_0^1 X^{\beta_1} dX = C \max(I, J)^{-\zeta - \beta_2} (1 + |J - I|)^{\beta_2}, \end{aligned}$$

because $\beta_1 \geq 0$. Again, there is a constant $C > 0$ such that

$$e^{-\frac{|J-I|}{2T_i}} (1 + |J - I|)^{\beta_2} \leq C e^{-\frac{|J-I|}{4T_i}}.$$

Moreover, as $\max(I, J) \geq 1$, we have $\max(I, J)^{-\zeta - \beta_2} \leq C(1 + \max(I, J))^{-\zeta - \beta_2}$, leading, in this case, to

$$R_2 \leq C e^{-\frac{|J-I|}{4T_i}} (\max(I, J) + 1)^{-\zeta - \beta_2}.$$

Case 2. If $\max(I, J) \geq 1$ and $|J - I| < 1$, then, still from (4.72) in Lemma 4.18 and (4.2),

$$\begin{aligned} &\int_0^1 \frac{(X + \max(I, J))^{\gamma/2}}{\overline{\mu_2}(X + \max(I, J))} \varphi(X) \varphi(X + |J - I|) dX \\ &\leq C \int_0^1 (X + \max(I, J))^{-\zeta - \beta_2} X^{\beta_1} (X + |J - I|)^{\beta_1} dX \\ &\leq C \max(I, J)^{-\zeta - \beta_2}, \end{aligned}$$

since $\beta_1 \geq 0$. Hence, also in this case,

$$R_2 \leq C e^{-\frac{|J-I|}{4T_i}} (\max(I, J) + 1)^{-\zeta - \beta_2}.$$

Case 3. Finally, if $\max(I, J) < 1$ then we also have $|J - I| < 1$, and, using (4.71) in Lemma 4.18 and (4.2), we get

$$\begin{aligned} &\int_0^1 \frac{(X + \max(I, J))^{\gamma/2}}{\overline{\mu_2}(X + \max(I, J))} \varphi(X) \varphi(X + |J - I|) dX \\ &\leq C \int_0^1 (X + \max(I, J))^{\frac{\gamma}{2} - 1} \frac{X^{\beta_1} (X + |J - I|)^{\beta_1}}{(X + \max(I, J))^{2\beta_1}} dX. \end{aligned}$$

Since $\beta_1 \geq 0$, it holds that $\frac{X^{\beta_1} (X+|J-I|)^{\beta_1}}{(X+\max(I,J))^{2\beta_1}} \leq 1$, and we obtain, after changing variables $E_i = X + \max(I, J)$,

$$R_2 \leq C' \int_{\max(I,J)}^2 E_i^{\frac{\gamma}{2}-1} dE_i.$$

Putting the previous bounds together yields the result. \square

From the previous lemma, we deduce the following corollary.

Corollary 4.6. • For any $\gamma \in (-2 - 2\beta_1, 2 + 2\beta_2)$, there exists $C > 0$ such that

$$\int_{\mathbb{R}_+} \kappa_i(I, J) d\mu(J) \leq C(1+I)^{-\zeta}, \quad \text{for a.e. } I \geq 0, \quad (4.33)$$

$$\int_{\mathbb{R}_+} \kappa_i(I, J) d\mu(I) \leq C(1+J)^{-\zeta}, \quad \text{for a.e. } J \geq 0, \quad (4.34)$$

where $\zeta = 1 + \beta_2 - \frac{\gamma}{2} > 0$.

Proof. Let $I \geq 0$. We split the integral into two parts,

$$\int_{\mathbb{R}_+} \kappa_i(I, J) d\mu(J) = \int_{\max(I,J) \geq 1} \kappa_i(I, J) d\mu(J) + \int_{\max(I,J) < 1} \kappa_i(I, J) d\mu(J).$$

For the first part, we use the fact that on the set $\{\max(I, J) \geq 1\}$, we have from (4.30) in Lemma 4.5, and as $\zeta > 0$ and $\beta_2 \geq 0$,

$$\begin{aligned} \kappa_i(I, J) &\leq C e^{-\frac{|J-I|}{4T_i}} (1 + \max(I, J))^{-\zeta - \beta_2} \\ &\leq C e^{-\frac{|J-I|}{4T_i}} (1 + I)^{-\zeta} (1 + J)^{-\beta_2}. \end{aligned}$$

Then, using the assumptions on φ , namely (4.2)-(4.3), we get

$$\begin{aligned} \int_{\max(I,J) \geq 1} \kappa_i(I, J) d\mu(J) &\leq C(1+I)^{-\zeta} \int_{\mathbb{R}_+} e^{-\frac{|J-I|}{4T_i}} (1+J)^{-\beta_2} \varphi(J) dJ \\ &\leq C(1+I)^{-\zeta} \left(\int_0^1 J^{\beta_1} dJ + \int_1^{+\infty} e^{-\frac{|J-I|}{4T_i}} (1+J)^{-\beta_2} J^{\beta_2} dJ \right) \\ &\leq C'(1+I)^{-\zeta}. \end{aligned}$$

On the other hand, using (4.31) in Lemma 4.5, we obtain, for all $I \geq 0$,

$$\begin{aligned} \int_{\max(I,J) < 1} \kappa_i(I, J) d\mu(J) &\leq C \mathbf{1}_{I < 1} \int_0^1 \int_{\max(I,J)}^2 E_i^{\gamma/2-1} dE_i J^{\beta_1} dJ \\ &\leq C \mathbf{1}_{I < 1} \int_0^1 \int_J^2 E_i^{\gamma/2-1} dE_i J^{\beta_1} dJ. \end{aligned}$$

We distinguish two cases. If $\gamma = 0$, the double integral in E_i and J becomes

$$\log(2) \int_0^1 J^{\beta_1} \, dJ - \int_0^1 \log(J) J^{\beta_1} \, dJ,$$

which is finite because $\beta_1 \geq 0$. Else, it equals

$$\frac{2}{\gamma} \int_0^1 (2^{\frac{\gamma}{2}} - J^{\frac{\gamma}{2}}) J^{\beta_1} \, dJ,$$

which is less than

$$C \left(\int_0^1 J^{\beta_1} \, dJ + \int_0^1 J^{\frac{\gamma}{2} + \beta_1} \, dJ \right),$$

which is itself finite as $\beta_1 \geq 0$ and $\frac{\gamma}{2} + \beta_1 > -1$. A symmetry argument in I and J ends the proof. \square

We are now in a position to deduce integrability properties of κ_i in L^2 .

Lemma 4.7. *The kernel κ_i belongs to $L^2_{loc}(\mathbb{R}_+, d\mu(I); L^2(\mathbb{R}_+, d\mu(J)))$.*

Proof. The proof is similar to the one of Corollary 4.6. For $I \geq 1$, we have, using (4.30) in Lemma 4.5 and (4.2)–(4.3) that

$$\begin{aligned} \int_{\mathbb{R}_+} \kappa_i(I, J)^2 \, d\mu(J) &\leq C \left(\int_0^1 e^{-\frac{|J-I|}{2T_i}} (1+J)^{-\beta_2} J^{\beta_1} \, dJ + \int_1^\infty e^{-\frac{|J-I|}{2T_i}} (1+J)^{-\beta_2} J^{\beta_2} \, dJ \right) \\ &\leq C \int_{\mathbb{R}} e^{-\frac{|J|}{2T_i}} \, dJ = C. \end{aligned}$$

Else, if $I < 1$, we split

$$\int_{\mathbb{R}_+} \kappa_i(I, J)^2 \, d\mu(J) = \int_0^1 \kappa_i(I, J)^2 \, d\mu(J) + \int_1^\infty \kappa_i(I, J)^2 \, d\mu(J) \leq \int_0^1 \kappa_i(I, J)^2 \, d\mu(J) + C,$$

where the fact that the integral from 1 to infinity is less than a constant is proven in the same manner as in the previous computation. Now using (4.31) in Lemma 4.5 and again (4.2)–(4.3) we get

$$\int_0^1 \kappa_i(I, J)^2 \, d\mu(J) \leq C \int_0^1 \left(\int_{\max(I, J)}^2 E_i^{\frac{\gamma}{2}-1} \, dE_i \right)^2 J^{\beta_1} \, dJ.$$

If $\gamma = 0$, then

$$\int_0^1 \kappa_i(I, J)^2 \, d\mu(J) \leq C \int_0^1 \left(\int_J^2 E_i^{-1} \, dE_i \right)^2 J^{\beta_1} \, dJ = C \int_0^1 (\log 2 - \log J)^2 J^{\beta_1} \, dJ,$$

which is finite as $\beta_1 \geq 0$. Else, we split

$$\int_0^1 \kappa_i(I, J)^2 \, d\mu(J) \leq \int_0^I \kappa_i(I, J)^2 \, d\mu(J) + \int_I^1 \kappa_i(I, J)^2 \, d\mu(J).$$

On the one hand,

$$\int_0^I \left(\int_I^2 E_i^{\frac{\gamma}{2}-1} dE_i \right)^2 J^{\beta_1} dJ \leq C(1+I^\gamma) \int_0^I J^{\beta_1} dJ \leq C(1+I^{\gamma+\beta_1+1}).$$

On the other hand,

$$\int_I^1 \left(\int_J^2 E_i^{\frac{\gamma}{2}-1} dE_i \right)^2 J^{\beta_1} dJ \leq C \int_I^1 (1+J^\gamma) J^{\beta_1} dJ \leq C(1+I^{\gamma+\beta_1+1}),$$

hence all in all,

$$\int_0^1 \kappa_i(I, J)^2 d\mu(J) \leq C(1+I^{\gamma+\beta_1+1}).$$

We conclude by observing that the function $I \mapsto 1+I^{\gamma+\beta_1+1}$ belongs to $L^1_{loc}(\mathbb{R}_+, d\mu(I))$, as $\beta_1 \geq 0$ and $\gamma+2\beta_1+1 > -1$. \square

4.4.2.4 Proof of uniform decay at infinity and equicontinuity property

We now combine the results on κ_i with the ones on κ_k , obtained from the monatomic case studied in Appendix 4.A.

Lemma 4.8. For $\gamma \in (-2-2\beta_1, 2+2\beta_2)$, we have

$$\iint_{\mathbb{R}^3 \times \mathbb{R}_+} \kappa_2(v, I, \eta, J) d\eta d\mu(J) \leq \frac{C}{(1+I+|v|)^{\min(1, \zeta)}}, \quad \text{for a.e. } (v, I) \in \mathbb{R}^3 \times \mathbb{R}_+, \quad (4.35)$$

$$\iint_{\mathbb{R}^3 \times \mathbb{R}_+} \kappa_2(v, I, \eta, J) dv d\mu(I) \leq C, \quad \text{for a.e. } (\eta, J) \in \mathbb{R}^3 \times \mathbb{R}_+, \quad (4.36)$$

where $\zeta = 1 + \beta_2 - \frac{\gamma}{2} > 0$.

Proof. From the bounds (4.66) and (4.33), we get

$$\begin{aligned} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \kappa_2(v, I, \eta, J) d\eta d\mu(J) &\leq \left(\int_{\mathbb{R}^3} \kappa_k(v, \eta) d\eta \right) \left(\int_{\mathbb{R}_+} \kappa_i(I, J) d\mu(J) \right) \\ &\leq \frac{C}{(1+|v|)(1+I)^\zeta} \leq \frac{C}{(1+|v|+I)^{\min(1, \zeta)}}, \end{aligned}$$

where $\zeta = 1 + \beta_2 - \frac{\gamma}{2} > 0$. A symmetry argument along with the fact that $1+|\eta|+J \geq 1$ allows to obtain (4.36). \square

The following lemma is then a straightforward consequence of Lemmas 4.4, 4.7 and 4.17.

Lemma 4.9. The kernel κ_2 belongs to $L^2_{loc}(\mathbb{R}^3 \times \mathbb{R}_+, dv d\mu(I); L^2(\mathbb{R}^3 \times \mathbb{R}_+, d\eta d\mu(J)))$.

All norms being equivalent in finite dimension, we can choose, on the space $\mathbb{R}^3 \times \mathbb{R}$, the norm $|(v, I)|_{\mathbb{R}^4} = |v| + |I|$, where $|v|$ is the Euclidean norm of v in \mathbb{R}^3 . In the following, \mathcal{B}_R is defined for any $R > 0$ by $\mathcal{B}_R = \{(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+ \text{ s.t. } |v| + I < R\}$. In the following Proposition 4.10, we prove the property of *uniform decay at infinity*.

Proposition 4.10. *There exists $C > 0$ such that, for all $g \in L^2(\mathbb{R}^3 \times \mathbb{R}_+, d\eta d\mu(J))$ and any $R > 0$,*

$$\|K_2 g\|_{L^2(\mathcal{B}_R^c, dv d\mu(I))}^2 \leq \frac{C}{(1+R)^{\min(1,\zeta)}} \|g\|_{L^2(\mathbb{R}^3 \times \mathbb{R}_+, d\eta d\mu(J))}^2. \quad (4.37)$$

Proof. Let $R > 0$. Using the Cauchy-Schwarz inequality and (4.35)–(4.36), we get

$$\begin{aligned} \|K_2 g\|_{L^2(\mathcal{B}_R^c, dv d\mu(I))}^2 &= \iint_{|v|+I \geq R} \left(\iint_{\mathbb{R}^3 \times \mathbb{R}_+} g(\eta, J) \kappa_2(v, I, \eta, J) d\eta d\mu(J) \right)^2 dv d\mu(I) \\ &\leq \iint_{|v|+I \geq R} \left(\int_{\mathbb{R}^3 \times \mathbb{R}_+} g(\eta, J)^2 \kappa_2(v, I, \eta, J) d\eta d\mu(J) \right) \left(\iint_{\mathbb{R}^3 \times \mathbb{R}_+} \kappa_2(v, I, \eta, J) d\eta d\mu(J) \right) dv d\mu(I) \\ &\leq \iint_{|v|+I \geq R} \left(\iint_{\mathbb{R}^3 \times \mathbb{R}_+} g(\eta, J)^2 \kappa_2(v, I, \eta, J) d\eta d\mu(J) \right) \frac{C}{(1+|v|+I)^{\min(1,\zeta)}} dv d\mu(I) \\ &\leq \frac{C}{(1+R)^{\min(1,\zeta)}} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} g(\eta, J)^2 \left(\iint_{\mathbb{R}^3 \times \mathbb{R}_+} \kappa_2(v, I, \eta, J) dv d\mu(I) \right) d\eta d\mu(J) \\ &\leq \frac{C}{(1+R)^{\min(1,\zeta)}} \|g\|_{L^2(\mathbb{R}^3 \times \mathbb{R}_+, d\eta d\mu(J))}^2, \end{aligned}$$

where C depends neither on R nor on g . □

From now on, we denote by $\tau_{(w,H)}$ the operator of translation by $(w, H) \in \mathbb{R}^3 \times \mathbb{R}_+$. In the following Proposition 4.11, we prove the property of *equicontinuity*.

Proposition 4.11. *For any $\varepsilon > 0$, there exists $s > 0$ such that, for any $g \in L^2(\mathbb{R}^3 \times \mathbb{R}_+, d\eta d\mu(J))$,*

$$\left\| \left((\tau_{(w,H)} - \text{Id}) K_2 \right) g \right\|_{L^2(\mathbb{R}^3 \times \mathbb{R}_+, dv d\mu(I))} \leq \varepsilon \|g\|_{L^2(\mathbb{R}^3 \times \mathbb{R}_+, d\eta d\mu(J))}, \quad \text{for a.e. } (w, H) \in \mathcal{B}_s.$$

Proof. Let $R > 0$. We have, for almost every $(w, H) \in \mathcal{B}_R$,

$$\begin{aligned} &\left\| \left((\tau_{(w,H)} - \text{Id}) K_2 \right) g \right\|_{L^2(\mathbb{R}^3 \times \mathbb{R}_+, dv d\mu(I))}^2 \\ &\leq \iint_{\mathcal{B}_{2R}} (K_2 g(v+w, I+H) - K_2 g(v, I))^2 dv d\mu(I) + \iint_{\mathcal{B}_R^c} K_2 g(v, I)^2 dv d\mu(I). \end{aligned} \quad (4.38)$$

Equation (4.37) ensures that the second integral is bounded by

$$\frac{C}{(1+R)^{\min(1,\zeta)}} \|g\|_{L^2(\mathbb{R}^3 \times \mathbb{R}_+, d\eta d\mu(J))}^2.$$

We choose R such that $\frac{C}{(1+R)^{\min(1,\zeta)}} \leq \frac{\varepsilon^2}{2}$.

Let us conclude, now that R is fixed. We notice that the first integral in (4.38) can be upper-bounded by

$$\|g\|_{L^2(\mathbb{R}^3 \times \mathbb{R}_+, d\eta d\mu(J))}^2 \iint_{\mathcal{B}_{2R}} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} (\kappa_2(v+w, I+H, \eta, J) - \kappa_2(v, I, \eta, J))^2 d\eta d\mu(J) dv d\mu(I).$$

Thanks to Lemma 4.9, we know that $\kappa_2 \in L^2_{loc}(\mathbb{R}^3 \times \mathbb{R}_+, dv d\mu(I); L^2(\mathbb{R}^3 \times \mathbb{R}_+, d\eta d\mu(J))$, consequently, there exists $s \in (0, R)$ such that, if $|w| + H \leq s$, then

$$\iint_{\mathcal{B}_{2R}} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} (\kappa_2(v+w, I+H, \eta, J) - \kappa_2(v, I, \eta, J))^2 d\eta d\mu(J) dv d\mu(I) \leq \frac{\varepsilon^2}{2},$$

which allows to conclude. \square

4.4.2.5 Conclusion to the compactness of K_2

As K_2 satisfies the properties of *uniform decay at infinity*, proven in Proposition 4.10, and *equicontinuity*, proven in Proposition 4.11, both relatively to the space $L^2(\mathbb{R}^3 \times \mathbb{R}_+, dv d\mu(I))$, we conclude to the compactness of K_2 as an operator on $L^2(\mathbb{R}^3 \times \mathbb{R}_+, dv d\mu(I))$.

4.4.3 Conclusion to the proof of Theorem 4.1

We now know that both K_1 and K_2 are compact on $L^2(\mathbb{R}^3 \times \mathbb{R}_+, dv d\mu(I))$, and then so does K_3 , as stated in the beginning of this Subsection. As a sum of three compact operators, K is also compact on this space, and this concludes the proof of Theorem 4.1.

4.A Grad's proof revisited

In this appendix, we aim to present a variant proof of Grad's, involving a geometric interpretation of the change of variables to obtain the kernel form, which allows to recover the compactness property.

Let us briefly recall the monatomic case. In this context, no internal energies are involved, and the collision rules are given by (4.9). We assume that the cross section B^m only depends on $|v - v_*|$ and $|\cos(\widehat{v_* - v}, \sigma)|$, in the same way as in (4.16), *i.e.* there exist $\delta_1 \in [0, 1)$, $\delta_2 \in [0, \frac{1}{2})$ and a constant C such that for almost every $\rho \geq 0$ and $\theta \in [0, 2\pi]$,

$$B^m(\rho, |\cos\theta|) \leq C \left(|\sin\theta| (\rho^2 + \rho^{-1}) + \rho + \rho^{-\delta_1} + |\sin\theta|^{-\delta_2} \right). \quad (4.39)$$

The difficult part of the compactness proof in the monatomic case mainly lies in the study of the operator K_2^m defined, for all measurable function h for which it makes sense and for almost every $v \in \mathbb{R}^3$, by

$$K_2^m h(v) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} h\left(\frac{v+v_*}{2} + \frac{|v-v_*|}{2}\sigma\right) M\left(\frac{v+v_*}{2} + \frac{|v-v_*|}{2}\sigma\right)^{-1/2} M(v)^{1/2} M(v_*) \quad (4.40)$$

$$B^m\left(|v-v_*|, \left|\cos\left(\widehat{v_*-v}, \sigma\right)\right|\right) d\sigma dv_*,$$

where we recall that $M(v) = c e^{-\frac{|v|^2}{2T_k}}$ for some constant $c > 0$.

It is worth noting that, thanks to an interpolation argument, the cross section $|\sin\theta|^\alpha \rho^{1+\alpha}$, $\alpha \in [0, 1]$, is also covered by Assumption (4.39). Indeed,

$$|\sin\theta|^\alpha \rho^{1+\alpha} = (|\sin\theta|\rho^2)^\alpha \rho^{1-\alpha} \leq \alpha |\sin\theta|\rho^2 + (1-\alpha)\rho \leq |\sin\theta|\rho^2 + \rho.$$

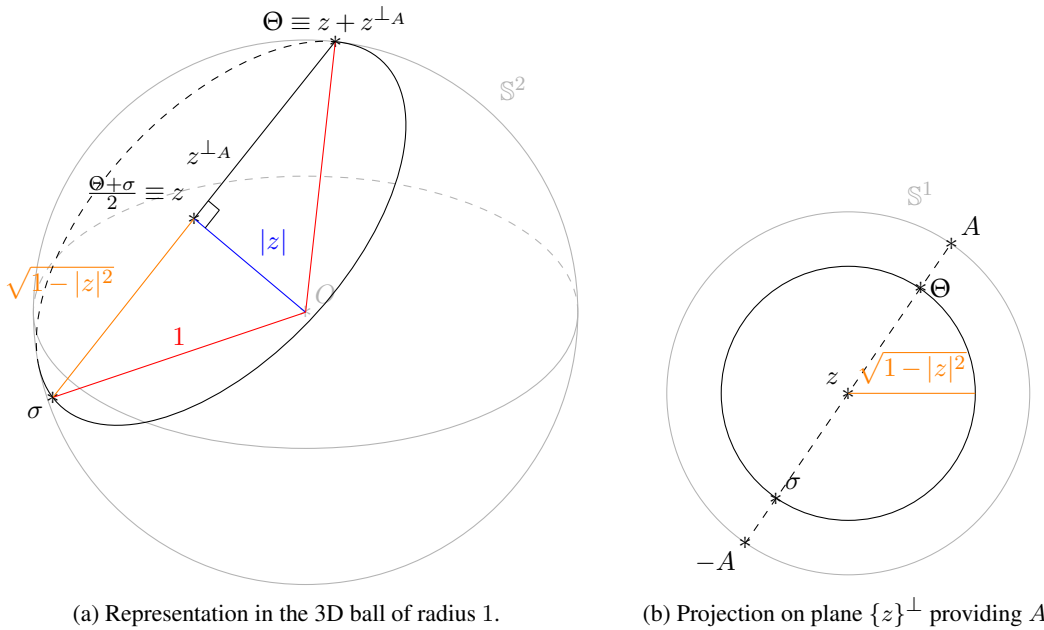
Similarly, for any $\alpha \in (0, 1)$, $\gamma_1 \in (-\alpha, \alpha]$ and $\gamma_2 \in [0, \frac{1-\alpha}{2})$, the cross section $|\sin\theta|^{-\gamma_2} \rho^{\gamma_1}$ is also covered.

4.A.1 Alternative change of variables

Let us first discuss the crucial change of variables which is used later on to obtain the kernel form of the operator K_2^m . The idea is to change a couple of angles in the two-dimensional sphere (Θ, σ) into a couple composed of an element of the three-dimensional open ball and an angle in the one-dimensional circle (z, A) .

On the one hand, if we take $\Theta \in \mathbb{S}^2$ and $\sigma \in \mathbb{S}^2 \setminus \{\Theta, -\Theta\}$, setting $z = \frac{\Theta + \sigma}{2}$, we remark that $0 < |z| < 1$, and that z is orthogonal to $\Theta - z$, see Fig. 4.1a.

On the other hand, for any $z \in \mathbb{R}^3$ such that $0 < |z| < 1$, the set of all $(\Theta, \sigma) \in (\mathbb{S}^2)^2$ such that $z = \frac{\Theta + \sigma}{2}$ is a (double) circle (represented on Fig. 4.1a) of center z , radius $\sqrt{1 - |z|^2}$, and inside in the plane $\{z\}^\perp$, which can be parametrized by $A \in \mathbb{S}^1$, see Fig. 4.1b. We denote by $z^\perp A$ the projection on $\{z\}^\perp$ of the vector of this circle corresponding to the parameter $A \in \mathbb{S}^1$. Then $(z + z^\perp A, z - z^\perp A)$ defines a unique couple $(\Theta, \sigma) \in (\mathbb{S}^2)^2 \setminus (\{(\Theta, \Theta) \mid \Theta \in \mathbb{S}^2\} \cup \{(\Theta, -\Theta) \mid \Theta \in \mathbb{S}^2\})$.



(a) Representation in the 3D ball of radius 1.

(b) Projection on plane $\{z\}^\perp$ providing A .

Figure 4.1 – Geometric configuration between σ , Θ and z .

It is worth noting that, for all $z \in \mathbb{R}^3$ such that $0 < |z| < 1$, the parametrization of the associated circle represented on Fig. 4.1b by $A \in \mathbb{S}^1$ is defined up to the choice of an additive constant. Without being explicit about this choice, we simply state that there is a consistent choice of angle such that the transformation $(\Theta, \sigma) \mapsto (z, A)$ is a C^1 -diffeomorphism from $(\mathbb{S}^2)^2 \setminus (\{(\Theta, \Theta) \mid \Theta \in \mathbb{S}^2\} \cup \{(\Theta, -\Theta) \mid \Theta \in \mathbb{S}^2\})$ to $\{z \in \mathbb{R}^3 \mid 0 < |z| < 1\} \times \mathbb{S}^1$, that is almost everywhere from $(\mathbb{S}^2)^2$ to $\mathcal{B}(0, 1) \times \mathbb{S}^1$, where $\mathcal{B}(0, 1)$ stands for the open ball of \mathbb{R}^3 of center 0 and radius 1.

Proposition 4.12. *The Jacobian of the (z, A) change of variables equals $4|z|^{-1}$.*

Proof. The (z, A) change of variables is geometrically natural, but tricky to write explicitly. Hence, we compute its Jacobian \mathcal{J} by studying the image measure associated with it and not by direct computation. Since a rotation induces no deformation, we can state that \mathcal{J} depends neither on A nor on $\frac{z}{|z|}$. Thus $\mathcal{J}(z, A)$ can be written as $\tilde{\mathcal{J}}(|z|)$.

Define, for all $r \in (0, 1)$,

$$S(r) = \iint_{(\mathbb{S}^2)^2} \mathbf{1}_{\left|\frac{\Theta+\sigma}{2}\right| \leq r} d\Theta d\sigma.$$

Applying the (z, A) change of variables, we have, on the one hand,

$$S(r) = \int_{B(0,1)} \int_{\mathbb{S}^1} \mathbf{1}_{|z| \leq r} \mathcal{J}(z, A) dA dz = \int_{B(0,1)} \int_{\mathbb{S}^1} \mathbf{1}_{|z| \leq r} \tilde{\mathcal{J}}(|z|) dA dz = 2\pi \times 4\pi \int_0^r \tilde{\mathcal{J}}(\rho) \rho^2 d\rho,$$

where we passed in spherical coordinates to obtain the last equality. On the other hand, we can explicitly compute $S(r)$. Indeed, we can write

$$\begin{aligned} S(r) &= \iint_{(\mathbb{S}^2)^2} \mathbf{1}_{\left|\frac{\Theta+\sigma}{2}\right| \leq r} d\Theta d\sigma = \left| \left\{ (\Theta, \sigma) \in (\mathbb{S}^2)^2 \text{ s.t. } \left| \frac{\Theta + \sigma}{2} \right| \leq r \right\} \right| \\ &= \left| \left\{ (\Theta, \sigma) \in (\mathbb{S}^2)^2 \text{ s.t. } |\Theta|^2 + |\sigma|^2 + 2\Theta \cdot \sigma \leq 4r^2 \right\} \right| = \left| \left\{ (\Theta, \sigma) \in (\mathbb{S}^2)^2 \text{ s.t. } \Theta \cdot \sigma \leq 2r^2 - 1 \right\} \right| \\ &= 4\pi \left| \left\{ \sigma \in \mathbb{S}^2 \text{ s.t. } \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \cdot \sigma \leq 2r^2 - 1 \right\} \right| = 4\pi (4\pi - 4\pi(1 - r^2)) \\ &= 16\pi^2 r^2, \end{aligned}$$

where the penultimate equality comes from the fact that the area of the spherical cap

$$\left\{ \sigma \in \mathbb{S}^2 \text{ s.t. } \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \cdot \sigma > 2r^2 - 1 \right\},$$

corresponding to the cap above the black circle on Fig. 4.2, equals $2\pi \times (2 - 2r^2)$.

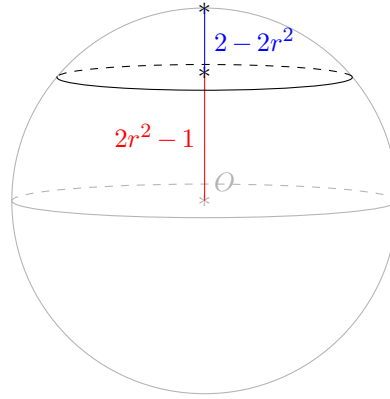


Figure 4.2 – Representation of the considered spherical cap.

We conclude that, for all $r \in (0, 1)$,

$$\int_0^r \tilde{\mathcal{J}}(\rho) \rho^2 d\rho = 2r^2.$$

Differentiating both sides with respect to r provides the required value. \square

4.A.2 Study of the kernel form of K_2^m

Recalling that, for almost every $v \in \mathbb{R}^3$,

$$K_2^m h(v) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} h\left(\frac{v+v_*}{2} + \frac{|v-v_*|}{2}\sigma\right) M\left(\frac{v+v_*}{2} + \frac{|v-v_*|}{2}\sigma\right)^{-1/2} M(v)^{1/2} M(v_*) \\ B^m\left(|v-v_*|, |\cos(\widehat{v_*-v}, \sigma)|\right) d\sigma dv_*,$$

we focus on the integration with respect to v_* , and perform the change of variable $V_* = v_* - v$ to obtain

$$K_2^m h(v) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} h\left(v + \frac{V_*}{2} + \frac{|V_*|}{2}\sigma\right) M\left(v + \frac{V_*}{2} + \frac{|V_*|}{2}\sigma\right)^{-1/2} M(v)^{1/2} M(V_* + v) \\ B^m(|V_*|, |\cos(\widehat{V_*}, \sigma)|) d\sigma dV_*.$$

With the spherical coordinates, $V_* = \rho\Theta$, $(\rho, \Theta) \in \mathbb{R}_+^* \times \mathbb{S}^2$, with Jacobian ρ^2 , it becomes

$$K_2^m h(v) = \int_{\mathbb{R}_+^*} \iint_{(\mathbb{S}^2)^2} h\left(v + \rho\left(\frac{\Theta + \sigma}{2}\right)\right) M\left(v + \rho\left(\frac{\Theta + \sigma}{2}\right)\right)^{-1/2} M(v)^{1/2} M(\rho\Theta + v) \\ B^m(\rho, |\cos(\widehat{\Theta}, \sigma)|) d\sigma d\Theta \rho^2 d\rho.$$

We now perform the (z, A) change of variables detailed in Subsection 4.A.1 with Jacobian $4|z|^{-1}$. Noticing that $z = \frac{\Theta + \sigma}{2}$, $\cos(\widehat{\Theta}, \sigma) = 2|z|^2 - 1$ and $\Theta = z + z^{\perp A}$, we thus obtain

$$K_2^m h(v) = \int_{\mathbb{R}_+^*} \int_{B(0,1)} \int_{\mathbb{S}^1} h(v + \rho z) M(v + \rho z)^{-1/2} M(v)^{1/2} M(\rho(z + z^{\perp A}) + v) \\ B^m(\rho, |2|z|^2 - 1|) dA 4|z|^{-1} dz \rho^2 d\rho. \quad (4.41)$$

Note that, in his proof [92, 93], Grad wrote

$$v' = v + p \quad \text{and} \quad v_* = v + p + q.$$

By identification to our case, we have in fact

$$p = \rho z \quad \text{and} \quad q = \rho z^{\perp A}.$$

Proposition 4.13. *Setting, for almost every $v, p, \eta \in \mathbb{R}^3$,*

$$\begin{aligned} \psi^m(v, p) &= 8\pi c \int_{\mathbb{R}_+} \exp\left(-\frac{r^2 + |v|^2 |\sin(\widehat{v, p})|^2}{2T_k}\right) \mathbb{I}_0\left(\frac{r|v| |\sin(\widehat{v, p})|}{T_k}\right) \\ &\quad \times B^m\left(\sqrt{r^2 + |p|^2}, \frac{|r^2 - |p|^2|}{r^2 + |p|^2}\right) \frac{r}{\sqrt{r^2 + |p|^2}} dr, \end{aligned} \quad (4.42)$$

$$\kappa^m(v, \eta) = e^{-\frac{|\eta-v|^2}{8T_k}} e^{-\frac{1}{8T_k} \frac{(|\eta|^2 - |v|^2)^2}{|\eta-v|^2}} |\eta-v|^{-1} \psi^m(v, \eta-v), \quad (4.43)$$

where \mathbb{I}_0 stands for the modified Bessel function of the first kind of order 0, defined in (4.24), then $K_2^m h$ can be written as

$$K_2^m h(v) = \int_{\mathbb{R}^3} h(\eta) \kappa^m(v, \eta) d\eta, \quad \text{for a.e. } v \in \mathbb{R}^3. \quad (4.44)$$

Proof. From (4.41), we immediately get

$$\begin{aligned} K_2^m h(v) &= 4c \int_{\mathbb{R}_+^*} \int_{B(0,1)} \int_{\mathbb{S}^1} h(v + \rho z) \exp\left(\frac{|v + \rho z|^2}{4T_k} - \frac{|v|^2}{4T_k} - \frac{|v + \rho z + \rho z^{\perp A}|^2}{2T_k}\right) \\ &\quad B^m(\rho, |2|z|^2 - 1|) |z|^{-1} \rho^2 dA dz d\rho. \end{aligned} \quad (4.45)$$

In the following, let us denote by w the orthogonal projection of v on $\{z\}^\perp$, i.e.

$$w = v - \left(v \cdot \frac{z}{|z|}\right) \frac{z}{|z|}.$$

Then, following the idea of [46], we can successively write

$$\begin{aligned} -\frac{1}{4}|v|^2 + \frac{1}{4}|v + \rho z|^2 - \frac{1}{2}|v + \rho z + \rho z^{\perp A}|^2 &= -\frac{1}{8}|\rho z|^2 - \frac{1}{2} \left| \rho z^{\perp A} + v + \frac{1}{2}\rho z \right|^2 \\ &= -\frac{1}{8}\rho^2 |z|^2 - \frac{1}{2} |\rho z^{\perp A} + w|^2 - \frac{1}{2} \left| \left(v \cdot \frac{z}{|z|}\right) \frac{z}{|z|} + \frac{1}{2}\rho z \right|^2 \\ &= -\frac{1}{8}\rho^2 |z|^2 - \frac{1}{2} |\rho z^{\perp A} + w|^2 - \frac{1}{2} \left(\left(v + \frac{1}{2}\rho z\right) \cdot \frac{z}{|z|} \right)^2, \end{aligned}$$

since both w and $z^{\perp A}$ are orthogonal to z . Thus (4.45) becomes

$$\begin{aligned} K_2^m h(v) &= 4c \int_{\mathbb{R}_+^*} \int_{B(0,1)} h(v + \rho z) e^{-\frac{\rho^2 |z|^2}{8T_k}} e^{-\frac{\left(\left(v + \frac{1}{2}\rho z\right) \cdot \frac{z}{|z|}\right)^2}{2T_k}} |z|^{-1} \int_{\mathbb{S}^1} e^{-\frac{|\rho z^{\perp A} + w|^2}{2T_k}} dA \\ &\quad B^m(\rho, |2|z|^2 - 1|) dz \rho^2 d\rho. \end{aligned} \quad (4.46)$$

We now focus on the integral in the variable A . We have

$$\begin{aligned} |\rho z^{\perp A} + w|^2 &= \rho^2 |z^{\perp A}|^2 + |w|^2 + 2\rho |z^{\perp A}| |w| \cos(\widehat{z^{\perp A}, w}) \\ &= \rho^2 (1 - |z|^2) + |w|^2 + 2\rho \sqrt{1 - |z|^2} |w| \cos(\widehat{z^{\perp A}, w}). \end{aligned}$$

Moreover, since w is the projection of v on the plane $\{z\}^\perp$, $|w| = |v| |\sin(\widehat{v, z})|$. Thus

$$|\rho z^{\perp A} + w|^2 = \rho^2(1 - |z|^2) + |v|^2 \sin(\widehat{v, z})^2 + 2\rho \sqrt{1 - |z|^2} |v| |\sin(\widehat{v, z})| \cos(\widehat{z^{\perp A}, w}).$$

For the sake of simplicity, let us momentarily denote

$$X = \frac{\rho \sqrt{1 - |z|^2} |v| |\sin(\widehat{v, z})|}{T_k},$$

which does not depend on A . Consequently, we can write

$$\int_{\mathbb{S}^1} \exp\left(-\frac{|\rho z^{\perp A} + w|^2}{2T_k}\right) dA = \exp\left(-\frac{\rho^2 - |\rho z|^2 + |v|^2 |\sin(\widehat{v, z})|^2}{2T_k}\right) \int_{\mathbb{S}^1} \exp\left(-X \cos(\widehat{z^{\perp A}, w})\right) dA. \quad (4.47)$$

Since the integration is performed on the whole unit circle \mathbb{S}^1 , and because w and $z^{\perp A}$ belong to the same plane $\{z\}^\perp$ (see Fig. 4.1a),

$$\int_{\mathbb{S}^1} \exp\left(-X \cos(\widehat{z^{\perp A}, w})\right) dA = \int_0^{2\pi} e^{X \cos \theta} d\theta = 2\pi \mathbb{I}_0(X). \quad (4.48)$$

Consequently, thanks to (4.47)–(4.48), (4.46) becomes

$$K_2^m h(v) = 8\pi c \int_{\mathbb{R}_+^*} \int_{\mathcal{B}(0,1)} h(v + \rho z) e^{-\frac{\rho^2 |z|^2}{8T_k}} e^{-\frac{((v + \frac{1}{2}\rho z) \cdot \frac{z}{|z|})^2}{2T_k}} \exp\left(-\frac{\rho^2 - |\rho z|^2 + |v|^2 \sin(\widehat{v, z})^2}{2T_k}\right) \mathbb{I}_0\left(\frac{\sqrt{\rho^2 - |\rho z|^2} |v| |\sin(\widehat{v, z})|}{T_k}\right) B^m(\rho, |2|z|^2 - 1) |z|^{-1} \rho^2 dz d\rho.$$

We now make the change of variable $p = \rho z$, $dp = \rho^3 dz$, and use Fubini's theorem to get

$$K_2^m h(v) = 8\pi c \int_{\mathbb{R}^3} h(v + p) e^{-\frac{|p|^2}{8T_k}} e^{-\frac{((v + \frac{1}{2}p) \cdot \frac{p}{|p|})^2}{2T_k}} |p|^{-1} \times \left[\int_{|p|}^{\infty} \exp\left(-\frac{\rho^2 - |p|^2 + |v|^2 \sin(\widehat{v, p})^2}{2T_k}\right) \mathbb{I}_0\left(\frac{\sqrt{\rho^2 - |p|^2} |v| |\sin(\widehat{v, p})|}{T_k}\right) B^m\left(\rho, \left|2\left|\frac{p}{\rho}\right|^2 - 1\right|\right) d\rho \right] dp. \quad (4.49)$$

When performing the change of variable $r = \sqrt{\rho^2 - |p|^2}$ of Jacobian $\frac{r}{\sqrt{r^2 + |p|^2}}$, the integral with respect to ρ in (4.49) becomes

$$\int_{\mathbb{R}_+} \exp\left(-\frac{r^2 + |v|^2 \sin(\widehat{v, p})^2}{2T_k}\right) \mathbb{I}_0\left(\frac{r |v| |\sin(\widehat{v, p})|}{T_k}\right) B^m\left(\sqrt{r^2 + |p|^2}, \frac{|r^2 - |p|^2|}{r^2 + |p|^2}\right) \frac{r}{\sqrt{r^2 + |p|^2}} dr.$$

Hence, using (4.42), (4.49) can be written as

$$K_2^m h(v) = \int_{\mathbb{R}^3} h(v + p) e^{-\frac{|p|^2}{8T_k}} e^{-\frac{((v + \frac{1}{2}p) \cdot \frac{p}{|p|})^2}{2T_k}} |p|^{-1} \psi^m(v, p) dp.$$

Finally, noticing that, for all $v, \eta \in \mathbb{R}^3$,

$$\left(v + \frac{1}{2}(\eta - v)\right) \cdot (\eta - v) = \frac{1}{2}(\eta + v) \cdot (\eta - v) = \frac{1}{2}(|\eta|^2 - |v|^2),$$

the change of variable $\eta = v + p$ allows to obtain (4.44). \square

Now that we have obtained a kernel form of the operator K_2^m , we study its kernel κ^m , for which we intend to find upper bounds. We start by focusing on the function ψ^m .

Lemma 4.14. *Let us denote, for all $\lambda \geq 0$ and $\alpha \in (-1, 1]$,*

$$\varphi_\alpha(\lambda) = \int_{\mathbb{R}_+} \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) \frac{r^\alpha}{1 + \sqrt{r\lambda}} dr, \quad (4.50)$$

Then there exists $C > 0$ such that, for almost every $v, p \in \mathbb{R}^3$, we have, setting $\lambda = |v| |\sin(\widehat{v, p})|$,

$$\psi^m(v, p) \leq C \left((1 + |p|) \varphi_1(\lambda) + 1 + \varphi_{-\delta_1}(\lambda) + |p|^{-\delta_2} \varphi_{\delta_2}(\lambda) \right). \quad (4.51)$$

Proof. Using the notation $\lambda = |v| |\sin(\widehat{v, p})|$, (4.42) becomes

$$\psi^m(v, p) = 8\pi c \int_{\mathbb{R}_+} \exp\left(-\frac{r^2 + \lambda^2}{2T_k}\right) \mathbb{I}_0\left(\frac{r\lambda}{T_k}\right) B^m\left(\sqrt{r^2 + |p|^2}, \frac{|r^2 - |p|^2|}{r^2 + |p|^2}\right) \frac{r}{\sqrt{r^2 + |p|^2}} dr. \quad (4.52)$$

We know from [1, Section 9.7.1, p. 377], that

$$\mathbb{I}_0(X) \underset{X \rightarrow +\infty}{\sim} \frac{e^X}{\sqrt{2\pi X}}. \quad (4.53)$$

It is moreover obvious that, for any $X \geq 0$,

$$\mathbb{I}_0(X) = \frac{1}{2\pi} \int_0^{2\pi} e^{X \cos \theta} d\theta \leq e^X. \quad (4.54)$$

Combining estimates (4.53)–(4.54), we conclude that there exists $C > 0$ such that, for any $X \geq 0$,

$$\mathbb{I}_0(X) \leq C \frac{e^X}{1 + \sqrt{X}}. \quad (4.55)$$

We then inject estimate (4.55) into (4.52) to obtain

$$\begin{aligned} \psi^m(v, p) &\leq C \int_{\mathbb{R}_+} \exp\left(-\frac{r^2 + \lambda^2 - 2r\lambda}{2T_k}\right) \frac{1}{1 + \sqrt{r\lambda}} B^m\left(\sqrt{r^2 + |p|^2}, \frac{|r^2 - |p|^2|}{r^2 + |p|^2}\right) \frac{r}{\sqrt{r^2 + |p|^2}} dr \\ &\leq C \int_{\mathbb{R}_+} \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) \frac{1}{1 + \sqrt{r\lambda}} B^m\left(\sqrt{r^2 + |p|^2}, \frac{|r^2 - |p|^2|}{r^2 + |p|^2}\right) \frac{r}{\sqrt{r^2 + |p|^2}} dr. \end{aligned}$$

Now, note that, if $|\cos \theta| = \frac{|r^2 - |p|^2|}{r^2 + |p|^2}$, then

$$|\sin \theta| = \sqrt{1 - \left(\frac{|r^2 - |p|^2|}{r^2 + |p|^2} \right)^2} = \sqrt{\frac{4r^2|p|^2}{(r^2 + |p|^2)^2}} = \frac{2r|p|}{r^2 + |p|^2}.$$

Thus it comes from the assumption (4.39) on the cross section that

$$B^m \left(\sqrt{r^2 + |p|^2}, \frac{|r^2 - |p|^2|}{r^2 + |p|^2} \right) \frac{r}{\sqrt{r^2 + |p|^2}} \leq C \left(r|p| + \frac{r|p|}{(r^2 + |p|^2)^{3/2}} + r + r^{-\delta_1} + r^{\delta_2} |p|^{-\delta_2} \right), \quad (4.56)$$

because $0 \leq \delta_1 < 1$, $0 \leq \delta_2 < \frac{1}{2}$, and using the fact that $r \leq \sqrt{r^2 + |p|^2}$. Injecting (4.56) in (4.52) ensures that

$$\begin{aligned} \psi^m(v, p) &\leq C(1+|p|) \int_{\mathbb{R}_+} \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) \frac{r}{1+\sqrt{r\lambda}} \mathrm{d}r + C \int_{\mathbb{R}_+} \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) \frac{r|p|}{(r^2 + |p|^2)^{3/2}} \mathrm{d}r \\ &\quad + C \int_{\mathbb{R}_+} \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) \frac{r^{-\delta_1}}{1+\sqrt{r\lambda}} \mathrm{d}r + \frac{C}{|p|^{\delta_2}} \int_{\mathbb{R}_+} \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) \frac{r^{\delta_2}}{1+\sqrt{r\lambda}} \mathrm{d}r. \end{aligned} \quad (4.57)$$

Finally, we notice that, for any $\lambda \geq 0$ and $p \in \mathbb{R}^3 \setminus \{0\}$,

$$\int_{\mathbb{R}_+} \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) \frac{r|p|}{(r^2 + |p|^2)^{3/2}} \mathrm{d}r \leq |p| \int_{\mathbb{R}_+} \frac{r}{(r^2 + |p|^2)^{3/2}} \mathrm{d}r = |p| \left[-(r^2 + |p|^2)^{-1/2} \right]_0^\infty = 1.$$

Plugging that previous estimate in (4.57) implies (4.51). \square

Lemma 4.15. *There exists $C > 0$ such that, for almost every $v, p \in \mathbb{R}^3$*

$$\psi^m(v, p) \leq C \left(|p| + |p|^{-\delta_2} \right). \quad (4.58)$$

Proof. We first focus on the functions φ_α defined by (4.50) and prove that for any $\alpha \in (-1, 1]$, there exists $C_\alpha > 0$ such that, for any $\lambda \geq 0$,

$$\varphi_\alpha(\lambda) \leq C_\alpha. \quad (4.59)$$

Let us first consider the case when $\alpha \in (-1, 0]$. Then, for any $\lambda \geq 0$,

$$\begin{aligned} \varphi_\alpha(\lambda) &\leq \int_{\mathbb{R}_+} r^\alpha \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) \mathrm{d}r \leq \int_0^1 r^\alpha \mathrm{d}r + \int_1^{+\infty} \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) \mathrm{d}r \\ &\leq \frac{1}{1+\alpha} + \int_{\mathbb{R}} \exp\left(-\frac{r^2}{2T_k}\right) \mathrm{d}r, \end{aligned} \quad (4.60)$$

which does not depend on λ . We now focus on the case $0 < \alpha \leq 1$. First, note that

$$\begin{aligned} \int_{\mathbb{R}_+} r^\alpha \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) \mathrm{d}r &\leq \int_{-\lambda}^\infty (r+\lambda)^\alpha \exp\left(-\frac{r^2}{2T_k}\right) \mathrm{d}r \\ &\leq \int_{\mathbb{R}} |r|^\alpha \exp\left(-\frac{r^2}{2T_k}\right) \mathrm{d}r + \lambda^\alpha \int_{\mathbb{R}} \exp\left(-\frac{r^2}{2T_k}\right) \mathrm{d}r \leq C_\alpha (1 + \lambda^\alpha). \end{aligned} \quad (4.61)$$

Consequently, we deduce, for any $\lambda \geq 0$, that

$$\varphi_\alpha(\lambda) \leq \int_{\mathbb{R}_+} r^\alpha \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) dr \leq C_\alpha(1 + \lambda^\alpha). \quad (4.62)$$

Besides, we have, for any $\lambda > 0$,

$$\varphi_\alpha(\lambda) \leq \frac{1}{\sqrt{\lambda}} \int_{\mathbb{R}_+} r^{\alpha-\frac{1}{2}} \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) dr. \quad (4.63)$$

When $\alpha \in (0, \frac{1}{2}]$, applying (4.60) for $\alpha - \frac{1}{2} \in (-\frac{1}{2}, 0]$ in (4.63) implies that, for any $\lambda > 0$,

$$\varphi_\alpha(\lambda) \leq \frac{C_\alpha}{\sqrt{\lambda}}. \quad (4.64)$$

Combining (4.62) and (4.64) thus yields, when $0 < \alpha \leq \frac{1}{2}$, that, for any $\lambda \geq 0$,

$$\varphi_\alpha(\lambda) \leq C_\alpha.$$

When $\frac{1}{2} < \alpha \leq 1$, applying (4.61) in (4.63) implies that, for any $\lambda \geq 0$,

$$\int_{\mathbb{R}_+} r^{\alpha-\frac{1}{2}} \exp\left(-\frac{(r-\lambda)^2}{2T_k}\right) dr \leq C_\alpha \left(1 + \lambda^{\alpha-\frac{1}{2}}\right),$$

so that

$$\varphi_\alpha(\lambda) \leq C_\alpha \left(\frac{1}{\sqrt{\lambda}} + \lambda^{\alpha-1}\right). \quad (4.65)$$

Combining (4.62) and (4.65) allows to obtain (4.59) when $\frac{1}{2} < \alpha \leq 1$.

Eventually, using jointly Lemma 4.14, and (4.59) with $\alpha \in \{1, -\delta_1, \delta_2\} \subset (-1, 1]$, we obtain (4.58). \square

The bound (4.58) obtained on ψ^m allows us to obtain both following propositions, implying the compactness of K_2^m , and also used in the main body of this paper for the proof of the compactness of the operator K_2 .

Proposition 4.16. *There exists $C > 0$ such that*

$$\int_{\mathbb{R}^3} \kappa^m(v, \eta) d\eta \leq \frac{C}{1 + |v|}, \quad \text{for a.e. } v \in \mathbb{R}^3, \quad (4.66)$$

$$\int_{\mathbb{R}^3} \kappa^m(v, \eta) dv \leq C, \quad \text{for a.e. } \eta \in \mathbb{R}^3. \quad (4.67)$$

Proof. By definition (4.43) of κ^m and from (4.58), we have

$$\kappa^m(v, \eta) \leq C e^{-\frac{|\eta-v|^2}{8T_k}} e^{-\frac{1}{8T_k} \frac{(|\eta|^2 - |v|^2)^2}{|\eta-v|^2}} (1 + |\eta - v|^{-1-\delta_2}). \quad (4.68)$$

Integrating (4.68) with respect to η and making the change of variable $\eta \mapsto \eta - v = p$ yield

$$\int_{\mathbb{R}^3} \kappa^m(v, \eta) d\eta \leq C \int_{\mathbb{R}^3} e^{-\frac{|p|^2}{8T_k}} e^{-\frac{(|p|+2|v|\cos(\widehat{v,p}))^2}{8T_k}} (1 + |p|^{-1-\delta_2}) dp.$$

Passing to spherical coordinates, the integral in p on the right-hand side writes

$$\begin{aligned} & \int_{\mathbb{R}_+} \int_0^{2\pi} \int_0^\pi (\rho^2 + \rho^{1-\delta_2}) e^{-\frac{\rho^2}{8T_k}} e^{-\frac{(\rho+2|v|\cos\theta)^2}{8T_k}} \sin\theta \, d\theta \, d\psi \, d\rho \\ &= 2\pi \int_{\mathbb{R}_+} (\rho^2 + \rho^{1-\delta_2}) e^{-\frac{\rho^2}{8T_k}} \left(\int_0^\pi e^{-\frac{(\rho+2|v|\cos\theta)^2}{8T_k}} \sin\theta \, d\theta \right) d\rho. \end{aligned}$$

Performing the change of variable $s = \cos\theta$, we obtain

$$\int_0^\pi e^{-\frac{(\rho+2|v|\cos\theta)^2}{8T_k}} \sin\theta \, d\theta \leq \int_{-1}^1 e^{-\frac{(\rho+2|v|s)^2}{8T_k}} ds \leq 2. \quad (4.69)$$

Besides, performing the change of variable $r = \rho + 2|v|s$, we obtain

$$\int_{-1}^1 e^{-\frac{(\rho+2|v|s)^2}{8T_k}} ds = \frac{1}{2|v|} \int_{\rho-2|v|}^{\rho+2|v|} e^{-\frac{r^2}{8T_k}} dr \leq \frac{1}{2|v|} \int_{\mathbb{R}} e^{-\frac{r^2}{8T_k}} dr = \frac{C}{|v|}. \quad (4.70)$$

Combining estimates (4.69)–(4.70) together yields

$$\int_0^\pi e^{-\frac{(\rho+2|v|\cos\theta)^2}{8T_k}} \sin\theta \, d\theta \leq \frac{C}{1+|v|}.$$

Hence

$$\int_{\mathbb{R}^3} \kappa^m(v, \eta) \, d\eta \leq \frac{C}{1+|v|} \int_{\mathbb{R}_+} (\rho^2 + \rho^{1-\delta_2}) e^{-\frac{\rho^2}{8T_k}} d\rho.$$

Since $1 - \delta_2 \geq 0$, we have $\int_{\mathbb{R}_+} (\rho^2 + \rho^{1-\delta_2}) e^{-\frac{\rho^2}{8T_k}} d\rho < \infty$, and we can conclude for (4.66). On the other hand, integrating (4.68) with respect to v and making the change of variable $v \mapsto v - \eta = p$ yields

$$\begin{aligned} \int_{\mathbb{R}^3} \kappa^m(v, \eta) \, dv &\leq C \int_{\mathbb{R}^3} e^{-\frac{|p|^2}{8T_k}} e^{-\frac{(|p|+2|p+\eta|\cos(\widehat{p+\eta,p}))^2}{8T_k}} (1+|p|^{-1-\delta_2}) \, dp \\ &\leq C \int_{\mathbb{R}^3} e^{-\frac{|p|^2}{8T_k}} (1+|p|^{-1-\delta_2}) \, dp. \end{aligned}$$

Since $-1 - \delta_2 > -3$, we have $\int_{\mathbb{R}^3} e^{-\frac{|p|^2}{8T_k}} (1+|p|^{-1-\delta_2}) \, dp < \infty$, which allows to conclude for (4.67). \square

Proposition 4.17. *The kernel κ^m belongs to $L^2_{loc}(\mathbb{R}^3, dv; L^2(\mathbb{R}^3, d\eta))$.*

The proof is similar to the one of Proposition 4.16, also remarking that $-2 - 2\delta_2 > -3$.

4.B A technical lemma

Lemma 4.18. *Under the assumptions (4.2)–(4.3), namely*

$$\varphi(I) \geq CI^{\beta_1}, \quad \text{for a.e. } I < 1,$$

$$\varphi(I) \geq C I^{\beta_2}, \quad \text{for a.e. } I \geq 1,$$

the function $\overline{\mu_2}$ defined by

$$\overline{\mu_2}(X) := \int_0^X \varphi(X-J) \varphi(J) \, dJ, \quad X \geq 0,$$

satisfies, for some constant C' ,

$$\overline{\mu_2}(X) \geq C' X^{2\beta_1+1}, \quad \text{for a.e. } X < 1, \quad (4.71)$$

$$\overline{\mu_2}(X) \geq C' X^{2\beta_2+1}, \quad \text{for a.e. } X \geq 1. \quad (4.72)$$

Proof. Let $X < 1$. As $\max(X-J, J) < 1$ for all $J \in (0, X)$, we have

$$\overline{\mu_2}(X) = \int_0^X \varphi(X-J) \varphi(J) \, dJ \geq C \int_0^X (X-J)^{\beta_1} J^{\beta_1} \, dJ.$$

Applying the change of variable $x = \frac{J}{X}$, we get

$$\overline{\mu_2}(X) \geq C X^{2\beta_1+1} \int_0^1 (1-x)^{\beta_1} x^{\beta_1} \, dx = C' X^{2\beta_1+1}.$$

Consider now $X \geq 3$. As $\min(X-J, J) \geq 1$ for all $J \in (1, X-1)$, we have in this case

$$\begin{aligned} \overline{\mu_2}(X) &= \int_0^X \varphi(X-J) \varphi(J) \, dJ \geq C \int_1^{X-1} (X-J)^{\beta_2} J^{\beta_2} \, dJ \\ &\geq C X^{2\beta_2+1} \left(\int_{\frac{1}{3}}^{\frac{2}{3}} (1-x)^{\beta_2} x^{\beta_2} \, dx \right) \geq C' X^{2\beta_2+1}. \end{aligned}$$

Finally, for $1 \leq X \leq 3$, we have

$$\overline{\mu_2}(X) \geq \int_0^1 (1-J)^{\beta_1} J^{\beta_1} \, dJ \equiv C \geq C \frac{X^{2\beta_2+1}}{3^{2\beta_2+1}},$$

ending the proof. □

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A Boltzmann model for polyatomic gases undergoing quasi-resonant collisions

Outline of the current chapter

Introduction	194
5.1 A Boltzmann model with quasi-resonant collisions	194
5.1.1 Quasi-resonance by collision truncation	195
5.1.2 Quasi-resonant Boltzmann operator and H -theorem	197
5.1.3 Resonant asymptotics	199
5.2 Expected properties of the model, Landau-Teller equations	201
5.2.1 Expected properties	201
5.2.2 Derivation of Landau-Teller type equations	202
5.3 Numerical experiments	206
5.3.1 The DSMC method	206
5.3.2 Result of the experiment and discussion	210
5.A Technical lemmas	212

Introduction

In this chapter, we propose a Boltzmann model for a single polyatomic gas, the molecules of which undergo *quasi-resonant* collisions. The previous Chapter 4 was concerned with exactly *resonant* collisions, and we intend to give more flexibility to the latter model, as an expected physical behaviour of the kind of considered collisions would rather be *quasi-resonant* than *exactly resonant*.

In Section 5.1, we build the model and propose a rigorous characterization of *quasi-resonance*, thanks to a *quasi-resonance parameter* $\varepsilon > 0$. After obtaining an *H*-theorem for this model, we prove some resonant asymptotics as ε goes to 0, confirming that the presented model characterizes quasi-resonance when ε is small.

In Section 5.2, from the obtained results, we informally deduce some expected properties of the model. We argue that a homogeneous quasi-resonant Boltzmann dynamics should be composed of two phases. In short time, the distribution may behave almost like in the resonant case and relax towards a two-temperature Maxwellian. After this phase, we expect the distribution to approximately stay in the form of a two-temperature Maxwellian. In long time, the two temperatures (kinetic and internal) should relax to each other.

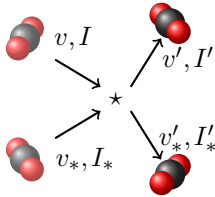
Assuming that the above behaviour indeed holds, we *explicitly* provide, for the second phase of the dynamics and for a wide family of collision kernels, an ODE system (approximately) satisfied by the kinetic and internal temperatures of the system, which is of *Landau-Teller* type (see for instance [137]).

Finally, in Section 5.3, we conduct a numerical experiment allowing to verify our claim on the kinetic and internal temperatures approximately satisfying the derived Landau-Teller type ODE system. Some technical lemmas are recast in Appendix 5.A.

5.1 A Boltzmann model with quasi-resonant collisions

We consider a single gas composed of polyatomic molecules, which are described, at the microscopic level, by their mass $m > 0$, velocity $v \in \mathbb{R}^3$ and energy level $I \in \mathbb{R}_+$ (we use the energy-level based description). The energy law of the molecules is provided by a measure μ on \mathbb{R}_+ , which is assumed to have a positive and continuous density φ with respect to the Lebesgue measure, *i.e.*

$$d\mu(I) = \varphi(I) dI, \quad I \in \mathbb{R}_+.$$



We consider two colliding molecules with respective incoming velocities $v, v_* \in \mathbb{R}^3$ and internal energies $I, I_* \in \mathbb{R}_+$ and their outgoing counterparts v', v_*, I', I_* . As the momentum and total energy of the two-particle (isolated) system are conserved during the collision, we have the microscopic conservation laws

$$v + v_* = v' + v'_*, \quad (5.1a)$$

$$\frac{1}{2}m|v|^2 + \frac{1}{2}m|v_*|^2 + I + I_* = \frac{1}{2}m|v'|^2 + \frac{1}{2}m|v'_*|^2 + I' + I'_*. \quad (5.1b)$$

Then (5.1a)–(5.1b) ensure the existence, as soon as

$$I' + I'_* \leq \frac{m}{4}|v - v_*|^2 + I + I_* =: E,$$

of $\sigma \in \mathbb{S}^2$ such that

$$v' = \frac{v + v_*}{2} + \frac{1}{2} \sqrt{E - (I' + I'_*)} \sigma, \quad v'_* = \frac{v + v_*}{2} - \frac{1}{2} \sqrt{E - (I' + I'_*)} \sigma. \quad (5.2)$$

Up to now, the setting is identical to the one of a usual polyatomic gas. We wish to implement, in a rigorous sense, the idea for the collision to be **quasi-resonant**, meaning that the kinetic and internal energies should be *almost separately conserved*. Morally, we are asking

$$|v'|^2 + |v'_*|^2 \approx |v|^2 + |v_*|^2,$$

or equivalently,

$$I' + I'_* \approx I + I_*.$$

To reach this goal, our approach, which we present in the next subsection, is to consider some *reference* polyatomic collisions, and to *remove* the ones that are “too far” from being resonant.

5.1.1 Quasi-resonance by collision truncation

In the Boltzmann model, the properties of collisions are embedded in the *collision kernel*. It is a positive function whose support (more precisely, domain of definition) is provided by the microscopic conservation laws (momentum and energy), and whose values correspond (formally) to some density of probability of possible collisions. Therefore, it is equivalent to saying that a collision is possible or that the collision kernel takes a positive value on the variables involved in the latter. In the following, in order to implement the idea of *quasi-resonance*, we shall consider a *quasi-resonance parameter* $\varepsilon > 0$, and as our quasi-resonant collision kernel B_ε , the multiplication of some reference polyatomic kernel B with a characteristic function χ_ε , the latter allowing to *remove* collisions that are too far from being resonant.

Reference collision kernel We introduce $B := B(v, v_*, I, I_*, I', I'_*, \sigma) \geq 0$ a reference polyatomic collision kernel, in the sense that it satisfies, for almost every $v, v_* \in \mathbb{R}^3$, $I, I_*, I', I'_* \in \mathbb{R}_+$, $\sigma \in \mathbb{S}^2$, a symmetry property

$$B(v, v_*, I, I_*, I', I'_*, \sigma) = B(v_*, v, I_*, I, I'_*, I', -\sigma), \quad (5.3)$$

a micro-reversibility one

$$|v - v_*| B(v, v_*, I, I_*, I', I'_*, \sigma) = |v' - v'_*| B(v', v'_*, I', I'_*, I, I_*, \sigma'), \quad (5.4)$$

and a positivity condition to authorize (only) physical collisions,

$$I' + I'_* \leq E \iff B(v, v_*, I, I_*, I', I'_*, \sigma) > 0, \quad (5.5)$$

with $E = \frac{1}{4}|v - v_*|^2 + I + I_*$. These assumptions may be found for instance in [37] and are compatible with other standard formulations as in [75, 86], as soon as the corresponding Boltzmann operator is defined accordingly.

Truncation function and quasi-resonant collision kernel We now construct a quasi-resonant collision kernel B_ε associated with the reference B . We introduce the following notations

$$R = \frac{m|v' - v'_*|^2}{4E} = 1 - \frac{I' + I'_*}{E}, \quad R' = \frac{m|v - v_*|^2}{4E} = 1 - \frac{I + I_*}{E}, \quad (5.6)$$

as in the Borgnakke-Larsen model, see [75] for instance. At the microscopic level, resonant collisions can thus be characterized by the property

$$R = R'.$$

Consequently, quasi-resonant collisions can be obtained by ensuring that R and R' are close to each other. We therefore consider the family of truncation functions $(\chi_\varepsilon)_{\varepsilon>0}$, defined for any $\varepsilon > 0$ by

$$\chi_\varepsilon(R, R') = \frac{c_\eta(R, R')}{2\varepsilon} \mathbb{1}_{\left[|\eta(R) - \eta(R')| \leq \varepsilon\right]}, \quad R, R' \in (0, 1), \quad (5.7)$$

where

$$\eta : (0, 1) \rightarrow \mathbb{R} \quad (5.8)$$

is a \mathcal{C}^1 -diffeomorphism, and c_η is a *normalizing factor*, satisfying a *symmetry* property (to later preserve micro-reversibility)

$$c_\eta(R, R') = c_\eta(R', R), \quad R, R' \in (0, 1), \quad (5.9)$$

and a *diagonal* one,

$$c_\eta(R, R) = \eta'(R), \quad R \in (0, 1), \quad (5.10)$$

which later allows to recover the resonant asymptotics as ε goes to 0.

Remark 5.1. Possible choices of c_η could be $c_\eta(R, R') = \sqrt{\eta'(R)\eta'(R')}$ or $c_\eta(R, R') = \frac{1}{2}(\eta'(R) + \eta'(R'))$.

We can now define the family of quasi-resonant collision kernels $(B_\varepsilon)_{\varepsilon>0}$ associated with the *reference kernel* B and the *truncation family* $(\chi_\varepsilon)_{\varepsilon>0}$, by, for any $\varepsilon > 0$, $v, v_* \in \mathbb{R}^3$, $\sigma \in \mathbb{S}^2$ and $I, I_*, I', I'_* \in \mathbb{R}_+$,

$$B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) = B(v, v_*, I, I_*, I', I'_*, \sigma) \times \chi_\varepsilon(R, R'), \quad (5.11)$$

where we used the notation (5.6) for R and R' . Thanks to (5.9), for any $\varepsilon > 0$, the kernel B_ε satisfies the symmetry and micro-reversibility properties, for any $v, v_*, \sigma, I, I_*, I', I'_*$,

$$B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) = B_\varepsilon(v_*, v, I_*, I, I'_*, I', -\sigma), \quad (5.12a)$$

$$|v - v_*| B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) = |v' - v'_*| B_\varepsilon(v', v'_*, I', I'_*, I, I_*, \sigma'), \quad (5.12b)$$

and thanks to (5.5), B_ε satisfies the following positivity property, which differs from (5.5) through the use of η and ε ,

$$\{I' + I'_* \leq E \quad \text{and} \quad |\eta(R) - \eta(R')| \leq \varepsilon\} \iff B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) > 0, \quad (5.13)$$

with $E = \frac{m}{4}|v - v_*|^2 + I + I_*$.

Remark 5.2. In the truncation function (5.7), we have introduced a \mathcal{C}^1 -diffeomorphism $\eta : (0, 1) \rightarrow \mathbb{R}$. This choice is made to provide flexibility to the model and to avoid boundary issues. In fact, it would not be precise to consider $\mathbb{1}_{\left[|R - R'| \leq \varepsilon\right]}$ in (5.7), as, for some fixed $R' < \varepsilon$, there is an asymmetry in the set $\{R \in (0, 1), |R - R'| \leq \varepsilon\}$ because of the requirement $R > 0$. Using $\mathbb{1}_{\left[|\eta(R) - \eta(R')| \leq \varepsilon\right]}$ instead avoids this issue. A typical choice of η (the one we later use in our explicit computations) would be

$$\eta : (0, 1) \rightarrow \mathbb{R}, \quad R \mapsto \log \left[\frac{R}{1 - R} \right],$$

which is an increasing smooth diffeomorphism from $(0, 1)$ to \mathbb{R} . The quasi-resonance is measured through the quantity $\eta(R) - \eta(R')$, which in this case corresponds to

$$\eta(R) - \eta(R') = [\log(E'_k) - \log(E'_i)] - [\log(E_k) - \log(E_i)],$$

with $E_k = \frac{m}{4}|v - v_*|^2$, $E_i = I + I_*$ and a similar definition, with prime variables, holds for E'_k and E'_i . The difference $\eta(R) - \eta(R')$ hence allows to simultaneously quantify the discrepancy between prime and non-prime energies, but also between kinetic and internal ones. Moreover, due to the presence of the log, the comparison is made through ratios instead of differences.

5.1.2 Quasi-resonant Boltzmann operator and H -theorem

Let us consider a family of quasi-resonant collision kernels $(B_\varepsilon)_{\varepsilon>0}$ defined as in the previous subsection. We set $(Q_\varepsilon)_{\varepsilon>0}$ to be the family of Boltzmann quasi-resonant collision operators, defined for any density $f \equiv f(v, I) \geq 0$ for which it makes sense, and $v \in \mathbb{R}^3$, $I \in \mathbb{R}_+$, by

$$Q_\varepsilon(f, f)(v, I) := \int_{\mathbb{R}^3} \iiint_{(\mathbb{R}_+)^3} \int_{\mathbb{S}^2} \{f' f'_* - f f_*\} B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) d\sigma \varphi(I') dI' \varphi(I'_*) dI'_* \varphi(I_*) dI_* dv_*, \quad (5.14)$$

where in the above equation, we used the standard short-hands $f \equiv f(v, I)$, $f_* \equiv f(v_*, I_*)$, $f' \equiv f(v', I')$, $f'_* \equiv f(v'_*, I'_*)$, and v' , v'_* are functions of the other variables, defined by (5.2).

Weak form of the operator Since the kernel B_ε satisfies the usual polyatomic symmetry and micro-reversibility conditions, we immediately obtain (see for instance [37]) that for any test function $\phi \equiv \phi(v, I)$ such that the following makes sense, we have, for any $\varepsilon > 0$,

$$\begin{aligned} & \int_{\mathbb{R}^3} \int_{\mathbb{R}_+} \phi(v, I) Q_\varepsilon(f, f)(v, I) \varphi(I) dI dv = \\ & \frac{1}{2} \iint_{(\mathbb{R}^3)^2} \iiint_{(\mathbb{R}_+)^4} \int_{\mathbb{S}^2} f f_* [\phi' + \phi'_* - \phi - \phi_*] B_\varepsilon d\sigma \varphi(I') dI' \varphi(I'_*) dI'_* \varphi(I) dI \varphi(I_*) dI_* dv dv_*, \end{aligned} \quad (5.15)$$

where, to simplify notations, we used the same short-hands as in (5.14) and did not write the arguments of the kernel B_ε . We deduce from the weak form (5.15) that, as usual, the operators Q_ε do conserve (at least formally) the mass, momentum and *total* energy: for any $\varepsilon > 0$ and $f \equiv f(v, I)$ such that it makes sense,

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}_+} Q_\varepsilon(f, f)(v, I) \begin{pmatrix} 1 \\ v \\ \frac{1}{2}m|v|^2 + I \end{pmatrix} dv \varphi(I) dI = 0. \quad (5.16)$$

Remark that the conservation properties of the quasi-resonant operators are the ones of the usual polyatomic case, and not of the resonant case (where moreover, kinetic and internal energy are separately conserved).

Collision invariants For some $\varepsilon > 0$ fixed, we say that $\psi : \mathbb{R}^3 \times \mathbb{R}_+ \rightarrow \mathbb{R}$ is an ε -quasi-resonant collision invariant if it is measurable and satisfies, for any $v, v_* \in \mathbb{R}^3$, $\sigma \in \mathbb{S}^2$ and $I, I_*, I', I'_* \in \mathbb{R}_+$,

$$\{I' + I'_* \leq E \quad \text{and} \quad |\eta(R) - \eta(R')| \leq \varepsilon\} \implies \{\psi(v', I') + \psi(v'_*, I'_*) = \psi(v, I) + \psi(v_*, I_*)\}, \quad (5.17)$$

where in the above, we used the notation $E = \frac{m}{4}|v - v_*|^2 + I + I_*$, v', v'_* are given by (5.2) and R, R' by (5.6).

Note that the definition of the ε -quasi-resonant collision invariants is slightly different from the one of the usual polyatomic collision invariants: there is the addition of the condition $|\eta(R) - \eta(R')| \leq \varepsilon$. Therefore, the set of collisions on which the invariance property is assumed to hold is *smaller* than in the usual polyatomic case. As a result, we cannot apply directly the known results of characterization of the collision invariants in the generic case; we provide this characterization in the following proposition, which is mostly based on [44, Lemma 3].

Proposition 5.1. Characterization of the invariants. *Let $\varepsilon > 0$ and assume ψ to be a continuous ε -quasi-resonant collision invariant, then there exists $a_1 \in \mathbb{R}$, $p \in \mathbb{R}^3$ and $a_2 \in \mathbb{R}$ such that for all $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$, we have*

$$\psi(v, I) = a_1 + p \cdot v + a_2 \left(\frac{m}{2} |v|^2 + I \right). \quad (5.18)$$

Notice that the collision invariants are here the same as in the usual polyatomic case (and not the ones of the resonant case). This is understandable, as (even if only very few) exchanges are allowed between the kinetic and internal energies.

Proof. As a collision invariant in the quasi-resonant case, ψ satisfies

$$\psi \left(\frac{v + v_*}{2} + \sqrt{\frac{E - I' - I'_*}{m}} \sigma, I' \right) + \psi \left(\frac{v + v_*}{2} - \sqrt{\frac{E - I' - I'_*}{m}} \sigma, I'_* \right) = \psi(v, I) + \psi(v_*, I_*) \quad (5.19)$$

for any $(v, v_*, I, I_*, I', I'_*, \sigma)$ such that $B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma)$ is non-zero. In particular, (5.19) holds whenever $R = R'$, using the notations defined in (5.6), *i.e.* in the resonant case. Using [44], there exist $a_1, a_2, a_3 \in \mathbb{R}$ and $p \in \mathbb{R}^3$ such that, for any (v, I) ,

$$\psi(v, I) = a_1 + p \cdot v + a_2 \frac{m}{2} |v|^2 + a_3 I.$$

Replacing ψ by its previous expression in (5.19), we obtain

$$p \cdot (v' + v'_*) + \frac{a_2}{2} (m|v'|^2 + m|v'_*|^2) + a_3(I' + I'_*) = p \cdot (v + v_*) + \frac{a_2}{2} (m|v|^2 + m|v_*|^2) + a_3(I + I_*).$$

Thanks to the microscopic conservations (5.1a)–(5.1b) of momentum and total energy, we get

$$(a_2 - a_3)(I' + I'_* - I - I_*) = 0.$$

Finally, we can choose $(v, v_*, I, I_*, I', I'_*, \sigma)$ such that $B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) \neq 0$ and $R \neq R'$ simultaneously, so that $I' + I'_* \neq I + I_*$, and subsequently obtain $a_2 = a_3$. \square

Having derived the weak form of the Boltzmann collision operator and characterized the collision invariants, we are now in a position to provide the H -Theorem associated with this model.

Theorem 5.1. H-Theorem for quasi-resonant Boltzmann model. For any density $f \equiv f(v, I) > 0$, it holds, at least formally, that

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}_+} \log f(v, I) Q_\varepsilon(f, f)(v, I) \, dv \varphi(I) \, dI \leq 0 \quad (5.20)$$

and

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}_+} \log f(v, I) Q_\varepsilon(f, f)(v, I) \, dv \varphi(I) \, dI = 0$$

$$\Downarrow$$

$$f(v, I) = \mathcal{M}(v, I) := \frac{\rho}{m} \left(\frac{2\pi T}{m} \right)^{-3/2} Z(1/T)^{-1} \exp\left(-\frac{m|v-u|^2}{2T} - \frac{I}{T} \right), \quad (5.21)$$

where Z is the partition function (see (4.4) in Chapter 4) and ρ , u and T are respectively the mass density, average velocity and average temperature associated with f (see (2.13) and the above equations in Chapter 2).

Notice that the equilibrium distributions in the quasi-resonant case are, as in the usual polyatomic case, Maxwellians with *one* temperature. We highlight the fact that in the resonant case, these distributions have *two* distinct temperatures (one kinetic and one internal).

The proof of Theorem 5.1 is straightforward once collision invariants are characterized (here, thanks to Proposition 5.1) and very standard, see for instance the proof of Theorem 2.3 in chapter 2.

5.1.3 Resonant asymptotics

In this subsection, we investigate the consistency of the quasi-resonant modeling by studying the behaviour of the collision kernel family (B_ε) as ε goes to 0. In order for us to ensure that our approach indeed describes the notion of *quasi-resonance*, we provide in the following a result of convergence towards *resonance* as ε goes to 0.

Proposition 5.2. Consider a family of quasi-resonant collision kernels $(B_\varepsilon)_\varepsilon$, and assume that their reference collision kernel B is continuous. Let $\varepsilon > 0$, and let $\psi := \psi(I', I'_*)$ be a continuous test-function with a compact support in $(\mathbb{R}_+)^2$. The tuple of variables $(v, v_*, I, I_*, \sigma) \in (\mathbb{R}^3)^2 \times (\mathbb{R}_+)^2 \times \mathbb{S}^2$ being fixed, we set

$$\mathcal{J}_\varepsilon = \iint_{(\mathbb{R}_+)^2} B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) \psi(I', I'_*) \varphi(I') \varphi(I'_*) \, dI' \, dI'_*.$$

Then $(\mathcal{J}_\varepsilon)$ converges, as ε goes to 0, towards

$$\mathcal{J}_0 = \int_{\mathbb{R}_+} B^{res}(v, v_*, I, I_*, I', \sigma) \psi(I', I + I_* - I') \varphi(I') \varphi(I + I_* - I') \, dI', \quad (5.22)$$

where the resonant collision kernel B^{res} associated with the reference kernel B is defined by

$$B^{res}(v, v_*, I, I_*, I', \sigma) := B(v, v_*, I, I_*, I', I + I_* - I', \sigma) E \mathbb{1}_{[I' \leq I + I_*]}, \quad (5.23)$$

with $E = \frac{m}{4}|v - v_*|^2 + I + I_*$.

In (5.22), we recover the *resonant integration measure* $\varphi(I') \varphi(I + I_* - I') \, dI'$ discussed in the previous chapter 4. This proposition confirms that, from a modeling point of view, considering a “small” ε in our approach indeed allows to describe the phenomenon of quasi-resonance.

Proof. Since, in the definition of \mathcal{J}_ε , the variables v, v_*, I, I_* and σ are fixed, we set, in the following, for the sake of clarity,

$$\Psi(I', I'_*) = B(v, v_*, I, I_*, I', I'_*, \sigma) \psi(I', I'_*) \varphi(I') \varphi(I'_*).$$

Using (5.11)–(5.7), we get

$$\mathcal{J}_\varepsilon = \frac{1}{2\varepsilon} \iint_{(0, +\infty)^2} c_\eta(R, R') \mathbf{1}_{[|\eta(R) - \eta(R')| \leq \varepsilon]} \Psi(I', I'_*) \, dI' \, dI'_*.$$

Remembering that R' only depends on some of the fixed variables, and not on I' nor I'_* , a convenient way to proceed is to use the Borgnakke-Larsen representation, that is to change variables (I', I'_*) into (R, r) with

$$R = 1 - \frac{I' + I'_*}{E}, \quad r = \frac{I'}{I' + I'_*}, \quad (5.24)$$

whose Jacobian equals $(1 - R)E^2$. Then we have

$$\begin{aligned} \mathcal{J}_\varepsilon = & \\ & \frac{1}{2\varepsilon} \iint_{(0,1)^2} c_\eta(R, R') \mathbf{1}_{[|\eta(R) - \eta(R')| \leq \varepsilon]} \Psi(r(1 - R)E, (1 - r)(1 - R)E) (1 - R)E^2 \, dR \, dr. \end{aligned} \quad (5.25)$$

Since, in the integral in R , both r and E are then considered to be fixed, let us set, for the sake of simplicity, for any R ,

$$\bar{\Psi}(R) = \Psi(r(1 - R)E, (1 - r)(1 - R)E) (1 - R)E^2,$$

which, with our assumptions, is clearly continuous. Let us focus, in (5.25), on the integral in R , that is

$$\frac{1}{2\varepsilon} \int_0^1 c_\eta(R, R') \mathbf{1}_{[|\eta(R) - \eta(R')| \leq \varepsilon]} \bar{\Psi}(R) \, dR.$$

We perform the change of variable $z = \eta(R)$, so that the above becomes, as η is a \mathcal{C}^1 -diffeomorphism from $(0, 1)$ to \mathbb{R} ,

$$\begin{aligned} & \frac{1}{2\varepsilon} \int_{\mathbb{R}} c_\eta(\eta^{-1}(z), R') \mathbf{1}_{[|z - \eta(R')| \leq \varepsilon]} \bar{\Psi}(\eta^{-1}(z)) (\eta^{-1})'(z) \, dz \\ & = \frac{1}{2\varepsilon} \int_{\eta(R') - \varepsilon}^{\eta(R') + \varepsilon} c_\eta(\eta^{-1}(z), R') \bar{\Psi}(\eta^{-1}(z)) (\eta^{-1})'(z) \, dz. \end{aligned} \quad (5.26)$$

Letting ε go to 0 in (5.26) and using the diagonal property of c_η , Equation (5.10), we get, at the limit,

$$c_\eta(R', R') \times \bar{\Psi}(R') \times (\eta^{-1})'(\eta(R')) = c_\eta(R', R') \times \bar{\Psi}(R') \times \frac{1}{\eta'(R')} = \bar{\Psi}(R').$$

Hence, by dominated convergence, $(\mathcal{J}_\varepsilon)$ converges, as ε goes to 0, towards

$$\int_0^1 \Psi(r(1 - R')E, (1 - r)(1 - R')E) (1 - R')E^2 \, dr,$$

which we denote \mathcal{J}_0 . Remembering that $(1 - R')E = I + I_*$, we finally perform the change of variable r

to I' with $I' = r(I + I_*)$, leading to

$$\mathcal{J}_0 = \int_0^{I+I_*} \Psi(I', I + I_* - I') E dI',$$

and thus to (5.22). \square

5.2 Expected properties of the model, Landau-Teller equations

In this section, we discuss what we can deduce from the H -Theorem 5.1 and the resonant asymptotics, Proposition 5.1.3. We consider from now on the *homogeneous quasi-resonant Boltzmann equation*, for some $\varepsilon > 0$,

$$\partial_t f(t, v, I) = Q_\varepsilon(f(t), f(t))(v, I), \quad f(0, v, I) = f_{\text{in}}(v, I), \quad (5.27)$$

for $t \geq 0$, $v \in \mathbb{R}^3$ and $I \in \mathbb{R}_+$.

5.2.1 Expected properties

Let us first discuss informally the properties of the quasi-resonant model we may expect, based on the results proven earlier. The H -Theorem 5.1 ensures that the equilibrium distributions of the *quasi-resonant* dynamics are of *Maxwellian form*, with **one** temperature. On the other hand, the resonant asymptotics, Proposition 5.1.3, ensures that, at least formally, when ε is very small, the *quasi-resonant* dynamics should behave *almost like* its associated resonant one. But we recall that *equilibrium distributions of the resonant dynamics are of Maxwellian form with two temperatures* like in (4.22).

Therefore, we expect the *quasi-resonant dynamics* to be composed of two phases, which we schematically represent in Figure 5.1.

1. First, in “short” time, the quasi-resonant dynamics behaves almost like its associated resonant dynamics. We should observe a relaxation towards a *two-temperature Maxwellian*.
2. Second, in “long” time, as the distribution is close to a two-temperature Maxwellian, its two temperatures should converge to each other. Moreover, we expect the distribution to *stay in the form of a two-temperature Maxwellian*, as the “resonant part” of the quasi-resonant collision operator is much stronger than its “mixing part”.

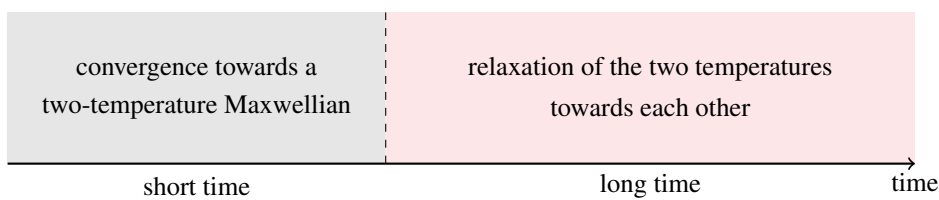


Figure 5.1 – Schematic representation of the expected behaviour of a quasi-resonant dynamics.

Let us highlight that we expect, *during the quasi-resonant dynamics* (5.27), that **if the initial distribution is approximately in the form of a two-temperature Maxwellian, it stays approximately of this form**. This is *not* the case in the generic polyatomic case, and is a specific feature of the present model. In particular, it allows to observe simple ODEs on the kinetic and internal temperatures (of the type of the so-called Landau-Teller equations, see for instance [137]).

Finally, we emphasize that the statements of this subsection are not rigorous. Nevertheless, we later perform numerical experiments, in Section 5.3, the results of which support the presented point of view.

5.2.2 Derivation of Landau-Teller type equations

In this subsection, we derive ODEs of Landau-Teller type on the kinetic and internal temperatures, which are *locally* satisfied (at time $t = 0$) by solutions to the quasi-resonant dynamics (5.27) with a *two-temperature Maxwellian initial distribution*.

In order to obtain an explicit result, we choose for the following

$$\varphi(I) = I^{\delta/2-1}, \quad I \geq 0, \quad (5.28)$$

with $\delta \geq 2$. This choice of energy law density corresponds to a *polytropic gas* with a number of internal degrees of freedom equal to δ , and is common in the literature, see [7, 47].

Moreover, we take

$$\eta(R) := \log \left[\frac{R}{1-R} \right], \quad R \in (0, 1), \quad (5.29)$$

which is indeed, as required in our model, an increasing \mathcal{C}^1 -diffeomorphism from $(0, 1)$ to \mathbb{R} . This peculiar choice is motivated by the following properties:

1. the difference $\eta(R) - \eta(R')$ is the log of the *ratio* between the post- and pre-collisional *ratios between kinetic and internal energies*,
2. the quantity $|\eta(R) - \eta(R')|$ is invariant by the change $(R, R') \mapsto (1-R, 1-R')$,
3. it seems to be one of the simplest ones for the explicit computations conducted in this subsection.

The considered quasi-resonant collision kernel We consider, for our upcoming computations, the family of quasi-resonant collision kernel $(B_\varepsilon)_{\varepsilon>0}$, defined, for any $\varepsilon > 0$, $v, v_* \in \mathbb{R}^3$, $\sigma \in \mathbb{S}^2$ and $I, I_*, I', I'_* \in \mathbb{R}_+$, by

$$B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) = C_B b(\sigma \cdot \sigma') E_k^{\beta_k - \frac{1}{2}} E_k^{\beta_k} E_i^{\beta_i} E_i^{\beta_i} E^\gamma \times \frac{\mathbb{1}_{[I'+I'_* \leq E]}}{\mathfrak{m}_\varphi(E)} \times \frac{\mathbb{1}_{[|\eta(R) - \eta(R')| \leq \varepsilon]}}{2\varepsilon}, \quad (5.30)$$

where we recall the notations

$$\begin{aligned} E_k &= \frac{m}{4} |v - v_*|^2, & E_i &= I + I_*, & E &= E_k + E_i, \\ E'_k &= \frac{m}{4} |v' - v'_*|^2, & E'_i &= I' + I'_*, \\ R &= \frac{E'_k}{E} = 1 - \frac{E'_i}{E}, & R' &= \frac{E_k}{E} = 1 - \frac{E_i}{E}, \end{aligned}$$

the velocities v' and v'_* are functions of the other variables given by (5.2), β_k, β_i and γ are real exponents, $C_B > 0$ is a constant, b is an angular kernel satisfying, for $\omega \in \mathbb{S}^2$,

$$\int_{\mathbb{S}^2} b(\sigma \cdot \omega) d\sigma = 1, \quad (5.31)$$

the function η is given by (5.29), the notation $\mathbb{1}_X$ is used for the characteristic function of the set X , and $\mathfrak{m}_\varphi(E)$ is the average value of $\mathbb{1}_{[I'+I'_* \leq E]}$ on $(\mathbb{R}_+)^2$ with respect to the internal energy distribution

measure, that is

$$\mathfrak{m}_\varphi(E) := \iint_{(\mathbb{R}_+)^2} \mathbb{1}_{[I'+I'_* \leq E]} \varphi(I') \varphi(I'_*) \, dI' \, dI'_*. \quad (5.32)$$

Explicitly, as we chose (5.28), we have

$$\mathfrak{m}_\varphi(E) = \frac{\Gamma(\delta/2)^2}{\Gamma(\delta+1)} E^\delta, \quad (5.33)$$

where Γ stands for the Gamma function.

One straightforwardly checks that the kernels B_ε defined by (5.30) satisfy all the required properties of quasi-resonant collision kernels (5.12a)–(5.13).

Remark 5.3. *Let us link the family of kernels defined by (5.30) with the general form of quasi-resonant kernels (5.11). Choose for instance*

$$c_\eta(R, R') = \sqrt{\eta'(R) \eta'(R')} = \frac{1}{\sqrt{R(1-R) R'(1-R')}},$$

which indeed satisfies (5.9)–(5.10). Then, for any $\varepsilon > 0$, the kernel B_ε defined by (5.30) has indeed the form (5.11), with the reference collision kernel B being equal to

$$B(v, v_*, I, I_*, I', I'_*, \sigma) = C_B b(\sigma \cdot \sigma') E_k^{\beta_k} E_k'^{\beta_k + \frac{1}{2}} E_i^{\beta_i + \frac{1}{2}} E_i'^{\beta_i + \frac{1}{2}} E^{\gamma-2} \frac{\mathbb{1}_{[I'+I'_* \leq E]}}{\mathfrak{m}_\varphi(E)},$$

using the same notations as in (5.30).

Local Landau-Teller equation We provide, in the next proposition, the first term in the expansion in ε of the derivative at time $t = 0$ of the internal temperature of a solution to the homogeneous quasi-resonant Boltzmann equation (5.27) with a two-temperature Maxwellian initial condition.

Proposition 5.3. *For $\varepsilon > 0$, consider f a solution to the homogeneous quasi-resonant Boltzmann equation (5.27) associated with φ , η and B_ε defined in (5.28)–(5.30), with $\gamma = \delta + 3$. Assume the initial condition f_{in} to be a two-temperature Maxwellian distribution (which form is given in (4.22)) associated with the mass density $\rho > 0$, the average velocity $u \in \mathbb{R}^3$ and the kinetic and internal temperatures $T_k^0 > 0$ and $T_i^0 > 0$. For $t \geq 0$, we denote*

$$T_k(t) = \frac{1}{3\rho} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} \frac{m}{2} |v - u|^2 f(t, v, I) \, dv \varphi(I) \, dI, \quad T_i(t) = \frac{1}{\delta\rho} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} I f(t, v, I) \, dv \varphi(I) \, dI, \quad (5.34)$$

respectively the kinetic and internal temperatures of the solution f at time t . Then

$$\left. \frac{dT_i(t)}{dt} \right|_{t=0} = \varepsilon^2 \rho C_{\delta, \beta_k, \beta_i} (T_k^0)^{2\beta_k + \frac{3}{2}} (T_i^0)^{2\beta_i + \delta + 1} (T_k^0 - T_i^0) + \mathcal{O}(\varepsilon^4), \quad (5.35)$$

with, recalling that Γ stands for the Gamma function,

$$C_{\delta, \beta_k, \beta_i} = \frac{C_B}{12} \times \frac{\Gamma(2\beta_k + 4) \Gamma(2\beta_i + 2\delta + 2)}{\Gamma(\frac{3}{2}) \Gamma(\delta)}. \quad (5.36)$$

Proof. Let us first notice that, as f solves (5.27), we have

$$\left. \frac{dT_i(t)}{dt} \right|_{t=0} = \frac{1}{\delta \rho} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} I Q_\varepsilon(f_{\text{in}}, f_{\text{in}})(v, I) \, dv \varphi(I) \, dI.$$

The whole proof therefore consists in evaluating the above integral. It comes from the weak form (5.15) of the operator Q_ε and the choice $\varphi(I) = I^{\frac{\delta}{2}-1}$ that

$$\begin{aligned} & \frac{1}{\delta \rho} \iint_{\mathbb{R}^3 \times \mathbb{R}_+} I Q_\varepsilon(f_{\text{in}}, f_{\text{in}})(v, I) \, dv \varphi(I) \, dI = \\ & \frac{1}{2\delta \rho} \iint_{(\mathbb{R}^3)^2} \iiint_{(\mathbb{R}_+)^4} \int_{\mathbb{S}^2} f_{\text{in}}(f_{\text{in}})_* [I' + I'_* - I - I_*] B_\varepsilon(\cdot) (II_* I' I'_*)^{\frac{\delta}{2}-1} \, d\sigma \, dI \, dI_* \, dI' \, dI'_* \, dv \, dv_*, \end{aligned}$$

where we used the short-hands $f_{\text{in}} \equiv f_{\text{in}}(v, I)$, $(f_{\text{in}})_* \equiv f_{\text{in}}(v_*, I_*)$ and $B_\varepsilon(\cdot) \equiv B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma)$. The above integral can be rewritten as

$$\begin{aligned} & \frac{1}{2\delta \rho} \iint_{(\mathbb{R}^3)^2} \iint_{(\mathbb{R}_+)^2} f_{\text{in}}(f_{\text{in}})_* \left\{ \iint_{(\mathbb{R}_+)^2} \int_{\mathbb{S}^2} [I' + I'_* - I - I_*] B_\varepsilon(\cdot) (I' I'_*)^{\frac{\delta}{2}-1} \, d\sigma \, dI' \, dI'_* \right\} \\ & \qquad \qquad \qquad \times (II_*)^{\frac{\delta}{2}-1} \, dI \, dI_* \, dv \, dv_*. \quad (5.37) \end{aligned}$$

Let us now focus on the term inside the braces. Using the explicit form of B_ε , Equation (5.30), as well as (5.31), it equals

$$\begin{aligned} & C_B E_k^{\beta_k - \frac{1}{2}} E_i^{\beta_i} E^\gamma \\ & \times \frac{1}{2\varepsilon \mathfrak{m}_\varphi(E)} \iint_{(\mathbb{R}_+)^2} (E'_i - E_i) (E - E'_i)^{\beta_k} E_i^{\beta_i} \mathbf{1}_{[I'+I'_* \leq E]} \mathbf{1}_{[|\eta(R) - \eta(R')| \leq \varepsilon]} (I' I'_*)^{\frac{\delta}{2}-1} \, dI' \, dI'_*, \end{aligned}$$

with the same notations as in (5.30), and since $E'_k = E - E'_i$. For $R' \in (0, 1)$ and $E \geq 0$ fixed, we set

$$\begin{aligned} \mathbf{I}_\varepsilon := & \frac{1}{2\varepsilon \mathfrak{m}_\varphi(E)} \iint_{(\mathbb{R}_+)^2} (E'_i - (1 - R')E) (E - E'_i)^{\beta_k} E_i^{\beta_i} \\ & \times \mathbf{1}_{[I'+I'_* \leq E]} \mathbf{1}_{[|\eta(R) - \eta(R')| \leq \varepsilon]} (I' I'_*)^{\frac{\delta}{2}-1} \, dI' \, dI'_*. \quad (5.38) \end{aligned}$$

By definition (5.32) of \mathfrak{m}_φ , we thus have (changing $x = I' + I'_*$)

$$\mathbf{I}_\varepsilon = \frac{1}{2\varepsilon \mathfrak{m}_\varphi(E)} \int_0^E (x - (1 - R')E) (E - x)^{\beta_k} x^{\beta_i} \mathbf{1}_{[|\eta(R) - \eta(R')| \leq \varepsilon]} \mathfrak{m}'_\varphi(x) \, dx,$$

with the notation $R = 1 - \frac{x}{E}$. Using the explicit form (5.33) of \mathfrak{m}_φ and performing the change of variable $x \mapsto R = 1 - \frac{x}{E}$, we obtain

$$\mathbf{I}_\varepsilon = -\delta E^{\beta_k + \beta_i + 1} \times \frac{1}{2\varepsilon} \int_0^1 (R - R') R^{\beta_k} (1 - R)^{\beta_i + \delta - 1} \mathbf{1}_{[|\eta(R) - \eta(R')| \leq \varepsilon]} \, dR. \quad (5.39)$$

Applying (5.56) of Lemma 5.4 in Appendix 5.A with the choice $\psi(R) = R^{\beta_k} (1 - R)^{\beta_i + \delta - 1}$, and η given

by (5.29), we obtain

$$\begin{aligned} \mathbb{I}_\varepsilon &= -\delta E^{\beta_k + \beta_i + 1} \times \\ &\quad \frac{\varepsilon^2}{6} (R')^{\beta_k + 2} (1 - R')^{\beta_i + \delta + 1} [2(\beta_k(1 - R') - (\beta_i + \delta - 1)R') - 3(R' - (1 - R'))] + \mathcal{O}(\varepsilon^4), \end{aligned}$$

where we used

$$\eta'(R) = \frac{1}{R(1-R)}, \quad \frac{\eta''(R)}{\eta'(R)} = \frac{R - (1-R)}{R(1-R)}, \quad \psi'(R) = \frac{\psi(R)}{R(1-R)} (\beta_k(1-R) - (\beta_i + \delta - 1)R).$$

Simplifying, and using the notations $E_k = R'E$, $E_i = (1-R')E$, it becomes

$$\mathbb{I}_\varepsilon = \varepsilon^2 \frac{\delta}{6} E^{-\delta-3} E_k^{\beta_k+2} E_i^{\beta_i+\delta+1} [(2\beta_i + 2\delta + 1)E_k - (2\beta_k + 3)E_i] + \mathcal{O}(\varepsilon^4).$$

Therefore, using (5.37), we have

$$\begin{aligned} \left. \frac{dT_i(t)}{dt} \right|_{t=0} &= \varepsilon^2 \frac{C_B}{12\rho} \iint_{(\mathbb{R}^3)^2} \iint_{(\mathbb{R}_+)^2} E_k^{2\beta_k + \frac{3}{2}} E_i^{2\beta_i + \delta + 1} [(2\beta_i + 2\delta + 1)E_k - (2\beta_k + 3)E_i] \\ &\quad \times f_{\text{in}}(f_{\text{in}})_* (II_*)^{\frac{\delta}{2}-1} dI dI_* dv dv_* + \mathcal{O}(\varepsilon^4). \end{aligned}$$

We highlight that the term $E^{\gamma-\delta-3}$ disappeared as we assumed $\gamma = \delta + 3$. Since f_{in} is a two-temperature Maxwellian distribution (with associated mass density ρ and kinetic and internal temperatures respectively T_k^0 and T_i^0), the above right-hand-side expression may be recast as

$$\begin{aligned} \varepsilon^2 \rho \frac{C_B}{12} &\left((2\beta_i + 2\delta + 1) \mathbf{m}_{2\beta_k + \frac{3}{2}}^k(T_k^0) \mathbf{m}_{2\beta_i + \delta + 1}^i[\delta](T_i^0) - (2\beta_k + 3) \mathbf{m}_{2\beta_k + \frac{3}{2}}^k(T_k^0) \mathbf{m}_{2\beta_i + \delta + 2}^i[\delta](T_i^0) \right) \\ &\quad + \mathcal{O}(\varepsilon^4), \quad (5.40) \end{aligned}$$

where \mathbf{m}^k and \mathbf{m}^i denote moments of the two-particle Maxwellian distribution and are defined, for $T > 0$ and $\beta > 0$ by

$$\mathbf{m}_\beta^k(T) := \left(\frac{2\pi T}{m} \right)^{-3} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} e^{-\frac{m}{2T}(|v|^2 + |v_*|^2)} \left(\frac{m}{4} |v - v_*|^2 \right)^\beta dv dv_*, \quad (5.41a)$$

$$\mathbf{m}_\beta^i[\delta](T) := \left(\iint_{(\mathbb{R}_+)^2} e^{-\frac{I+I_*}{T}} (II_*)^{\frac{\delta}{2}-1} dI dI_* \right)^{-1} \iint_{(\mathbb{R}_+)^2} e^{-\frac{I+I_*}{T}} (I+I_*)^\beta (II_*)^{\frac{\delta}{2}-1} dI dI_*. \quad (5.41b)$$

Using their explicit expression given in (5.58)–(5.59) in Lemma 5.5, we deduce that (5.40) can be rewritten as

$$\varepsilon^2 \rho \frac{C_B}{12} \times \frac{\Gamma(2\beta_k + 4) \Gamma(2\beta_i + \delta + 2)}{\Gamma(\frac{3}{2}) \Gamma(\delta)} \times (T_k^0)^{2\beta_k + \frac{3}{2}} (T_i^0)^{2\beta_i + \delta + 1} (T_k^0 - T_i^0) + \mathcal{O}(\varepsilon^4), \quad (5.42)$$

ending the proof. \square

Global Landau-Teller equations in the quasi-resonant case In the previous Proposition 5.3, we obtained an explicit formula, for small ε , of the derivative around time $t = 0$ of the internal temperature of a solution to the homogeneous quasi-resonant Boltzmann equation (5.27) with a two-temperature Maxwellian initial condition. Following the discussion on the expected properties of solutions to the homogeneous quasi-resonant Boltzmann equation in Subsection 5.2.1, such a solution is expected to *stay close* to the two-temperature Maxwellian form.

Therefore, one can extrapolate, from the expected properties of the quasi-resonant model and Proposition 5.3 that, if f is a solution to (5.27) associated with the kernel B_ε defined in (5.30), for a small ε , and with an initial condition close to a two-temperature Maxwellian, we have for any time $t \geq 0$,

$$\frac{dT_i(t)}{dt} \approx \varepsilon^2 \rho C_{\delta, \beta_k, \beta_i} T_k(t)^{2\beta_k + \frac{3}{2}} T_i(t)^{2\beta_i + \delta + 1} (T_k(t) - T_i(t)). \quad (5.43)$$

where the notations are the same as in Proposition 5.3.

We emphasize that we have not proven (5.43) rigorously (it is in itself a non-rigorous statement). The goal of the next section is to *verify*, via numerical experiments, the *validity* of (5.43).

5.3 Numerical experiments

In this section, we conduct a first numerical experiment to check the validity of our statement (5.43), providing an equation on the relaxation of the kinetic and internal temperatures towards each other, in a quasi-resonant context.

In order to achieve this goal, we do the following.

1. We simulate the 3D homogeneous Boltzmann equation (5.27) associated with the collision kernel (5.30), with a two-temperature Maxwellian initial condition. We denote the kinetic and internal temperatures of the solution at time t by $T_k(t)$ and $T_i(t)$.
2. We numerically solve the ODE system (with the same notations as in Proposition 5.3)

$$\bar{T}'_i(t) = \varepsilon^2 \rho C_{\delta, \beta_k, \beta_i} \bar{T}_k(t)^{2\beta_k + \frac{3}{2}} \bar{T}_i(t)^{2\beta_i + \delta + 1} (\bar{T}_k(t) - \bar{T}_i(t)), \quad t \geq 0, \quad (5.44a)$$

$$\frac{3}{2} \bar{T}'_k(t) + \frac{\delta}{2} \bar{T}'_i(t) = 0, \quad t \geq 0, \quad (5.44b)$$

$$(\bar{T}_i(0), \bar{T}_k(0)) = (T_i(0), T_k(0)). \quad (5.44c)$$

3. We compare $t \mapsto T_i(t)$ with $t \mapsto \bar{T}_i(t)$: if the two curves globally coincide, we can conclude, from an experimental point of view, to the validity of (5.43).

Numerically solving (5.44a)–(5.44c) is straightforward with the solver `solve_ivp` from the python package `scipy.integrate`. We present, in the next subsection, the method we use to simulate the 3D homogeneous Boltzmann equation.

5.3.1 The DSMC method

The DSMC (Direct Simulation Monte Carlo) method is a *probabilistic* and *particle-based* approach for the simulation of the Boltzmann equation, created by Bird in the 1960s, see [22, 23]. It consists in the simulation of a system of *representative particles*. Each particle is endowed with its internal state, here its velocity $v \in \mathbb{R}^3$ and internal energy level $I \in \mathbb{R}_+$ (actually, we rather use its *energy quantile* $q \in \mathbb{R}_+$, see Subsubsection 1.2.2.2).

At each time step, a set of particle couples is selected *randomly* and *uniformly* (corresponding to the chaos property of the Boltzmann equation). The time step is linked to an *upper-bound on the collision kernel*, denoted here by $B_{\max} > 0$. These particle couples are *potential candidates* for binary collision. Each couple is then *selected for collision* with a probability linked to a ratio between a kernel related to both particle states and B_{\max} . When a couple is selected for collision, we update the states of the two selected molecules randomly, *according to a probability law* given by the collision kernel, ending the time step.

In our simulations, we consider the functions φ , η and for some $\varepsilon > 0$, a kernel B_ε of the form (5.28)–(5.30), with $\gamma = \delta + 3$, as in Proposition 5.3. We moreover assume

$$2\beta_k + \frac{1}{2} \geq 0, \quad \beta_i + \delta \geq 0. \quad (5.45)$$

We simulate the homogeneous quasi-resonant Boltzmann equation (5.27), the solution of which is denoted $f \equiv f(t, v, I)$. The mass density, average velocity, average temperature, kinetic and internal temperatures of $f(t)$ are respectively denoted $\rho > 0$, $u \in \mathbb{R}^3$, $T_{eq} > 0$ (these quantities are constant in time) and $T_k(t)$ and $T_i(t)$ (these depend on time). In particular, for all $t \geq 0$,

$$3T_k(t) + \delta T_i(t) = (3 + \delta)T_{eq}.$$

We consider, for the following, $N \gg 1$ numerical particles.

Collision frequency As the kernel B_ε satisfies the angular cut-off assumption (5.31), the Boltzmann operator Q_ε can be split into gain Q_ε^+ and loss Q_ε^- terms. The latter, applied to f , writes, for any $t \geq 0$, $v \in \mathbb{R}^3$ and $I \in \mathbb{R}_+$,

$$Q_\varepsilon^-(f(t), f(t))(v, I) = \nu_f^\varepsilon(t, v, I) f(t, v, I),$$

where ν_f^ε is called the *collision frequency*

$$\nu_f^\varepsilon(t, v, I) := \int_{\mathbb{R}_+} \int_{\mathbb{R}^3} f(t, v, I) \overline{B}_\varepsilon(v, v_*, I, I_*) \, dv_* I_*^{\frac{\delta}{2}-1} \, dI_*,$$

and \overline{B}_ε is the *averaged kernel*, defined by

$$\overline{B}_\varepsilon(v, v_*, I, I_*) := \iint_{(\mathbb{R}_+)^2} \int_{\mathbb{S}^2} B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) \, d\sigma (I' I'_*)^{\frac{\delta}{2}-1} \, dI' \, dI'_*.$$

In particular, combining (5.30) with (5.31) and $\gamma = \delta + 3$, we have

$$\begin{aligned} \overline{B}_\varepsilon(v, v_*, I, I_*) &= C_B E_k^{\beta_k - \frac{1}{2}} E_i^{\beta_i} E^{\delta+3} \\ &\quad \times \frac{1}{\mathfrak{m}_\varphi(E) 2\varepsilon} \iint_{I'+I'_* \leq E} (E - E'_i)^{\beta_k} E_i'^{\beta_i} \mathbb{1}_{[|\eta(R) - \eta(R')| \leq \varepsilon]} (I' I'_*)^{\frac{\delta}{2}-1} \, dI' \, dI'_*, \end{aligned}$$

with the same notations as in (5.30). Changing $x = I' + I'_*$ thanks to the definition of \mathfrak{m}_φ , using its explicit expression (5.33) and then performing the change of variable $R = 1 - \frac{x}{E}$, we obtain

$$\overline{B}_\varepsilon(v, v_*, I, I_*) = C_B E_k^{\beta_k - \frac{1}{2}} E_i^{\beta_i} E^{\beta_k + \beta_i + \delta + 3} \times \frac{\delta}{2\varepsilon} \int_{R_\varepsilon^-}^{R_\varepsilon^+} R^{\beta_k} (1 - R)^{\beta_i + \delta - 1} \, dR, \quad (5.46)$$

where we denoted

$$R_\varepsilon^\pm := \frac{R'}{R' + e^{\mp\varepsilon}(1 - R')}.$$

Expanding (5.46) in $\varepsilon > 0$, we obtain

$$\bar{B}_\varepsilon(v, v_*, I, I_*) = \bar{B}_0(v, v_*, I, I_*) + \mathcal{O}(\varepsilon^2), \quad (5.47)$$

with

$$\bar{B}_0(v, v_*, I, I_*) = C_B \delta E_k^{2\beta_k + \frac{1}{2}} E_i^{2\beta_i + \delta} E^2. \quad (5.48)$$

In our simulations, we *approximate the collision frequency* ν_f^ε by

$$\nu_f^0(t, v, I) := \int_{\mathbb{R}_+} \int_{\mathbb{R}^3} f(t, v_*, I_*) \bar{B}_0(v, v_*, I, I_*) dv_* I_*^{\frac{\delta}{2} - 1} dI_*, \quad (5.49)$$

as $\nu_0 > 0$ and, by (5.47),

$$\nu_f^\varepsilon = \nu_f^0 + \mathcal{O}(\varepsilon^2).$$

Selecting the pairs of particles to collide Let us consider some time t and a time step $\Delta t > 0$. A numerically efficient way of drawing pairs of numerical particles to collide between t and $t + \Delta t$ according to the collision frequency ν_f^0 consists in first *over-estimating* the number of colliding pairs and then go through an *accept or reject* process.

We denote, for any numerical particle labelled by $n \in \llbracket 1, N \rrbracket$, by $v^n \in \mathbb{R}^3$ its velocity and $I^n \in \mathbb{R}_+$ its internal energy, and we consider the upper-bounds

$$\Delta v_{\max}(t) = \max_{1 \leq n_1, n_2 \leq N} |v^{n_1} - v^{n_2}|^1, \quad I_{\max}(t) = \max_{1 \leq n \leq N} I^n.$$

We thus have, from (5.48)–(5.49), that

$$\nu_f^0(t, v, I) \leq \nu_{\max}(t),$$

with

$$\nu_{\max}(t) := \rho \bar{B}_{\max}(t) \quad (5.50)$$

and

$$\bar{B}_{\max}(t) = C_B \delta \left(\frac{m}{4} (\Delta v_{\max}(t))^2 \right)^{2\beta_k + \frac{1}{2}} (2I_{\max}(t))^{2\beta_i + \delta} \left(\frac{m}{4} (\Delta v_{\max}(t))^2 + 2I_{\max}(t) \right)^2. \quad (5.51)$$

We are now ready for the selection of pairs of numerical particles to collide.

- We uniformly draw

$$\left\lfloor \Delta t \times \nu_{\max}(t) \times \frac{N}{2} \right\rfloor$$

pairs of numerical particles as *potential candidates* to collide between times t and $t + \Delta t$, where $\lfloor \cdot \rfloor$ stands for the integer part.²

1. In practice, we consider a cheaper-to-compute upper-bound.

2. In practice, we rather choose the number of pairs of potential candidates, typically $\lfloor N/2 \rfloor$, and deduce the corresponding time step Δt .

• As $\nu_{\max}(t)$ is an *over-estimation* of the collision frequency, we go through an *accept or reject process*. For each pair of drawn numerical particles, we *uniformly draw* a number $U \in (0, 1)$. Denoting respectively by (v, I) and (v_*, I_*) their states,

— we accept the collision if

$$U \leq \frac{\overline{B}_0(v, v_*, I, I_*)}{\overline{B}_{\max}(t)},$$

— otherwise we reject the collision.

Updating the states of the colliding particles We consider a pair of numerical particles that we have selected for collision, which pre-collisional states are respectively denoted by (v, I) and (v_*, I_*) . We update their states to the post-collisional ones (v', I') and (v'_*, I'_*) by *drawing the post-collisional quantities* $R = 1 - \frac{I' + I'_*}{E}$, $r = \frac{I'}{I' + I'_*}$ and σ .

• We first draw $R = 1 - \frac{I' + I'_*}{E}$. The law of the *post-collisional total internal energy* $I' + I'_*$ (seen as a random variable) on $(\mathbb{R}_+)^2$ conditionally to v, v_*, I and I_* and drawn according to the collision kernel B_ε is

$$\frac{\int_{\mathbb{S}^2} B_\varepsilon(v, v_*, I, I_*, I', I'_*, \sigma) d\sigma}{\overline{B}_\varepsilon(v, v_*, I, I_*)} (I' I'_*)^{\frac{\delta}{2}-1} dI' dI'_*.$$

Remembering (5.46), it explicitly rewrites

$$\delta^{-1} \frac{E_k^{\beta_k} E_i^{\beta_i}}{E^{\beta_k + \beta_i}} \times \left(\int_{R_\varepsilon^-}^{R_\varepsilon^+} R_*^{\beta_k} (1 - R_*)^{\beta_i + \delta - 1} dR_* \right)^{-1} \frac{\mathbb{1}_{[I' + I'_* \leq E]} \mathbb{1}_{[|\eta(R) - \eta(R')| \leq \varepsilon]}}{m_\varphi(E)} (I' I'_*)^{\frac{\delta}{2}-1} dI' dI'_*,$$

where we recall the notation $R_\varepsilon^\pm := \frac{R'}{R' + e^{\mp \varepsilon}(1 - R')}$. By definition (5.32) of m_φ , the law of the quantity $x = I' + I'_*$ on \mathbb{R}_+ is thus

$$\delta^{-1} \frac{(E - x)^{\beta_k} x^{\beta_i}}{E^{\beta_k + \beta_i}} \times \left(\int_{R_\varepsilon^-}^{R_\varepsilon^+} R_*^{\beta_k} (1 - R_*)^{\beta_i + \delta - 1} dR_* \right)^{-1} \frac{\mathbb{1}_{[x \leq E]} \mathbb{1}_{[|\eta(R) - \eta(R')| \leq \varepsilon]}}{m_\varphi(E)} m'_\varphi(x) dx.$$

Therefore, the ratio $R = 1 - \frac{x}{E}$ is associated with the probability measure, on $(R_\varepsilon^-, R_\varepsilon^+)$,

$$\frac{R^{\beta_k} (1 - R)^{\beta_i + \delta - 1}}{\int_{R_\varepsilon^-}^{R_\varepsilon^+} R_*^{\beta_k} (1 - R_*)^{\beta_i + \delta - 1} dR_*} dR, \quad (5.52)$$

In order to draw R according to (5.52), one may compute the inverse of the corresponding cumulative function, which is defined for any $y \in (R_\varepsilon^-, R_\varepsilon^+)$ by

$$F_\varepsilon^{R'}(y) := \frac{\int_{R_\varepsilon^-}^y R^{\beta_k} (1 - R)^{\beta_i + \delta - 1} dR}{\int_{R_\varepsilon^-}^{R_\varepsilon^+} R^{\beta_k} (1 - R)^{\beta_i + \delta - 1} dR}.$$

We then *uniformly draw* $U \in (0, 1)$ and set $R = (F_\varepsilon^{R'})^{-1}(U)$.

• We *uniformly draw* $r \in (0, 1)$.

- We draw $\sigma \in \mathbb{S}^2$ according to the probability density b , the angular kernel.³

We finally set

$$I' = r(1-R)E, \quad I'_* = (1-r)(1-R)E, \quad (5.53)$$

$$v' = \frac{v+v_*}{2} + \sqrt{\frac{(1-R)E}{m}}\sigma, \quad v'_* = \frac{v+v_*}{2} - \sqrt{\frac{(1-R)E}{m}}\sigma, \quad (5.54)$$

and this ends the state-updating phase.

Remark 5.4. *In our simulations, for the sake of simplicity, we choose $\beta_k = 0$, $\beta_i = -1$ and $\delta = 2$, so that the inverse function of $F_\varepsilon^{R'}$ writes, for any $U \in (0, 1)$,*

$$(F_\varepsilon^{R'})^{-1}(U) = R_\varepsilon^- + U(R_\varepsilon^+ - R_\varepsilon^-). \quad (5.55)$$

Implementation We implemented the DSMC algorithm in `python`, using the libraries `numpy`, `scipy`, `matplotlib` and `numba`, the latter allowing to speed up the simulations, also by parallelizing the computations. Significant results can be obtained within a few minutes on my personal computer.

5.3.2 Result of the experiment and discussion

We perform a numerical experiment with the following physical parameters

$$C_B = 2, \quad b = \frac{1}{4\pi}, \quad m = 1, \quad \rho = 1, \quad \delta = 2, \quad \beta_k = 0, \quad \beta_i = -1.$$

We take $N = 10^5$ numerical particles, and set the initial temperatures⁴ to be

$$T_k^0 = 1, \quad T_i^0 = 50.$$

In particular, the equilibrium temperature is $T_{eq} = 20.6$.

Quasi-resonant experiment We first conduct a numerical experiment in a quasi-resonant setting, taking $\varepsilon = 10^{-1}$, and with $4 \cdot 10^6$ time steps (the final time is approximately $3.3 \cdot 10^{-2}$). We show in Figure 5.2 the result of the simulation, which took approximately 40 minutes to run on my personal computer.

The black curve describes the time evolution of the internal temperature T_i of the system simulated through the DSMC algorithm, while the white dashed curve is obtained by solving the ODE system (5.44a)–(5.44c) with the solver `solve_ivp` from the `python` package `scipy.integrate`. The grey dashed-dotted line is set at the equilibrium temperature T_{eq} .

3. In our simulations, we take a constant b .

4. There are no restrictions (for instance, of closeness) on the initial temperatures to consider.

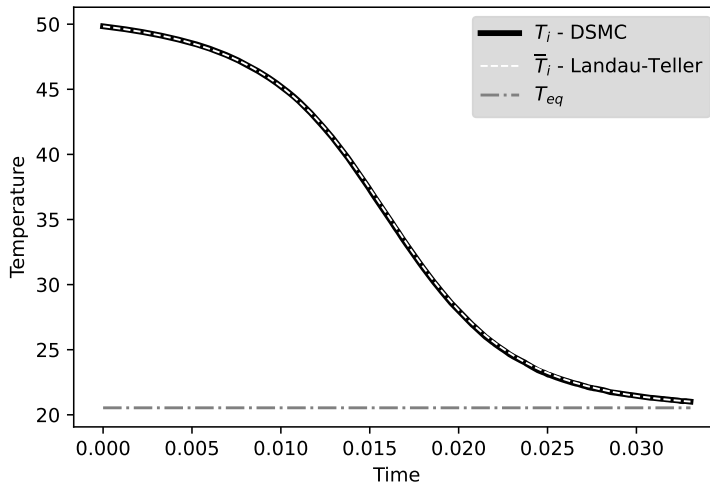


Figure 5.2 – Graph of the internal temperature of the system simulated through the DSMC algorithm and of the one obtained by solving (5.44a)–(5.44c), with $\varepsilon = 10^{-1}$.

We have plotted on Figure 5.3 the graph of $|T_i - \bar{T}_i|/\bar{T}_i$ in semi-log scale, the relative error between T_i (DSMC) and \bar{T}_i (Landau-Teller), with respect to time. The total L^2 relative error is approximately $2.2 \cdot 10^{-3}$.

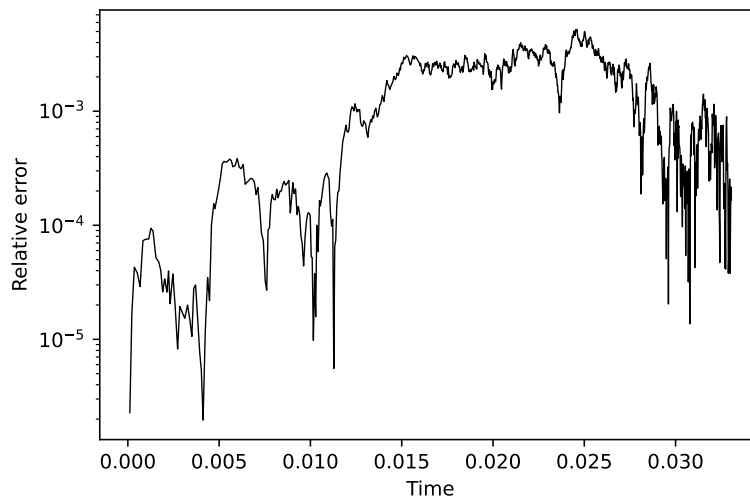


Figure 5.3 – Graph of the relative error $|T_i - \bar{T}_i|/\bar{T}_i$ related to Figure 5.2 in semi-log scale with respect to time.

Far-from-resonance experiment We conduct another experiment in a far-from-resonance setting, considering $\varepsilon = 10$, with in this case only $4 \cdot 10^3$ time steps (the final time is approximately 10^{-5}). We show the result of the simulation in Figure 5.4, which took 3 seconds to run on my personal computer.

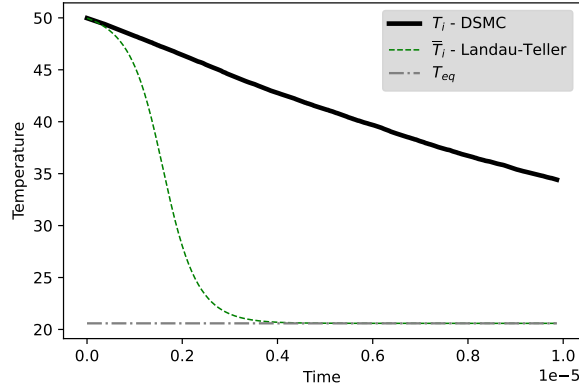


Figure 5.4 – Graph of the temperature associated with the internal energy with respect to time with $\varepsilon = 10$.

Again, the black curve describes the time evolution of the internal temperature T_i of the system simulated through the DSMC algorithm, while the green dashed curve is obtained by solving the ODE system (5.44a)–(5.44c).

Discussion on the result We observe on Figures 5.2 and 5.3 a firm agreement of the two curves of T_i (DSMC) and \bar{T}_i (Landau-Teller) in a quasi-resonant setting (with $\varepsilon = 10^{-1}$), while it is clear on Figure 5.4 that, as expected, the curves do not match at all in a far-from-resonant setting (with $\varepsilon = 10$).

This seems to numerically confirm, at least for our chosen set of parameters, our statement of Subsection 5.2.2: the kinetic and internal temperatures of a solution to the homogeneous quasi-resonant Boltzmann equation, associated with the kernel B_ε defined in (5.28), for some ε small and two-temperature Maxwellian initial condition, do approximately satisfy the Landau-Teller ODE system (5.44a)–(5.44c).

This moreover somehow provides a numerical validation on the expected behaviour of the quasi-resonant dynamics detailed in Subsection 5.2.1: it does appear reasonable to understand the latter as composed of two parts, a resonant-like dynamics in short-time making the distribution relax towards a two-temperature Maxwellian, and then a relaxation of the two temperatures towards each other driven by a Landau-Teller type ODE system.

5.A Technical lemmas

The following lemma is key in the derivation of Landau-Teller equations at small quasi-resonance parameter ε .

Lemma 5.4. *Let $\psi \in C^1((0, 1))$ and $\eta : (0, 1) \rightarrow \mathbb{R}$ a smooth diffeomorphism with $\eta' > 0$. Then, for any $R_0 \in (0, 1)$, we have*

$$\begin{aligned} \frac{1}{2\varepsilon} \int_0^1 (R - R_0) \psi(R) \mathbf{1}_{|\eta(R) - \eta(R_0)| \leq \varepsilon} \, dR \\ \stackrel{\varepsilon \rightarrow 0}{=} \frac{\varepsilon^2}{6\eta'(R_0)^3} \left[2\psi'(R_0) - 3\psi(R_0) \frac{\eta''(R_0)}{\eta'(R_0)} \right] + \mathcal{O}(\varepsilon^4). \end{aligned} \quad (5.56)$$

Proof. Let $R_0 \in (0, 1)$, denote by Ψ an antiderivative of $R \mapsto (R - R_0)\psi(R)$, and set, for any $x \in \mathbb{R}$,

$$g(x) = \eta^{-1}(\eta(R_0) + x),$$

and notice that g is as smooth as η (as $\eta' > 0$). Then we can write, for any $\varepsilon > 0$,

$$\frac{1}{2\varepsilon} \int_0^1 (R - R_0) \psi(R) \mathbb{1}_{\left[|\eta(R) - \eta(R_0)| \leq \varepsilon\right]} \mathrm{d}R = \frac{1}{2\varepsilon} \int_{g(-\varepsilon)}^{g(\varepsilon)} (R - R_0) \psi(R) \mathrm{d}R.$$

Straightforward Taylor expansions of $\Psi \circ g$ near 0 yield

$$\frac{1}{2\varepsilon} \int_{g(-\varepsilon)}^{g(\varepsilon)} (R - R_0) \psi(R) \mathrm{d}R \underset{\varepsilon \rightarrow 0}{=} (\Psi \circ g)'(0) + \frac{\varepsilon^2}{6} (\Psi \circ g)'''(0) + \mathcal{O}(\varepsilon^4). \quad (5.57)$$

The zeroth-order (in ε) term in (5.57) is null as $(\Psi \circ g)'(0) = \Psi'(R_0)g'(0) = 0$. The second-order term involves

$$(\Psi \circ g)'''(0) = \Psi'(R_0)g'''(0) + 3\Psi''(R_0)g'(0)g''(0) + \Psi'''(R_0)g'(0)^3.$$

By direct computations,

$$\Psi'(R_0) = 0, \quad \Psi''(R_0) = \psi(R_0), \quad \Psi'''(R_0) = 2\psi'(R_0).$$

Moreover, we also have, remembering that $\eta' > 0$,

$$g'(0) = \frac{1}{\eta'(R_0)}, \quad g''(0) = -\frac{\eta''(R_0)}{\eta'(R_0)^3}.$$

Putting everything together, we finally obtain (5.56). \square

The second result required in the derivation of the Landau-Teller equations concerns moments of the Maxwellian distribution and is provided in the following lemma.

Lemma 5.5. *For any $\beta > -3$ and $T_k > 0$, we have*

$$\begin{aligned} \mathbf{m}_{\beta}^k(T_k) &:= \left(\frac{2\pi T_k}{m}\right)^{-3} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} e^{-\frac{m}{2T_k}(|v|^2 + |v_*|^2)} \left(\frac{m}{4}|v - v_*|^2\right)^{\beta} \mathrm{d}v \mathrm{d}v_* \\ &= \frac{\Gamma(\beta + \frac{3}{2})}{\Gamma(\frac{3}{2})} T_k^{\beta}. \end{aligned} \quad (5.58)$$

On the other hand for any $\delta > 0$, $\beta > -\delta$ and $T_i > 0$, we have

$$\begin{aligned} \mathbf{m}_{\beta}^i[\delta](T_i) &:= \left(\iint_{(\mathbb{R}_+)^2} e^{-\frac{I+I_*}{T_i}} (II_*)^{\frac{\delta}{2}-1} \mathrm{d}I \mathrm{d}I_*\right)^{-1} \iint_{(\mathbb{R}_+)^2} e^{-\frac{I+I_*}{T_i}} (I+I_*)^{\beta} (II_*)^{\frac{\delta}{2}-1} \mathrm{d}I \mathrm{d}I_* \\ &= \frac{\Gamma(\beta + \delta)}{\Gamma(\delta)} T_i^{\beta}. \end{aligned} \quad (5.59)$$

Proof. We start by proving (5.58). One easily checks that, through the change of variables $(v, v_*) \mapsto (g, G) = (v - v_*, \frac{v+v_*}{2})$, we have

$$\begin{aligned} \left(\frac{2\pi T_k}{m}\right)^{-3} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} e^{-\frac{m}{2T_k}(|v|^2 + |v_*|^2)} \left(\frac{m}{4}|v - v_*|^2\right)^\beta \mathbf{d}v \mathbf{d}v_* = \\ \left(\frac{4\pi T_k}{m}\right)^{-3/2} \int_{\mathbb{R}^3} e^{-\frac{m|g|^2}{4T_k}} \left(\frac{m}{4}|g|^2\right)^\beta \mathbf{d}g. \end{aligned}$$

Changing to polar coordinates, the above right-hand-side integral becomes

$$\left(\frac{4\pi T_k}{m}\right)^{-3/2} |\mathbb{S}^2| \int_0^\infty e^{-\frac{mr^2}{4T_k}} \left(\frac{m}{4}r^2\right)^\beta r^2 \mathbf{d}r.$$

Changing variables $r \mapsto x = \frac{mr^2}{4T_k}$, we thus obtain

$$\begin{aligned} \mathbf{m}_\beta^k(T_k) &= \left(\frac{4\pi T_k}{m}\right)^{-3/2} |\mathbb{S}^2| \int_0^\infty e^{-x} (x T_k)^\beta \left(\frac{4T_k}{m}\right) x \sqrt{\frac{T_k}{m}} \frac{\mathbf{d}x}{\sqrt{x}} \\ &= \frac{2}{\sqrt{\pi}} T_k^\beta \int_0^\infty e^{-x} x^{\beta + \frac{1}{2}} \mathbf{d}x, \end{aligned}$$

allowing to recover the announced (5.58).

As for \mathbf{m}_β^i , we have by definition of \mathbf{m}_φ (with $x = I + I_*$), and using its explicit form (5.33),

$$\iint_{(\mathbb{R}_+)^2} e^{-\frac{I+I_*}{T_i}} (I + I_*)^\beta (II_*)^{\frac{\delta}{2}-1} \mathbf{d}I \mathbf{d}I_* = \int_0^\infty e^{-\frac{x}{T_i}} x^\beta \mathbf{m}'_\varphi(x) \mathbf{d}x = \frac{\Gamma(\delta/2)^2}{\Gamma(\delta)} \int_0^\infty e^{-\frac{x}{T_i}} x^{\beta+\delta-1} \mathbf{d}x.$$

Applying the change of variable $y = \frac{x}{T_i}$, the above transforms into

$$\frac{\Gamma(\delta/2)^2}{\Gamma(\delta)} T_i^{\beta+\delta} \int_0^\infty e^{-y} y^{\beta+\delta-1} \mathbf{d}y = \frac{\Gamma(\delta/2)^2}{\Gamma(\delta)} \Gamma(\beta + \delta) T_i^{\beta+\delta}. \quad (5.60)$$

Then (5.59) comes by taking the quotient of the right-hand-side of (5.60) with its value at $\beta = 0$. \square

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Part III

On relaxation towards equilibrium for the Boltzmann-Fermi-Dirac equation

Overview

In this part, composed of Chapters 6 and 7, we study the long-time behaviour of solutions to the homogeneous Boltzmann-Fermi-Dirac equation. Chapter 6 is the reproduction of [36] and Chapter 7 of [39]. In this part, the notation ε stands for the quantum parameter.

This work deals with **functional analysis** and **analysis of PDEs**.

ABSTRACT OF CHAPTER 6. We establish a connection between the relative classical entropy and the relative Fermi-Dirac entropy, allowing us to transpose, in the context of the Boltzmann or Landau equations, any entropy-entropy production inequality from one case to the other, therefore providing entropy-entropy production inequalities for the Boltzmann-Fermi-Dirac operator, similar to the ones of the classical Boltzmann operator. We also provide a generalized version of the Csiszár-Kullback-Pinsker inequality to weighted L^p norms, $1 \leq p \leq 2$, and a wide class of entropies.

ABSTRACT OF CHAPTER 7. We provide the first quantitative result of convergence to equilibrium in the context of the spatially homogeneous Boltzmann-Fermi-Dirac equation associated with hard potential interactions under the angular cutoff assumption, providing an explicit-algebraic-rate of convergence to Fermi-Dirac steady solutions. This result complements the quantitative convergence result of Liu and Lu [118] and is based upon new L^∞ bounds on the solutions uniformly with respect to time and ε .

Articles reproduced in this chapter

- [36] T. Borsoni. « Extending Cercignani's conjecture results from Boltzmann to Boltzmann-Fermi-Dirac equation ». Accepted in: *J. Stat. Phys.* (2024). URL: <https://hal.science/hal-04079527>.
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Extending Cercignani’s conjecture results from Boltzmann to Boltzmann-Fermi-Dirac

Outline of the current chapter

6.1 Introduction	223
6.1.1 The Boltzmann-Fermi-Dirac operator	223
6.1.2 Macroscopic quantities and equilibrium distribution	225
6.1.3 Fermi-Dirac entropy	226
6.1.4 Entropy production	228
6.1.5 Trend to equilibrium and Cercignani’s conjecture	228
6.2 Main results	230
6.2.1 Comparison of the Fermi-Dirac and Classical relative entropies	230
6.2.2 Entropy-entropy production inequalities for the Boltzmann-Fermi-Dirac (BFD) equation	230
6.2.3 About the Csiszár-Kullback-Pinsker inequality	231
6.2.4 Convergence towards equilibrium	233
6.3 Proof of Theorem 6.1 and Proposition 6.2	234
6.3.1 Key element of the proof	234
6.3.2 Continuity at zero	238
6.3.3 Final proof of Theorem 6.1	239
6.3.4 Final proof of Proposition 6.2	240
6.4 Proof of Corollary 6.3	243
6.4.1 Super quadratic kernels	243
6.4.2 General kernels	244
6.4.3 Inverse result	245
6.5 About the Landau-Fermi-Dirac equation	247
6.6 L^1-L^2 weighted Csiszár-Kullback-Pinsker inequality	249
6.A Similar results in the Bose-Einstein case	253

6.B A general discussion about entropies and equilibria	255
6.C Technical results	260
6.C.1 L^∞ bound for the Fermi-Dirac statistics	260
6.C.2 Regularity in ε of the coefficients of the Fermi-Dirac statistics	262
Acknowledgements	265

6.1 Introduction

In the study of quantum dilute gases, Nordheim [138], Uehling and Uhlenbeck [154] proposed in the early 1930s a kinetic approach, with a modified Boltzmann equation - bearing the names Nordheim equation, quantum Boltzmann equation, or Boltzmann-Fermi-Dirac equation (for fermions). Quoting Villani [156, Chapter 5.3], this description "does not rest on the traditional quantum formalism, [...] it is rather a classical description of interacting particles with quantum features", which nevertheless allows to recover the expected Fermi-Dirac statistics (in the context of fermions) and Bose-Einstein statistics (in the context of bosons). In this paper, we focus on the case of fermions in which Pauli's exclusion principle is taken into account.

In the context of the study of trend to equilibrium, the use of entropy-entropy production inequalities, allowing to obtain explicit rates of convergence, has been increasing in the recent years. We mention the results of Villani [157] for the Classical Boltzmann operator, Desvillettes [71], Desvillettes and Villani [78], Carrapatoso, Desvillettes and He [58] for the Landau operator, Alonso, Bagland, Desvillettes and Lods [4, 3] and Alonso, Bagland, and Lods [2] for the Landau-Fermi-Dirac (LFD) operator. We also refer the reader to the reviews [156, 77]. Up to now, no such results were known for the Boltzmann-Fermi-Dirac (BFD) operator, and the initial goal of this work was to fill this gap. In doing so, we actually established a connection between the Classical and Fermi-Dirac cases, allowing to transpose any entropy-entropy production result from one setting to the other under suitable conditions. Entropy-entropy production estimates for the BFD operator then directly follow from the ones of Villani [157] for the Classical Boltzmann operator - the same procedure can be applied to transpose entropy-entropy production estimates for the Landau operator to ones for the LFD operator.

This paper is constructed as follows. In the rest of this section, we introduce our mathematical setting, useful definitions and further discuss our motivations. In Section 6.2, we state our main results, which are the connection between the Fermi-Dirac and Classical relative entropies (Theorem 6.1 and Proposition 6.2), the entropy-entropy production estimates for the BFD operator (Corollary 6.3), and a generalization of the Csiszár-Kullback-Pinsker inequality (Proposition 6.4). We provide the proof of Theorem 6.1 in Section 6.3, of Corollary 6.3 in Section 6.4, discuss the case of the Landau / LFD equation in Section 6.5 and provide the proof of Proposition 6.4 (along with a more precise result and discussions) in Section 6.6. We very briefly discuss the case of bosons in Appendix 6.A. Considerations about a wider class of entropies (with a generalization of Proposition 6.4) are provided in Appendix 6.B. In particular, we provide in Proposition 6.15 a general formula for the minimizer of a general entropy under the constraints given by general conserved quantities, under a sole condition of existence. There are links with the results of [48] where equilibria of collision kernels of type two particles give two particles appearing in weak turbulence theory are rigorously obtained. In fact, Proposition 6.15 does not replace a rigorous study of equilibria, such as in [48], but gives insights, in a general setting, on to which distributions we should be expected to be equilibria. Finally, technical results relevant to our study are proven in Appendix 6.C.

6.1.1 The Boltzmann-Fermi-Dirac operator

The spatially homogeneous Boltzmann-Fermi-Dirac (BFD) equation writes

$$\partial_t f = Q_\varepsilon(f, f), \quad f(0, \cdot) = f^{in}, \quad (6.1)$$

where $f \equiv f(t, v) \geq 0$ represents a density of fermions (quantum particles of half-integer spin, e.g. electrons), depending on time $t \geq 0$ and velocity $v \in \mathbb{R}^3$, $f^{in} \equiv f^{in}(v) \geq 0$ is an initial distribution and Q_ε stands for the BFD operator. We refer the reader to [67, 80, 123, 124] for results on the Cauchy problem

associated with (6.1). In this paper, we focus on the operator Q_ε and, if not specified otherwise, discard the time variable t , considering $f \equiv f(v) \geq 0$.

In dimension 3, the BFD operator writes, for $\varepsilon > 0$ and measurable $f : \mathbb{R}^3 \rightarrow [0, \varepsilon^{-1}]$,

$$Q_\varepsilon(f, f)(v) := \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \left[f' f'_* (1 - \varepsilon f)(1 - \varepsilon f_*) - f f_* (1 - \varepsilon f')(1 - \varepsilon f'_*) \right] B(v, v_*, \sigma) d\sigma dv_*, \quad (6.2)$$

where we used the standard shorthands $f \equiv f(v)$, $f_* \equiv f(v_*)$, $f' \equiv f(v')$, $f'_* \equiv f(v'_*)$ and

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2} \sigma, \quad v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2} \sigma. \quad (6.3)$$

We insist that any physically meaningful solution f to (6.1) should be such that $1 - \varepsilon f \geq 0$. As a consequence of time micro-reversibility and Galilean invariance properties, the collision kernel $B \geq 0$ is assumed to satisfy, for $(v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3$ and $\sigma \in \mathbb{S}^2$,

$$B(v, v_*, \sigma) \equiv B(|v - v_*|, \cos \theta), \quad (6.4)$$

with $\cos \theta = \sigma \cdot \frac{v - v_*}{|v - v_*|}$. At this level of generality, no other assumption is made on B . Formally choosing $\varepsilon = 0$ in (6.2) yields the Classical Boltzmann operator

$$Q_0(f, f)(v) := \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \left[f' f'_* - f f_* \right] B(v, v_*, \sigma) d\sigma dv_*, \quad (6.5)$$

with the same shorthands as in (6.2). Now for $\varepsilon \geq 0$, define

$$\varphi_\varepsilon(x) := \frac{x}{1 - \varepsilon x}, \quad \text{for } x \in \mathbb{R}_+ \text{ s.t. } 1 - \varepsilon x > 0. \quad (6.6)$$

Remark that when $\varepsilon = 0$, corresponding to the classical case, we have $\varphi_0 = \text{Id}_{\mathbb{R}_+}$. Moreover, φ_ε is a C^1 -diffeomorphism from $[0, \varepsilon^{-1})$ to \mathbb{R}_+ , with $\varphi_\varepsilon^{-1} = \varphi_{-\varepsilon}$.

Then, when f is such that $1 - \varepsilon f > 0$ almost everywhere, Equation (6.2) can be rewritten in the following form resembling the Classical Boltzmann operator (6.5),

$$Q_\varepsilon(f, f)(v) := \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \left[\varphi_\varepsilon(f)' \varphi_\varepsilon(f)'_* - \varphi_\varepsilon(f) \varphi_\varepsilon(f)_* \right] B_\varepsilon^f(v, v_*, \sigma) d\sigma dv_*, \quad (6.7)$$

using the same shorthands as in (6.2), and

$$B_\varepsilon^f(v, v_*, \sigma) = (1 - \varepsilon f(v))(1 - \varepsilon f(v_*))(1 - \varepsilon f(v'))(1 - \varepsilon f(v'_*)) B(v, v_*, \sigma), \quad (6.8)$$

The collision kernel B_ε^f straightforwardly satisfies the usual assumptions of symmetry and micro-reversibility which imply the weak form of the classical Boltzmann operator, (see for instance [67]), so that for any test function $\psi : \mathbb{R}^3 \rightarrow \mathbb{R}$,

$$\begin{aligned} \int_{\mathbb{R}^3} \psi(v) Q_\varepsilon(f, f)(v) dv = \\ - \frac{1}{4} \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} \left[\varphi_\varepsilon(f)' \varphi_\varepsilon(f)'_* - \varphi_\varepsilon(f) \varphi_\varepsilon(f)_* \right] \left(\psi' + \psi'_* - \psi - \psi_* \right) B_\varepsilon^f d\sigma dv dv_*, \end{aligned} \quad (6.9)$$

still using the same shorthands as in (6.2) for $\varphi_\varepsilon(f)$ and ψ . Formally taking $\psi(v) = 1$, $\psi(v) = v_i$ for

$i = 1, 2, 3$ and $\psi(v) = \frac{1}{2}|v|^2$ in (6.9) yields the conservation of mass, momentum and energy

$$\int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ \frac{1}{2}|v|^2 \end{pmatrix} Q_\varepsilon(f, f)(v) \, dv = 0. \quad (6.10)$$

In the following, we define, for $p \geq 1$ and $s \in \mathbb{R}$, the weighted L_s^p norm of some function g by

$$\|g\|_{L_s^p} := \left(\int_{\mathbb{R}^3} |g(v)|^p (1 + |v|^2)^{\frac{ps}{2}} \, dv \right)^{\frac{1}{p}}, \quad (6.11)$$

and its essential supremum by $\|g\|_\infty$.

6.1.2 Macroscopic quantities and equilibrium distribution

Throughout this paper, for any nonnegative $f \in L_2^1(\mathbb{R}^3) \setminus \{0\}$, we denote $(\rho, u, T) \in \mathbb{R}_+^* \times \mathbb{R}^3 \times \mathbb{R}_+^*$ respectively the density, mean velocity and temperature associated with f , in the sense that

$$\int_{\mathbb{R}^3} f(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \, dv = \begin{pmatrix} \rho \\ \rho u \\ 3\rho T + \rho|u|^2 \end{pmatrix}. \quad (6.12)$$

We also define the minimal directional temperature of f ,

$$T_*(f) := \frac{1}{\rho} \inf_{e \in \mathbb{S}^2} \int_{\mathbb{R}^3} f(v) (v \cdot e)^2 \, dv, \quad (6.13)$$

as well as the so-called Fermi temperature associated with ρ and $\varepsilon > 0$,

$$T_F(\rho, \varepsilon) := \frac{1}{2} \left(\frac{3\varepsilon\rho}{4\pi} \right)^{\frac{2}{3}}, \quad (6.14)$$

and the ratio

$$\gamma := \frac{T}{T_F(\rho, \varepsilon)}, \quad (6.15)$$

with the convention $\gamma = +\infty$ when $\varepsilon = 0$. The adimensional number γ is thus the ratio between the actual temperature of the system and its Fermi temperature. In [123], Lu proved that

$$1 - \varepsilon f \geq 0 \implies \gamma \geq \frac{2}{5}, \quad (6.16)$$

as well as, for any fixed $\varepsilon > 0$,

$$\left(1 - \varepsilon f \geq 0 \text{ and } \gamma = \frac{2}{5} \right) \iff f \equiv F_\varepsilon^\rho := \varepsilon^{-1} \mathbf{1}_{|\cdot - u| \leq \left(\frac{3\varepsilon\rho}{4\pi}\right)^{\frac{1}{3}}}, \quad (6.17)$$

$\left(1 - \varepsilon f \geq 0 \text{ and } \gamma > \frac{2}{5}\right) \iff$ there exists a unique ε -Fermi-Dirac distribution $\mathcal{M}_\varepsilon^f$ such that (6.18)

$$\int_{\mathbb{R}^3} \mathcal{M}_\varepsilon^f(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = \begin{pmatrix} \rho \\ \rho u \\ 3\rho T + \rho|u|^2 \end{pmatrix},$$

where we recall that the ε -Fermi-Dirac distributions are the ones which are such that $\varphi_\varepsilon(\mathcal{M}_\varepsilon^f)$ is a Maxwellian distribution. Equivalently, ε -Fermi-Dirac distributions are the distributions defined by

$$\mathcal{M}_\varepsilon^f(v) = \frac{e^{a_\varepsilon + b_\varepsilon|v - u_\varepsilon|^2}}{1 + \varepsilon e^{a_\varepsilon + b_\varepsilon|v - u_\varepsilon|^2}}, \quad a_\varepsilon \in \mathbb{R}, u_\varepsilon \in \mathbb{R}^3, b_\varepsilon < 0. \quad (6.19)$$

In particular, a *characterisation* of the Fermi-Dirac (or of the Maxwellian, when $\varepsilon = 0$) distribution $\mathcal{M}_\varepsilon^f$ is that $\log \circ \varphi_\varepsilon(\mathcal{M}_\varepsilon^f)$ is a linear combination of $v \mapsto 1$, $v \mapsto v$ and $v \mapsto |v|^2$ (that is, of the conserved quantities). The interested reader shall find further discussions on this matter in Appendix 6.B.

As proven in [123], F_ε^ρ and $\mathcal{M}_\varepsilon^f$ are the only two possible equilibria of the (spatially homogeneous) BFD dynamic (6.1). Contrary to $\mathcal{M}_\varepsilon^f$ (called first equilibrium in [123]), which is an attractor, the distribution F_ε^ρ (called second equilibrium in [123]) is not, and corresponds to a degenerate state, which can actually occur for very cold gases (note that (6.16)–(6.17) imply that F_ε^ρ is of “lowest” temperature).

From now on, we denote by M^g the Maxwellian distribution associated with a distribution g , in the sense that

$$M^g \equiv \mathcal{M}_0^g.$$

6.1.3 Fermi-Dirac entropy

We now define the ε -entropy of the distribution f .

Definition 6.1. We define, for any $\varepsilon \geq 0$ and $x \in \mathbb{R}_+$ such that $1 - \varepsilon x \geq 0$,

$$\Phi_\varepsilon(x) := \int_0^x \log \varphi_\varepsilon(y) dy, \quad (6.20)$$

where φ_ε is defined in (6.6). The function Φ_ε is well-defined as $\log \in L_{loc}^1(\mathbb{R}_+)$. For any nonnegative $f, g \in L_2^1(\mathbb{R}^3)$ such that $1 - \varepsilon f \geq 0$ and $1 - \varepsilon g \geq 0$, we define the ε -entropy of f by

$$H_\varepsilon(f) := \int_{\mathbb{R}^3} \Phi_\varepsilon(f)(v) dv, \quad (6.21)$$

as well as the relative ε -entropy of f and g by

$$H_\varepsilon[f|g] := H_\varepsilon(f) - H_\varepsilon(g). \quad (6.22)$$

Remark 6.1. Our definition of entropy slightly differs from the usual ones, but is actually equivalent in the problems that we consider. We choose to define the entropy with (6.20)–(6.21) because, our study relying on a Taylor expansion, it is here the more natural definition. Let us detail the link between the ε -entropy and usual definitions.

- **Classical entropy.** If $\varepsilon = 0$, then $\Phi_0(x) = x \log x - x$ with the convention $0 \log 0 = 0$, the condition $1 - \varepsilon f \geq 0$ is always satisfied, and

$$H_0(f) = \int_{\mathbb{R}^3} (f \log f - f) \, dv.$$

Note that often (consider for instance [157]), the classical entropy is defined by

$$\tilde{H}_0(f) = \int_{\mathbb{R}^3} f \log f \, dv \equiv \int_{\mathbb{R}^3} \tilde{\Phi}_0(f) \, dv,$$

with $\tilde{\Phi}_0(x) = x \log x$.

- **Fermi-Dirac entropy.** If $\varepsilon > 0$, then $\Phi_\varepsilon(x) = x \log x + \varepsilon^{-1}(1 - \varepsilon x) \log(1 - \varepsilon x)$ with the convention $0 \log 0 = 0$, and the condition $1 - \varepsilon f \geq 0$ is satisfied if and only if $f \leq \varepsilon^{-1}$. In this case, we have

$$H_\varepsilon(f) = \int_{\mathbb{R}^3} f \log f + \varepsilon^{-1}(1 - \varepsilon f) \log(1 - \varepsilon f) \, dv.$$

Note that for instance in [4] (up to a minus sign, which is just a choice of convention), the Fermi-Dirac entropy is defined by

$$\tilde{H}_\varepsilon(f) = \varepsilon^{-1} \int_{\mathbb{R}^3} (\varepsilon f) \log(\varepsilon f) + (1 - \varepsilon f) \log(1 - \varepsilon f) \, dv \equiv \int_{\mathbb{R}^3} \tilde{\Phi}_\varepsilon(f) \, dv,$$

with $\tilde{\Phi}_\varepsilon(x) = \varepsilon^{-1}(\varepsilon x \log(\varepsilon x) + (1 - \varepsilon x) \log(1 - \varepsilon x))$.

As we are only interested in the relative (Classical of Fermi-Dirac) entropy between f and its associated equilibrium distribution $\mathcal{M}_\varepsilon^f$ (defined in (6.18)), we see in the following Proposition 6.1 that only Φ_ε'' is actually relevant to the definition. From $\tilde{\Phi}_\varepsilon'' = \Phi_\varepsilon''$, we then obtain $\tilde{H}_\varepsilon[f|\mathcal{M}_\varepsilon^f] = H_\varepsilon[f|\mathcal{M}_\varepsilon^f]$, ensuring the announced equivalence.

Proposition 6.1. For any $\varepsilon \geq 0$ and nonnegative $f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq 0$ and either $\gamma > \frac{2}{5}$ if $\varepsilon > 0$ or $f \in L \log L(\mathbb{R}^3)$ if $\varepsilon = 0$, denoting by $\mathcal{M}_\varepsilon^f$ the Fermi-Dirac (or Maxwellian if $\varepsilon = 0$) distribution associated with f , we have the following representation of the relative ε -entropy between f and $\mathcal{M}_\varepsilon^f$,

$$H_\varepsilon[f|\mathcal{M}_\varepsilon^f] = \int_0^1 (1 - \tau) \left[\int_{\mathbb{R}^3} (f - \mathcal{M}_\varepsilon^f)^2 \Phi_\varepsilon'' \left((1 - \tau)\mathcal{M}_\varepsilon^f + \tau f \right) \, dv \right] \, d\tau \quad (6.23)$$

$$= \int_{\mathbb{R}^3} \int_{\mathcal{M}_\varepsilon^f(v)}^{f(v)} \frac{f(v) - x}{\varphi_\varepsilon(x)} \varphi_\varepsilon'(x) \, dx \, dv. \quad (6.24)$$

It holds that

$$H_\varepsilon[f|\mathcal{M}_\varepsilon^f] \geq 0 \quad \text{and} \quad (H_\varepsilon[f|\mathcal{M}_\varepsilon^f] = 0 \iff f = \mathcal{M}_\varepsilon^f). \quad (6.25)$$

The reader will find the proof of (6.23) and (6.25) in Appendix 6.B - see Proposition 6.15. We just point out here that this comes straightforwardly from a Taylor expansion of the function Φ_ε , and that (6.25) is a direct consequence of (6.23) because $\Phi_\varepsilon'' > 0$ on $(0, \varepsilon^{-1})$. Equation (6.24) comes directly from $\Phi_\varepsilon'' = \frac{\varphi_\varepsilon'}{\varphi_\varepsilon}$ and the change of variable, for fixed v , $x = (1 - \tau)\mathcal{M}_\varepsilon^f(v) + \tau f(v)$ inside (6.23).

Remark 6.2. We point out that for any $0 < x < \varepsilon^{-1}$, we have

$$\Phi_\varepsilon''(x) = \frac{\varphi_\varepsilon'(x)}{\varphi_\varepsilon(x)} = \frac{1}{x(1-\varepsilon x)}.$$

Hence for any $\tau \in (0, 1)$, $(1-\tau)\mathcal{M}_\varepsilon^f + \tau f \in (0, \varepsilon^{-1})$, and $\Phi_\varepsilon''((1-\tau)\mathcal{M}_\varepsilon^f + \tau f)$ is thus well-defined.

Moreover, with $\varepsilon = 0$ (Classical case), Equations (6.23)–(6.24) write

$$H_0[f|M^f] = \int_0^1 (1-\tau) \left[\int_{\mathbb{R}^3} \frac{(f-M^f)^2}{(1-\tau)M^f + \tau f} dv \right] d\tau \quad (6.26)$$

$$= \int_{\mathbb{R}^3} \int_{M^f(v)}^{f(v)} \frac{f(v)-x}{x} dx dv. \quad (6.27)$$

6.1.4 Entropy production

We finally define the entropy production \mathcal{D}_ε of the BFD operator by

$$\mathcal{D}_\varepsilon(f) := - \int_{\mathbb{R}^3} \log \varphi_\varepsilon(f) Q_\varepsilon(f, f)(v) dv. \quad (6.28)$$

We get, taking $\psi = \log \varphi_\varepsilon(f)$ in (6.9),

$$\mathcal{D}_\varepsilon(f) = \frac{1}{4} \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} \left[\varphi_\varepsilon(f)' \varphi_\varepsilon(f)'_* - \varphi_\varepsilon(f) \varphi_\varepsilon(f)_* \right] \log \left(\frac{\varphi_\varepsilon(f)' \varphi_\varepsilon(f)'_*}{\varphi_\varepsilon(f) \varphi_\varepsilon(f)_*} \right) B_\varepsilon^f d\sigma dv dv_* \geq 0. \quad (6.29)$$

Formally, a solution f to the BFD equation (6.1) satisfies

$$\frac{d}{dt} H_\varepsilon(f(t, \cdot)) = -\mathcal{D}_\varepsilon(f(t, \cdot)),$$

or, using the relative entropy,

$$\frac{d}{dt} H_\varepsilon[f(t, \cdot) | \mathcal{M}_\varepsilon^{f^{in}}] = -\mathcal{D}_\varepsilon(f(t, \cdot)). \quad (6.30)$$

The nonnegativity of \mathcal{D}_ε then ensures the second principle of thermodynamics.

6.1.5 Trend to equilibrium and Cercignani's conjecture

The relative entropy between a solution at a given time t and its associated equilibrium is a very useful quantity to estimate how close to equilibrium the system is, and (6.25) in Proposition 6.1 makes it a suitable tool into proving convergence towards equilibrium. Indeed, if one shows for some solution f that

$$H_\varepsilon[f(t, \cdot) | \mathcal{M}_\varepsilon^{f^{in}}] \xrightarrow{t \rightarrow \infty} 0,$$

then the Csiszár-Kullback-Pinsker (CKP) inequalities, discussed below in Proposition 6.4 and Section 6.6 yield

$$\|f(t, \cdot) - \mathcal{M}_\varepsilon^{f^{in}}\|_{L^1_2} \xrightarrow{t \rightarrow \infty} 0,$$

with a rate of convergence related to the one of the relative entropy. In the study of large-time behaviour of the solutions to the (Classical or Fermi-Dirac) Boltzmann equation, the relative entropy is thus a major tool. The idea of entropy-entropy production methods is to prove an inequality of the type

$$\mathcal{D}_\varepsilon(f) \geq \Theta(H_\varepsilon[f|\mathcal{M}_\varepsilon^f]),$$

for some suitable function Θ (typically, a linear or power law function), allowing to obtain, combined with (6.30) and using a Grönwall-type argument, an explicit rate of the convergence towards 0 of the relative entropy - thus of the L_2^1 distance, using the CKP inequality.

In the early 80's, Cercignani conjectured in [59], *in the context of the Classical Boltzmann equation* with suitable collision kernels, that for any distribution f , there exists some $\lambda > 0$ depending only on density, temperature and upper bound on the entropy of f (this is called the strong form of Cercignani's conjecture) such that

$$\mathcal{D}_0(f) \geq \lambda \rho H_0[f|M^f],$$

where we recall that ρ is the density associated with f , \mathcal{D}_0 is the entropy production in the classical case, H_0 the classical entropy and M^f the Maxwellian associated with f . It is now known that this is false in general (see the negative result of Bobylev and Cercignani [31]), however Villani proved in [157] the strong form of this conjecture when the collision kernel B is "super-quadratic", as well as a weak form $\mathcal{D}_0(f) \geq C(f) H_0[f|M^f]^{1+\delta}$, holding for all $\delta > 0$, for general collision kernels (and $C(f)$ depending on various quantities related to f). We mention the cornerstone papers of Toscani and Villani [153, 152] on this topic, and refer the reader to [77] for a review of Cercignani's conjecture results for the Boltzmann and Landau equations.

Similar ideas hold in the study of the Landau equation (we shall talk about Cercignani's conjecture for the Landau equation), this topic is further addressed in Section 6.5.

The motivation of this work is to provide Cercignani's conjecture type results in the case of the Boltzmann-Fermi-Dirac equation, uniformly with respect to $\varepsilon > 0$.

The simple yet fundamental idea which is at the root of this work is the fact that, whenever $\varepsilon > 0$, assuming $1 - \varepsilon f \geq \kappa_0$ for some $\kappa_0 \in (0, 1)$ straightforwardly implies

$$B(v, v_*, \sigma) \geq B_\varepsilon^f(v, v_*, \sigma) \geq \kappa_0^4 B(v, v_*, \sigma),$$

so that, as log is nonincreasing,

$$\mathcal{D}_0(\varphi_\varepsilon(f)) \geq \mathcal{D}_\varepsilon(f) \geq \kappa_0^4 \mathcal{D}_0(\varphi_\varepsilon(f)). \quad (6.31)$$

Therefore, relatively to κ_0 , the quantity $\mathcal{D}_\varepsilon(f)$ (the Fermi-Dirac entropy production associated with f) behaves like $\mathcal{D}_0(\varphi_\varepsilon(f))$ (the Classical entropy production associated with $\varphi_\varepsilon(f)$). Our main results, Theorem 6.1 and Proposition 6.2, allow to state a similar property for the relative entropies. We find that, relatively to κ_0 , the quantity $H_\varepsilon[f|\mathcal{M}_\varepsilon^f]$ (the Fermi-Dirac relative-entropy between f and $\mathcal{M}_\varepsilon^f$) behaves like $H_0[\varphi_\varepsilon(f)|M^{\varphi_\varepsilon(f)}]$ (the Classical relative entropy between $\varphi_\varepsilon(f)$ and $M^{\varphi_\varepsilon(f)}$). This entails that **any entropy-entropy production inequality in the Classical case yields the same inequality** (with an almost identical constant) **in the Fermi-Dirac case**; this corresponds to Corollary 6.3 (and Proposition 6.8 for the Landau/Landau-Fermi-Dirac adaptation). The same holds for counter-examples to entropy-entropy production inequalities.

6.2 Main results

In this section, we state our main results.

6.2.1 Comparison of the Fermi-Dirac and Classical relative entropies

Theorem 6.1 is the main contribution of this work, as it establishes a strong link between the different entropies, allowing to transfer “positive” Cercignani's conjecture results from the classical to the fermionic case.

Theorem 6.1. Lower-bound inequality. *For any $\varepsilon > 0$ and nonnegative $f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that*

$$1 - \varepsilon f > 0 \quad \text{and} \quad \frac{f}{1 - \varepsilon f} \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3),$$

we have

$$H_0 \left[\frac{f}{1 - \varepsilon f} \middle| M^{\frac{f}{1 - \varepsilon f}} \right] \geq H_\varepsilon[f | \mathcal{M}_\varepsilon^f]. \quad (6.32)$$

The hypotheses of Theorem 6.1 are actually the minimal ones to ensure that every term in (6.32) makes sense. The following Proposition 6.2 allows to transfer “negative” Cercignani's conjecture results from the classical to the fermionic case.

Proposition 6.2. Upper-bound inequality. *For any $\kappa_0 \in (0, 1)$, any $\varepsilon > 0$ and nonnegative $f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that*

$$1 - \varepsilon f \geq \kappa_0, \quad (6.33)$$

we have

$$H_0 \left[\frac{f}{1 - \varepsilon f} \middle| M^{\frac{f}{1 - \varepsilon f}} \right] \leq C_0(\kappa_0) H_\varepsilon[f | \mathcal{M}_\varepsilon^f], \quad (6.34)$$

with $C_0(\kappa_0) = \exp(16(\kappa_0^{-1} - 1))$.

Remark 6.3. *Inequality (6.32) becomes reversed in the Bose-Einstein case. We refer the interested reader to Proposition 6.12 in Appendix 6.A. In fact, we expect that both inequalities, but reversed (and probably with a different constant C_0), hold in the Bose-Einstein case, as the core of the proof would be the exact same in this case, only changing ε into $-\varepsilon$ (hence the reversal of the inequalities).*

6.2.2 Entropy-entropy production inequalities for the Boltzmann-Fermi-Dirac (BFD) equation

As a corollary to Theorem 6.1 and Proposition 6.2, adapting the main results found in Villani [157], we obtain the following entropy-entropy production estimates.

Corollary 6.3. • Cercignani's conjecture result for the BFD operator with super-quadratic kernels (adaptation of [157, Theorem 2.1]). *Assume that B satisfies (6.4) and*

$$B(v, v_*, \sigma) \geq 1 + |v - v_*|^2.$$

Then, for any $\kappa_0 \in (0, 1)$, $\varepsilon \geq 0$ and nonnegative $f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq \kappa_0$, we have

$$\mathcal{D}_\varepsilon(f) \geq K(f) H_\varepsilon[f|\mathcal{M}_\varepsilon^f], \quad (6.35)$$

with

$$K(f) = \frac{2\pi}{7} \kappa_0^5 \min(1, T) \rho T_*(f), \quad (6.36)$$

where $\rho, T, T_*(f)$ are defined in (6.12)–(6.13), $\mathcal{D}_\varepsilon, H_\varepsilon$ and $\mathcal{M}_\varepsilon^f$ are given respectively in (6.28)–(6.29), (6.21)–(6.22) and (6.18) (note that $T_*(f)$ can be bounded below using the entropy or an L^∞ bound [78, Proposition 2]).

• **Super-linear Cercignani’s conjecture result for the BFD operator with general kernels** (adaptation of [157, Theorem 4.1]). Assume the existence of $B_0 > 0$ and $\beta_+, \beta_- \geq 0$ such that

$$B(v, v_*, \sigma) \geq B_0 \min(|v - v_*|^{\beta_+}, |v - v_*|^{-\beta_-}), \quad (6.37)$$

and B satisfies (6.4). We consider $\kappa_0 \in (0, 1)$, $0 \leq f \in L_2^1(\mathbb{R}^3) \setminus \{0\}$ and $\varepsilon \geq 0$ such that $1 - \varepsilon f \geq \kappa_0$ and

$$\forall v \in \mathbb{R}^3, \quad f(v) \geq K_0 e^{-A_0|v|^{q_0}} \quad (K_0 > 0, \quad A_0 > 0, \quad q_0 \geq 2). \quad (6.38)$$

Then for any $\alpha \in (0, 1)$ there exists an explicit constant $K_\alpha(f)$ depending on α, B_0 , an upper bound of ε and on f only through ρ, T, q_0 , and upper bounds on $A_0, 1/K_0, 1/\kappa_0, \|f\|_{L_s^1}$ and $\|f\|_{H^k}$, where $s = s(\alpha, q_0, \beta_-, \beta_+)$ and $k = k(\alpha, s, \beta_-, \beta_+)$, such that

$$\mathcal{D}_\varepsilon(f) \geq K_\alpha(f) H_\varepsilon[f|\mathcal{M}_\varepsilon^f]^{1+\alpha}. \quad (6.39)$$

• **Counter-example to Cercignani’s conjecture for the BFD operator with sub-quadratic kernels** (weak adaptation of [31] and [157, Theorem 1.1]). Assume that B satisfies (6.4) and that there exists $B_0 > 0$ and $0 \leq \beta < 2$ such that

$$\int_{\mathbb{S}^2} B(v, v_*, \sigma) d\sigma \leq B_0 (1 + |v - v_*|^\beta).$$

Then for any $\varepsilon \in (0, \frac{1}{2})$, we have

$$\inf \left\{ \frac{\mathcal{D}_\varepsilon(f)}{H_\varepsilon[f|\mathcal{M}_\varepsilon^f]} \mid f \in \mathcal{C}_{1,0,1}^\varepsilon \text{ and } f(v) \geq \frac{1}{2} (2\pi)^{-3/2} e^{-|v|^2}, \quad v \in \mathbb{R}^3 \right\} = 0,$$

with

$$f \in \mathcal{C}_{1,0,1}^\varepsilon \iff 0 \leq f \in L_2^1(\mathbb{R}^3), \quad 1 - \varepsilon f \geq 0, \quad 1 \leq \rho \leq 1 + 2\varepsilon, \quad |u| \leq 4\sqrt{3}\varepsilon, \quad \frac{1}{1 + 2\varepsilon} \leq T \leq 1 + 2\varepsilon.$$

We recall that ρ, u and T are defined in (6.12). The last part of the corollary (the counter-example) is a weak version of [31, Theorem 1], due to the presence of $\mathcal{C}_{1,0,1}^\varepsilon$ instead of the more expected $\mathcal{C}_{1,0,1}^0$ (the set of normalized functions) and the lack of a condition on the $\|\cdot\|_{L_s^1}$ and $\|\cdot\|_{H^k}$ norms. One could probably replace $\mathcal{C}_{1,0,1}^\varepsilon$ by $\mathcal{C}_{1,0,1}^0$ and add the $\|\cdot\|_{L_s^1}$ and $\|\cdot\|_{H^k}$ conditions with further technical work.

6.2.3 About the Csiszár-Kullback-Pinsker inequality

The Csiszár-Kullback-Pinsker (CKP) inequality is a well-known link between the total variation distance of two probability measures and their relative entropy, which is often used to transform a convergence

in relative entropy into a convergence in an actual norm, such as L^1 or L^1_2 . In conducting our study, we were led to prove Proposition 6.4 (or the optimal Proposition 6.10), which are generalizations of the CKP inequality.

A generalization of the CKP inequality allowing for a weight in the total variation distance, called "weighted Csiszár-Kullback-Pinsker inequalities" was already provided by Bolley and Villani in [33, Theorem 2.1]. However our inequality does differ from theirs. On the one hand, as far as drawbacks are concerned, we need the reference measure to be an equilibrium distribution while it is not the case in [33], and our constant depends on f while it doesn't in the inequality in [33]. On the other hand, for the improvements, our constant seems more precise and a great deal smaller (possibly the constant in Proposition 6.10 is optimal), in the sense that choosing a weight equal to $|v|^\alpha$ with $\alpha > 2$ yields a finite constant in our case but an infinite one in [33, Theorem 2.1]. In particular, remark that by Jensen's inequality, $\|M \varpi^2\|_{L^1} \leq \log \int e^{\varpi^2} M \, dv$.

In another direction, in the study of the Vlasov-Poisson system, Cáceres et al. provided a generalization of the CKP inequality to L^p norms with $1 \leq p \leq 2$ in [55, Proposition 3.1] (specifically in the note [54]) for various different entropies, which formulation and proof is quite close to our result. However, as far as the standard entropy is concerned, their result works only for $p = 1$, is without weights, and their constant is not optimal. I am not aware of other such generalizations of the CKP inequality in the literature.

Finally, the main idea of our proof of this inequality was already present in Jüngel's [111, proof of Theorem A.2], and he also proposed a generalization in [111, Theorem A.3], which differs from ours and holds for the L^1 norm.

In the following Proposition 6.4 (and in Proposition 6.10 in Section 6.6), we propose an extension the CKP inequality to weighted L^p distances for $p \in [1, 2]$, as well as to other entropies than the Classical entropy (typically, the Fermi-Dirac and the Bose-Einstein entropies), which could be seen as a extension of the previously mentioned three generalizations. We denote this extension by L^1 - L^2 weighted Csiszár-Kullback-Pinsker inequality.

We moreover wish to highlight the fact that the proof of these inequalities, which is the same as in [111, Theorem A.2], but with the addition of weights and of considering L^p , $1 \leq p \leq 2$, relies on a Hölder inequality. In particular, our proof of the original CKP inequality relies on a Taylor expansion and a Cauchy-Schwarz argument, instead of the tricky inequality (see for instance [88]) $x \log x - x + 1 \geq \frac{3}{2} \times \frac{(x-1)^2}{x+2}$.

For the sake of readability, we present hereafter a simplified non-optimal version of the proposition, and refer the reader to Section 6.6 for the refined and more general version of it, where it is also extended to the Bose-Einstein case and further discussed. We also extend it to a broader class of general entropies (Φ -entropies in the text) in Proposition 6.16 of Appendix 6.B.

Proposition 6.4. *L^1 - L^2 weighted Csiszár-Kullback-Pinsker inequality related to the Classical and Fermi-Dirac relative entropies. [simplified]*

Let $\varpi : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ be measurable, and $r \in [1, 2]$.

• **Classical CKP inequality.** For any $0 \leq f \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3) \setminus \{0\}$, assuming that the norms below are finite, it holds

$$\left\| (f - M^f) \varpi \right\|_{L^r}^2 \leq 2 \max \left(\left\| M^f \varpi^2 \right\|_{L^{\frac{r}{2-r}}}, \left\| f \varpi^2 \right\|_{L^{\frac{r}{2-r}}} \right) H_0[f|M^f], \quad (6.40)$$

where M^f is the Maxwellian associated with f .

• **Fermi-Dirac CKP inequality.** For any $\varepsilon > 0$ and $0 \leq f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq 0$ and $\gamma > \frac{2}{5}$, assuming that the norms below are finite,

$$\left\| (f - \mathcal{M}_\varepsilon^f) \varpi \right\|_{L^r}^2 \leq 2 \max \left(\left\| \mathcal{M}_\varepsilon^f \varpi^2 \right\|_{L^{\frac{r}{2-r}}}, \left\| f \varpi^2 \right\|_{L^{\frac{r}{2-r}}} \right) H_\varepsilon[f | \mathcal{M}_\varepsilon^f], \quad (6.41)$$

where $\mathcal{M}_\varepsilon^f$ is the ε -Fermi-Dirac distribution associated with f .

In the above proposition, when $r = 2$, $L^{\frac{r}{2-r}}$ should be understood as L^∞ .

6.2.4 Convergence towards equilibrium

A result like Corollary 6.3 constitutes the core of the proof of convergence towards equilibrium of solutions to the Boltzmann-Fermi-Dirac equation, based on an entropy method. The proof is then complete provided that the solution satisfies a variety of bounds. This is addressed in Chapter 7.¹

Proposition 6.5. Let $\varepsilon > 0$ and $f^{in} \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that $0 \leq f^{in} \leq \varepsilon^{-1}$. We consider a collision kernel B satisfying the symmetry and micro-reversibility assumptions, thus having the form (6.4), as well as, for some $B_0 > 0$ and $\beta^+, \beta^- \geq 0$,

$$B(|v - v_*|, \cos \theta) \geq B_0 \min \left(|v - v_*|^{\beta^+}, |v - v_*|^{-\beta^-} \right).$$

We assume the existence of a solution $f \equiv f(t, v)$ to the spatially homogeneous Boltzmann-Fermi-Dirac equation (6.1) associated with the quantum parameter ε , the collision kernel B and the initial distribution f^{in} . Assume that there exists an explicit time $t_0 > 0$ depending only on ε , B and f^{in} such that

- $\exists \kappa_0 \in (0, 1)$ depending only on ε , B and f^{in} such that $1 - \varepsilon f(t, v) \geq \kappa_0$ for any $(t, v) \in [t_0, +\infty) \times \mathbb{R}^3$,
- $\exists K_0, A_0 > 0$ depending only on ε , B and f^{in} such that $f(t, v) \geq K_0 e^{-A_0 |v|^2}$ for any $(t, v) \in [t_0, +\infty) \times \mathbb{R}^3$,
- $\forall k, l \in \mathbb{N}$, there exist $C_k, \tilde{C}_l > 0$ depending only on ε , B and f^{in} such that $\sup_{t \geq t_0} \|f(t, \cdot)\|_{L^1_k} \leq C_k$ and $\sup_{t \geq t_0} \|f(t, \cdot)\|_{H^l} \leq \tilde{C}_l$.

Then for any $p \geq 1$, $l \geq 0$ and $\alpha > 0$ there exists an explicit constant $\mathbf{C}_{p,l,\alpha} > 0$ depending only on p, l, ε , B and f^{in} such that for any $t \geq t_0$,

$$\left\| f(t, \cdot) - \mathcal{M}_\varepsilon^{f^{in}} \right\|_{L^p_t} \leq \mathbf{C}_{p,l,\alpha} (1+t)^{-1/\alpha}. \quad (6.42)$$

Proof. The assumptions on the solution f allow to apply Corollary 6.3, more specifically Equation (6.39), yielding the fact that for any $t \geq t_0$ and $\alpha > 0$, there is an explicit constant $K_\alpha(f(t, \cdot))$ depending only on α , B_0 , an upper bound of ε and on $f(t, \cdot)$ only through ρ , T (its density and temperature, defined by (6.12)), and upper bounds on A_0 , $1/K_0$, $1/\kappa_0$, $\|f(t, \cdot)\|_{L^1_s}$ and $\|f(t, \cdot)\|_{H^k}$, where $s = s(\alpha, q_0, \beta_-, \beta_+)$ and $k = k(\alpha, s, \beta_-, \beta_+)$, such that

$$\mathcal{D}_\varepsilon(f(t, \cdot)) \geq K_\alpha(f(t, \cdot)) H_\varepsilon[f(t, \cdot) | \mathcal{M}_\varepsilon^{f(t, \cdot)}]^{1+\alpha}. \quad (6.43)$$

From our assumptions, we observe that $K_\alpha(f(t, \cdot))$ can be upper-bounded by a constant \hat{K}_α depending only on ε , B and f^{in} (in particular not on time t). Moreover, since f solves (6.1), we have for all $t \geq 0$

1. Cette phrase a été modifiée par rapport à [36].

that $\mathcal{M}_\varepsilon^{f(t,\cdot)} = \mathcal{M}_\varepsilon^{f^{in}}$ and, at least formally, that

$$\frac{d}{dt} H_\varepsilon[f(t,\cdot)|\mathcal{M}_\varepsilon^{f^{in}}] = -\mathcal{D}_\varepsilon(f(t,\cdot)).$$

Then (6.43) implies

$$\frac{d}{dt} H_\varepsilon[f(t,\cdot)|\mathcal{M}_\varepsilon^{f^{in}}] \leq -\hat{K}_\alpha H_\varepsilon[f(t,\cdot)|\mathcal{M}_\varepsilon^{f^{in}}]^{1+\alpha}.$$

Integrating this equation between t_0 and $t > t_0$ yields

$$H_\varepsilon[f(t,\cdot)|\mathcal{M}_\varepsilon^{f^{in}}] \leq \left(H_\varepsilon[f(t_0,\cdot)|\mathcal{M}_\varepsilon^{f^{in}}]^\alpha + \alpha \hat{K}_\alpha (t - t_0) \right)^{-1/\alpha}.$$

We then conclude that for any $t \geq t_0$, (even if $H_\varepsilon[f(t_0,\cdot)|\mathcal{M}_\varepsilon^{f^{in}}] = 0$, in which case $H_\varepsilon[f(t,\cdot)|\mathcal{M}_\varepsilon^{f^{in}}] = 0$)

$$H_\varepsilon[f(t,\cdot)|\mathcal{M}_\varepsilon^{f^{in}}] \leq \hat{C}_\alpha (1+t)^{-1/\alpha}, \quad (6.44)$$

where $\hat{C}_\alpha > 0$ is explicit and depends only on α, ε, B and f^{in} . Finally, we recall the CKP inequalities provided in Proposition 6.4, Equation (6.41) in the Fermi-Dirac context, for weighted L^1 norms, implying that for any $k \geq 0$ we have for any $t \geq t_0$

$$\left\| f(t,\cdot) - \mathcal{M}_\varepsilon^{f^{in}} \right\|_{L_k^1}^2 \leq 2 \max \left(\left\| \mathcal{M}_\varepsilon^{f^{in}} \right\|_{L_{2k}^1}, \left\| f(t,\cdot) \right\|_{L_{2k}^1} \right) H_\varepsilon[f(t,\cdot)|\mathcal{M}_\varepsilon^{f^{in}}].$$

Since by assumption $\left\| f(t,\cdot) \right\|_{L_{2k}^1} \leq C_{2k}$, we conclude that there exists an explicit C'_k depending only on ε, B and f^{in} such that

$$\left\| f(t,\cdot) - \mathcal{M}_\varepsilon^{f^{in}} \right\|_{L_k^1}^2 \leq C'_k H_\varepsilon[f(t,\cdot)|\mathcal{M}_\varepsilon^{f^{in}}] \leq C'_k \hat{C}_\alpha (1+t)^{-1/\alpha}.$$

Then (6.42) for the L_k^1 norm is finally obtained with $\mathbf{C}_{1,k,\alpha} = \sqrt{C'_k \hat{C}_\alpha}$ and L_l^p norms follow, as $\mathcal{M}_\varepsilon^{f^{in}} \in L^\infty(\mathbb{R}^3)$ and $f \in L^\infty(\mathbb{R}_+ \times \mathbb{R}^3)$. \square

6.3 Proof of Theorem 6.1 and Proposition 6.2

This section is devoted to the proof of Theorem 6.1 and Proposition 6.2. We make use of Proposition 6.1, which is later proven in Appendix 6.B - see Proposition 6.15.

6.3.1 Key element of the proof

The main argument in the proofs of Theorem 6.1 and Proposition 6.2 lies in the following proposition.

Proposition 6.6. *Let $0 \leq g \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3) \setminus \{0\}$ and define, for $\varepsilon \geq 0$,*

$$R_g(\varepsilon) := H_\varepsilon \left[\varphi_\varepsilon^{-1}(g) \middle| \mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}(g)} \right]. \quad (6.45)$$

Then $\varepsilon \mapsto R_g(\varepsilon)$ is \mathcal{C}^1 on \mathbb{R}_+^* , with, for any $\varepsilon > 0$,

$$R'_g(\varepsilon) = \int_{\mathbb{R}^3} \int_{M_\varepsilon(v)}^{g(v)} \frac{\partial_\varepsilon(\varphi_\varepsilon^{-1})(g(v)) - \partial_\varepsilon(\varphi_\varepsilon^{-1})(y)}{y} \mathbf{d}y \mathbf{d}v, \quad (6.46)$$

where we used the shorthand $M_\varepsilon = \varphi_\varepsilon(\mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}}(g))$.

The striking point of (6.46) lies in the fact that it immediately proves that, for any $\varepsilon > 0$, the global monotonicity of $x \mapsto \partial_\varepsilon(\varphi_\varepsilon^{-1})(x)$ translates into the same monotonicity of R_g at the point ε , as the integral in y in (6.46) is automatically nonnegative if $x \mapsto \partial_\varepsilon(\varphi_\varepsilon^{-1})(x)$ is nondecreasing, or nonpositive if $x \mapsto \partial_\varepsilon(\varphi_\varepsilon^{-1})(x)$ is nonincreasing. Moreover, this proposition generalises to any family of entropies and any conserved quantities (provided a suitable differentiability property for R_g), as all key arguments rely only the generic framework we present in Appendix 6.B, and the specificity of the Fermi-Dirac case is used only for the study of the differentiability of R_g .

Proof. Using the relative entropy representation (6.24) in Proposition 6.1, we have, for any $\varepsilon > 0$,

$$R_g(\varepsilon) = \int_{\mathbb{R}^3} \int_{\mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}}(g)(v)}^{\varphi_\varepsilon^{-1}(g(v))} (\varphi_\varepsilon^{-1}(g(v)) - x) \frac{\varphi'_\varepsilon(x)}{\varphi_\varepsilon(x)} \mathbf{d}x \mathbf{d}v.$$

Changing variables $y = \varphi_\varepsilon(x)$, with then $\mathbf{d}y = \varphi'_\varepsilon(x) \mathbf{d}x$ and $x = \varphi_\varepsilon^{-1}(y)$, we obtain

$$R_g(\varepsilon) = \int_{\mathbb{R}^3} \int_{M_\varepsilon(v)}^{g(v)} \frac{\varphi_\varepsilon^{-1}(g(v)) - \varphi_\varepsilon^{-1}(y)}{y} \mathbf{d}y \mathbf{d}v.$$

where we denoted $M_\varepsilon = \varphi_\varepsilon(\mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}}(g))$ for convenience of notations. We fix $v \in \mathbb{R}^3$ and set, for $(\varepsilon, z) \in (\mathbb{R}_+^*)^2$,

$$K(\varepsilon, z) := \int_z^{g(v)} \frac{\varphi_\varepsilon^{-1}(g(v)) - \varphi_\varepsilon^{-1}(y)}{y} \mathbf{d}y. \quad (6.47)$$

Note that if $g(v) = 0$ then $K(\varepsilon, z) = \varepsilon^{-1} \log(1 + \varepsilon z)$. The application K is clearly \mathcal{C}^1 on $(\mathbb{R}_+^*)^2$, and straightforward computations can provide that differentiation in ε under the integral in y is valid. We find that

$$\begin{aligned} \partial_\varepsilon K(\varepsilon, z) &= \int_z^{g(v)} \frac{\partial_\varepsilon(\varphi_\varepsilon^{-1}(g(v))) - \partial_\varepsilon(\varphi_\varepsilon^{-1}(y))}{y} \mathbf{d}y, \\ \partial_z K(\varepsilon, z) &= -\frac{\varphi_\varepsilon^{-1}(g(v)) - \varphi_\varepsilon^{-1}(z)}{z}. \end{aligned}$$

As a result of Lemma 6.21 in Appendix 6.C, the application $\varepsilon \mapsto M_\varepsilon(v)$ is \mathcal{C}^1 on \mathbb{R}_+^* (as a composition of \mathcal{C}^1 applications), hence so is $\varepsilon \mapsto K(\varepsilon, M_\varepsilon(v))$, and we have, for any $\varepsilon > 0$ and $v \in \mathbb{R}^3$,

$$\frac{\mathbf{d}}{\mathbf{d}\varepsilon} K(\varepsilon, M_\varepsilon(v)) = \int_{M_\varepsilon(v)}^{g(v)} \frac{\partial_\varepsilon(\varphi_\varepsilon^{-1})(g(v)) - \partial_\varepsilon(\varphi_\varepsilon^{-1})(y)}{y} \mathbf{d}y - (\partial_\varepsilon M_\varepsilon(v)) \frac{\varphi_\varepsilon^{-1}(g(v)) - \varphi_\varepsilon^{-1}(M_\varepsilon(v))}{M_\varepsilon(v)}. \quad (6.48)$$

Now note that

$$R'_g(\varepsilon) = \int_{\mathbb{R}^3} K(\varepsilon, M_\varepsilon(v)) \mathbf{d}v. \quad (6.49)$$

Then R_g is indeed \mathcal{C}^1 on \mathbb{R}_+^* , and differentiation under the integral is valid, if we can prove that for any $\varepsilon > 0$, there is a $\delta \in (0, \varepsilon)$ such that

$$\int_{\mathbb{R}^3} \sup_{\varepsilon_* \in (\varepsilon - \delta, \varepsilon + \delta)} \left| \frac{d}{d\varepsilon_*} K(\varepsilon_*, M_{\varepsilon_*}(v)) \right| dv < \infty. \quad (6.50)$$

For the sake of clarity, we continue our computations assuming (6.50) for now, and show (6.50) after we have obtained our claimed result (6.46).

Differentiating (6.49) in ε under the integral in v , using (6.48), yields for any $\varepsilon > 0$ (omitting to write the dependence in v for clarity)

$$R'_g(\varepsilon) = \int_{\mathbb{R}^3} \int_{M_\varepsilon}^g \frac{\partial_\varepsilon(\varphi_\varepsilon^{-1})(g) - \partial_\varepsilon(\varphi_\varepsilon^{-1})(y)}{y} dy dv - \int_{\mathbb{R}^3} (\partial_\varepsilon M_\varepsilon) \times \frac{\varphi_\varepsilon^{-1}(g) - \varphi_\varepsilon^{-1}(M_\varepsilon)}{M_\varepsilon} dv. \quad (6.51)$$

Now remark that

$$\frac{\partial_\varepsilon M_\varepsilon}{M_\varepsilon} = \partial_\varepsilon \left(\log \circ \varphi_\varepsilon \left(\mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}(g)} \right) \right). \quad (6.52)$$

Since $\mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}(g)}$ is a Fermi-Dirac statistics, we have, denoting its coefficients by a_ε , u_ε and b_ε (as in (6.19)), that for any $v \in \mathbb{R}^3$,

$$\log \circ \varphi_\varepsilon \left(\mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}(g)} \right) (v) = \alpha_\varepsilon + \beta_\varepsilon \cdot v + b_\varepsilon |v|^2, \quad (6.53)$$

where $\alpha_\varepsilon = a_\varepsilon + b_\varepsilon |u_\varepsilon|^2$ and $\beta_\varepsilon = -2b_\varepsilon u_\varepsilon$. Lemma 6.21 in Appendix 6.C ensures that the application $\varepsilon \mapsto (a_\varepsilon, u_\varepsilon, b_\varepsilon)$ is \mathcal{C}^1 on \mathbb{R}_+^* , hence so is the above expression pointwise in v , and we conclude that $\frac{\partial_\varepsilon M_\varepsilon}{M_\varepsilon}$ is a linear combination of the functions $v \mapsto 1$, $v \mapsto v$ and $v \mapsto |v|^2$. By construction, $\varphi_\varepsilon^{-1}(g)$ and $\varphi_\varepsilon^{-1}(M_\varepsilon) = \mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}(g)}$ share the same normalization in $v \mapsto 1$, $v \mapsto v$ and $v \mapsto |v|^2$, hence

$$\int_{\mathbb{R}^3} (\varphi_\varepsilon^{-1}(g) - \varphi_\varepsilon^{-1}(M_\varepsilon)) \frac{\partial_\varepsilon M_\varepsilon}{M_\varepsilon} dv = 0,$$

and (6.51) becomes the announced (6.46).

We now show (6.50), ensuring the validity of the differentiation in ε under the integral in Equation (6.49), by dominated convergence. The previous computations imply that for any $\varepsilon > 0$,

$$\left| \frac{d}{d\varepsilon} K(\varepsilon, M_\varepsilon(v)) \right| \leq \left| \int_{M_\varepsilon}^g \frac{\partial_\varepsilon(\varphi_\varepsilon^{-1})(g) - \partial_\varepsilon(\varphi_\varepsilon^{-1})(y)}{y} dy \right| + \left| \frac{\partial_\varepsilon M_\varepsilon}{M_\varepsilon} (\varphi_\varepsilon^{-1}(g) - \varphi_\varepsilon^{-1}(M_\varepsilon)) \right|.$$

On the one hand, using (6.52)–(6.53), we get, for any $v \in \mathbb{R}^3$,

$$\begin{aligned} \left| \frac{\partial_\varepsilon M_\varepsilon}{M_\varepsilon} (\varphi_\varepsilon^{-1}(g) - \varphi_\varepsilon^{-1}(M_\varepsilon)) \right| &\leq (|\partial_\varepsilon \alpha_\varepsilon| + |\partial_\varepsilon \beta_\varepsilon| + |\partial_\varepsilon b_\varepsilon|) (1 + |v|^2) |\varphi_\varepsilon^{-1}(g(v)) - \varphi_\varepsilon^{-1}(M_\varepsilon(v))| \\ &\leq (|\partial_\varepsilon \alpha_\varepsilon| + |\partial_\varepsilon \beta_\varepsilon| + |\partial_\varepsilon b_\varepsilon|) (1 + |v|^2) \{g(v) + M_\varepsilon(v)\}, \end{aligned}$$

where for the last inequality, we used the inequalities $|x - y| \leq x + y$ and $\varphi_\varepsilon^{-1}(x) \leq x$ for $x, y \geq 0$.

On the other hand, remarking that

$$\forall x \geq 0, \quad \partial_\varepsilon(\varphi_\varepsilon^{-1})(x) = \partial_\varepsilon\left(\frac{x}{1+\varepsilon x}\right) = -\left(\frac{x}{1+\varepsilon x}\right)^2 = -\varphi_\varepsilon^{-1}(x)^2, \quad (6.54)$$

we obtain, as $x \mapsto \varphi_\varepsilon^{-1}(x)^2$ is increasing,

$$\left| \int_{M_\varepsilon}^g \frac{\partial_\varepsilon(\varphi_\varepsilon^{-1})(g) - \partial_\varepsilon(\varphi_\varepsilon^{-1})(y)}{y} \, dy \right| = \int_{M_\varepsilon}^g \frac{\varphi_\varepsilon^{-1}(g)^2 - \varphi_\varepsilon^{-1}(y)^2}{y} \, dy.$$

In the last equation, as well as in the four following ones, we omit writing the dependence of g and M_ε in v for clarity. From the identity $|x^2 - y^2| = (x+y)|x-y|$, for $x, y \geq 0$, the fact that $\|\varphi_\varepsilon^{-1}\|_\infty = \varepsilon^{-1}$ and that φ_ε^{-1} is increasing, we get

$$\int_{M_\varepsilon}^g \frac{\varphi_\varepsilon^{-1}(g)^2 - \varphi_\varepsilon^{-1}(y)^2}{y} \, dy \leq 2\varepsilon^{-1} \int_{M_\varepsilon}^g \frac{\varphi_\varepsilon^{-1}(g) - \varphi_\varepsilon^{-1}(y)}{y} \, dy,$$

which, using the bound $|\varphi_\varepsilon^{-1}(x) - \varphi_\varepsilon^{-1}(y)| \leq |x-y|$ for $x, y \geq 0$ and $\varepsilon > 0$, is less than

$$2\varepsilon^{-1} \int_{M_\varepsilon}^g \frac{g-y}{y} \, dy.$$

By direct integration, the latter equals

$$2\varepsilon^{-1} (g \log g - g \log M_\varepsilon - g + M_\varepsilon),$$

which, recalling that $M_\varepsilon(v) = \exp(a_\varepsilon + |v - u_\varepsilon|^2)$ and $g \geq 0$, is itself less than

$$2\varepsilon^{-1} (g \log g - a_\varepsilon g + M_\varepsilon).$$

All in all, as $-a_\varepsilon g \leq |a_\varepsilon|g$, we have for any $\varepsilon > 0$ and $v \in \mathbb{R}^3$ that

$$\left| \frac{d}{d\varepsilon} K(\varepsilon, M_\varepsilon(v)) \right| \leq 2\varepsilon^{-1} \{g \log g(v) + |a_\varepsilon|g(v) + M_\varepsilon(v)\} + (|\partial_\varepsilon \alpha_\varepsilon| + |\partial_\varepsilon \beta_\varepsilon| + |\partial_\varepsilon b_\varepsilon|)(1 + |v|^2) \{g(v) + M_\varepsilon(v)\}. \quad (6.55)$$

Let us now fix $\varepsilon > 0$ and an arbitrary $\delta \in (0, \varepsilon)$. Since the application $\varepsilon \mapsto (\alpha_\varepsilon, \beta_\varepsilon, b_\varepsilon)$ is \mathcal{C}^1 on \mathbb{R}_+^* , there exists $c_0 > 0$ such that

$$\sup_{\varepsilon_* \in (\varepsilon - \delta, \varepsilon + \delta)} (|\partial_{\varepsilon_*} \alpha_{\varepsilon_*}| + |\partial_{\varepsilon_*} \beta_{\varepsilon_*}| + |\partial_{\varepsilon_*} b_{\varepsilon_*}|) \leq c_0.$$

Moreover, as $\varepsilon \mapsto a_\varepsilon$ is continuous on \mathbb{R}_+ , there is a $c_1 > 0$ such that

$$\sup_{\varepsilon_* \in (\varepsilon - \delta, \varepsilon + \delta)} |a_{\varepsilon_*}| \leq c_1.$$

Finally, from Lemma 6.22 in Appendix 6.C (with $\bar{\varepsilon} = \varepsilon + \delta$ in the lemma), there exist $c_2 > 0$ and $\eta > 0$ such that for any $v \in \mathbb{R}^3$,

$$\sup_{\varepsilon_* \in [0, \varepsilon + \delta]} M_{\varepsilon_*}(v) \leq c_2 e^{-\eta|v|^2}.$$

Then (6.55) implies that for any $v \in \mathbb{R}^3$,

$$\sup_{\varepsilon_* \in (\varepsilon - \delta, \varepsilon + \delta)} \left| \frac{d}{d\varepsilon_*} K(\varepsilon_*, M_{\varepsilon_*}(v)) \right| \leq 2(\varepsilon - \delta)^{-1} \left(g \log g(v) + c_1 g(v) + c_2 e^{-\eta|v|^2} \right) + c_0(1 + |v|^2) \left\{ g(v) + c_2 e^{-\eta|v|^2} \right\}.$$

Since $g \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3)$, the right-hand side of the above equation is integrable, and we conclude, by dominated convergence, to the differentiability of R_g and the validity of the differentiation in ε under the integral, ending the proof. \square

6.3.2 Continuity at zero

The second and last argument required in the proofs of Theorem 6.1 and Proposition 6.2 is the continuity of $\varepsilon \mapsto R_g(\varepsilon)$ at the point $\varepsilon = 0$, which is given in the following lemma.

Lemma 6.7. *Let $0 \leq g \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3) \setminus \{0\}$. Then the function $\varepsilon \in \mathbb{R}_+ \mapsto R_g(\varepsilon)$ defined in (6.45) is continuous at the point $\varepsilon = 0$.*

Proof. We write $R_g(\varepsilon)$ as

$$R_g(\varepsilon) = H_\varepsilon \left(\frac{g}{1 + \varepsilon g} \right) - H_\varepsilon \left(\mathcal{M}_\varepsilon^{\frac{g}{1 + \varepsilon g}} \right). \quad (6.56)$$

We show that both terms, in the right-hand-side, are continuous at the point $\varepsilon = 0$. Firstly, by definition of the Fermi-Dirac entropy, it holds for any $\varepsilon > 0$ that

$$\begin{aligned} H_\varepsilon \left(\frac{g}{1 + \varepsilon g} \right) &= \int_{\mathbb{R}^3} \left\{ \frac{g}{1 + \varepsilon g} \log \left(\frac{g}{1 + \varepsilon g} \right) + \varepsilon^{-1} \left(1 - \varepsilon \frac{g}{1 + \varepsilon g} \right) \log \left(1 - \varepsilon \frac{g}{1 + \varepsilon g} \right) \right\} dv \\ &= \int_{\mathbb{R}^3} \left\{ \frac{g}{1 + \varepsilon g} \log g - \varepsilon^{-1} \log(1 + \varepsilon g) \right\} dv. \end{aligned}$$

As $g \geq 0$, we have for any $\varepsilon > 0$ that

$$\left| \frac{g}{1 + \varepsilon g} \log g \right| \leq g |\log g| \quad \text{and} \quad \left| -\varepsilon^{-1} \log(1 + \varepsilon g) \right| \leq g,$$

Since by hypothesis $0 \leq g \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3)$, the function $g |\log g| + g$ is integrable, and, by dominated convergence, we then conclude to the limit

$$H_\varepsilon \left(\frac{g}{1 + \varepsilon g} \right) \xrightarrow{\varepsilon \rightarrow 0} \int_{\mathbb{R}^3} \{g \log g - g\} dv = H_0(g).$$

Secondly, going through the same computations as for the first term, we have, for any $\varepsilon > 0$,

$$H_\varepsilon \left(\mathcal{M}_\varepsilon^{\frac{g}{1 + \varepsilon g}} \right) = \int_{\mathbb{R}^3} \left\{ \frac{M_\varepsilon}{1 + \varepsilon M_\varepsilon} \log M_\varepsilon - \varepsilon^{-1} \log(1 + \varepsilon M_\varepsilon) \right\} dv,$$

where we denoted $M_\varepsilon = \varphi_\varepsilon \left(\mathcal{M}_\varepsilon^{\frac{g}{1 + \varepsilon g}} \right)$. Lemma 6.22 in Appendix 6.C (with $\bar{\varepsilon} = 1$ in the lemma) provides the existence of $C, \eta > 0$ such that for all $0 \leq \varepsilon \leq 1$,

$$|\log M_\varepsilon(v)| \leq C(1 + |v|^2) \quad \text{and} \quad M_\varepsilon(v) \leq C e^{-\eta|v|^2}.$$

Hence, for any $0 \leq \varepsilon \leq 1$ and $v \in \mathbb{R}^3$,

$$\left| \frac{M_\varepsilon(v)}{1 + \varepsilon M_\varepsilon(v)} \log M_\varepsilon(v) \right| \leq C^2 e^{-\eta|v|^2} (1 + |v|^2), \quad \text{and} \quad |\varepsilon^{-1} \log(1 + \varepsilon M_\varepsilon(v))| \leq M_\varepsilon(v) \leq C e^{-\eta|v|^2}.$$

By dominated convergence, it thus comes that

$$\lim_{\varepsilon \rightarrow 0} H_\varepsilon \left(\mathcal{M}_\varepsilon^{\frac{g}{1+\varepsilon g}} \right) = \int_{\mathbb{R}^3} \lim_{\varepsilon \rightarrow 0} \left(\frac{M_\varepsilon}{1 + \varepsilon M_\varepsilon} \log M_\varepsilon - \varepsilon^{-1} \log(1 + \varepsilon M_\varepsilon) \right) dv.$$

As Lemma 6.20 ensures that $\lim_{\varepsilon \rightarrow 0} M_\varepsilon(v) = \mathcal{M}_0^g(v)$ for all $v \in \mathbb{R}^3$, the above limit becomes

$$\int_{\mathbb{R}^3} \mathcal{M}_0^g \log \mathcal{M}_0^g - \mathcal{M}_0^g dv,$$

that is $H_0(\mathcal{M}_0^g)$, ending the proof. \square

We can finally conclude to the announced inequalities of Theorem 6.1 and Proposition 6.2.

6.3.3 Final proof of Theorem 6.1

Let $\varepsilon > 0$ and $0 \leq f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that

$$g := \frac{f}{1 - \varepsilon f} \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3) \setminus \{0\}.$$

Proposition 6.6 ensures that the application R_g defined by (6.45) is \mathcal{C}^1 on \mathbb{R}^*_+ , and combining (6.46) with (6.54) yields, for any $\varepsilon_* > 0$,

$$R'_g(\varepsilon_*) = - \int_{\mathbb{R}^3} \int_{M_{\varepsilon_*}}^g \frac{\varphi_{\varepsilon_*}^{-1}(g)^2 - \varphi_{\varepsilon_*}^{-1}(y)^2}{y} dy dv.$$

As, for any $\varepsilon_* > 0$, the application $x \mapsto \varphi_{\varepsilon_*}^{-1}(x)^2$ is increasing, the integral in y is nonnegative, hence so is the integral in y and v , therefore

$$\forall \varepsilon_* > 0, \quad R'_g(\varepsilon_*) \leq 0.$$

Combining this result with Lemma 6.7, which states that $\varepsilon_* \mapsto R_g(\varepsilon_*)$ is continuous at the point $\varepsilon_* = 0$, R_g is then nonincreasing on \mathbb{R}_+ , which implies in particular that

$$R_g(0) \geq R_g(\varepsilon),$$

that is

$$H_0[g | M^g] \geq H_\varepsilon \left[\varphi_\varepsilon^{-1}(g) \middle| \mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}(g)} \right],$$

or the announced inequality (6.32),

$$H_0 \left[\frac{f}{1 - \varepsilon f} \middle| M^{\frac{f}{1 - \varepsilon f}} \right] \geq H_\varepsilon \left[f \middle| \mathcal{M}_\varepsilon^f \right].$$

6.3.4 Final proof of Proposition 6.2

Let us fix $\varepsilon > 0$, $\kappa_0 \in (0, 1)$ and $0 \leq f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq \kappa_0$. We let

$$g := \frac{f}{1 - \varepsilon f}.$$

Then $0 \leq g \in L^1_2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3) \setminus \{0\}$, which is in particular included in $L \log L(\mathbb{R}^3)$. We apply the results of Proposition 6.6 and Lemma 6.7 with the function g , ensuring that the application R_g , defined by (6.45), is continuous on \mathbb{R}_+ and C^1 on \mathbb{R}_+^* with, combining (6.46) with (6.54),

$$\forall \varepsilon_* > 0, \quad R'_g(\varepsilon_*) = - \int_{\mathbb{R}^3} \int_{M_{\varepsilon_*}}^g \frac{\varphi_{\varepsilon_*}^{-1}(g)^2 - \varphi_{\varepsilon_*}^{-1}(y)^2}{y} \, dy \, dv.$$

For $\varepsilon_* > 0$, $v \in \mathbb{R}^3$ and any y between $M_{\varepsilon_*}(v)$ and $g(v)$, one has (omitting the dependencies in v for clarity)

$$|\varphi_{\varepsilon_*}^{-1}(g)^2 - \varphi_{\varepsilon_*}^{-1}(y)^2| = (\varphi_{\varepsilon_*}^{-1}(g) + \varphi_{\varepsilon_*}^{-1}(y)) |\varphi_{\varepsilon_*}^{-1}(g) - \varphi_{\varepsilon_*}^{-1}(y)| \leq c_g(\varepsilon_*) |\varphi_{\varepsilon_*}^{-1}(g) - \varphi_{\varepsilon_*}^{-1}(y)|,$$

where we denoted

$$c_g(\varepsilon_*) := \|\varphi_{\varepsilon_*}^{-1}(g)\|_\infty + \max \left(\|\varphi_{\varepsilon_*}^{-1}(g)\|_\infty, \|\mathcal{M}_{\varepsilon_*}^{\varphi_{\varepsilon_*}^{-1}(g)}\|_\infty \right).$$

As both $z \mapsto \varphi_{\varepsilon_*}^{-1}(z)^2$ and $z \mapsto \varphi_{\varepsilon_*}^{-1}(z)$ are increasing, we thus have

$$R'_g(\varepsilon_*) \geq -c_g(\varepsilon_*) \int_{\mathbb{R}^3} \int_{M_{\varepsilon_*}}^g \frac{\varphi_{\varepsilon_*}^{-1}(g) - \varphi_{\varepsilon_*}^{-1}(y)}{y} \, dy \, dv = -c_g(\varepsilon_*) R_g(\varepsilon_*).$$

Noticing that

$$c_g(\varepsilon_*) \leq \|g\|_\infty + \max \left(\|g\|_\infty + \|\mathcal{M}_{\varepsilon_*}^{\varphi_{\varepsilon_*}^{-1}(g)}\|_\infty \right),$$

we conclude to the relationship, for any $\varepsilon_* > 0$,

$$R'_g(\varepsilon_*) \geq - \left(\|g\|_\infty + \max \left(\|g\|_\infty + \|\mathcal{M}_{\varepsilon_*}^{\varphi_{\varepsilon_*}^{-1}(g)}\|_\infty \right) \right) R_g(\varepsilon_*). \quad (6.57)$$

By hypothesis, it holds that $1 - \varepsilon f \geq \kappa_0$, hence

$$\|g\|_\infty \leq \varepsilon^{-1} (\kappa_0^{-1} - 1), \quad (6.58)$$

and we have for any $\varepsilon_* > 0$ that

$$\varepsilon_* \varphi_{\varepsilon_*}^{-1}(g) = \frac{\varepsilon_* g}{1 + \varepsilon_* g} \leq \left(1 + \frac{1}{\varepsilon_* \|g\|_\infty} \right)^{-1} \leq \left(1 + \frac{\varepsilon}{\varepsilon_*} (\kappa_0^{-1} - 1)^{-1} \right)^{-1}. \quad (6.59)$$

Let us use the notation

$$\gamma_{\varepsilon_*} = \frac{T_*}{T_F(\rho_*, \varepsilon_*)},$$

where ρ_* and T_* are respectively the density and temperature associated with the distribution $\varphi_{\varepsilon_*}^{-1}(g)$ defined as in (6.12), and $T_F(\rho_*, \varepsilon_*) = \frac{1}{2} \left(\frac{3\rho_*\varepsilon_*}{4\pi} \right)^{2/3}$ is the corresponding ε_* -Fermi temperature.

Using Equation (6.117) in Proposition 6.18 in Appendix 6.C and the fact that $\mathcal{M}_{\varepsilon_*}^{\varphi_{\varepsilon_*}^{-1}(g)} \leq \varphi_{\varepsilon_*} \left(\mathcal{M}_{\varepsilon_*}^{\varphi_{\varepsilon_*}^{-1}(g)} \right)$, we have, whenever $\gamma_{\varepsilon_*} \geq \gamma^\dagger = \left(\frac{4}{\pi}\right)^{\frac{1}{3}} \left(\frac{5}{3}\right)^{\frac{5}{3}}$,

$$\varepsilon_* \|\mathcal{M}_{\varepsilon_*}^{\varphi_{\varepsilon_*}^{-1}(g)}\|_\infty \leq \frac{2}{3} \left(\frac{\gamma_{\varepsilon_*}}{\gamma^\dagger} \right)^{-3/2}. \quad (6.60)$$

We now notice that [123, Proposition 4] actually implies

$$\gamma_{\varepsilon_*} \geq \frac{2}{5} (\varepsilon_* \|\varphi_{\varepsilon_*}^{-1}(g)\|_\infty)^{-2/3},$$

which, combined with (6.59), yields

$$\gamma_{\varepsilon_*} \geq \frac{2}{5} \left(1 + \frac{\varepsilon}{\varepsilon_*} (\kappa_0^{-1} - 1)^{-1} \right)^{2/3}. \quad (6.61)$$

We define

$$\varepsilon^\dagger := \left(\left(\frac{5}{2} \gamma^\dagger \right)^{\frac{3}{2}} - 1 \right)^{-1} (\kappa_0^{-1} - 1)^{-1} \varepsilon. \quad (6.62)$$

Then, for any $\varepsilon_* \in (0, \varepsilon^\dagger]$, combining (6.61) with (6.62) yields

$$\gamma_{\varepsilon_*} \geq \frac{2}{5} \left(1 + \frac{\varepsilon}{\varepsilon^\dagger} (\kappa_0^{-1} - 1)^{-1} \right)^{2/3} = \gamma^\dagger.$$

Applying (6.60), along with (6.61) and the fact that

$$\frac{2}{3} \left(\frac{5}{2} \gamma^\dagger \right)^{\frac{3}{2}} = \frac{2}{3} \left(\frac{5}{2} \right)^{\frac{3}{2}} \left(\frac{4}{\pi} \right)^{\frac{1}{2}} \left(\frac{5}{3} \right)^{\frac{5}{2}} \leq 11,$$

gives, for any $\varepsilon_* \in (0, \varepsilon^\dagger]$,

$$\|\mathcal{M}_{\varepsilon_*}^{\varphi_{\varepsilon_*}^{-1}(g)}\|_\infty \leq \frac{11}{\varepsilon_* + \varepsilon (\kappa_0^{-1} - 1)^{-1}} \leq 11 \varepsilon^{-1} (\kappa_0^{-1} - 1).$$

Therefore, recalling (6.58), we have for any $\varepsilon_* \in (0, \varepsilon^\dagger]$ that

$$\|g\|_\infty + \max \left(\|g\|_\infty, \|\mathcal{M}_{\varepsilon_*}^{\varphi_{\varepsilon_*}^{-1}(g)}\|_\infty \right) \leq \varepsilon^{-1} (\kappa_0^{-1} - 1) + 11 \varepsilon^{-1} (\kappa_0^{-1} - 1) = 12 \varepsilon^{-1} (\kappa_0^{-1} - 1),$$

implying, with the relationship (6.57), that for any $\varepsilon_* \in (0, \varepsilon^\dagger]$,

$$R'_g(\varepsilon_*) \geq -12 \varepsilon^{-1} (\kappa_0^{-1} - 1) R_g(\varepsilon_*). \quad (6.63)$$

Applying a Grönwall argument over (6.63) and using the continuity of $\varepsilon_* \mapsto R_g(\varepsilon_*)$ at the point $\varepsilon_* = 0$

provided by Lemma 6.7, we obtain

$$\forall \varepsilon_* \in (0, \varepsilon^\dagger], \quad R_g(0) \leq \exp\left(12 \frac{\varepsilon_*}{\varepsilon} (\kappa_0^{-1} - 1)\right) R_g(\varepsilon_*). \quad (6.64)$$

On the one hand, if $\varepsilon \leq \varepsilon^\dagger$, we take $\varepsilon_* = \varepsilon$ in (6.64) to get

$$R_g(0) \leq \exp(12(\kappa_0^{-1} - 1)) R_g(\varepsilon). \quad (6.65)$$

On the other hand, if $\varepsilon \geq \varepsilon^\dagger$, we apply (6.64) with $\varepsilon_* = \varepsilon^\dagger$ to get

$$R_g(0) \leq \exp\left(12 \frac{\varepsilon^\dagger}{\varepsilon} (\kappa_0^{-1} - 1)\right) R_g(\varepsilon^\dagger). \quad (6.66)$$

Since it holds for any $\varepsilon_* > 0$ that $\|\mathcal{M}_{\varepsilon_*}^{\varphi_{\varepsilon_*}^{-1}(g)}\|_\infty \leq \varepsilon_*^{-1}$, we have in particular that, for any $\varepsilon_* \in [\varepsilon^\dagger, \varepsilon]$,

$$\|\mathcal{M}_{\varepsilon_*}^{\varphi_{\varepsilon_*}^{-1}(g)}\|_\infty \leq (\varepsilon^\dagger)^{-1},$$

which, combined with (6.57) and (6.58), leads to

$$\forall \varepsilon_* \in [\varepsilon^\dagger, \varepsilon], \quad R'_g(\varepsilon_*) \geq -\varepsilon^{-1} \left((\kappa_0^{-1} - 1) + \max\left(\kappa_0^{-1} - 1, \frac{\varepsilon}{\varepsilon^\dagger}\right) \right) R_g(\varepsilon_*). \quad (6.67)$$

By a Grönwall argument over (6.67), we obtain

$$R_g(\varepsilon^\dagger) \leq \exp\left(\frac{\varepsilon - \varepsilon^\dagger}{\varepsilon} \left(\kappa_0^{-1} - 1 + \max\left(\kappa_0^{-1} - 1, \frac{\varepsilon}{\varepsilon^\dagger}\right) \right)\right) R_g(\varepsilon). \quad (6.68)$$

Recalling that ε^\dagger is defined by (6.62), we have

$$\frac{\varepsilon}{\varepsilon^\dagger} = \left(\left(\frac{5}{2} \gamma^\dagger \right)^{\frac{3}{2}} - 1 \right) (\kappa_0^{-1} - 1).$$

As $\gamma^\dagger = \left(\frac{4}{\pi}\right)^{\frac{1}{3}} \left(\frac{5}{3}\right)^{\frac{5}{3}}$, we have $\left(\frac{5}{2} \gamma^\dagger\right)^{\frac{3}{2}} - 1 \leq 15$, therefore

$$\left(\kappa_0^{-1} - 1 + \max\left(\kappa_0^{-1} - 1, \frac{\varepsilon}{\varepsilon^\dagger}\right) \right) \leq 16(\kappa_0^{-1} - 1). \quad (6.69)$$

Combining (6.68) with (6.69), we get

$$R_g(\varepsilon^\dagger) \leq \exp\left(\frac{\varepsilon - \varepsilon^\dagger}{\varepsilon} 16(\kappa_0^{-1} - 1)\right) R_g(\varepsilon). \quad (6.70)$$

Finally, combining (6.66) with (6.70), we obtain, in this case where we assumed $\varepsilon \geq \varepsilon^\dagger$,

$$R_g(0) \leq \exp\left(\left\{12 \frac{\varepsilon^\dagger}{\varepsilon} + 16 \frac{\varepsilon - \varepsilon^\dagger}{\varepsilon}\right\} (\kappa_0^{-1} - 1)\right) R_g(\varepsilon) \leq \exp(16(\kappa_0^{-1} - 1)) R_g(\varepsilon).$$

We thus conclude, with (6.65), that in any case, we have

$$R_g(0) \leq \exp(16(\kappa_0^{-1} - 1)) R_g(\varepsilon),$$

yielding the required result as $R_g(0) = H_0 \left[\frac{f}{1-\varepsilon f} \middle| M^{1-\varepsilon f} \right]$ and $R_g(\varepsilon) = H_\varepsilon \left[f \middle| \mathcal{M}_\varepsilon^f \right]$.

6.4 Proof of Corollary 6.3

This section is devoted to the proof of Corollary 6.3. Throughout this section, we use the notation

$$\begin{pmatrix} \rho_\varepsilon \\ \rho_\varepsilon u_\varepsilon \\ 3\rho_\varepsilon T_\varepsilon + \rho_\varepsilon |u_\varepsilon|^2 \end{pmatrix} = \int_{\mathbb{R}^3} \varphi_\varepsilon(f)(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv, \quad \begin{pmatrix} \rho \\ \rho u \\ 3\rho T + \rho |u|^2 \end{pmatrix} = \int_{\mathbb{R}^3} f(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv. \quad (6.71)$$

In the following, we use the bound

$$1 - \varepsilon f \geq \kappa_0 \implies T_\varepsilon \geq \kappa_0 T. \quad (6.72)$$

This comes by first remarking that, if $1 - \varepsilon f \geq \kappa_0$,

$$\begin{aligned} 3\rho_\varepsilon T_\varepsilon &= \int_{\mathbb{R}^3} \varphi_\varepsilon(f)(v) |v - u_\varepsilon|^2 dv \geq \int_{\mathbb{R}^3} f(v) |v - u_\varepsilon|^2 dv = \int_{\mathbb{R}^3} f(v) |v - u - (u_\varepsilon - u)|^2 dv \\ &= 3\rho T + \rho |u_\varepsilon - u|^2, \end{aligned}$$

implying $\rho_\varepsilon T_\varepsilon \geq \rho T$, and the fact that

$$\rho_\varepsilon = \int_{\mathbb{R}^3} \varphi_\varepsilon(f)(v) dv \leq \kappa_0^{-1} \int_{\mathbb{R}^3} f(v) dv = \kappa_0^{-1} \rho. \quad (6.73)$$

6.4.1 Super quadratic kernels

Proof. Let $\kappa_0 \in (0, 1)$, $\varepsilon > 0$ and $0 \leq f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq \kappa_0$. We have from (6.31) that

$$\mathcal{D}_\varepsilon(f) \geq \kappa_0^4 \mathcal{D}_0(\varphi_\varepsilon(f)). \quad (6.74)$$

We apply [157, Theorem 2.1] to the function $\varphi_\varepsilon(f)$, adapted (since it is written for normalized functions) with the change of variable $w = \sqrt{T_\varepsilon} v + u_\varepsilon$, and obtain

$$\mathcal{D}_0(\varphi_\varepsilon(f)) \geq \min(1, T_\varepsilon) \frac{|\mathbb{S}^2|}{28} (3\rho_\varepsilon T_\varepsilon - \rho_\varepsilon T^*(\varphi_\varepsilon(f))) H_0 \left[\varphi_\varepsilon(f) \middle| M^{\varphi_\varepsilon(f)} \right],$$

where $T^*(g)$ stands for the maximal directional temperature of g , defined by $\frac{\sup_{e \in \mathbb{S}^2} \int_{\mathbb{R}^3} g(v) (v \cdot e)^2 dv}{\int_{\mathbb{R}^3} g(v) dv}$. Since in particular,

$$3\rho_\varepsilon T_\varepsilon - \rho_\varepsilon T^*(\varphi_\varepsilon(f)) \geq 2\rho_\varepsilon T_*(\varphi_\varepsilon(f)),$$

where $T_*(g)$ stands for the minimal directional temperature of g , defined in (6.13), we obtain

$$\mathcal{D}_0(\varphi_\varepsilon(f)) \geq \min(1, T_\varepsilon) \frac{2\pi}{7} \rho_\varepsilon T_*(\varphi_\varepsilon(f)) H_0 \left[\varphi_\varepsilon(f) \middle| M^{\varphi_\varepsilon(f)} \right]. \quad (6.75)$$

Applying Theorem 6.1's lower-bound inequality (6.32), we obtain

$$H_0 \left[\varphi_\varepsilon(f) \middle| M^{\varphi_\varepsilon(f)} \right] \geq H_\varepsilon[f | \mathcal{M}_\varepsilon^f]. \quad (6.76)$$

Combining (6.74)–(6.76) yields

$$\mathcal{D}_\varepsilon(f) \geq \frac{2\pi}{7} \kappa_0^4 \min(1, T_\varepsilon) \rho_\varepsilon T_*(\varphi_\varepsilon(f)) H_\varepsilon[f | \mathcal{M}_\varepsilon^f].$$

The required result is obtained after remarking that, from (6.72), $T_\varepsilon \geq \kappa_0 T$, and

$$\rho_\varepsilon T_*(\varphi_\varepsilon(f)) = \inf_{e \in \mathbb{S}^2} \int_{\mathbb{R}^3} \varphi_\varepsilon(f)(v) (v \cdot e)^2 \, dv \geq \inf_{e \in \mathbb{S}^2} \int_{\mathbb{R}^3} f(v) (v \cdot e)^2 \, dv = \rho T_*(f).$$

□

6.4.2 General kernels

Proof. Let $\kappa_0 \in (0, 1)$, $\varepsilon > 0$ and $0 \leq f \in L_2^1(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq \kappa_0$. Again, (6.31) yields

$$\mathcal{D}_\varepsilon(f) \geq \kappa_0^4 \mathcal{D}_0(\varphi_\varepsilon(f)).$$

Remarking that $\varphi_\varepsilon(f)(v) \geq f(v) \geq K_0 e^{-A_0|v|^{q_0}}$, we apply [157, Theorem 4.1] to the function $\varphi_\varepsilon(f)$ and obtain for any $\alpha \in (0, 1)$ the existence of some $\overline{K}_\alpha(\varphi_\varepsilon(f))$ depending only on α , upper and lower bounds on $\rho_\varepsilon, T_\varepsilon$ (see Remark 6.4 below), q_0 and upper bounds on $A_0, 1/K_0, \|\varphi_\varepsilon(f)\|_{L_s^1}$ and $\|\varphi_\varepsilon(f)\|_{H^k}$ where $s = s(\alpha, q_0, \beta_+, \beta_-)$ and $k = k(\alpha, s, \beta_+, \beta_-)$ such that

$$\mathcal{D}_0(\varphi_\varepsilon(f)) \geq \overline{K}_\alpha(\varphi_\varepsilon(f)) H_0 \left[\varphi_\varepsilon(f) \middle| M^{\varphi_\varepsilon(f)} \right]^{1+\alpha}.$$

Again, Theorem 6.1's lower-bound inequality (6.32) implies

$$H_0 \left[\varphi_\varepsilon(f) \middle| M^{\varphi_\varepsilon(f)} \right] \geq H_\varepsilon[f | \mathcal{M}_\varepsilon^f],$$

so that

$$\mathcal{D}_\varepsilon(f) \geq \kappa_0^4 \overline{K}_\alpha(\varphi_\varepsilon(f)) H_\varepsilon[f | \mathcal{M}_\varepsilon^f]^{1+\alpha}.$$

Moreover, we can upper-bound $\|\varphi_\varepsilon(f)\|_{L_s^1}$ by $\kappa_0^{-1} \|f\|_{L_s^1}$, and $\|\varphi_\varepsilon(f)\|_{H^k}$ by a polynomial in $(\|f\|_{H^l})_{l \leq k}$, κ_0^{-1} and an upper bound on ε , since for $l \geq 1$, and x such that $1 - \varepsilon x \geq \kappa_0$,

$$|\varphi_\varepsilon^{(l)}(x)| = \frac{l! \varepsilon^{l-1}}{(1 - \varepsilon x)^{l+1}} \leq l! \kappa_0^{-l-1} \varepsilon^{l-1}.$$

We end the proof by using

- Equations (6.72)–(6.73) stating that $\rho_\varepsilon \leq \kappa_0^{-1} \rho$ and $T_\varepsilon \geq \kappa_0 T$,
- the fact that $\rho \leq \rho_\varepsilon$, coming from

$$\int_{\mathbb{R}^3} f \, dv \leq \int_{\mathbb{R}^3} \frac{f}{1 - \varepsilon f} \, dv,$$

— the fact that $T_\varepsilon \leq \kappa_0^{-1}T$, coming from

$$3\rho_\varepsilon T_\varepsilon + \rho_\varepsilon |u_\varepsilon - u|^2 = \int_{\mathbb{R}^3} \varphi_\varepsilon(f)(v) |v - u|^2 \, dv \leq \kappa_0^{-1} \int_{\mathbb{R}^3} f(v) |v - u|^2 \, dv = \kappa_0^{-1} 3\rho T.$$

implying $\rho_\varepsilon T_\varepsilon \leq \kappa_0^{-1} \rho T$ hence $T_\varepsilon \leq \kappa_0^{-1} \frac{\rho}{\rho_\varepsilon} T \leq \kappa_0^{-1} T$. □

Remark 6.4. In [157, Theorem 4.1], the constant $\bar{K}_\alpha(\varphi_\varepsilon(f))$ is said to depend on $\rho_\varepsilon, T_\varepsilon$. Having a look at the proof there, this dependence can be relaxed into a dependence on upper and lower bounds of those quantities.

6.4.3 Inverse result

Let $\varepsilon \in (0, \frac{1}{2})$, $B_0 > 0$ and $0 \leq \beta < 2$. We assume that

$$\int_{\mathbb{S}^2} B(v, v_*, \sigma) \, d\sigma \leq B_0 (1 + |v - v_*|^\beta).$$

Relying on Bobylev and Cercignani's [31, Theorem 1], and the nice formulation of this theorem by Villani [157, Theorem 1.1], we know that there exists a family of normalized functions (g_l) , in the sense that for any l ,

$$\int_{\mathbb{R}^3} g_l(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \, dv = \begin{pmatrix} 1 \\ 0 \\ 3 \end{pmatrix}, \quad (6.77)$$

such that (taking $\delta = 1 - \frac{1+2\varepsilon}{2} > 0$ in [157, Theorem 1.1])

$$\forall v \in \mathbb{R}^3, \quad 2 \geq g_l(v) \geq \frac{1+2\varepsilon}{2} (2\pi)^{-3/2} e^{-|v|^2}, \quad (6.78)$$

and

$$\frac{\mathcal{D}_0(g_l)}{H_0[g_l | M^{g_l}]} \xrightarrow{l \rightarrow \infty} 0. \quad (6.79)$$

We now consider

$$f_l^\varepsilon = \frac{g_l}{1 + \varepsilon g_l} \equiv \varphi_\varepsilon^{-1}(g_l).$$

As φ_ε^{-1} is increasing, and from (6.78), we have

$$f_l^\varepsilon(v) \equiv \frac{g_l(v)}{1 + \varepsilon g_l(v)} \geq \frac{g_l(v)}{1 + 2\varepsilon} \geq \frac{1 + 2\varepsilon}{2(1 + 2\varepsilon)} (2\pi)^{-3/2} e^{-|v|^2} = \frac{1}{2} (2\pi)^{-3/2} e^{-|v|^2}.$$

We denote

$$\int_{\mathbb{R}^3} f_l^\varepsilon(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \, dv = \begin{pmatrix} \rho_\varepsilon^l \\ \rho_\varepsilon^l u_\varepsilon^l \\ 3\rho_\varepsilon^l T_\varepsilon^l + \rho_\varepsilon^l |u_\varepsilon^l|^2 \end{pmatrix},$$

We have, from $f_l^\varepsilon = \frac{g_l}{1+\varepsilon g_l}$ and $g_l \leq 2$,

$$\frac{1}{1+2\varepsilon} \int_{\mathbb{R}^3} g_l(v) \, dv \leq \int_{\mathbb{R}^3} f_l^\varepsilon(v) \, dv \leq \int_{\mathbb{R}^3} g_l(v) \, dv,$$

that is

$$\frac{1}{1+2\varepsilon} \leq \rho_\varepsilon^l \leq 1.$$

Secondly,

$$3\rho_\varepsilon^l T_\varepsilon^l \leq 3\rho_\varepsilon^l T_\varepsilon^l + \rho_\varepsilon^l |u_\varepsilon^l|^2 = \int_{\mathbb{R}^3} f_l^\varepsilon(v) |v|^2 \, dv \leq \int_{\mathbb{R}^3} g_l(v) |v|^2 \, dv = 3,$$

that is $\rho_\varepsilon^l T_\varepsilon^l \leq 1$, hence

$$T_\varepsilon^l \leq \frac{1}{\rho_\varepsilon^l} \leq 1+2\varepsilon.$$

On the other hand, since g_l is normalized by (6.77), we have

$$3\rho_\varepsilon^l T_\varepsilon^l = \int_{\mathbb{R}^3} f_l^\varepsilon(v) |v - u_\varepsilon^l|^2 \, dv \geq \frac{1}{1+2\varepsilon} \int_{\mathbb{R}^3} g_l(v) |v - u_\varepsilon^l|^2 \, dv = \frac{3 + |u_\varepsilon^l|^2}{1+2\varepsilon} \geq \frac{3}{1+2\varepsilon},$$

that is $\rho_\varepsilon^l T_\varepsilon^l \geq \frac{1}{1+2\varepsilon}$, hence

$$T_\varepsilon^l \geq \frac{1}{\rho_\varepsilon^l} \times \frac{1}{1+2\varepsilon} \geq \frac{1}{1+2\varepsilon}.$$

Finally, since $f_l^\varepsilon = g_l - \varepsilon \frac{g_l^2}{1+\varepsilon g_l}$, g_l is normalized by (6.77) and $g_l \leq 2$, we have

$$\begin{aligned} \rho_\varepsilon^l |u_\varepsilon^l| &= \left| \int_{\mathbb{R}^3} f_l^\varepsilon(v) v \, dv \right| = \varepsilon \left| \int_{\mathbb{R}^3} \frac{g_l(v)^2}{1+\varepsilon g_l(v)} v \, dv \right| \leq \varepsilon \int_{\mathbb{R}^3} \frac{g_l(v)^2}{1+\varepsilon g_l(v)} |v| \, dv \leq 2\varepsilon \int_{\mathbb{R}^3} g_l(v) |v| \, dv \\ &\leq 2\varepsilon \left(\int_{\mathbb{R}^3} g_l(v) \, dv \right)^{1/2} \left(\int_{\mathbb{R}^3} g_l(v) |v|^2 \, dv \right)^{1/2} = 2\sqrt{3}\varepsilon, \end{aligned}$$

where the last inequality is a Cauchy-Schwarz argument. We then conclude, since $\varepsilon \in (0, \frac{1}{2})$, that

$$|u_\varepsilon^l| \leq \frac{1}{\rho_\varepsilon^l} 2\sqrt{3}\varepsilon \leq 2\sqrt{3}(1+2\varepsilon)\varepsilon \leq 4\sqrt{3}\varepsilon.$$

All in all, we proved that for any l , $f_l^\varepsilon \in \mathcal{C}_{1,0,1}^\varepsilon$.

We now apply Equation (6.31) to get

$$\mathcal{D}_\varepsilon(f_l^\varepsilon) \leq \mathcal{D}_0(g_l),$$

and Proposition 6.2's upper-bound inequality, Equation (6.34), which gives, for any $\varepsilon \in (0, \frac{1}{2})$, and denoting $\kappa_0^\varepsilon = 1 - 2\varepsilon$ (so that $1 - \varepsilon f_l^\varepsilon \geq \kappa_0^\varepsilon$),

$$H_\varepsilon \left[f_l^\varepsilon \left| \mathcal{M}_\varepsilon^{f_l^\varepsilon} \right. \right] \geq \frac{1}{C_0(\kappa_0^\varepsilon)} H_0 \left[\frac{f_l^\varepsilon}{1 - \varepsilon f_l^\varepsilon} \left| M^{\frac{f_l^\varepsilon}{1 - \varepsilon f_l^\varepsilon}} \right. \right] = \frac{1}{C_0(\kappa_0^\varepsilon)} H_0[g_l | M^{g_l}].$$

We finally obtain that, for any $\varepsilon \in (0, \frac{1}{2})$,

$$\frac{\mathcal{D}_\varepsilon(f_l^\varepsilon)}{H_\varepsilon[f_l^\varepsilon | \mathcal{M}_\varepsilon^{f_l^\varepsilon}]} \leq \frac{1}{C_0(\kappa_0^\varepsilon)} \times \frac{\mathcal{D}_0(g_l)}{H_0[g_l | M^{g_l}]} \xrightarrow{l \rightarrow \infty} 0. \quad (6.80)$$

6.5 About the Landau-Fermi-Dirac equation

A study of the entropy-entropy production relationship for the Landau-Fermi-Dirac equation for various cross sections was recently conducted by Alonso, Bagland, Desvillettes and Lods in [4, 3] (see also Desvillettes [73] and Alonso, Bagland, Lods [2]) and we do not (intend to) provide here any new result on this side. We refer the interested reader to these papers and the references therein for a detailed study of the Landau-Fermi-Dirac equation. Nevertheless, using the exact same strategy of transposing results from the Classical towards the Fermi-Dirac case that we used in the Boltzmann-Fermi-Dirac case (Corollary 6.3), we obtain an original proof of inequalities reminiscent of the ones stated in [4, 3] and [73], namely [4, Theorem 1.4], the first inequality in the proof of [3, Proposition 5.8] and [73, Proposition 2]. Let us first briefly introduce the Landau-Fermi-Dirac equation.

In dimension 3, the Landau-Fermi-Dirac operator writes, for $\varepsilon \geq 0$ and nonnegative $f \in L^1_2(\mathbb{R}^3)$ such that $1 - \varepsilon f \geq 0$,

$$\mathcal{D}_\varepsilon^L(f)(v) := \nabla_v \cdot \int_{\mathbb{R}^3} \Psi(|v - v_*|) \Pi(v - v_*) \left[f_*(1 - \varepsilon f_*) \nabla f - f(1 - \varepsilon f) \nabla f_* \right] dv_*. \quad (6.81)$$

The case $\varepsilon = 0$ corresponds to the classical Landau operator. In (6.81), we used the common short-hands $f \equiv f(v)$ and $f_* \equiv f(v_*)$, $\Pi(z)$ denotes the orthogonal projection on $(\mathbb{R}z)^\perp$, whose components are

$$\Pi_{ij}(z) = \delta_{ij} - \frac{z_i z_j}{|z|^2},$$

and Ψ is sometimes called the kinetic potential. The entropy production associated with the Landau-Fermi-Dirac operator writes

$$\mathcal{D}_\varepsilon^L(f) = \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \Psi(|v - v_*|) f f_* (1 - \varepsilon f) (1 - \varepsilon f_*) \left| \Pi(v - v_*) \left(\frac{\nabla f}{f(1 - \varepsilon f)} - \frac{\nabla f_*}{f_*(1 - \varepsilon f_*)} \right) \right|^2 dv dv_*. \quad (6.82)$$

We notice that (6.82) can be rewritten (where φ_ε is defined in (6.6))

$$\begin{aligned} \mathcal{D}_\varepsilon^L(f) &= \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \Psi(|v - v_*|) \varphi_\varepsilon(f) \varphi_\varepsilon(f)_* (1 - \varepsilon f)^2 (1 - \varepsilon f_*)^2 \\ &\quad \times \left| \Pi(v - v_*) \left(\frac{\nabla \varphi_\varepsilon(f)}{\varphi_\varepsilon(f)} - \frac{\nabla \varphi_\varepsilon(f)_*}{\varphi_\varepsilon(f)_*} \right) \right|^2 dv dv_*. \end{aligned}$$

This directly implies that for any $\kappa_0 \in (0, 1)$, $\varepsilon > 0$ and nonnegative $f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq \kappa_0$,

$$\mathcal{D}_0^L(\varphi_\varepsilon(f)) \geq \mathcal{D}_\varepsilon^L(f) \geq \kappa_0^4 \mathcal{D}_0^L(\varphi_\varepsilon(f)). \quad (6.83)$$

This inequality, similar to (6.31), allows to apply the same strategy as in the Boltzmann-Fermi-Dirac case. Adapting the entropy-entropy production inequalities known for the Landau equation [156, Chapter 3, Theorem 14] and [73, Remark 1], we get the following proposition.

Proposition 6.8. Entropy-entropy production inequalities for the Landau-Fermi-Dirac operator (adaptation of [156, Chapter 3, Theorem 14] and [73, Remark 1]). We recall that $\mathcal{D}_\varepsilon^L$, H_ε and $T_*(f)$ are defined respectively in (6.82), (6.21)–(6.22) and (6.13).

• **Over-Maxwellian case [Adaptation of [156, Chapter 3, Theorem 14, (i)]]**. Assume $\Psi(|z|) \geq |z|^2$. Then, for any $\kappa_0 \in (0, 1)$, $\varepsilon \geq 0$ and $0 \leq f \in L_2^1(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq \kappa_0$, we have

$$\mathcal{D}_\varepsilon^L(f) \geq 4\kappa_0^4 \rho T_*(f) H_\varepsilon[f|\mathcal{M}_\varepsilon^f], \quad (6.84)$$

• **Soft potentials [Adaptation of [156, Chapter 3, Theorem 14, (ii)]]**. Assume $\Psi(|z|) \geq |z|^2(1 + |z|)^{-\beta}$ with $\beta > 0$. Then, for any $\kappa_0 \in (0, 1)$, $\varepsilon \geq 0$ and $0 \leq f \in L_2^1(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq \kappa_0$, for any $s > 0$, there exists a constant $C_s^L(f)$, explicit and depending on f only via ρ , T , κ_0 , an upper bound on ε and an upper bound on $H_\varepsilon(f)$ such that

$$\mathcal{D}_\varepsilon^L(f) \geq C_s^L(f) \left(\|f\|_{L_{s+2}^1} + \|\nabla \sqrt{f}\|_{L_{1+\frac{s}{2}}^2} \right)^{-\frac{\beta}{s}} H_\varepsilon[f|\mathcal{M}_\varepsilon^f]^{1+\frac{\beta}{s}}. \quad (6.85)$$

• **Hard potentials [Adaptation of [73, Remark 1]]**. Assume $\Psi(|z|) \geq |z|^{2+\beta}$ with $\beta \in (0, 1]$. Then, for any $\kappa_0 \in (0, 1)$, $\varepsilon \geq 0$ and $0 \leq f \in L_2^1(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq \kappa_0$, there exist two explicit constants $K_1^L(f)$ and $K_2^L(f)$ which depend on β , on f only via ρ , T , κ_0 and on an upper bound on $\|f\|_{L_6^2}^2$ such that

$$\mathcal{D}_\varepsilon^L(f) \leq K_1^L(f) \implies \mathcal{D}_\varepsilon^L(f) \geq K_2^L(f) H_\varepsilon[f|\mathcal{M}_\varepsilon^f]. \quad (6.86)$$

We briefly discuss here the qualitative difference of our results with respect to the ones in [4, 3] and [73]. The inequality we obtain in the over-Maxwellian case (6.84) is almost identical to the one in [4, Theorem 1.4], with however an extra quantity in the constant in their inequality. As for the soft potentials case, the inequality in the proof of [3, Proposition 5.8] involves the hard potential of order $\eta > 0$ entropy production (for some chosen $\eta > 0$), which relates in (6.85) with the $\|\nabla \sqrt{f}\|_{L_{1+\frac{s}{2}}^2}^2$ norm (for some chosen $s > 0$). We

also point out that, while [3, Proposition 5.8] holds for soft potentials of order at most $-\frac{4}{3}$, there is no such restriction in (6.85). As far as hard potentials are concerned, the result we obtain (which could actually be more precise, but somewhat more complicated, by using [73, Theorem 1] instead of [73, Remark 1]) is very similar to the one obtained by Desvillettes in [73, Proposition 2], with the difference that his result involves the relative Fisher information instead of the relative entropy (hence yielding a stronger result); our methodology only gives another proof to obtain it. Also, the inequality obtained in [4, Theorem 1.4] comes with a more complicated constant than in [73, Proposition 2] (similarly, than (6.86)), but holds without any assumption of smallness on $\mathcal{D}_\varepsilon^L(f)$. We mention that a statement of the type (6.86) entails an exponential decay with explicit constants (if $K_1^L(f)$ and $K_2^L(f)$ are controlled below) as shown in [73, Lemma 1]. Finally, we can also obtain inequalities for hard potentials of order $\beta > 1$ by adapting [156, Chapter 3, Theorem 14, (iii)].

Remark 6.5. We want to mention [71] which bounds below the entropy production with a weighted version of the Fisher information, which would lead to a weighted relative entropy with power one in the right-hand-side of (6.85). A similar result for hard potentials was proven in [58]. We refer the interested reader to [74] (in french) for a discussion on the entropic structure of the Landau operator. However our method of adapting results from the Classical to the Fermi-Dirac situation breaks here, as we did not prove any link between weighted entropies.

Convergence towards equilibrium. As an example of application of Proposition 6.8, we provide a convergence to equilibrium proposition in the hard potential case. We remind that this type of result was

already obtained in [4] (and in [3] for soft potentials), although the constants that we obtain do differ, and our proof is shorter.

Proposition 6.9. Hard potentials case. *Assume $\Psi(|z|) = |z|^{2+\beta}$ with $\beta \in (0, 1]$. Consider $0 \leq f^{in} \in L^1_{s_\beta}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ with $s_\beta = \max\left(\frac{3\beta}{2}, 4 - \beta\right)$. Then there exists $\varepsilon^{in} > 0$ depending only on f^{in} such that for any $\varepsilon \in (0, \varepsilon^{in}]$, there exists a solution f^ε to the homogeneous Landau-Fermi-Dirac equation (associated with the collision operator Q_ε^L defined in (6.81) and the initial distribution f^{in}) and two constants $C_1, C_2 > 0$ such that for any $t \geq 0$,*

$$\|f^\varepsilon(t, \cdot) - \mathcal{M}_\varepsilon^{f^{in}}\|_{L^1_2} \leq C_1 e^{-C_2 t}. \quad (6.87)$$

Proof. The proof is similar to the one of Proposition 6.5, to which we refer the reader, and we only outline here the crucial points. First, we rely on [2, Corollary 3.7] to obtain the existence of $\varepsilon^{in} > 0$ depending only on f^{in} such that for any $\varepsilon \in (0, \varepsilon^{in}]$, the solution f^ε associated with LFD_ε satisfies

$$\sup_{t \geq 1} (1 - \varepsilon \|f^\varepsilon(t, \cdot)\|_\infty) \geq \frac{1}{2}.$$

We are now able to use (6.86). In order for the proof to be complete, we must ensure that the coefficient that multiplies the relative entropy can be lower bounded uniformly in time. It amounts to upper bound the L^2_θ norm of $f^\varepsilon(t, \cdot)$ uniformly in time. This is possible as we have a uniform-in-time L^∞ bound and [4, Theorem 1.3] ensures the generation and uniform-in-time boundedness of all moments at some explicit time. Then the same argument as in [73, Lemma 1] provides the announced exponential decay to equilibrium. \square

6.6 L^1 - L^2 weighted Csiszár-Kullback-Pinsker inequality

In this section, we discuss an optimized version of the L^1 - L^2 weighted Csiszár-Kullback-Pinsker (CKP) inequality presented in Proposition 6.4. For a discussion on the CKP inequality and its previous generalizations, we refer the reader to the paragraph preceding Proposition 6.4 in Subsection 6.2.3.

We highlight that the idea of the proof of (6.90) in the case $r = 1$, $\varpi = 1$, can be found in [123], and the proof of (6.104) (Bose-Einstein case) for $r = 1$, $\varpi = 1$ was also done with the same approach by Lu [122]. Notice moreover that we consider here the case when f is defined on \mathbb{R}^3 , but (6.89)–(6.90) and (6.104) do hold in the broader setting where f and ϖ are defined on an arbitrary measured set, as long as the equilibrium distribution is well-defined. This is further detailed in Appendix 6.B. Finally, we inform the reader that the Bose-Einstein case is briefly discussed in Appendix 6.A, where useful definitions may be found.

Proposition 6.10. L^1 - L^2 weighted Csiszár-Kullback-Pinsker inequality. [optimal]

Let $\varpi : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ be measurable, and $r \in [1, 2]$. Denote

$$\Lambda(\lambda) := \begin{cases} 2 & \text{if } \lambda = 1, \\ \frac{(\lambda - 1)^2}{\lambda \log \lambda - \lambda + 1} & \text{if } \lambda \in \mathbb{R}_+ \setminus \{1\}. \end{cases} \quad (6.88)$$

- **Classical CKP inequality.** For any $0 \leq f \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3) \setminus \{0\}$, assuming that the norms

below are finite,

$$\|(f - M)\varpi\|_{L^r}^2 \leq \|M\varpi^2\|_{L^{\frac{r}{2-r}}} \Lambda \left(\frac{\|f\varpi^2\|_{L^{\frac{r}{2-r}}}}{\|M\varpi^2\|_{L^{\frac{r}{2-r}}}} \right) H_0[f|M], \quad (6.89)$$

where we denoted $M \equiv M^f$ the Maxwellian distribution associated with f and H_0 is defined in (6.21)–(6.22) (with $\varepsilon = 0$).

• **Fermi-Dirac CKP inequality.** For any $\varepsilon > 0$ and $0 \leq f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq 0$ and $\gamma > \frac{2}{5}$, assuming that the norms below are finite,

$$\|(f - \mathcal{M})\varpi\|_{L^r}^2 \leq \|\mathcal{M}\varpi^2\|_{L^{\frac{r}{2-r}}} \Lambda \left(\frac{\|f\varpi^2\|_{L^{\frac{r}{2-r}}}}{\|\mathcal{M}\varpi^2\|_{L^{\frac{r}{2-r}}}} \right) H_\varepsilon[f|\mathcal{M}], \quad (6.90)$$

where we denoted $\mathcal{M} \equiv \mathcal{M}_\varepsilon^f$ the ε -Fermi-Dirac distribution associated with f and H_ε is defined in (6.21)–(6.22).

The announced inequalities (6.40)–(6.41) of Proposition 6.4 are then consequence of Proposition 6.10 and the fact that for any $a \geq 0$ and $b > 0$,

$$b \Lambda \left(\frac{a}{b} \right) \leq 2 \max(a, b). \quad (6.91)$$

The latter inequality can be deduced from the following ones. We claim that in fact,

$$\Lambda(\lambda) \leq 1 + \lambda^{2/3}, \quad \lambda \in [0, 1], \quad (6.92)$$

$$\Lambda(\lambda) \leq \frac{2}{3}(2 + \lambda), \quad \lambda \in (1, 10) \quad (6.93)$$

$$\Lambda(\lambda) \leq \frac{\lambda}{\log(\lambda) - 1}, \quad \lambda \geq 10. \quad (6.94)$$

Notice the improvement of (6.94) over (6.91) by a factor $\frac{1}{2(\log a - \log b - 1)}$ when $\lambda = \frac{a}{b}$ is large, which, even if slowly, converges towards 0 as a goes to infinity. The second inequality (6.93) is well-known, and is actually the one used in the standard proof of the usual CKP inequality (see for instance [88]). As for the third one (6.94), we have for $\lambda \geq 10$,

$$\Lambda(\lambda) = \frac{(\lambda - 1)^2}{\lambda \log \lambda - \lambda + 1} = \frac{\lambda - 1}{\frac{\lambda}{\lambda - 1} \log \lambda - 1} \leq \frac{\lambda}{\log(\lambda) - 1}.$$

Finally, the proof of the first inequality (6.92) is trickier and was suggested to me by Matthieu Dolbeault. Changing variables $x = \lambda^{1/3}$, it is enough to show that for any $x \in [0, 1]$,

$$(1 + x^2)(3x^3 \log x - x^3 + 1) - (1 - x^3)^2 \geq 0.$$

Developing, the above term actually equals $x^2 g(x)$, where

$$g(x) = 1 + x - x^3 - x^4 + 3(x + x^3) \log x.$$

We can then conclude once we prove that g is nonnegative on $(0, 1)$. We compute its first four derivatives,

$$\begin{aligned} g'(x) &= 4 - 4x^3 + (3 + 9x^2) \log x, & g''(x) &= \frac{3}{x} + 9x - 12x^2 + 18x \log x, \\ g'''(x) &= 27 - \frac{3}{x^2} - 24x + 18 \log x, & g^{(4)}(x) &= 6(-4 + x^{-3} + 3x^{-1}). \end{aligned}$$

The function $g^{(4)}$ is clearly nonnegative on $(0, 1)$, hence g''' is nondecreasing on $(0, 1)$. But $g'''(1) = 0$, hence g''' is nonpositive on $(0, 1)$, thus g'' is nonincreasing on $(0, 1)$. Again, $g''(1) = 0$ hence g'' is nonnegative, thus g' is nondecreasing. Again, $g'(1) = 0$ hence g' is nonpositive, thus g is nonincreasing on $(0, 1)$. Finally, $g(1) = 0$, so that g is nonnegative on $(0, 1)$.

Let us now prove Proposition 6.10.

Proof. This proposition is a consequence of the general inequality (6.114) in Corollary 6.17 in Appendix 6.B. We prove both inequalities (6.89)–(6.90) simultaneously, as the first one corresponds to the limit case $\varepsilon = 0$ of the second. Let us then consider $\varepsilon \geq 0$.

We apply Corollary 6.17 with $\Phi(x) \equiv \Phi_\varepsilon(x) = \int_0^x \log \varphi_\varepsilon(y) \, dy$, $J = (0, \varepsilon^{-1})$ and

$$\mathcal{F} = \left\{ 0 \leq g \in L^1_2(\mathbb{R}^3) \mid 1 - \varepsilon g \geq 0, \int_{\mathbb{R}^3} g(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \, dv = \begin{pmatrix} \rho \\ \rho u \\ 3\rho T + \rho|u|^2 \end{pmatrix} \right\},$$

with ρ, T and ε such that $\gamma > \frac{2}{5}$ (ensuring the existence of $\mathcal{M}_\varepsilon^f$). Then (6.114) writes, since $H_{\Phi_\varepsilon} \equiv H_\varepsilon$ the ε -Fermi (or Classical in the case $\varepsilon = 0$) entropy, and $\frac{1}{\Phi_\varepsilon''}(x) = x(1 - \varepsilon x) \leq x$,

$$\|(f - \mathcal{M}_\varepsilon^f) \varpi\|_{L^r}^2 \leq \left(\int_0^1 (1 - \tau) \left\| ((1 - \tau)\mathcal{M}_\varepsilon^f + \tau f) \varpi^2 \right\|_{L^{\frac{r}{2-\tau}}}^{-1} \, d\tau \right)^{-1} H_\varepsilon[f | \mathcal{M}_\varepsilon^f].$$

We focus on the integral in the variable τ . From Minkowski's inequality, we have

$$\begin{aligned} \left(\int_0^1 \frac{1 - \tau}{\left\| ((1 - \tau)\mathcal{M}_\varepsilon^f + \tau f) \varpi^2 \right\|_{L^{\frac{r}{2-\tau}}}^2} \, d\tau \right)^{-1} &\leq \left(\int_0^1 \frac{1 - \tau}{(1 - \tau) \left\| \mathcal{M}_\varepsilon^f \varpi^2 \right\|_{L^{\frac{r}{2-\tau}}}^2 + \tau \|f \varpi^2\|_{L^{\frac{r}{2-\tau}}}^2} \, d\tau \right)^{-1} \\ &= \left\| \mathcal{M}_\varepsilon^f \varpi^2 \right\|_{L^{\frac{r}{2-\tau}}} \Lambda \left(\frac{\|f \varpi^2\|_{L^{\frac{r}{2-\tau}}}}{\left\| \mathcal{M}_\varepsilon^f \varpi^2 \right\|_{L^{\frac{r}{2-\tau}}}} \right), \end{aligned}$$

where Λ is defined in (6.88). Indeed, this last equality comes from the Taylor expansion of $\lambda \mapsto \lambda \log \lambda - \lambda$ around 1,

$$\lambda \log \lambda - \lambda = -1 + (\lambda - 1) \log 1 + (\lambda - 1)^2 \int_0^1 \frac{1 - \tau}{(1 - \tau) + \tau \lambda} \, d\tau,$$

that is

$$\int_0^1 \frac{1 - \tau}{(1 - \tau) + \tau \lambda} \, d\tau = \begin{cases} \frac{1}{2} & \text{if } \lambda = 1, \\ \frac{\lambda \log \lambda - \lambda + 1}{(\lambda - 1)^2} & \text{if } \lambda \in \mathbb{R}_+ \setminus \{1\} \end{cases} = \frac{1}{\Lambda(\lambda)}.$$

□

Finally, as a corollary to Proposition 6.10 come the standard Csiszár-Kullback-Pinsker inequalities.

Corollary 6.11. Standard Csiszár-Kullback-Pinsker inequalities.

For any real number $x \in \mathbb{R}$, we denote in the following $x_+ = \max(0, x)$.

- **Standard Classical CKP inequalities.** For any $\alpha \geq 0$ and $0 \leq f \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3) \setminus \{0\}$,

$$\|f - M\|_{L^1}^2 \leq 2 \|M\|_{L^1} H_0[f|M], \quad (6.95)$$

$$\|(M - f)_+\|_{L^1_\alpha}^2 \leq 2 \|M\|_{L^1_{2\alpha}} H_0[f|M], \quad (6.96)$$

$$\|f - M\|_{L^1_2}^2 \leq 8 \|M\|_{L^1_4} H_0[f|M], \quad (6.97)$$

where we denoted $M \equiv M^f$ the Maxwellian distribution associated with f .

- **Standard Fermi-Dirac CKP inequalities.** For any $\varepsilon > 0$, $\alpha \geq 0$ and $0 \leq f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that $1 - \varepsilon f \geq 0$ and $\gamma > \frac{2}{5}$,

$$\|f - \mathcal{M}\|_{L^1}^2 \leq 2 \|\mathcal{M}\|_{L^1} H_\varepsilon[f|\mathcal{M}], \quad (6.98)$$

$$\|(\mathcal{M} - f)_+\|_{L^1_\alpha}^2 \leq 2 \|\mathcal{M}\|_{L^1_{2\alpha}} H_\varepsilon[f|\mathcal{M}], \quad (6.99)$$

$$\|f - \mathcal{M}\|_{L^1_2}^2 \leq 8 \|\mathcal{M}\|_{L^1_4} H_\varepsilon[f|\mathcal{M}], \quad (6.100)$$

where we denoted $\mathcal{M} \equiv \mathcal{M}_\varepsilon^f$ the ε -Fermi-Dirac distribution associated with f .

Proof. We only prove (6.98)–(6.100) as (6.95)–(6.97) can be seen as a limit case of the previous ones when $\varepsilon \rightarrow 0$.

- *Proof of (6.98).* Applying Proposition 6.10, specifically Equation (6.90), with $r = 1$ and $\varpi = 1$, we obtain

$$\|f - \mathcal{M}\|_{L^1}^2 \leq \|\mathcal{M}\|_{L^1} \Lambda \left(\frac{\|f\|_{L^1}}{\|\mathcal{M}\|_{L^1}} \right) H_\varepsilon[f|\mathcal{M}].$$

Since $\|f\|_{L^1} = \|\mathcal{M}\|_{L^1}$ and $\Lambda(1) = 2$, we obtain (6.98).

- *Proof of (6.99).* Applying Proposition 6.10, specifically Equation (6.90), with the choices $\varpi(v) = (1 + |v|^2)^{\alpha/2} \mathbf{1}_{f \leq \mathcal{M}}$ and $r = 1$, we obtain

$$\|(\mathcal{M} - f)_+\|_{L^1_\alpha}^2 \leq \|\mathcal{M} \mathbf{1}_{f \leq \mathcal{M}}\|_{L^1_{2\alpha}} \Lambda \left(\frac{\|f \mathbf{1}_{f \leq \mathcal{M}}\|_{L^1_{2\alpha}}}{\|\mathcal{M} \mathbf{1}_{f \leq \mathcal{M}}\|_{L^1_{2\alpha}}} \right) H_\varepsilon[f|\mathcal{M}].$$

Since $\|f \mathbf{1}_{f \leq \mathcal{M}}\|_{L^1_{2\alpha}} \leq \|\mathcal{M} \mathbf{1}_{f \leq \mathcal{M}}\|_{L^1_{2\alpha}}$ and, from (6.92), $\Lambda \leq 2$ on $[0, 1]$, we obtain (6.99) after upper bounding $\|\mathcal{M} \mathbf{1}_{f \leq \mathcal{M}}\|_{L^1_{2\alpha}}$ by $\|\mathcal{M}\|_{L^1_{2\alpha}}$.

- *Proof of (6.100).* We remark that $|f - \mathcal{M}| = f - \mathcal{M} + 2(\mathcal{M} - f)_+$, and

$$\int_{\mathbb{R}^3} (f - \mathcal{M})(v) (1 + |v|^2) \, dv = 0,$$

so that

$$\|f - \mathcal{M}\|_{L^1_2}^2 = 4\|(\mathcal{M} - f)_+\|_{L^1_2}^2.$$

We apply (6.99) with $\alpha = 2$ and obtain (6.100). □

6.A Similar results in the Bose-Einstein case

An upper-bound inequality similar to (6.34) can also be obtained in the Bose-Einstein case. This latter case formally corresponds to taking $-\varepsilon$ instead of ε in our formulas. First define for any $x \in \mathbb{R}_+$ and $\varepsilon > 0$,

$$\varphi_\varepsilon^{BE}(x) := \frac{x}{1 + \varepsilon x}, \quad \Phi_\varepsilon^{BE}(x) := \int_0^x \log \varphi_\varepsilon^{BE}(y) \, dy,$$

and the Bose-Einstein entropy of $0 \leq f \in L^1_2(\mathbb{R}^3)$:

$$H_\varepsilon^{BE}(f) := \int_{\mathbb{R}^3} \Phi_\varepsilon^{BE}(f) \, dv.$$

Lu proved in [121] that, under the condition

$$T \geq \frac{\zeta(\frac{5}{2})}{\zeta(\frac{3}{2})} T_c, \quad T_c := \frac{1}{2\pi} \left(\frac{\rho\varepsilon}{\zeta(\frac{3}{2})} \right)^{2/3}, \tag{6.101}$$

where ζ is the Riemann Zêta function and T_c is called the critical temperature, there exists a unique ε -Bose-Einstein statistics $\mathcal{M}_\varepsilon^{BE,f}$ associated with f - that is a distribution such that $\log \varphi_\varepsilon^{BE}(\mathcal{M}_\varepsilon^{BE,f})$ is a linear combination of $v \mapsto 1$, $v \mapsto v$ and $v \mapsto |v|^2$ and sharing the same normalization in $v \mapsto 1$, $v \mapsto v$ and $v \mapsto |v|^2$ as f . We can obtain from Proposition 6.15 in Appendix 6.B that, denoting $H_\varepsilon^{BE}[f|\mathcal{M}_\varepsilon^{BE,f}] := H_\varepsilon^{BE}(f) - H_\varepsilon^{BE}(\mathcal{M}_\varepsilon^{BE,f})$, we have

$$\begin{aligned} H_\varepsilon^{BE}[f|\mathcal{M}_\varepsilon^{BE,f}] &= \int_0^1 (1 - \tau) \left(\int_{\mathbb{R}^3} (f(v) - \mathcal{M}_\varepsilon^{BE,f}(v))^2 \Phi_\varepsilon^{BE''} \left((1 - \tau)\mathcal{M}_\varepsilon^{BE,f}(v) + \tau f(v) \right) \, dv \right) \, d\tau \\ &= \int_{\mathbb{R}^3} \int_{\mathcal{M}_\varepsilon^{BE,f}(v)}^{f(v)} \frac{f(v) - x}{\varphi_\varepsilon^{BE}(x)} \varphi_\varepsilon^{BE'}(x) \, dx \, dv, \end{aligned} \tag{6.102}$$

where the last equality comes from $\Phi_\varepsilon^{BE''} = \frac{\varphi_\varepsilon^{BE'}}{\varphi_\varepsilon^{BE}}$ and the change of variables $x = \mathcal{M}_\varepsilon^{BE,f}(v) + \tau(f(v) - \mathcal{M}_\varepsilon^{BE,f}(v))$.

In the following Proposition, we provide a link between the relative entropies to equilibrium of the Bose-Einstein and the classical cases. Although I believe that both inequalities could be obtained, we only present here the ‘‘upper-bound’’ inequality as its proof is rather short. Further work may allow to obtain the lower-bound inequality, with a constant that probably depends on an L^∞ bound on f . This constitutes another reason why we did not investigate this other inequality, as, although L^∞ bounds are natural to use in the Fermi-Dirac context, due to Pauli’s exclusion principle, they are not in the Bose-Einstein one, due to the phenomenon of condensation.

Proposition 6.12. Upper-bound in the Bose-Einstein case. *For any $\varepsilon > 0$ and nonnegative $f \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3) \setminus \{0\}$ which density and temperature satisfy (6.101), we have*

$$H_0 \left[\frac{f}{1 + \varepsilon f} \middle| M^{\frac{f}{1 + \varepsilon f}} \right] \leq H_\varepsilon^{BE} [f|\mathcal{M}_\varepsilon^{BE,f}]. \tag{6.103}$$

Proof. The starting point of the proof are Equation (6.102) and the inequality $|y - z| \geq |\varphi_\varepsilon^{BE}(y) -$

$\varphi_\varepsilon^{BE}(z)$ for all $(y, z) \in \mathbb{R}_+^2$, yielding

$$\begin{aligned} H_\varepsilon^{BE} [f | \mathcal{M}_\varepsilon^{BE, f}] &= \int_{\mathbb{R}^3} \int_{\mathcal{M}_\varepsilon^{BE, f}}^f \frac{f-x}{\varphi_\varepsilon^{BE}(x)} \varphi_\varepsilon^{BE'}(x) \, dx \, dv \\ &\geq \int_{\mathbb{R}^3} \int_{\mathcal{M}_\varepsilon^{BE, f}}^f \frac{\varphi_\varepsilon^{BE}(f) - \varphi_\varepsilon^{BE}(x)}{\varphi_\varepsilon^{BE}(x)} \varphi_\varepsilon^{BE'}(x) \, dx \, dv. \end{aligned}$$

Applying the change of variables $y = \varphi_\varepsilon^{BE}(x)$ and using formula (6.27), we obtain

$$H_\varepsilon^{BE} [f | \mathcal{M}_\varepsilon^{BE, f}] \geq H_0 [\varphi_\varepsilon^{BE}(f) | M^{\varphi_\varepsilon^{BE}(f)}] + \int_{\mathbb{R}^3} \int_{\varphi_\varepsilon^{BE}(\mathcal{M}_\varepsilon^{BE, f})}^{M^{\varphi_\varepsilon^{BE}(f)}} \frac{\varphi_\varepsilon^{BE}(f) - y}{y} \, dy \, dv.$$

Remark that, as $\log M^{\varphi_\varepsilon^{BE}(f)} - \log \varphi_\varepsilon^{BE}(\mathcal{M}_\varepsilon^{BE, f})$ is a linear combination of conserved quantities (namely, $v \mapsto 1$, $v \mapsto v$ and $v \mapsto |v|^2$), we have by definition of $M^{\varphi_\varepsilon^{BE}(f)}$ that

$$\int_{\mathbb{R}^3} \varphi_\varepsilon^{BE}(f) \log \left(\frac{M^{\varphi_\varepsilon^{BE}(f)}}{\varphi_\varepsilon^{BE}(\mathcal{M}_\varepsilon^{BE, f})} \right) \, dv = \int_{\mathbb{R}^3} M^{\varphi_\varepsilon^{BE}(f)} \log \left(\frac{M^{\varphi_\varepsilon^{BE}(f)}}{\varphi_\varepsilon^{BE}(\mathcal{M}_\varepsilon^{BE, f})} \right) \, dv,$$

so that

$$\int_{\mathbb{R}^3} \int_{\varphi_\varepsilon^{BE}(\mathcal{M}_\varepsilon^{BE, f})}^{M^{\varphi_\varepsilon^{BE}(f)}} \frac{\varphi_\varepsilon^{BE}(f) - y}{y} \, dy \, dv = \int_{\mathbb{R}^3} \int_{\varphi_\varepsilon^{BE}(\mathcal{M}_\varepsilon^{BE, f})}^{M^{\varphi_\varepsilon^{BE}(f)}} \frac{M^{\varphi_\varepsilon^{BE}(f)} - y}{y} \, dy \, dv \geq 0,$$

ending the proof. \square

Proposition 6.13. Bose-Einstein CKP inequality. Let $\varpi : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ be measurable, and $r \in [1, 2]$. We recall the definition (6.88) of the function Λ ,

$$\Lambda(\lambda) := \begin{cases} 2 & \text{if } \lambda = 1, \\ \frac{(\lambda - 1)^2}{\lambda \log \lambda - \lambda + 1} & \text{if } \lambda \in \mathbb{R}_+ \setminus \{1\}. \end{cases}$$

Then for any $\varepsilon > 0$ and $0 \leq f \in L_2^1(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3) \setminus \{0\}$ which density and temperature satisfy (6.101), assuming that the norms below are finite,

$$\|(f - \mathcal{M}) \varpi\|_{L^r}^2 \leq \|\mathcal{M}(1 + \varepsilon \mathcal{M}) \varpi^2\|_{L^{\frac{r}{2-r}}} \Lambda \left(\frac{\|f(1 + \varepsilon f) \varpi^2\|_{L^{\frac{r}{2-r}}}}{\|\mathcal{M}(1 + \varepsilon \mathcal{M}) \varpi^2\|_{L^{\frac{r}{2-r}}}} \right) H_\varepsilon^{BE} [f | \mathcal{M}], \quad (6.104)$$

where we denoted $\mathcal{M} \equiv \mathcal{M}_\varepsilon^{BE, f}$ the ε -Bose-Einstein distribution associated with f , and H_ε^{BE} is the Bose-Einstein entropy. When $r = 2$, $L^{\frac{r}{2-r}}$ shall be understood as L^∞ .

Proof. The proof is similar to the one of Proposition 6.10. Let $\varepsilon > 0$.

We apply Corollary 6.17 with $\Phi(x) \equiv \Phi_\varepsilon^{BE}(x) = \int_0^x \log \frac{y}{1+\varepsilon y} dy$, $J = \mathbb{R}_+^*$ and

$$\mathcal{F} = \left\{ 0 \leq g \in L^1_2(\mathbb{R}^3) \left| \int_{\mathbb{R}^3} g(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = \begin{pmatrix} \rho \\ \rho u \\ 3\rho T + \rho|u|^2 \end{pmatrix} \right. \right\},$$

with ρ, T and ε such that (6.101) is satisfied, ensuring the existence of $\mathcal{M}_\varepsilon^{BE,f}$. In the rest of this proof, we denote for the sake of clarity $\mathcal{M} \equiv \mathcal{M}_\varepsilon^{BE,f}$. Then (6.114) writes, since $H_{\Phi_\varepsilon^{BE}} \equiv H_\varepsilon^{BE}$ the ε -Bose-Einstein entropy, and $\frac{1}{\Phi_\varepsilon^{BE}''}(x) = x(1 + \varepsilon x)$ is convex,

$$\|(f - \mathcal{M}) \varpi\|_{L^r}^2 \leq \left(\int_0^1 (1 - \tau) \|((1 - \tau)\mathcal{M}(1 + \varepsilon\mathcal{M}) + \tau f(1 + \varepsilon f)) \varpi^2\|_{L^{\frac{r}{2-\tau}}}^{-1} d\tau \right)^{-1} H_\varepsilon^{BE}[f|\mathcal{M}].$$

We focus on the term with the integral in τ . From Minkowski's inequality, it is smaller than

$$\begin{aligned} & \left(\int_0^1 \frac{1 - \tau}{(1 - \tau) \|\mathcal{M}(1 + \varepsilon\mathcal{M}) \varpi^2\|_{L^{\frac{r}{2-\tau}}} + \tau \|f(1 + \varepsilon f) \varpi^2\|_{L^{\frac{r}{2-\tau}}} } d\tau \right)^{-1} \\ &= \|\mathcal{M}(1 + \varepsilon\mathcal{M}) \varpi^2\|_{L^{\frac{r}{2-\tau}}} \Lambda \left(\frac{\|f(1 + \varepsilon f) \varpi^2\|_{L^{\frac{r}{2-\tau}}}}{\|\mathcal{M}(1 + \varepsilon\mathcal{M}) \varpi^2\|_{L^{\frac{r}{2-\tau}}}} \right), \end{aligned}$$

where Λ is defined in (6.88) and appears thanks to a Taylor expansion of $\lambda \mapsto \lambda \log \lambda - \lambda$ around 1 like in the proof of Proposition 6.10, allowing to conclude. \square

From the previous proposition, we easily deduce the following standard inequalities.

Corollary 6.14. Standard Bose-Einstein CKP inequalities. For any $\varepsilon > 0$, $\alpha \geq 0$ and $0 \leq f \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3) \setminus \{0\}$ satisfying (6.101),

$$\|(\mathcal{M} - f)_+\|_{L^1_\alpha}^2 \leq 2 \left(\|\mathcal{M}\|_{L^1_{2\alpha}} + \varepsilon \|\mathcal{M}\|_{L^2_\alpha}^2 \right) H_\varepsilon^{BE}[f|\mathcal{M}], \tag{6.105}$$

$$\|f - \mathcal{M}\|_{L^1}^2 \leq 8 \left(\|\mathcal{M}\|_{L^1} + \varepsilon \|\mathcal{M}\|_{L^2}^2 \right) H_\varepsilon^{BE}[f|\mathcal{M}], \tag{6.106}$$

$$\|f - \mathcal{M}\|_{L^1_2}^2 \leq 8 \left(\|\mathcal{M}\|_{L^1_4} + \varepsilon \|\mathcal{M}\|_{L^2_2}^2 \right) H_\varepsilon^{BE}[f|\mathcal{M}], \tag{6.107}$$

where we denoted for clarity $\mathcal{M} \equiv \mathcal{M}_\varepsilon^{BE,f}$ the ε -Bose-Einstein distribution associated with f .

We prove the above inequalities similarly as we did for Corollary 6.11. For (6.105) we apply Proposition 6.13 with $r = 1$ and $\varpi(v) = (1 + |v|^2)^{\frac{\alpha}{2}} \mathbf{1}_{f \leq \mathcal{M}}$ and notice that $\Lambda \leq 2$ on $[0, 1]$. We then obtain (6.106)–(6.107) by decomposing $|f - \mathcal{M}| = f - \mathcal{M} + 2(\mathcal{M} - f)_+$, using the fact that f and \mathcal{M} share the same normalization in $v \mapsto 1$, $v \mapsto v$ and $v \mapsto |v|^2$, and (6.105) with respectively $\alpha = 0$ and $\alpha = 2$.

6.B A general discussion about entropies and equilibria

In this section we intend to provide general considerations on the entropy, which are much more general than the scope of this paper, but give a good understanding of the notions we used, and could also be helpful in the study of weak turbulence, where various kinds of unusual entropies can emerge (see [48]).

Our setting is laid down quite generally, and is similar to the one of Chafaï [64] (in terms of relative Φ -entropy). Consider a measured space $(\mathcal{E}, \mathcal{A}, \mu)$, an open interval $J \subset \mathbb{R}$ which closure we denote by \bar{J} , and a function $\Phi \in \mathcal{C}^2(J) \cap \mathcal{C}^0(\bar{J})$ such that $\Phi'' > 0$ on J . Remark that Φ' is then a \mathcal{C}^1 -diffeomorphism from J onto $\Phi'(J)$.

Entropy. We define the Φ -entropy, for any $(\mathcal{A}, \text{Bor}(\bar{J}))$ -measurable $f : \mathcal{E} \rightarrow \bar{J}$ such that the following integral makes sense and is finite, by

$$H_{\Phi}(f) := \int_{\mathcal{E}} \Phi(f(\zeta)) \, \mathrm{d}\mu(\zeta), \quad (6.108)$$

and we denote by E_{Φ} the set of such f . We let the relative Φ -entropy of f and g to be

$$H_{\Phi}[f|g] = H_{\Phi}(f) - H_{\Phi}(g). \quad (6.109)$$

We also define, for $(\mathcal{A}, \text{Bor}(\bar{J}))$ -measurable $f, g : \mathcal{E} \rightarrow \bar{J}$, the Φ -relative-entropy (which in general differs from the relative Φ -entropy) of f and g by

$$\mathcal{H}_{\Phi}[f|g] := \int_0^1 (1-\tau) \left(\int_{g \in J} (f-g)^2 \Phi''((1-\tau)g + \tau f) \, \mathrm{d}\mu(\zeta) \right) \, \mathrm{d}\tau. \quad (6.110)$$

Note that $\mathcal{H}_{\Phi}[f|g]$ is possibly infinite, but always well-defined, as

$$g \in J \implies \forall \tau \in (0, 1), \quad (1-\tau)g + \tau f \in J,$$

and that $\mathcal{H}_{\Phi}[f|g]$ is always nonnegative. The following Proposition 6.15 gives a quite simple but general result linking entropies, conserved quantities and equilibrium distributions, under a sole existence assumption.

Proposition 6.15. *Let I be a countable set, $(\phi_i)_{i \in I}$ a family of measurable real functions, $(\omega_i)_{i \in I}$ a family of real numbers, and*

$$\mathcal{F} = \left\{ f \in E_{\Phi} \text{ s.t. } \forall i \in I, \int_{\mathcal{E}} |f(\zeta)| |\phi_i(\zeta)| \, \mathrm{d}\mu(\zeta) < \infty \text{ and } \int_{\mathcal{E}} f(\zeta) \phi_i(\zeta) \, \mathrm{d}\mu(\zeta) = \omega_i \right\}.$$

Assume that $\Phi'(J) = \mathbb{R}$, and that there exists $(\alpha_i(\omega)) \in \mathbb{R}^I$ such that $M_{\Phi}^{\mathcal{F}} \in \mathcal{F}$, where

$$M_{\Phi}^{\mathcal{F}} := (\Phi')^{-1} \left(\sum_{i \in I} \alpha_i(\omega) \phi_i \right). \quad (6.111)$$

Then the following four propositions are equivalent. Let $g \in \mathcal{F}$.

- (i) $g \in J$ μ -a.e. and $\forall f \in \mathcal{F}$, $H_{\Phi}[f|g] = \mathcal{H}_{\Phi}[f|g]$,
- (ii) $g \in J$ μ -a.e. and $\forall f \in \mathcal{F}$, $\mathcal{H}_{\Phi}[f|g] < \infty$ and $\int_{\mathcal{E}} (f-g) \Phi'(g) \, \mathrm{d}\mu(\zeta) = 0$,
- (iii) $H_{\Phi}(g) = \min_{h \in \mathcal{F}} H_{\Phi}(h)$,
- (iv) $g = M_{\Phi}^{\mathcal{F}}$ μ -a.e.

In particular, $M_{\Phi}^{\mathcal{F}}$ is the unique minimizer of H_{Φ} under the constraints of the set \mathcal{F} .

The above proposition actually proves the following (under the assumptions $\Phi'(J) = \mathbb{R}$ and of existence

of $M_{\Phi}^{\mathcal{F}}$). An admissible distribution g is an equilibrium relative to the conserved quantities ϕ_i , in the sense of the minimization of the Φ -entropy [(iii)], if and only if $\Phi'(g)$ is a linear combination of the functions ϕ_i [(iv)], if and only if the relative Φ -entropy between any admissible distribution f and g is given by (6.110) [(i)], if and only if the quantity $\Phi'(g)$ is conserved amongst all admissible distributions [(ii)] - indeed, (ii) is equivalent, assuming the following integrals make sense, to $\forall f_1, f_2 \in \mathcal{F}, \int_{\mathcal{E}} f_1 \Phi'(g) d\mu(\zeta) = \int_{\mathcal{E}} f_2 \Phi'(g) d\mu(\zeta)$.

The reader may notice that the Classical case corresponds to the choice $\Phi(x) \equiv \Phi_0(x) = x \log x - x$, for which $(\Phi'_0)^{-1} = \exp$, hence $M_{\Phi}^{\mathcal{F}}$ is in this case a Maxwellian, since the conserved quantities (corresponding to the functions ϕ_i in the proposition) are $v \mapsto 1, v \mapsto v$ and $v \mapsto |v|^2$.

Moreover, the Fermi-Dirac case corresponds to the choice $\Phi(x) \equiv \Phi_{\varepsilon}(x) \equiv \int_0^x \log \frac{y}{1-\varepsilon y} dy$, for which

$(\Phi'_{\varepsilon})^{-1}(x) = \frac{e^x}{1+\varepsilon e^x}$, hence $M_{\Phi}^{\mathcal{F}}$ is in this case a Fermi-Dirac distribution, since again, the conserved quantities (corresponding to the functions ϕ_i in the proposition) are $v \mapsto 1, v \mapsto v$ and $v \mapsto |v|^2$. Proposition 6.1 then comes as a corollary to Proposition 6.15 with $\mathcal{E} = \mathbb{R}^3$ endowed with the Lebesgue measure, $J = (0, \varepsilon^{-1}), \Phi(x) \equiv \Phi_{\varepsilon}(x) \equiv \int_0^x \log \varphi_{\varepsilon}(y) dy, M_{\Phi}^{\mathcal{F}} \equiv \mathcal{M}_{\varepsilon}^f$ and

$$\mathcal{F} = \left\{ 0 \leq f \in L^1_2(\mathbb{R}^3) \mid 1 - \varepsilon f \geq 0, \int_{\mathbb{R}^3} f(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = \begin{pmatrix} \rho \\ \rho u \\ 3\rho T + \rho |u|^2 \end{pmatrix} \right\},$$

with ρ, T and ε such that $\gamma > \frac{2}{5}$ (ensuring the existence of $\mathcal{M}_{\varepsilon}^f$, as proven in [123]).

Remark 6.6. The Bose-Einstein case is also recovered with $\Phi(x) \equiv \Phi_{\varepsilon}^{BE}(x) \equiv \int_0^x \log \frac{y}{1+\varepsilon y} dy$, for

which $(\Phi'_{-\varepsilon})^{-1}(x) = \frac{e^x}{1-\varepsilon e^x}$, hence $M_{\Phi}^{\mathcal{F}}$ is in this case a Bose-Einstein distribution (when it exists).

Proof. We start by proving (i) \iff (ii). Let $f, g \in \mathcal{F}$ such that $g \in J$ μ -almost everywhere and $\mathcal{H}_{\Phi}[f|g] < \infty$. Using a Taylor expansion followed by Fubini's Theorem, we get

$$\begin{aligned} H_{\Phi}[f|g] &= \int_{\mathcal{E}} (\Phi(f) - \Phi(g)) d\mu(\zeta) = \int_{g \in J} (\Phi(f) - \Phi(g)) d\mu(\zeta) \\ &= \int_{g \in J} \left((f-g)\Phi'(g) + (f-g)^2 \int_0^1 (1-\tau)\Phi''((1-\tau)g + \tau f) d\tau \right) d\mu(\zeta) \\ &= \int_{g \in J} (f-g)\Phi'(g) d\mu(\zeta) + \mathcal{H}_{\Phi}[f|g], \end{aligned}$$

thus proving the announced equivalence. Remark that in the last equality we used the fact that $\mathcal{H}_{\Phi}[f|g] < \infty$ to ensure that $\int_{g \in J} (f-g)\Phi'(g) d\mu(\zeta)$ is well-defined. We now show (iv) \implies (ii). Since $\text{Im}(\Phi'^{-1}) = J$, we do have $M_{\Phi}^{\mathcal{F}} \in J$ μ -almost everywhere, and

$$\begin{aligned} \int_{M_{\Phi}^{\mathcal{F}} \in J} (f - M_{\Phi}^{\mathcal{F}}) \Phi'(M_{\Phi}^{\mathcal{F}}) d\mu(\zeta) &= \int_{\mathcal{E}} (f - M_{\Phi}^{\mathcal{F}}) \sum_i \alpha_i(\omega_i) \phi_i d\mu(\zeta) \\ &= \sum_i \alpha_i(\omega_i) \left(\int_{\mathcal{E}} f \phi_i d\mu(\zeta) - \int_{\mathcal{E}} M_{\Phi}^{\mathcal{F}} \phi_i d\mu(\zeta) \right) = 0, \end{aligned}$$

where the last equality comes from the fact that both f and $M_\Phi^{\mathcal{F}}$ belong to \mathcal{F} . We now focus on (ii) \implies (iv). Assume the existence of $g \in \mathcal{F}$ such that $g \in J$ μ -almost everywhere and

$$\forall f \in \mathcal{F}, \quad \int_{g \in J} (f - g) \Phi'(g) \, d\mu(\zeta) = 0.$$

Since we also have $M_\Phi^{\mathcal{F}} \in \mathcal{F}$, then $M_\Phi^{\mathcal{F}} \in J$ μ -almost everywhere and we just proved that

$$\int_{M_\Phi^{\mathcal{F}} \in J} (g - M_\Phi^{\mathcal{F}}) \Phi'(M_\Phi^{\mathcal{F}}) \, d\mu(\zeta) = 0,$$

allowing to deduce that

$$\int_{\mathcal{E}} (g - M_\Phi^{\mathcal{F}}) (\Phi'(g) - \Phi'(M_\Phi^{\mathcal{F}})) \, d\mu(\zeta) = 0.$$

Since Φ' is increasing, this implies that $g = M_\Phi^{\mathcal{F}}$ μ -almost everywhere. We now focus on (iv) \implies (iii). Since we already proved (iv) \implies (ii) \implies (i), we have for any $f \in \mathcal{F}$,

$$H_\Phi[f|M_\Phi^{\mathcal{F}}] = \mathcal{H}_\Phi[f|M_\Phi^{\mathcal{F}}] \geq 0,$$

thus

$$H_\Phi(f) \geq H_\Phi(M_\Phi^{\mathcal{F}}).$$

Finally, we prove (iii) \implies (iv). Assume $H_\Phi(g) = \min_{h \in \mathcal{F}} H_\Phi(h)$. We just proved that $H_\Phi(M_\Phi^{\mathcal{F}}) = \min_{h \in \mathcal{F}} H_\Phi(h)$, hence $H_\Phi(g) = H_\Phi(M_\Phi^{\mathcal{F}})$ and $H_\Phi[g|M_\Phi^{\mathcal{F}}] = 0$. Since we also proved (iv) \implies (i), we know that

$$\mathcal{H}_\Phi[g|M_\Phi^{\mathcal{F}}] = H_\Phi[g|M_\Phi^{\mathcal{F}}],$$

hence $\mathcal{H}_\Phi[g|M_\Phi^{\mathcal{F}}] = 0$, that is

$$\int_0^1 (1 - \tau) \left(\int_{M_\Phi^{\mathcal{F}} \in J} (g - M_\Phi^{\mathcal{F}})^2 \Phi''((1 - \tau)M + \tau g) \, d\mu(\zeta) \right) \, d\tau = 0.$$

This implies, since $M_\Phi^{\mathcal{F}} \in J$ and $(1 - \tau)M_\Phi^{\mathcal{F}} + \tau g \in J$ μ -almost everywhere for any $\tau \in (0, 1)$, and $\Phi'' > 0$ on J , that $g = M_\Phi^{\mathcal{F}}$ μ almost everywhere. \square

General Csiszár-Kullback-Pinsker inequality. The famous Csiszár-Kullback-Pinsker inequality, linking the squared L^1 distance of two probabilities with their relative Classical entropy can in fact be generalized to the whole family of Φ -entropies, and for weighted L^r , $1 \leq r \leq 2$ distances, by the following Proposition 6.16, and more specifically, in the context of convergence towards equilibrium, by Corollary 6.17. Again, such inequalities may be useful in the study of weak turbulence [48].

Proposition 6.16. *Let some $(\mathcal{A}, \text{Bor}(\bar{J}))$ -measurable $\varpi : \mathcal{E} \rightarrow \bar{J}$ and $r \in [1, 2]$. Then for any $(\mathcal{A}, \text{Bor}(\bar{J}))$ -measurable $f, g : \mathcal{E} \rightarrow \bar{J}$ such that all terms below are finite, we have*

$$\|(f - g) \varpi\|_{L^r(g \in J)}^2 \leq \left(\int_0^1 (1 - \tau) \left\| \frac{\varpi^2}{\Phi''((1 - \tau)g + \tau f)} \right\|_{L^{\frac{r}{2 - \tau}}(g \in J)}^{-1} \, d\tau \right)^{-1} \mathcal{H}_\Phi[f|g], \quad (6.112)$$

where \mathcal{H}_Φ is the Φ -relative-entropy defined in (6.110).

Proof. Let us recall the definition of $\mathcal{H}_\Phi[f|g]$, that is

$$\mathcal{H}_\Phi[f|g] = \int_0^1 (1-\tau) \left(\int_{g \in J} (f-g)^2 \Phi''((1-\tau)g + \tau f) d\mu(\zeta) \right) d\tau.$$

We fix $\tau \in (0, 1)$. Let $p = \frac{2}{r} \in [1, 2]$ and $q = \frac{2}{2-r} \in [2, +\infty]$, so that $\frac{1}{p} + \frac{1}{q} = 1$. By Hölder's inequality, we have

$$\begin{aligned} \int_{g \in J} |f-g|^{\frac{2}{p}} \varpi^{\frac{2}{p}} d\mu(\zeta) &= \int_{g \in J} |f-g|^{\frac{2}{p}} \Phi''((1-\tau)g + \tau f)^{\frac{1}{p}} \left[\frac{\varpi^2}{\Phi''((1-\tau)g + \tau f)} \right]^{\frac{1}{p}} d\mu(\zeta) \\ &\leq \left(\int_{g \in J} (f-g)^2 \Phi''((1-\tau)g + \tau f) d\mu(\zeta) \right)^{\frac{1}{p}} \left\| \left[\frac{\varpi^2}{\Phi''((1-\tau)g + \tau f)} \right]^{\frac{1}{p}} \right\|_{L^q(g \in J)}. \end{aligned}$$

Raising the above inequality to the power p , we obtain

$$\begin{aligned} \left(\int_{g \in J} |f-g|^{\frac{2}{p}} \varpi^{\frac{2}{p}} d\mu(\zeta) \right)^p &\leq \\ &\left(\int_{g \in J} (f-g)^2 \Phi''((1-\tau)g + \tau f) d\mu(\zeta) \right) \left\| \frac{\varpi^2}{\Phi''((1-\tau)g + \tau f)} \right\|_{L^{\frac{q}{p}}(g \in J)}, \end{aligned} \quad (6.113)$$

where we used the fact that $\|\cdot\|_{L^q}^{\frac{1}{p}} = \|\cdot\|_{L^{\frac{q}{p}}}$. Since $\frac{2}{p} = r$ and $\frac{q}{p} = \frac{r}{2-r}$, (6.113) actually writes

$$\|(f-g)\varpi\|_{L^r(g \in J)}^2 \leq \left(\int_{g \in J} (f-g)^2 \Phi''((1-\tau)g + \tau f) d\mu(\zeta) \right) \left\| \frac{\varpi^2}{\Phi''((1-\tau)g + \tau f)} \right\|_{L^{\frac{r}{2-r}}(g \in J)}.$$

If ϖ is zero μ -almost everywhere on $\{g \in J\}$, then the proposition is trivial. Else, since $\Phi'' > 0$ on $\{g \in J\}$ and $(1-\tau)g + \tau f \in J$ on $\{g \in J\}$ for any $\tau \in (0, 1)$, we know that $\left\| \frac{\varpi^2}{\Phi''((1-\tau)g + \tau f)} \right\|_{L^{\frac{r}{2-r}}(g \in J)}$ is non zero. Since we assumed that the quantity

$$\left(\int_0^1 (1-\tau) \left\| \frac{\varpi^2}{\Phi''((1-\tau)g + \tau f)} \right\|_{L^{\frac{r}{2-r}}(g \in J)}^{-1} d\tau \right)^{-1}$$

is finite, we also know that for almost every $\tau \in (0, 1)$ we have $\left\| \frac{\varpi^2}{\Phi''((1-\tau)g + \tau f)} \right\|_{L^{\frac{r}{2-r}}(g \in J)} < \infty$.

For these values of τ , we then have

$$\|(f-g)\varpi\|_{L^r(g \in J)}^2 \frac{1-\tau}{\left\| \frac{\varpi^2}{\Phi''((1-\tau)g + \tau f)} \right\|_{L^{\frac{r}{2-r}}(g \in J)}} \leq (1-\tau) \left(\int_{g \in J} (f-g)^2 \Phi''((1-\tau)g + \tau f) d\mu(\zeta) \right).$$

Integrating in τ yields

$$\|(f-g)\varpi\|_{L^r(g \in J)}^2 \left(\int_0^1 (1-\tau) \left\| \frac{\varpi^2}{\Phi''((1-\tau)g + \tau f)} \right\|_{L^{\frac{r}{2-r}}(g \in J)}^{-1} d\tau \right) \leq \mathcal{H}_\Phi[f|g].$$

Since, again by hypothesis, the integral in τ is nonzero (its inverse is finite), we obtain (6.112). \square

Remarking that $\{M_\Phi^{\mathcal{F}} \in J\} = \mathcal{E}$ and that for any $f \in \mathcal{F}$, $\mathcal{H}_\Phi[f|M_\Phi^{\mathcal{F}}] = H_\Phi[f|M_\Phi^{\mathcal{F}}]$ (see Proposition 6.15), we straightforwardly obtain the following corollary.

Corollary 6.17. *Let some $(\mathcal{A}, \text{Bor}(\bar{J}))$ -measurable $\varpi : \mathcal{E} \rightarrow \bar{J}$ and $r \in [1, 2]$. With the same notations as in Proposition 6.15, assuming $M_\Phi^{\mathcal{F}}$ exists, we have for any $f \in \mathcal{F}$ such that the integral term below is finite,*

$$\|(f - M_\Phi^{\mathcal{F}})\varpi\|_{L^r}^2 \leq \left(\int_0^1 (1-\tau) \left\| \frac{\varpi^2}{\Phi''((1-\tau)M_\Phi^{\mathcal{F}} + \tau f)} \right\|_{L^{\frac{r}{2-\tau}}}^{-1} d\tau \right)^{-1} H_\Phi[f|M_\Phi^{\mathcal{F}}], \quad (6.114)$$

where H_Φ is defined in (6.108)–(6.109) and $M_\Phi^{\mathcal{F}}$ is the equilibrium associated with Φ and the set \mathcal{F} , defined in (6.111).

6.C Technical results

In this section, we consider $\mathcal{M}_\varepsilon^f$, the Fermi-Dirac distribution associated with some $\varepsilon > 0$ and $0 \leq f \in L_2^1(\mathbb{R}^3)$ such that $1 - \varepsilon f \geq 0$. The existence of $\mathcal{M}_\varepsilon^f$ is provided by assuming $\gamma > \frac{2}{5}$ (see [123]), where we recall the notation

$$\gamma := \frac{T}{T_F(\rho, \varepsilon)}, \quad (6.115)$$

where $T_F(\rho, \varepsilon) = \frac{1}{2} \left(\frac{3\rho\varepsilon}{4\pi} \right)^{2/3}$ is the Fermi temperature associated with ρ and ε ; and ρ, T are respectively the density and temperature associated with the distribution f , defined in (6.12). We also recall the notation, for $x \in [0, \varepsilon^{-1})$,

$$\varphi_\varepsilon(x) = \frac{x}{1 - \varepsilon x}.$$

6.C.1 L^∞ bound for the Fermi-Dirac statistics

In this subsection, we provide an L^∞ bound on the Fermi-Dirac statistics. The following result is very similar to [2, Lemma A.1].

Proposition 6.18. *Let $\varepsilon > 0$ and $f \in L_2^1(\mathbb{R}^3)$ be a nonnegative distribution such that $1 - \varepsilon f \geq 0$ and $\gamma \geq \gamma^\dagger$, where γ is given by (6.115) and*

$$\gamma^\dagger := \left(\frac{4}{\pi} \right)^{\frac{1}{3}} \left(\frac{5}{3} \right)^{\frac{5}{3}}. \quad (6.116)$$

Then the quantity $\varepsilon \|\varphi_\varepsilon(\mathcal{M}_\varepsilon^f)\|_\infty$ satisfies

$$\varepsilon \|\varphi_\varepsilon(\mathcal{M}_\varepsilon^f)\|_\infty \leq \frac{2}{3} \left(\frac{\gamma}{\gamma^\dagger} \right)^{-3/2}. \quad (6.117)$$

Proof. Our proof is based on [123, proof of Proposition 3]. We introduce, for $s \geq 0$,

$$I_s(t) := \int_0^\infty \frac{r^s}{1 + te^{r^2}} dr, \quad P(t) := I_4(t)[I_2(t)]^{-5/3}, \quad t > 0.$$

It is proven in [123, proof of Proposition 3] that P is continuous and increasing on \mathbb{R}_+ , and that

$$P\left(\frac{1}{\varepsilon\|\varphi_\varepsilon(\mathcal{M}_\varepsilon^f)\|_\infty}\right) = 3\rho^{-2/3}T(4\pi\varepsilon^{-1})^{2/3} \equiv \frac{3^{5/3}}{2}\gamma.$$

Let $\alpha > 0$ and

$$t = \alpha^{-1} \times \frac{3\sqrt{\pi}}{4} \gamma^{3/2}.$$

As, for any $r \geq 0$, it holds that

$$\frac{e^{-r^2}}{1+t} \leq \frac{1}{1+te^{r^2}} \leq \frac{e^{-r^2}}{t},$$

we have

$$P(t) \leq \left(\frac{1}{t} \int_0^\infty r^4 e^{-r^2} dr\right) \left(\frac{1}{1+t} \int_0^\infty r^2 e^{-r^2} dr\right)^{-5/3} = \frac{(1+t)^{5/3}}{t} \left(\frac{1}{2}\Gamma\left(\frac{5}{2}\right)\right) \left(\frac{1}{2}\Gamma\left(\frac{3}{2}\right)\right)^{-5/3},$$

that is

$$P(t) \leq \frac{(1+t)^{5/3}}{t} \times \frac{3 \times 2^{1/3}}{\pi^{1/3}}.$$

We define

$$\gamma^\alpha := \left(\frac{4}{3\sqrt{\pi}} \times \frac{\alpha}{\alpha^{2/5}-1}\right)^{2/3}.$$

Then, whenever $\gamma \geq \gamma^\alpha$, we have $t \geq \frac{1}{\alpha^{2/5}-1}$, so that $1+t \leq \alpha^{2/5}t$, implying

$$P(t) \leq t^{2/3} \times \frac{3 \times 2^{1/3} \alpha^{2/3}}{\pi^{1/3}} = \alpha^{-2/3} \times \left(\frac{3\sqrt{\pi}}{4}\right)^{2/3} \gamma \times \frac{3 \times 2^{1/3} \alpha^{2/3}}{\pi^{1/3}} = \frac{3^{5/3}}{2} \gamma = P\left(\frac{1}{\varepsilon\|\varphi_\varepsilon(\mathcal{M}_\varepsilon^f)\|_\infty}\right).$$

Since P is increasing, we deduce that, whenever $\gamma \geq \gamma^\alpha$, we have

$$\alpha^{-1} \times \frac{3\sqrt{\pi}}{4} \gamma^{3/2} = t \leq \frac{1}{\varepsilon\|\varphi_\varepsilon(\mathcal{M}_\varepsilon^f)\|_\infty},$$

that is

$$\varepsilon\|\varphi_\varepsilon(\mathcal{M}_\varepsilon^f)\|_\infty \leq \alpha \times \frac{4}{3\sqrt{\pi}} \gamma^{-3/2}. \quad (6.118)$$

By computing the derivative of $\alpha \mapsto \frac{\alpha}{\alpha^{2/5}-1}$, we can minimize $\alpha \mapsto \gamma^\alpha$ and find that the minimum value is

$$\gamma^\dagger = \left(\frac{4}{\pi}\right)^{\frac{1}{3}} \left(\frac{5}{3}\right)^{\frac{5}{3}},$$

reached for $\alpha^\dagger = \left(\frac{5}{3}\right)^{5/2}$, and, combined with (6.118), this proves (6.117).

□

6.C.2 Regularity in ε of the coefficients of the Fermi-Dirac statistics

In this last subsection, for any $\varepsilon \geq 0$ and $0 \leq g \in L_2^1(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3)$, we denote by $\mathcal{M}_\varepsilon \equiv \mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}(g)}$ the ε -Fermi distribution associated with $\varphi_\varepsilon^{-1}(g)$. In particular, in the limit case $\varepsilon = 0$, \mathcal{M}_0 is the Maxwellian distribution associated with g . We also denote $a_\varepsilon, b_\varepsilon, \bar{u}_\varepsilon$ and $\rho_\varepsilon, u_\varepsilon, T_\varepsilon$ the quantities such that, letting

$$\mathcal{M}_\varepsilon \equiv \mathcal{M}_\varepsilon^{\frac{g}{1+\varepsilon g}}, \quad M_\varepsilon = \frac{\mathcal{M}_\varepsilon}{1-\varepsilon \mathcal{M}_\varepsilon}, \quad (6.119)$$

we have, for any $v \in \mathbb{R}^3$,

$$M_\varepsilon(v) = \exp(a_\varepsilon + b_\varepsilon |v - \bar{u}_\varepsilon|^2), \quad (6.120)$$

and

$$\int_{\mathbb{R}^3} \frac{g}{1+\varepsilon g} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = \begin{pmatrix} \rho_\varepsilon \\ \rho_\varepsilon u_\varepsilon \\ 3\rho_\varepsilon T_\varepsilon + \rho_\varepsilon |u_\varepsilon|^2 \end{pmatrix}. \quad (6.121)$$

Lemma 6.19. *Let $0 \leq g \in L_2^1(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3)$. Using the notation (6.121), the application $\varepsilon \mapsto (\rho_\varepsilon, u_\varepsilon, T_\varepsilon)$ is continuous on \mathbb{R}_+ and \mathcal{C}^1 on \mathbb{R}_+^* .*

Proof. The continuity of $\varepsilon \mapsto (\rho_\varepsilon, u_\varepsilon, T_\varepsilon)$ on \mathbb{R}_+ comes by dominated convergence, as it holds for any $\varepsilon \geq 0$ and $v \in \mathbb{R}^3$ that

$$\frac{g}{1+\varepsilon g} (1+|v|^2) \leq g(1+|v|^2),$$

and by hypothesis $0 \leq g \in L_2^1(\mathbb{R}^3)$. Similarly, for any $\varepsilon > 0$ and $v \in \mathbb{R}^3$ we have

$$\left| \partial_\varepsilon \frac{g}{1+\varepsilon g} \right| (1+|v|^2) = \left(\frac{g}{1+\varepsilon g} \right)^2 (1+|v|^2) \leq \varepsilon^{-1} g(1+|v|^2).$$

Therefore, for any $\varepsilon > 0$, we have

$$\sup_{\varepsilon_* \in (\varepsilon/2, 3\varepsilon/2)} \left| \partial_{\varepsilon_*} \frac{g}{1+\varepsilon_* g} \right| (1+|v|^2) \leq 2\varepsilon^{-1} g(1+|v|^2).$$

The differentiability of $\varepsilon \mapsto (\rho_\varepsilon, u_\varepsilon, T_\varepsilon)$ on \mathbb{R}_+^* then comes by dominated convergence, as $g \in L_2^1(\mathbb{R}^3)$. \square

The following lemmas provide the continuity of $\varepsilon \mapsto (a_\varepsilon, b_\varepsilon, \bar{u}_\varepsilon)$ at the point $\varepsilon = 0$ and its differentiability on \mathbb{R}_+^* .

Lemma 6.20. *Let $0 \leq g \in L_2^1(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3)$. Using the notations (6.119)–(6.120), the application $\varepsilon \mapsto (a_\varepsilon, b_\varepsilon, \bar{u}_\varepsilon)$ is continuous at the point $\varepsilon = 0$.*

Proof. Using the notations (6.119) and (6.121), we have

$$\begin{aligned} \left| \int_{\mathbb{R}^3} M_\varepsilon \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv - \int_{\mathbb{R}^3} \mathcal{M}_\varepsilon \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv \right| &= \left| \int_{\mathbb{R}^3} \frac{\varepsilon \mathcal{M}_\varepsilon^2}{1+\varepsilon \mathcal{M}_\varepsilon} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv \right| \leq \varepsilon \|M_\varepsilon\|_\infty \int_{\mathbb{R}^3} \mathcal{M}_\varepsilon \begin{pmatrix} 1 \\ |v| \\ |v|^2 \end{pmatrix} dv \\ &\leq \varepsilon \|M_\varepsilon\|_\infty (\rho_\varepsilon + 3\rho_\varepsilon T_\varepsilon + \rho_\varepsilon |u_\varepsilon|^2). \end{aligned} \quad (6.122)$$

Recall the notation, in this case,

$$\gamma_\varepsilon = \frac{T_\varepsilon}{T_F(\rho_\varepsilon, \varepsilon)},$$

where $T_F(\rho_\varepsilon, \varepsilon) = \frac{1}{2} \left(\frac{3\rho_\varepsilon \varepsilon}{4\pi} \right)^{2/3}$. By continuity at the point $\varepsilon = 0$ of the application $\varepsilon \mapsto (\rho_\varepsilon, T_\varepsilon)$, given by Lemma 6.19, we have

$$\gamma_\varepsilon \xrightarrow{\varepsilon \rightarrow 0} +\infty.$$

Thereby, there exists $\varepsilon^* > 0$ such that $\gamma_\varepsilon \geq \gamma^\dagger$ for any $\varepsilon \in (0, \varepsilon^*)$, where γ^\dagger is a universal constant defined in Proposition 6.18. Then, from (6.117) in Proposition 6.18, for any $\varepsilon \in (0, \varepsilon^*)$,

$$\varepsilon \|M_\varepsilon\|_\infty \leq \frac{2}{3} \left(\frac{\gamma_\varepsilon}{\gamma_*} \right)^{-\frac{3}{2}},$$

which vanishes as $\varepsilon \rightarrow 0$, since γ_ε tends to $+\infty$ in this limit. Combining this result, the continuity of $\varepsilon \mapsto (\rho_\varepsilon, u_\varepsilon, T_\varepsilon)$ at $\varepsilon = 0$, given by Lemma 6.19, and Equation (6.122), we obtain

$$\left| \int_{\mathbb{R}^3} M_\varepsilon \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv - \int_{\mathbb{R}^3} \mathcal{M}_\varepsilon \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv \right| \xrightarrow{\varepsilon \rightarrow 0} 0.$$

The continuity of $\varepsilon \mapsto (\rho_\varepsilon, u_\varepsilon, T_\varepsilon)$ at $\varepsilon = 0$ being equivalent to the statement

$$\int_{\mathbb{R}^3} \mathcal{M}_\varepsilon \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv \xrightarrow{\varepsilon \rightarrow 0} \int_{\mathbb{R}^3} \mathcal{M}_0 \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv,$$

we finally conclude that

$$\int_{\mathbb{R}^3} M_\varepsilon \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv \xrightarrow{\varepsilon \rightarrow 0} \int_{\mathbb{R}^3} \mathcal{M}_0 \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv.$$

Both M_ε and \mathcal{M}_0 are gaussian distributions, which coefficients are continuously defined by the above moments, allowing to conclude to the continuity of these coefficients at the point $\varepsilon = 0$. \square

Lemma 6.21. *Let $0 \leq g \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3)$. Using the notations (6.119)–(6.120), the application $\varepsilon \mapsto (a_\varepsilon, b_\varepsilon, \bar{u}_\varepsilon)$ is \mathcal{C}^1 on \mathbb{R}^*_+ .*

Proof. Since the distribution $M_\varepsilon(\cdot + \bar{u}_\varepsilon)$ is radially symmetric, so is $\mathcal{M}_\varepsilon(\cdot + \bar{u}_\varepsilon)$, hence $\bar{u}_\varepsilon = u_\varepsilon$, which, by Lemma 6.19, is \mathcal{C}^1 on \mathbb{R}^*_+ . We then define

$$g_\varepsilon := g(\cdot + u_\varepsilon), \quad \mathcal{N}_\varepsilon := \mathcal{M}_\varepsilon(\cdot + u_\varepsilon) \equiv \mathcal{M}_\varepsilon^{\varphi_\varepsilon^{-1}(g_\varepsilon)} \quad \text{and} \quad N_\varepsilon := M_\varepsilon(\cdot + u_\varepsilon),$$

so that, for any $\varepsilon > 0$, it holds that

$$N_\varepsilon = \exp(a_\varepsilon + b_\varepsilon |v|^2).$$

As in (6.121), we let $\rho_\varepsilon, T_\varepsilon > 0$ be such that

$$\int_{\mathbb{R}^3} \frac{g_\varepsilon}{1 + \varepsilon g_\varepsilon} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = \begin{pmatrix} \rho_\varepsilon \\ 0 \\ 3\rho_\varepsilon T_\varepsilon \end{pmatrix}.$$

Let us now show that $\varepsilon \mapsto (a_\varepsilon, b_\varepsilon)$ is \mathcal{C}^1 on \mathbb{R}_+^* . It is proven in [123, proof of Proposition 3] that, letting

$$I_s(\tau) := \int_0^\infty \frac{r^s}{1 + \tau e^{r^2}} dr, \quad P(\tau) := I_4(\tau) I_2(\tau)^{-5/3}, \quad \tau \in \mathbb{R}_+^*,$$

the function P is an increasing \mathcal{C}^1 function from \mathbb{R}_+^* to $\left(\frac{3^{5/3}}{5}, +\infty\right)$, with $P' > 0$ on \mathbb{R}_+^* . Therefore it is invertible, and P^{-1} is also \mathcal{C}^1 . All the more, a dominated convergence argument ensures that I_2 is \mathcal{C}^1 on \mathbb{R}_+^* . It is moreover shown in [123, proof of Proposition 3] that

$$\left(\frac{\varepsilon}{4\pi}\right)^{2/3} P\left(\frac{1}{\varepsilon e^{a_\varepsilon}}\right) = \frac{3\rho_\varepsilon T_\varepsilon}{\rho_\varepsilon^{5/3}}, \quad b_\varepsilon = -\left(\frac{4\pi}{\varepsilon \rho_\varepsilon} I_2\left(\frac{1}{\varepsilon e^{a_\varepsilon}}\right)\right)^{\frac{2}{3}}.$$

By Lemma 6.19, the application $\varepsilon \mapsto (\rho_\varepsilon, T_\varepsilon)$ is \mathcal{C}^1 on \mathbb{R}_+^* , hence so is the application $\varepsilon \mapsto (a_\varepsilon, b_\varepsilon)$, as a composition of \mathcal{C}^1 applications. \square

Lemma 6.22. *Let $0 \leq g \in L^1_2(\mathbb{R}^3) \cap L \log L(\mathbb{R}^3)$. Using the notation (6.119), for any $\bar{\varepsilon} > 0$, there exist $C > 0$ and $\eta > 0$ such that for any $\varepsilon \in [0, \bar{\varepsilon}]$ and $v \in \mathbb{R}^3$, we have*

$$M_\varepsilon(v) \leq C e^{-\eta|v|^2}, \quad (6.123)$$

and

$$|\log M_\varepsilon(v)| \leq C(1 + |v|^2). \quad (6.124)$$

Proof. We denote

$$\underline{a} = \sup_{\varepsilon \in [0, \bar{\varepsilon}]} |a_\varepsilon|, \quad \underline{b} = -\sup_{\varepsilon \in [0, \bar{\varepsilon}]} |b_\varepsilon|, \quad \bar{b} = -\inf_{\varepsilon \in [0, \bar{\varepsilon}]} |b_\varepsilon| \quad \text{and} \quad \underline{u} = \sup_{\varepsilon \in [0, \bar{\varepsilon}]} |u_\varepsilon|.$$

Combining the results of Lemmas 6.20 and 6.21, the application $\varepsilon \mapsto (a_\varepsilon, b_\varepsilon, u_\varepsilon)$ is continuous on \mathbb{R}_+ , from which we deduce that \underline{a} , \underline{b} and \underline{u} are finite.

Moreover, as $M_\varepsilon \in L^1(\mathbb{R}^3)$ for all $\varepsilon \in [0, \bar{\varepsilon}]$, the application $\varepsilon \mapsto b_\varepsilon$ is (strictly) negative on $[0, \bar{\varepsilon}]$, so that, as $\varepsilon \mapsto b_\varepsilon$ is continuous on $[0, \bar{\varepsilon}]$, we have $\bar{b} < 0$.

Therefore, for any $0 \leq \varepsilon \leq \bar{\varepsilon}$ and $v \in \mathbb{R}^3$, we have

$$|\log M_\varepsilon(v)| = |a_\varepsilon + b_\varepsilon|v - u_\varepsilon|^2| \leq \underline{a} + 2|\underline{b}|\underline{u}^2 + 2|\underline{b}||v|^2,$$

and, since $|v - u_\varepsilon|^2 \geq \frac{1}{2}|v|^2 - |u_\varepsilon|^2 \geq \frac{1}{2}|v|^2 - \underline{u}^2$ and $\bar{b} < 0$,

$$M_\varepsilon(v) = e^{a_\varepsilon + b_\varepsilon|v - u_\varepsilon|^2} \leq e^{\underline{a} + \bar{b}|v - u_\varepsilon|^2} \leq e^{\underline{a} + |\bar{b}|\underline{u}^2 + \frac{1}{2}\bar{b}|v|^2}.$$

Letting $\eta = -\frac{1}{2}\bar{b}$ and $C = \max\left(\underline{a} + 2|\underline{b}|\underline{u}^2, e^{\underline{a} + |\bar{b}|\underline{u}^2}\right)$ yields the result. \square

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Quantitative relaxation towards equilibrium for solutions to the Boltzmann-Fermi-Dirac equation with cutoff hard potentials

Outline of the current chapter

7.1 Introduction and main results	271
7.1.1 The Boltzmann-Fermi-Dirac equation	271
7.1.2 Notations	272
7.1.3 Relaxation to equilibrium	273
7.1.4 The role of relative entropy	275
7.1.5 Main results	278
7.1.6 Organization of the paper	280
7.2 Uniform-in-ε L^∞ bound: proof of Theorem 7.3	281
7.2.1 A link between the Fermi-Dirac and the classical cases	281
7.2.2 General estimates on $Q_{\gamma,b}^+$	283
7.2.3 Key estimates on $Q_{\gamma,b}^+$, $\Gamma_{\gamma,b}$ and $Q_{\gamma,b}^-$	285
7.2.4 Derivation of L_γ^2 bounds	290
7.2.5 Conclusion to the proof of Theorem 7.3	293
7.3 Explicit rate of convergence to equilibrium: proof of Theorem 7.4	295
7.3.1 Maxwellian pointwise lower bound	295
7.3.2 Conclusion to the proof of Theorem 7.4	295
7.A More physically relevant models	299
7.A.1 Quantum collision kernels	299
7.A.2 Main mathematical changes induced by quantum collision kernels	300
7.B Known results about (BFD Eq.) and the Fermi-Dirac entropy	301
7.B.1 Cauchy problem and moment estimates	301

7.B.2 Csiszár-Kullback-Pinsker inequalities	302
7.C Explicit and uniform-in-ε bounds for Fermi-Dirac statistics	303
Acknowledgments	306

7.1 Introduction and main results

7.1.1 The Boltzmann-Fermi-Dirac equation

The scope of the present paper is to derive the *first explicit rate* of convergence to equilibrium for solutions to the spatially homogeneous Boltzmann-Fermi-Dirac equation (7.1) for hard potentials under the Grad cutoff assumption. The Boltzmann-Fermi-Dirac equation (**BFD Eq.**) in the rest of the paper) is a modification of the classical Boltzmann equation and describes the interactions between quantum particles satisfying Pauli's exclusion principle (fermions). In the spatially homogeneous setting we are considering here, it takes the form

$$\partial_t f = \mathcal{Q}_B^\varepsilon(f, f), \quad f(0, \cdot) = f^{\text{in}}, \quad (7.1)$$

where $f \equiv f(t, v) \geq 0$ represents a density of fermions (quantum particles of half-integer spin, e.g. electrons), depending on time $t \geq 0$ and velocity $v \in \mathbb{R}^3$ while the initial datum f^{in} is a given nonnegative distribution density. The Boltzmann-Fermi-Dirac collision operator $\mathcal{Q}_B^\varepsilon$ is modelling the interactions between particles and is given, for $\varepsilon > 0$ and a suitably integrable $f \geq 0$ such that $1 - \varepsilon f \geq 0$, by

$$\begin{aligned} \mathcal{Q}_B^\varepsilon(f, f)(v) := & \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \left[f' f'_* (1 - \varepsilon f)(1 - \varepsilon f_*) - f f_* (1 - \varepsilon f')(1 - \varepsilon f'_*) \right] \times \\ & \times B(v, v_*, \sigma) \, d\sigma \, dv_*, \end{aligned} \quad (7.2)$$

where we used the standard shorthands $f \equiv f(v)$, $f_* \equiv f(v_*)$, $f' \equiv f(v')$, $f'_* \equiv f(v'_*)$ and

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2} \sigma, \quad v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2} \sigma, \quad \sigma \in \mathbb{S}^2. \quad (7.3)$$

The collision kernel $B(v, v_*, \sigma)$ is providing the rate at which a given combination of in-going velocities results in a given set of outgoing velocities. In the classical case (for which all quantum effects are neglected), the exact form of the collision kernel can be derived explicitly in the case of interaction driven by inverse power laws repulsive forces and hard-spheres particles [67]. For Fermi-Dirac particles, the situation is much more involved and several models co-exist. In particular, for semi-conductor applications, the velocity range is restricted to a subset of \mathbb{R}^3 (periodically repeated Brillouin zones) whereas, in the so-called “parabolic band” approximation in semi-conductor, the velocity range is indeed \mathbb{R}^3 . For the sake of simplicity, we choose to present our results in the present form for collision kernels B which assumes the same form for both classical and quantum particles. Considering hard-potential interactions, this corresponds to the choice

$$B(v, v_*, \sigma) \equiv b(\cos \theta) |v - v_*|^\gamma, \quad \text{for } (v, v_*) \in \mathbb{R}^3 \times \mathbb{R}^3 \text{ and } \sigma \in \mathbb{S}^2, \quad (7.4a)$$

with $\cos \theta = \sigma \cdot \frac{v - v_*}{|v - v_*|}$ and the mapping $b : (-1, 1) \rightarrow \mathbb{R}^+$ is assumed to satisfy the cutoff assumption

$$\|b\|_1 := \|b\|_{L^1(\mathbb{S}^2)} := 2\pi \int_0^\pi b(\cos \theta) \sin \theta \, d\theta = 2\pi \int_{-1}^1 b(s) \, ds < \infty. \quad (7.4b)$$

With a slight abuse of notation, in the above (7.4b), we identify the function b (defined over $(-1, 1)$) to a function defined over the sphere \mathbb{S}^2 through the identification $\sigma \rightarrow \cos \theta$ here above. We consider *hard potential* interactions for which

$$\gamma \in (0, 1]. \quad (7.4c)$$

For collision kernel B of the form (7.4a), we will use the shorthand notation

$$\mathcal{Q}_{\gamma,b}^\varepsilon(f, f) = \mathcal{Q}_B^\varepsilon(f, f).$$

We are aware that restricting ourselves to the case of collision kernel B defined by (7.4a) (valid for both classical and quantum particles) is an important restriction of our analysis and we are confident that most of the results of the present paper can be extended to more physically relevant collision kernels of the form described in [105, 160]. We refer to Appendix 7.A for more details about this.

As readily seen, the main difference between the classical Boltzmann equation and its quantum counterpart (**BFD Eq.**) lies in the presence of the *quantum parameter*

$$\varepsilon := \frac{(2\pi\hbar)^3}{m^3\beta} > 0$$

which depends on the reduced Planck constant $\hbar \approx 1.054 \times 10^{-34} \text{ m}^2 \text{ kg s}^{-1}$, the mass m and the statistical weight β of the particles species, see [67, Chapter 17]. For instance, in the case of electrons $\varepsilon \approx 1.93 \times 10^{-10} \ll 1$. The parameter ε quantifies the quantum effects of the model and more precisely ensures the Pauli exclusion principle from which solution $f = f(t, v)$ to (**BFD Eq.**) satisfies the *a priori* bound

$$1 - \varepsilon f(t, v) \geq 0.$$

Formally choosing $\varepsilon = 0$ in (7.2) yields the classical Boltzmann operator

$$\mathcal{Q}_B(f, f) = \mathcal{Q}_B^0(f, f)(v) := \iint_{\mathbb{R}^3 \times \mathbb{S}^2} [f'f'_* - ff_*] B(v, v_*, \sigma) \, d\sigma \, dv_*, \quad (7.5)$$

with the same shorthands as in (7.2). In particular, for collision kernel of the form (7.4a), we will use for *classical* Boltzmann operator the shorthand notation

$$\mathcal{Q}_{\gamma,b}(f, f) = \mathcal{Q}_{\gamma,b}^0(f, f) = \mathcal{Q}_B^0(f, f).$$

We refer the reader to [123] for results about the Cauchy problem associated to (7.1) for hard potentials with cutoff, as well as [67, 80] for more results the Cauchy problem associated with (**BFD Eq.**). We briefly recall in Appendix 7.B the results of the Cauchy problem we use in this paper.

7.1.2 Notations

In the following, we define, for $p \geq 1$ and $k \in \mathbb{R}$, the Lebesgue space $L_k^p = L_k^p(\mathbb{R}^3)$ through the norm

$$\|f\|_{L_k^p} := \left(\int_{\mathbb{R}^3} |f(v)|^p \langle v \rangle^{kp} \, dv \right)^{\frac{1}{p}}, \quad L_k^p(\mathbb{R}^3) := \left\{ f : \mathbb{R}^3 \rightarrow \mathbb{R} ; \|f\|_{L_k^p} < \infty \right\}, \quad (7.6)$$

where $\langle v \rangle := \sqrt{1 + |v|^2}$, $v \in \mathbb{R}^3$. For $k = 0$, we simply denote $\|\cdot\|_p$ the L^p -norm. For $p = \infty$, $\|\cdot\|_\infty$ will denote the usual essential supremum of a given measurable function. We also define, for $k \in \mathbb{R}$, the Orlicz space $L_k^1 \log L(\mathbb{R}^3)$ as

$$L_k^1 \log L(\mathbb{R}^3) = \left\{ f : \mathbb{R}^3 \rightarrow \mathbb{R} ; \int_{\mathbb{R}^3} \langle v \rangle^k |f(v)| \log^+ |f(v)| \, dv < \infty \right\},$$

as well as the quantity

$$\|f\|_{L_k^1 \log L} := \int_{\mathbb{R}^3} \langle v \rangle^k |f(v)| |\log |f(v)|| \, dv,$$

which we highlight is not a norm on the Orlicz space, but is finite as soon as there is an $s > 0$ such that $f \in L_{k+s}^1(\mathbb{R}^3) \cap L_k^1 \log L(\mathbb{R}^3)$. As usual, for $k = 0$, we simply write $\|\cdot\|_{L \log L} = \|\cdot\|_{L_0^1 \log L}$ and $L \log L(\mathbb{R}^3) = L_0^1 \log L(\mathbb{R}^3)$.

7.1.3 Relaxation to equilibrium

In contrast to what occurs for classical gases, quantum gases of fermions exhibit *two* distinct families of steady states. First, $Q_B^\varepsilon(\mathcal{M}_\varepsilon) = 0$ when \mathcal{M}_ε is the following Fermi-Dirac statistics:

Definition 7.1 (Fermi-Dirac statistics). Given $\varrho > 0, u \in \mathbb{R}^3, E > 0$ and $\varepsilon > 0$ satisfying

$$5E > \left(\frac{3\varepsilon\varrho}{4\pi}\right)^{\frac{2}{3}}, \tag{7.7}$$

we denote by \mathcal{M}_ε the unique Fermi-Dirac statistics

$$\mathcal{M}_\varepsilon(v) = \frac{\exp(a_\varepsilon + b_\varepsilon|v - u|^2)}{1 + \varepsilon \exp(a_\varepsilon + b_\varepsilon|v - u|^2)} =: \frac{M_\varepsilon(v)}{1 + \varepsilon M_\varepsilon(v)}, \tag{7.8}$$

with $a_\varepsilon \in \mathbb{R}$ and $b_\varepsilon < 0$ defined in such a way that

$$\int_{\mathbb{R}^3} \mathcal{M}_\varepsilon(v) \begin{pmatrix} 1 \\ v \\ |v - u|^2 \end{pmatrix} \, dv = \begin{pmatrix} \varrho \\ \varrho u \\ 3\varrho E \end{pmatrix}.$$

The existence and uniqueness of Fermi-Dirac statistics satisfying (7.7) has been established in [123, Proposition 3]. Note that M_ε is here a suitable Maxwellian distribution that allows to recover in the classical limit $\varepsilon \rightarrow 0$ the Maxwellian equilibrium.

Besides the Fermi-Dirac statistics (7.8), the distribution

$$F_\varepsilon(v) = \begin{cases} \varepsilon^{-1} & \text{if } |v - u| \leq \left(\frac{3\varrho\varepsilon}{4\pi}\right)^{\frac{1}{3}}, \\ 0 & \text{if } |v - u| > \left(\frac{3\varrho\varepsilon}{4\pi}\right)^{\frac{1}{3}}, \end{cases} \tag{7.9}$$

can also be a stationary state, as $Q_B^\varepsilon(F_\varepsilon) = 0$. Such a degenerate state, referred to as a *saturated Fermi-Dirac* stationary state, can occur for very cold gases (with an explicit condition on the gas temperature). More precisely, for any $\varepsilon > 0$, one can define the *Fermi temperature* associated to $\varrho > 0, \varepsilon > 0$, as

$$T(\varrho, \varepsilon) := \frac{1}{2} \left(\frac{3\varepsilon\varrho}{4\pi}\right)^{\frac{2}{3}}.$$

Then, given $0 \leq f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ with

$$\int_{\mathbb{R}^3} f(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = \begin{pmatrix} \varrho \\ \varrho u \\ 3\varrho E + \varrho |u|^2 \end{pmatrix} \quad (7.10)$$

and $\varepsilon > 0$, the ratio r_E between the actual temperature of f and its Fermi temperature defined as

$$r_E := \frac{E}{T(\varrho, \varepsilon)}$$

is an a -dimensional number which plays a crucial role in the dynamic of **(BFD Eq.)**. Indeed, it has been shown in [123] that, given $\varepsilon > 0$, the following holds

$$1 - \varepsilon f \geq 0 \implies r_E \geq \frac{2}{5}$$

with moreover the following dichotomy:

1. $1 - \varepsilon f \geq 0$ and $r_E = \frac{2}{5}$ if and only if $f = F_\varepsilon$ as defined in (7.9);
2. $1 - \varepsilon f \geq 0$ and $r_E > \frac{2}{5}$ if and only if there exists a unique Fermi-Dirac statistics $\mathcal{M}_\varepsilon = \mathcal{M}_\varepsilon^f$ with same mass, momentum and energy that f .

Observe here that

$$r_E = \frac{2}{5} \iff \varepsilon = \varepsilon_{\text{sat}} = \frac{4\pi (5E)^{\frac{3}{2}}}{3\varrho} \quad (7.11)$$

whereas the inequality (7.7) exactly means that $\varepsilon \in (0, \varepsilon_{\text{sat}})$. In all the sequel, for given $\varrho, E > 0$, we will always implicitly assume that $\varepsilon \in (0, \varepsilon_{\text{sat}})$.

As we will see in the next section, the fact that an initial distribution close to such degenerate state makes $1 - \varepsilon f$ arbitrarily small in non-negligible sets affects drastically the speed of convergence and one of the crucial points of our analysis will be to show that, for suitable initial datum f^{in} , there exist $c \in (0, 1)$ and κ_0 (depending on c) such that solutions f^ε to **(BFD Eq.)** satisfy

$$1 - \varepsilon f^\varepsilon(t, v) \geq \kappa_0, \quad \forall \varepsilon \in (0, c\varepsilon_{\text{sat}}).$$

*In all the sequel, we will always consider solutions to (7.1) associated to the operator $\mathcal{Q}_B^\varepsilon = \mathcal{Q}_{\gamma, b}^\varepsilon$, i.e. considering kernels B of the form (7.4). We also always consider nonnegative initial datum $f^{\text{in}} \in L^1_2(\mathbb{R}^3)$ and (conservative) solutions f^ε to **(BFD Eq.)** associated to f^{in} whose existence and uniqueness are recalled in Appendix 7.B. In particular,*

$$\int_{\mathbb{R}^3} f^\varepsilon(t, v) \begin{pmatrix} 1 \\ v \\ |v - u^{\text{in}}|^2 \end{pmatrix} dv = \int_{\mathbb{R}^3} f^{\text{in}}(v) \begin{pmatrix} 1 \\ v \\ |v - u^{\text{in}}|^2 \end{pmatrix} dv = \begin{pmatrix} \varrho^{\text{in}} \\ \varrho^{\text{in}} u^{\text{in}} \\ 3\varrho^{\text{in}} E^{\text{in}} \end{pmatrix} \quad \forall t \geq 0$$

with $\varrho^{\text{in}} > 0$, $u^{\text{in}} \in \mathbb{R}^3$ and $E^{\text{in}} > 0$. We will also, unless otherwise stated, consider the associated

Fermi-Dirac statistics $\mathcal{M}_\varepsilon = \mathcal{M}_\varepsilon^{f^{\text{in}}}$ sharing the same mass, momentum and kinetic energy as f^{in} , i.e.

$$\int_{\mathbb{R}^3} \mathcal{M}_\varepsilon^{f^{\text{in}}}(v) \begin{pmatrix} 1 \\ v \\ |v - u^{\text{in}}|^2 \end{pmatrix} dv = \begin{pmatrix} \varrho^{\text{in}} \\ \varrho^{\text{in}} u^{\text{in}} \\ 3\varrho^{\text{in}} E^{\text{in}} \end{pmatrix}.$$

For such solutions, non-quantitative results about the long-time behaviour of solutions to **(BFD Eq.)** have already been obtained in the literature. In particular, we have the following recent result from [119]:

Theorem 7.1 (Liu & Lu (2023)). Assume that the collision kernel $B = B(v, v_*, \sigma)$ satisfies (7.4) with moreover

$$b(\cos \theta) \geq \sum_{n=0}^{\infty} a_n \cos^{2n}(\theta), \quad \theta \in (0, \pi), \quad a_n \geq 0 \quad \forall n \in \mathbb{N}. \tag{7.12}$$

For any initial datum $f^{\text{in}} \in L^1_2(\mathbb{R}^3)$ with $0 \leq f^{\text{in}} \leq \varepsilon^{-1}$, the unique conservative (mild) solution $f^\varepsilon = f^\varepsilon(t, v)$ to **(BFD Eq.)** with initial datum f^{in} is such that

$$\lim_{t \rightarrow \infty} \|f^\varepsilon(t) - \mathcal{M}_\varepsilon\|_{L^1_2} = 0$$

where \mathcal{M}_ε is the unique Fermi-Dirac statistics with the same mass, momentum and kinetic energy as f^{in} .

Remark 7.1. The additional assumption (7.12) on the angular kernel $b = b(\cos \theta)$ in the above theorem means that, as a function of $\cos^2(\theta)$, $b(\cos \theta)$ is completely positive. It is of course satisfied for instance if $b(\cos \theta)$ is bounded by below away from zero (corresponding to $a_0 = \inf_\theta b(\cos \theta)$ and $a_n = 0$ for $n \geq 1$) which is the simplified setting in which our main result (see Theorem 7.4) will hold.

As mentioned earlier, up to our knowledge, no quantitative estimates for the rate of convergence towards \mathcal{M}_ε exist in the literature and it is the purpose of our work to fill this blank.

7.1.4 The role of relative entropy

As very well documented, the main tool to provide *quantitative* rate of relaxation to equilibrium is related to entropy/entropy production. For $\varepsilon > 0$, we introduce the Fermi-Dirac entropy:

$$\mathcal{H}_\varepsilon(f) = \int_{\mathbb{R}^3} [f \log f + \varepsilon^{-1}(1 - \varepsilon f) \log(1 - \varepsilon f)] dv, \tag{7.13}$$

well-defined for any $0 \leq f \leq \varepsilon^{-1}$. One can then show that $\mathcal{H}_\varepsilon(f)$ is a Lyapunov function for (7.1), i.e.

$$\frac{d}{dt} \mathcal{H}_\varepsilon(f(t)) =: -\mathcal{D}_\varepsilon(f(t)) \leq 0$$

for any suitable solution to (7.1) where the entropy production is defined, assuming $1 - \varepsilon f > 0$ almost everywhere, by

$$\begin{aligned} \mathcal{D}_\varepsilon(f) := & \frac{1}{4} \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} [\varphi_\varepsilon(f') \varphi_\varepsilon(f'_*) - \varphi_\varepsilon(f) \varphi_\varepsilon(f_*)] \log \left(\frac{\varphi_\varepsilon(f') \varphi_\varepsilon(f'_*)}{\varphi_\varepsilon(f) \varphi_\varepsilon(f_*)} \right) \times \\ & \times (1 - \varepsilon f)(1 - \varepsilon f_*)(1 - \varepsilon f')(1 - \varepsilon f'_*) B(v, v_*, \sigma) dv dv_* d\sigma, \end{aligned} \tag{7.14}$$

where

$$\varphi_\varepsilon(x) = \frac{x}{1 - \varepsilon x}, \quad x \in [0, \varepsilon^{-1}]. \tag{7.15}$$

In particular, introducing the *relative entropy*

$$\mathcal{H}_\varepsilon(f|\mathcal{M}_\varepsilon) = \mathcal{H}_\varepsilon(f) - \mathcal{H}_\varepsilon(\mathcal{M}_\varepsilon)$$

which is nonnegative if f and \mathcal{M}_ε share the same mass, momentum and kinetic energy, one has, for any suitable solution to **(BFD Eq.)**,

$$\frac{d}{dt} \mathcal{H}_\varepsilon(f(t)|\mathcal{M}_\varepsilon) = -\mathcal{D}_\varepsilon(f(t)) \leq 0. \quad (7.16)$$

According to Csiszár-Kullback-Pinsker inequality (see Appendix 7.B), the relative entropy controls the L_k^1 -norm of the difference $f(t) - \mathcal{M}_\varepsilon$ and this is what makes entropy/entropy production estimate a powerful tool for proving the convergence towards equilibrium. Indeed, if one can prove a *functional inequality* of the form

$$\mathcal{D}_\varepsilon(f) \geq \Theta(\mathcal{H}_\varepsilon(f|\mathcal{M}_\varepsilon)), \quad \forall f \in \mathcal{C}$$

where \mathcal{C} is a suitable class of functions $0 \leq f \in L_2^1(\mathbb{R}^3)$ with $0 \leq f \leq \varepsilon^{-1}$ and a *superlinear* mapping $\Theta : \mathbb{R}^+ \rightarrow \mathbb{R}^+$, Eq. (7.16) implies

$$\frac{d}{dt} \mathcal{H}_\varepsilon(f(t)|\mathcal{M}_\varepsilon) \leq -\Theta(\mathcal{H}_\varepsilon(f|\mathcal{M}_\varepsilon))$$

provided solutions to **(BFD Eq.)** belong to the class \mathcal{C} . Then, a Grönwall-type argument provides a rate of convergence to equilibrium of the relative entropy. For instance, if the entropy production controls the relative entropy in a linear way, corresponding to $\Theta(u) = \lambda u$, for some $\lambda > 0$ and any $u \geq 0$, then one would get the exponential relaxation to equilibrium

$$\mathcal{H}_\varepsilon(f(t)|\mathcal{M}_\varepsilon) \leq \exp(-\lambda t) \mathcal{H}_\varepsilon(f(0)|\mathcal{M}_\varepsilon), \quad \forall t \geq 0.$$

provided one is able to show that solutions to **(BFD Eq.)** belong to the class \mathcal{C} . Such a decay, combined with Csiszár-Kullback-Pinsker inequality, yields an explicit rate of convergence of $f(t)$ towards \mathcal{M}_ε in L_k^1 (or even L_k^p , $p > 1$) topology. Other kinds of functional Θ can of course be considered and such a strategy has been efficiently applied to the study of the long-time behavior for classical gases, corresponding to $\varepsilon = 0$, for which suitable functional inequalities linking the Boltzmann relative entropy

$$\mathcal{H}_0(f|\mathcal{M}_0) = \int_{\mathbb{R}^3} f \log f \, dv - \int_{\mathbb{R}^3} \mathcal{M}_0 \log \mathcal{M}_0 \, dv$$

and the entropy production

$$\mathcal{D}_0(f) := \frac{1}{4} \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} [f' f'_* - f f_*] \log \left(\frac{f' f'_*}{f f_*} \right) B(v, v_*, \sigma) \, dv \, dv_* \, d\sigma,$$

have been obtained, starting with the pioneering works [59, 57, 153] and culminating with a celebrated result in [157]. An improvement of the result of [157] (reducing the required regularity of f , up to the mere L^p or even $L \log L$ estimate) has been derived in [10] and can be formulated as

Theorem 7.2. *Assume the existence of $b_0 > 0$ and $\beta_\pm \geq 0$ such that*

$$B(v, v_*, \sigma) \geq b_0 \min \left(|v - v_*|^{\beta_+}, |v - v_*|^{-\beta_-} \right), \quad B(v, v_*, \sigma) = B(|v - v_*|, \cos \theta).$$

Given $K_0 > 0, A_0 > 0, q_0 \geq 2$, we consider the class of functions

$$\mathcal{C}_0 = \left\{ g \in L^1_2(\mathbb{R}^3) \text{ such that } g(v) \geq K_0 \exp(-A_0|v|^{q_0}), \quad \forall v \in \mathbb{R}^3 \right\}.$$

Then, given $1 < p < \infty$ and $\delta > 0$, defining $s = 2 + \frac{2+\beta_-}{\delta}$, for any

$$g \in L^p(\mathbb{R}^3) \cap L^1_s \log L(\mathbb{R}^3) \cap \mathcal{C}_0 \cap L^1_{s+q_0}(\mathbb{R}^3)$$

it holds

$$\mathcal{D}_0(g) \geq A_{\delta,p}(g) \mathcal{H}_0(g|\mathcal{M}_0^g)^\alpha \tag{7.17}$$

where $\alpha = (1+\delta)(1 + \frac{p\beta_+}{3(p-1)})$ and $A_{\delta,p}(f)$ depend on the parameters $K_0, q_0, A_0, \beta_\pm, p$, upper and lower bounds to $\|g\|_1$ and $\|g\|_{L^1_2}$, as well as upper bounds for $\|g\|_{L^1_s \log L(\mathbb{R}^3)}, \|g\|_p, \|g\|_{L^1_{s+q_0}}$.

Remark 7.2. Notice that the above assumption on B is satisfied for collision kernel of the form (7.4) with $\beta_+ = \gamma, \beta_- = 0$ provided that $b(\cos\theta) \geq b_0$. We also wish to point out that we will apply the above result to

$$g = \varphi_\varepsilon(f(t)) = \frac{f(t)}{1 - \varepsilon f(t)}, \quad f(t) \text{ solution to (7.1),}$$

and we can check easily that, in such a case, if $1 - \varepsilon f(t) \geq \kappa_0$, then $A_{\delta,p}(\varphi_\varepsilon(f(t)))$ can be bounded away from zero uniformly with respect to time (and ε). See the proof of Theorem 7.4.

Such a result has been recently adapted by the first author in [36] to the case of the Fermi-Dirac entropy thanks to a suitable link between the Boltzmann relative entropy $\mathcal{H}_0(\varphi_\varepsilon(f)|\mathcal{M}_{\varphi_\varepsilon(f)})$ and the Fermi-Dirac relative entropy $\mathcal{H}_\varepsilon(f|\mathcal{M}_\varepsilon)$. Typically,

Proposition 7.1. Given $\kappa_0 \in (0, 1)$, there is a positive constant $C(\kappa_0) > 0$, that could be made explicit, such that, for any $\varepsilon > 0$ and nonnegative $f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ such that

$$1 - \varepsilon f \geq \kappa_0,$$

it holds

$$\mathcal{H}_\varepsilon(f|\mathcal{M}_\varepsilon^f) \leq \mathcal{H}_0(\varphi_\varepsilon(f)|\mathcal{M}_0^{\varphi_\varepsilon(f)}) \leq C(\kappa_0) \mathcal{H}_\varepsilon(f|\mathcal{M}_\varepsilon^f)$$

and

$$\kappa_0^4 \mathcal{D}_0(\varphi_\varepsilon(f)) \leq \mathcal{D}_\varepsilon(f) \leq \mathcal{D}_0(\varphi_\varepsilon(f)),$$

where we recall that we defined $\varphi_\varepsilon(x) = \frac{x}{1-\varepsilon x}$ for $x \in [0, \varepsilon^{-1})$ in (7.15).

The comparison provided in Proposition 7.1 is the key point of our analysis as it allows us to deduce suitable entropy/entropy production estimates in the Fermi-Dirac case. To that purpose, for any $\varepsilon > 0$, and $\kappa_0 > 0, K_0 > 0, A_0 > 0, q_0 \geq 2, E > 0, \varrho > 0, u \in \mathbb{R}^3$, we introduce the class

$$\mathcal{C}_\varepsilon = \left\{ f \in L^1_2(\mathbb{R}^3) \text{ satisfying (7.10) and such that } \right. \\ \left. f(v) \geq K_0 \exp(-A_0|v|^{q_0}) \text{ and } 1 - \varepsilon f(v) \geq \kappa_0, \quad \forall v \in \mathbb{R}^3 \right\}. \tag{7.18}$$

One can easily deduce from Theorem 7.2 that, for any $\varepsilon, \delta > 0$ and $1 < p < \infty$, an estimate of the type

$$\mathcal{D}_\varepsilon(f) \geq \tilde{A}_{\delta,p}(f) \mathcal{H}_\varepsilon(f | \mathcal{M}_\varepsilon)^\alpha \quad \forall f \in \mathcal{C}_\varepsilon \cap L^p(\mathbb{R}^3) \cap L_s^1 \log L(\mathbb{R}^3)$$

where $\tilde{A}_{\delta,p}(f)$ depends explicitly on $\kappa_0, K_0, A_0, q_0, \varrho, E$ and upper bounds on $\|f\|_{L_s^1 \log L}, \|f\|_p$ with s defined in Theorem 7.2. As in the classical case, the key point to apply such a functional inequality to solutions to **(BFD Eq.)** is then to determine suitable conditions on the initial distribution f^{in} ensuring that the unique solution $f^\varepsilon = f^\varepsilon(t, v)$ to (7.1) satisfies

$$f^\varepsilon(t, \cdot) \in \mathcal{C}_\varepsilon \cap L^p(\mathbb{R}^3) \cap L_s^1 \log L(\mathbb{R}^3) \quad \forall t \geq 0.$$

The main technical difficulty, which explains as already mentioned why the quantitative rate of convergence for **(BFD Eq.)** has not been obtained yet, is of course to create or propagate the lower bound

$$1 - \varepsilon f^\varepsilon(t, v) \geq \kappa_0 \quad \forall t > 0, \quad v \in \mathbb{R}^3. \tag{7.19}$$

In the study of the Landau-Fermi-Dirac equation, such pointwise lower bounds have been obtained by improving the mere L^∞ bounds thanks to the regularisation mechanism induced by the diffusive nature of the collision operator. This allows to prove the *appearance* of some L^∞ bound, *independent of ε* for the solution to the Landau-Fermi-Dirac equation and, up to reducing slightly the parameter ε , to obtain the lower bound (7.19).

When trying to adapt such a strategy to **(BFD Eq.)**, the major difficulty lies in the fact that, for *cut-off* interactions (see (7.4b)), no smoothing effect of the solution is expected and a new route has to be followed to deduce the non-saturation estimate.¹ We insist on the fact that, as already observed in [124, 119], such a non-saturation estimate is the crucial argument to provide a quantitative rate of convergence to equilibrium for the quantum Boltzmann equation.

We now describe in more detail our main results in the next subsection.

7.1.5 Main results

Recall that we are dealing with solutions to **(BFD Eq.)** as constructed in Theorem 7.6 in Appendix 7.B. As mentioned earlier, one of the main aspects of our strategy is to derive L^∞ bounds for solutions to **(BFD Eq.)** which are independent of ε . Besides its fundamental role in the long-time behaviour of solutions to **(BFD Eq.)**, such a result has its own independent interest and is one of the main results of our contribution

Theorem 7.3 (Uniform-in- ε L^∞ bound). *Let $\gamma \in (0, 1]$ and an angular kernel b satisfying the cutoff assumption (7.4b). Let $0 \leq f^{\text{in}} \in L^1_3(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. Then there exists an explicit $\mathbf{C}_\infty > 0$, depending only on γ, b and f^{in} only through $\varrho^{\text{in}}, E^{\text{in}}$ and upper-bounds on its L^∞ and L^1_3 norms, such that for any $\varepsilon \in (0, \|f^{\text{in}}\|_\infty^{-1})$, the unique solution f^ε to (7.1) associated to ε , the collision kernel defined by (7.4) and initial datum f^{in} satisfies*

$$\sup_{t \geq 0} \|f^\varepsilon(t)\|_\infty \leq \mathbf{C}_\infty. \tag{7.20}$$

Remark 7.3. *The assumption of f^{in} belonging to L^1_3 in Theorem 7.3 could be actually recast into f^{in} belonging to L^1_s for some arbitrary s such that $s > 2$ and $s \geq 3\gamma$. In this case, \mathbf{C}_∞ would also depend on s .*

1. We mention that a result of uniform-in-time L^∞ bound was already proposed in [160] (with $\varepsilon = 1$ and different kinds of collision kernels), however it seems to us that counter-examples to that result can be constructed. In particular, choosing $a = b, \beta = 0$ in [160, Theorem 1.7], one could consider an initial distribution f_0 with L^∞ norm equal to 1, and [160, Theorem 1.7] would imply that solutions $f(t)$ to **(BFD Eq.)** are such that $\|f(t)\|_\infty \leq \frac{1}{6}$ for all time $t \geq 0$.

The peculiarity of the result presented in Theorem 7.3 lies in the fact that the bound is *independent of* ε . This is one of the main points of the strategy we adopt here, reminiscent of a similar one in [2] (see also [3]). The clear advantage of such a bound is that, for a given *fixed* $f^{\text{in}} \in L^\infty(\mathbb{R}^3)$, one can always choose a small enough ε such that the non-saturation condition (7.19) holds for any time $t \geq 0$:

Corollary 7.2. *Consider the assumptions of Theorem 7.3 along with the same notations. Then for any $\kappa_0 \in (0, 1)$ and $\varepsilon \in (0, (1 - \kappa_0)\mathbf{C}_\infty^{-1}]$, the mentioned solution f^ε to (7.1) is such that*

$$1 - \varepsilon f^\varepsilon(t, v) \geq \kappa_0, \quad \forall (t, v) \in \mathbb{R}_+ \times \mathbb{R}^3. \tag{7.21}$$

This non-saturation property allows to greatly simplify various studies on the equation: in this event, and especially in the cutoff case (that is, when (7.4b) holds), very large parts of the study of solutions to the Boltzmann-Fermi-Dirac equation can be recast into the study of the classical Boltzmann equation thanks to a suitable comparison argument (see Proposition 7.1). To name two examples particularly important for our analysis, this allows to transfer the entropy inequalities from the classical to the fermionic case thanks to Proposition 7.1 and also to deduce straightforwardly a Maxwellian lower bound on the solutions to **(BFD Eq.)** by simply resuming the proof of [143] valid in the classical case (see Subsection 7.3.1).

We insist here on the fact that our approach consists in choosing *first* an initial datum f^{in} and subsequently pick $\varepsilon^{\text{in}} > 0$ small enough for the rest of our analysis to apply uniformly with respect to $\varepsilon \in (0, \varepsilon^{\text{in}}]$. It seems possible to adopt a similar viewpoint by choosing first $\varepsilon > 0$ and then determine the class of all initial data for which the results of the paper do hold. We did not pursue this line of investigation.

With this at hand, we can easily deduce the main result for the long-time behaviour of the solutions, where we recall that we consider solutions to (7.1) as constructed in [123] (see Appendix 7.B):

Theorem 7.4 (Explicit rate of convergence to equilibrium). *Let B be a collision kernel of the form (7.4) with $\gamma \in (0, 1]$ and an angular kernel b satisfying the cutoff assumption (7.4b) and such that $b \geq b_0$ for some $b_0 > 0$. Let $0 \leq f^{\text{in}} \in L^1_3(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. Then there exist some explicit $\mathbf{C}_\mathcal{H} > 0$ and $\varepsilon^{\text{in}} > 0$, depending only on $\gamma, b, \varrho^{\text{in}}, u^{\text{in}}, E^{\text{in}}, \|f^{\text{in}}\|_{L^1_3}$ and $\|f^{\text{in}}\|_\infty$, such that for any $\varepsilon \in (0, \varepsilon^{\text{in}}]$, the unique solution f^ε to (7.1) associated to ε and the initial datum f^{in} satisfies, for all $t \geq 0$,*

$$\mathcal{H}_\varepsilon(f^\varepsilon(t) | \mathcal{M}_\varepsilon^{f^{\text{in}}}) \leq \mathbf{C}_\mathcal{H} (1 + t)^{-\frac{1}{\gamma}}. \tag{7.22}$$

In particular, for any $p \geq 1$ and $k \geq 0$, there exist $\mathbf{C}_{\mathcal{H},p,k} > 0$, with the same properties as $\mathbf{C}_\mathcal{H}$, such that for all $t \geq 0$,

$$\left\| f^\varepsilon(t) - \mathcal{M}_\varepsilon^{f^{\text{in}}} \right\|_{L^p_k} \leq \mathbf{C}_{\mathcal{H},p,k} (1 + t)^{-\frac{1}{2p\gamma}}. \tag{7.23}$$

Remark 7.4. *Notice that (7.22) holds true with the choice*

$$\varepsilon^{\text{in}} = (1 - \kappa_0)\mathbf{C}_\infty^{-1}$$

and the same choice applies to (7.23) in the case $p = 1, k = 0$. In the case $k > 0$ or $p > 1$, additional smallness restriction is required on the parameter ε since an additional control of $\|\mathcal{M}_\varepsilon^{f^{\text{in}}}\|_\infty$ or $\|\mathcal{M}_\varepsilon^{f^{\text{in}}}\|_{L^1_{2k}}$ is actually needed. For the same reason, the constants actually depend on u^{in} only in the case of the L^p_k norm with $k > 0$. We refer to Section 7.3 for more details.

Remark 7.5. *We point out right away that the rate of convergence to equilibrium established in Theorem 7.4 is clearly not the optimal rate of convergence. As well-known for kinetic equations associated*

with hard-potentials (recall here $\gamma \in (0, 1]$), such a rate of convergence can be upgraded into an exponential relaxation governed by the spectral gap of the linearized collision operator. To implement such an upgrade, one would need to adopt the following strategy

1. Show a quantitative exponential rate of convergence to \mathcal{M}_ε for close-to-equilibrium initial state. This means that one can construct $\lambda > 0$ and an explicit $\delta > 0$ such that

$$\|f^{\text{in}} - \mathcal{M}_\varepsilon^{f^{\text{in}}}\|_{L_k^1} \leq \delta \implies \|f^\varepsilon(t) - \mathcal{M}_\varepsilon^{f^{\text{in}}}\|_{L_k^1} \leq C \exp(-\lambda t)$$

for some $k > 0$ large enough and some explicit $C > 0$ (depending on f^{in}).

2. Second, using Theorem 7.4, one can explicit the time $T > 0$ needed for general solutions f^ε to enter the neighbourhood of $\mathcal{M}_\varepsilon^{f^{\text{in}}}$ determined by δ . Then, restarting the evolution from time $T > 0$, we get that the rate of convergence to equilibrium is exponential.

A full analysis of the close-to-equilibrium solutions to **(BFD Eq.)** (i.e. full proof of the above point (a)) is still missing and is based upon a careful spectral analysis of the linearized operator associated with $\mathcal{Q}_B^\varepsilon$ around $\mathcal{M}_\varepsilon^{f^{\text{in}}}$. We are confident that it can be implemented, deriving first a spectral gap estimate in a Hilbert setting and extending then this spectral analysis to the L_k^1 by factorization and enlargement techniques following the line of [101, 134]. Notice that such an approach has been successfully applied in the study of the Landau-Fermi-Dirac equation in [2].

As mentioned already, such a Theorem is, to our knowledge, the first result providing an explicit and quantitative rate of convergence to equilibrium for solutions to **(BFD Eq.)** whereas several qualitative results were available in the literature. As said before, the crucial ideas of our strategy are the following:

- First, thanks to the L^∞ -bound independent of the quantum parameter ε , one can, for a given initial datum f^{in} , determine a whole family of ε for which the non-saturation estimate (7.19) holds true uniformly in time.
- Second, taking profit of this non-saturation condition, we can exploit several new and insightful comparison arguments – specially tailored for our analysis and with their own independent interest – which allow to deduce results regarding **(BFD Eq.)** from the analog ones already obtained in the classical case as exposed in the comprehensive survey [8] (see also [10]).

Not only does such an approach allow, in some sense, to treat in the same formalism the quantum and classical Boltzmann equations, but it also appears quite straightforward and elegant, fully exploiting the tools developed in [8] for the study of kinetic equations with hard potentials and cut-off assumptions. As mentioned in the last remark, we decided to focus on the main mathematical challenge for the rate of convergence, which is the control of the relative entropy, discarding in our analysis the optimality of the rate of convergence which should be easy to deduce from our result thanks to the recent methods developed in [101].

7.1.6 Organization of the paper

The paper is organized as follows: after this Introduction, we present in Section 7.2 the full proof of the main estimates for solutions to (7.1) culminating with the proof of Theorem 7.3. It is obtained from the representation of solutions to **(BFD Eq.)** as suitable “sub-solutions” (in the sense of (7.30)) to an equation very similar to the classical Boltzmann equation. We first describe such a representation in Subsection 7.2.1, then deduce suitable Young’s type estimates for the collision operator associated with such an equation, in the spirit of the fundamental results in [5, 6] (following the more recent exposition in [10, 8]). In particular, L_γ^2 bounds for solutions to **(BFD Eq.)** are deduced, uniformly with respect to $\varepsilon > 0$ and time, in Proposition 7.16 and, as in [8], this allows us to derive the full proof of Theorem 7.3. We then provide, in Section 7.3, the complete proof of our main convergence result, Theorem 7.4. It is deduced

from the results of Section 7.2 combined with suitable pointwise lower bounds, well-known for the classical Boltzmann equation [143] and easily adapted to **(BFD Eq.)** in Proposition 7.17. In Appendix 7.A, we present examples of physically relevant collision kernels for quantum kinetic equations and describe how the results of the paper could be adapted to such general collision models. In Appendix 7.B, we briefly recall results regarding existence and uniqueness of solutions to (7.1) as well as several important properties (moment estimates and entropy dissipation). The results of this Appendix are extracted from [119, 123, 124]. In a final Appendix 7.C, we provide explicit and uniform-in- ε upper-bounds on quantities related to the Fermi-Dirac statistics relevant to our study.

7.2 Uniform-in- ε L^∞ bound: proof of Theorem 7.3

This section is devoted to the derivation of L^∞ -bounds for solutions to **(BFD Eq.)** which are *uniform in time and independent of ε* , proving Theorem 7.3. Our study is largely inspired from [8] in which very similar bounds are obtained in the context of the classical Boltzmann equation. The strategy we employ in this paper is to use the fact that a solution to the Boltzmann-Fermi-Dirac equation (7.1) for some parameter ε is a “sub-solution” (in the sense of (7.30)) to an equation very much resembling the Boltzmann equation (with a modified gain operator), and in particular, free of any dependence in ε . This observation allows to completely transpose the estimates and techniques present in [8] to our problem and obtain without much trouble an L^∞ bound on the solution to (7.1) which is *independent of ε* .

7.2.1 A link between the Fermi-Dirac and the classical cases

We present in this section the crucial simplification that allows us to pass from a study on the Boltzmann-Fermi-Dirac operator to a study on the classical Boltzmann operator. This is made possible thanks to the Grad cutoff assumption (7.4b). Recall that, under such an assumption, the classical Boltzmann operator $\mathcal{Q}_{\gamma,b}$ can be split into two parts

$$\mathcal{Q}_{\gamma,b} = \mathcal{Q}_{\gamma,b}^+ - \mathcal{Q}_{\gamma,b}^- \quad (7.24a)$$

where

$$\begin{cases} \mathcal{Q}_{\gamma,b}^+(f,g)(v) &= \int_{\mathbb{R}^3 \times \mathbb{S}^2} f' g'_* B(v - v_*, \sigma) dv_* d\sigma, \\ \mathcal{Q}_{\gamma,b}^-(f,g)(v) &= f(v) \int_{\mathbb{R}^3 \times \mathbb{S}^2} g_* B(v - v_*, \sigma) dv_*. \end{cases} \quad (7.24b)$$

A similar splitting can be made for \mathcal{Q}_ε . Indeed, for any $\varepsilon > 0$ and $0 \leq f \in L^1_2(\mathbb{R}^3)$ such that $1 - \varepsilon f \geq 0$, defining

$$\begin{cases} \mathcal{Q}_{\gamma,b}^{\varepsilon,+}(f,f) &= \iint_{\mathbb{R}^3 \times \mathbb{S}^2} f' f'_* (1 - \varepsilon f)(1 - \varepsilon f_*) B dv_* d\sigma \\ \mathcal{Q}_{\gamma,b}^{\varepsilon,-}(f,f) &= f \iint_{\mathbb{R}^3 \times \mathbb{S}^2} f_* (1 - \varepsilon f')(1 - \varepsilon f'_*) B dv_* d\sigma. \end{cases} \quad (7.25a)$$

the cutoff assumption (7.4b) imply that $\mathcal{Q}_{\gamma,b}^{\varepsilon,+}(f,f) < \infty$, $\mathcal{Q}_{\gamma,b}^{\varepsilon,-}(f,f) < \infty$ and

$$\mathcal{Q}_{\gamma,b}^\varepsilon(f,f) = \mathcal{Q}_{\gamma,b}^{\varepsilon,+}(f,f) - \mathcal{Q}_{\gamma,b}^{\varepsilon,-}(f,f). \quad (7.25b)$$

Moreover, for any measurable and nonnegative $g, h : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ and $f \in L^\infty(\mathbb{R}^3)$, we define

$$\Gamma_{\gamma,b}(g, h)(v) := \int_{\mathbb{R}^3 \times \mathbb{S}^2} g_*(h' + h'_*) B(v - v_*, \sigma) dv_* d\sigma, \quad (7.26)$$

and

$$\tilde{\mathcal{Q}}_{\gamma,b}^+[f](g, h) := \mathcal{Q}_{\gamma,b}^+(g, h) + \frac{f}{\|f\|_\infty} \Gamma_{\gamma,b}(g, h). \quad (7.27)$$

Under the hypothesis that g, h are such that $\mathcal{Q}_{\gamma,b}^-(g, h) < \infty$, we can then define

$$\tilde{\mathcal{Q}}_{\gamma,b}[f](g, h) := \tilde{\mathcal{Q}}_{\gamma,b}^+[f](g, h) - \mathcal{Q}_{\gamma,b}^-(g, h). \quad (7.28)$$

One then has the fundamental proposition where we recall that, in all the paper, assumption (7.4b) is in force:

Proposition 7.3. *Let $\varepsilon > 0$ and $0 \leq f \in L^1_2(\mathbb{R}^3)$ such that $1 - \varepsilon f \geq 0$. Then*

$$\mathcal{Q}_{\gamma,b}^\varepsilon(f, f) \leq \tilde{\mathcal{Q}}_{\gamma,b}[f](f, f). \quad (7.29)$$

Remark 7.6. *Proposition 7.3 implies that any suitable solution to (7.1) is such that*

$$\partial_t f \leq \tilde{\mathcal{Q}}_{\gamma,b}[f](f, f). \quad (7.30)$$

Equation (7.30) is close to the classical Boltzmann equation, with the difference that the gain part of the collision operator is now $\tilde{\mathcal{Q}}_{\gamma,b}^+$ in place of $\mathcal{Q}_{\gamma,b}^+$, and that it is an inequation. Interestingly, the arguments and techniques present in [8], where the classical Boltzmann equation is studied, work even with the differences we mentioned, which will allow us to conclude. The most notable point is of course that (7.30) is free from any dependence on ε .

Proof. Let $\varepsilon > 0$ and $0 \leq f \in L^1_2(\mathbb{R}^3)$ such that $1 - \varepsilon f \geq 0$. We use the splitting (7.25b) and also set

$$\Upsilon_\varepsilon := \varepsilon^2 \iint_{\mathbb{R}^3 \times \mathbb{S}^2} f f_* f' f'_* B dv_* d\sigma$$

where we notice that Υ_ε appears in both $\mathcal{Q}_{\gamma,b}^{\varepsilon,+}$ and $\mathcal{Q}_{\gamma,b}^{\varepsilon,-}$. Namely, expanding the term $(1 - \varepsilon f)(1 - \varepsilon f_*)$ in $\mathcal{Q}_{\gamma,b}^{\varepsilon,+}(f, f)$ one has, using that $f \geq 0$ so that $1 - \varepsilon f - \varepsilon f_* \leq 1$,

$$\mathcal{Q}_{\gamma,b}^{\varepsilon,+}(f, f) = \iint_{\mathbb{R}^3 \times \mathbb{S}^2} f' f'_* (1 - \varepsilon f - \varepsilon f_*) B dv_* d\sigma + \Upsilon_\varepsilon \leq \mathcal{Q}_{\gamma,b}^+(f, f) + \Upsilon_\varepsilon$$

whereas

$$\begin{aligned} \mathcal{Q}_{\gamma,b}^{\varepsilon,-}(f, f) &= \iint_{\mathbb{R}^3 \times \mathbb{S}^2} f f_* B dv_* d\sigma - \varepsilon \iint_{\mathbb{R}^3 \times \mathbb{S}^2} f f_* (f' + f'_*) B dv_* d\sigma + \Upsilon_\varepsilon \\ &= \mathcal{Q}_{\gamma,b}^-(f, f) - \varepsilon f \Gamma_{\gamma,b}(f, f) + \Upsilon_\varepsilon. \end{aligned}$$

Taking the difference and noticing that $\varepsilon f \leq \frac{f}{\|f\|_\infty}$ yields the result. \square

The crucial property on which our estimates will rely is the fact that the operator $\Gamma_{\gamma,b}$ defined in (7.26) is adjoint to the (symmetrized version) of $\mathcal{Q}_{\gamma,b}^+$ in the following sense:

Lemma 7.4. *For any measurable nonnegative functions f, g, h on \mathbb{R}^3 , we have*

$$\int_{\mathbb{R}^3} f \Gamma_{\gamma,b}(g, h) \, dv = \int_{\mathbb{R}^3} h \left[\mathcal{Q}_{\gamma,b}^+(f, g) + \mathcal{Q}_{\gamma,b}^+(g, f) \right] \, dv.$$

Proof. Using first the micro-reversibility property of B and then its symmetry property, we get

$$\begin{aligned} \int_{\mathbb{R}^3} f \Gamma_{\gamma,b}(g, h) \, dv &= \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} f g_* (h' + h'_*) B \, dv \, dv_* \, d\sigma \\ &= \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} f' g'_* (h + h_*) B \, dv \, dv_* \, d\sigma \\ &= \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} f' g'_* h B \, dv \, dv_* \, d\sigma + \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} f'_* g' h B \, dv \, dv_* \, d\sigma \\ &= \int_{\mathbb{R}^3} h \left[\mathcal{Q}_{\gamma,b}^+(f, g) + \mathcal{Q}_{\gamma,b}^+(g, f) \right] \, dv, \end{aligned}$$

which is the desired result. \square

Lemma 7.4 allows to transfer well-known estimates on $\mathcal{Q}_{\gamma,b}^+$ directly to $\Gamma_{\gamma,b}$ and hence to $\tilde{\mathcal{Q}}_{\gamma,b}^+$. The reader may now see how the combination of Proposition 7.3 and Lemma 7.4 allows to easily transfer techniques on the classical Boltzmann operator to the Boltzmann-Fermi-Dirac operator.

7.2.2 General estimates on $\mathcal{Q}_{\gamma,b}^+$

In this subsection, we recall the already known estimates on $\mathcal{Q}_{\gamma,b}^+$ that we later use in our study. First comes the following proposition, extracted from [5, Theorem 2] (see also [8, Theorem 28]) which deals with collision kernel only depending on $b(\cos\theta)$, i.e. associated to $\gamma = 0$.

Proposition 7.5 (Young's type inequality). *Consider an angular kernel b satisfying (7.4b). Let $r \in [1, +\infty]$ and $p, q \in [1, r]$ such that*

$$\frac{1}{p} + \frac{1}{q} = 1 + \frac{1}{r}.$$

Then

$$\left\| \mathcal{Q}_{0,b}^+(g, h) \right\|_r \leq C_b(p, q) \|g\|_p \|h\|_q, \quad (7.31)$$

where, with p', q', r' respectively the conjugates to p, q and r and $e_1 = (1 \ 0 \ 0)^T$,

$$C_b(p, q) = \left(\int_{\mathbb{S}^2} \left(\frac{1 + e_1 \cdot \sigma}{2} \right)^{-\frac{3}{2r'}} b(e_1 \cdot \sigma) \, d\sigma \right)^{\frac{r'}{p'}} \left(\int_{\mathbb{S}^2} \left(\frac{1 - e_1 \cdot \sigma}{2} \right)^{-\frac{3}{2r'}} b(e_1 \cdot \sigma) \, d\sigma \right)^{\frac{r'}{q'}}. \quad (7.32)$$

In the case $p = q = r = 1$, the constant $C_b(1, 1)$ is understood as

$$C_b(1, 1) = \int_{\mathbb{S}^2} b(e_1 \cdot \sigma) \, d\sigma = \|b\|_{L^1(\mathbb{S}^2)},$$

and in the cases that $p = 1$ or $q = 1$, one interprets $(\cdot)^{\frac{r'}{p'}}$ = 1 and $(\cdot)^{\frac{r'}{q'}}$ = 1 respectively. As a consequence, for any $p \in [1, +\infty]$ and $f \in L^1(\mathbb{R}^3) \cap L^p(\mathbb{R}^3)$, we have

$$\left\| \mathcal{Q}_{0,b}^+(f, f) \right\|_p \leq 2^{\frac{3}{2p'}} \|b\|_1 \|f\|_1 \|f\|_p. \quad (7.33)$$

Remark 7.7. Inequality (7.33) has been derived in [8, Equation (6.11)] (we point out a misprint in [8, Eq. (6.11)] where the parameter s should be replaced with s').

One deduces easily the following estimate from Proposition 7.5:

Corollary 7.6. Consider a bounded angular kernel $b \in L^\infty((-1, 1))$. Then for $(f, g) \in L^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$, we have

$$\left\| \mathcal{Q}_{0,b}^+(f, g) \right\|_2 \leq 8 \|b\|_\infty \|f\|_1 \|g\|_2. \quad (7.34)$$

Proof. We use Young's inequality (7.31) with $p = 1, q = 2$ to obtain, for any $f \in L^1(\mathbb{R}^3), g \in L^2(\mathbb{R}^3)$

$$\left\| \mathcal{Q}_{0,b}^+(f, g) \right\|_2 \leq C_b(1, 2) \|f\|_1 \|g\|_2.$$

Since

$$C_2(1, 2) \leq \|b\|_\infty \int_{-1}^1 \left(\frac{1-s}{2} \right)^{-\frac{3}{4}} ds = 8 \|b\|_\infty,$$

we obtain (7.34). \square

The last crucial estimate on $\mathcal{Q}_{\gamma,b}^+$ is the following ‘‘gain of integrability’’ property, mostly extracted from [8, Equation (6.19)] and adapted to hard potentials.

Proposition 7.7. (Gain of integrability). Consider $\gamma \in (0, 1)$, a bounded angular kernel $b \in L^\infty((-1, 1))$, $f \in L^1(\mathbb{R}^3)$ and $g \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. Then

$$\max \left(\left\| \mathcal{Q}_{\gamma,b}^+(g, f) \right\|_2, \left\| \mathcal{Q}_{\gamma,b}^+(f, g) \right\|_2 \right) \leq 16 \|b\|_\infty \|f\|_1 \|g\|_1^{\frac{2\gamma}{3}} \|g\|_2^{1-\frac{2\gamma}{3}}. \quad (7.35)$$

Proof. Let $\delta > 0$, notice that for any $u \in \mathbb{R}^3$,

$$|u|^\gamma = |u|^\gamma \mathbf{1}_{|u| \geq \delta} + |u|^\gamma \mathbf{1}_{|u| \leq \delta} \leq \frac{|u|}{\delta^{1-\gamma}} \mathbf{1}_{|u| \geq \delta} + \delta^\gamma \mathbf{1}_{|u| \leq \delta} \leq \frac{|u|}{\delta^{1-\gamma}} + \delta^\gamma,$$

so that

$$\mathcal{Q}_{\gamma,b}^+(f, g) \leq \delta^{\gamma-1} \mathcal{Q}_{1,b}^+(f, g) + \delta^\gamma \mathcal{Q}_{0,b}^+(f, g).$$

Applying [8, Equation (6.19)] (in dimension 3), we have

$$\left\| \mathcal{Q}_{1,b}^+(f, g) \right\|_2 \leq C_3 \|b\|_\infty \|f\|_1 \|g\|_{\frac{6}{5}}, \quad (7.36)$$

where C_3 comes from a Hardy-Littlewood-Sobolev inequality (see the last lines of the proof of [8, Proposition 30]). Using [118, Theorem 3.1, Equation (3.2)] with here $C_3 = N_{\frac{6}{5}, 1, 3}$, we have in fact

$$C_3 = \pi^{\frac{1}{2}} \frac{\Gamma(\frac{3}{2} - \frac{1}{2})}{\Gamma(2 - \frac{1}{2})} \left(\frac{\Gamma(\frac{3}{2})}{\Gamma(3)} \right)^{-1 + \frac{1}{3}} = \pi^{\frac{1}{2}} \frac{\Gamma(1)}{\Gamma(\frac{5}{2})} \left(\frac{\Gamma(\frac{3}{2})}{\Gamma(3)} \right)^{-\frac{2}{3}} = \frac{4^{5/3}}{3\pi^{1/3}},$$

where, only in the above equation, Γ stands for the Gamma function. In particular, it holds that $C_3 \leq 3$. Moreover, by interpolation,

$$\|g\|_{\frac{6}{5}} \leq \|g\|_1^{\frac{2}{3}} \|g\|_2^{\frac{1}{3}},$$

therefore (7.36) implies

$$\|\mathcal{Q}_{1,b}^+(f,g)\|_2 \leq 3 \|b\|_\infty \|f\|_1 \|g\|_1^{\frac{2}{3}} \|g\|_2^{\frac{1}{3}}. \quad (7.37)$$

On the other hand, it comes from Equation (7.34) in Corollary 7.6 that

$$\|\mathcal{Q}_{0,b}^+(f,g)\|_2 \leq 8 \|b\|_\infty \|f\|_1 \|g\|_2.$$

All in all, we obtain, for any $\delta > 0$,

$$\begin{aligned} \|\mathcal{Q}_{\gamma,b}^+(f,g)\|_2 &\leq \delta^{\gamma-1} \|\mathcal{Q}_{1,b}^+(f,g)\|_2 + \delta^\gamma \|\mathcal{Q}_{0,b}^+(f,g)\|_2 \\ &\leq \|b\|_\infty \|f\|_1 \|g\|_2^{\frac{1}{3}} \left(\delta^{\gamma-1} 3 \|g\|_1^{\frac{2}{3}} + \delta^\gamma 8 \|g\|_2^{\frac{2}{3}} \right). \end{aligned}$$

Choosing $\delta = \frac{3 \|g\|_1^{\frac{2}{3}}}{8 \|g\|_2^{\frac{2}{3}}}$ and noting that $3^\gamma \times 8^{1-\gamma} \leq 8$ for any $\gamma \in (0, 1]$ yields (7.35) with $\|\mathcal{Q}_{\gamma,b}^+(f,g)\|_2$

in place of the left-hand-side. Let us show now the bound for $\|\mathcal{Q}_{\gamma,b}^+(g,f)\|_2$. The change of variable $\sigma \rightarrow -\sigma$ directly proves that

$$\mathcal{Q}_{\gamma,b}^+(g,f) = \mathcal{Q}_{\gamma,\tilde{b}}^+(f,g)$$

with $\tilde{b}(\cos\theta) = b(-\cos\theta)$. Since $\|\tilde{b}\|_\infty = \|b\|_\infty$, we deduce the estimate for $\|\mathcal{Q}_{\gamma,b}^+(g,f)\|_2$ from the first part of the proof. \square

7.2.3 Key estimates on $\mathcal{Q}_{\gamma,b}^+$, $\Gamma_{\gamma,b}$ and $\mathcal{Q}_{\gamma,b}^-$

7.2.3.1 Estimates on $\mathcal{Q}_{\gamma,b}^+$

Relying on the general estimates on $\mathcal{Q}_{\gamma,b}^+$ stated above, we provide here two useful bounds that we later use in order to obtain L_γ^2 bounds on the solutions to (7.1).

Proposition 7.8. *Consider a bounded angular kernel $b \in L^\infty((-1, 1))$ and $\gamma \in (0, 1]$. Then for any $f \in L_{3\gamma}^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, we have*

$$\int_{\mathbb{R}^3} \mathcal{Q}_{\gamma,b}^+(f,f) f(v) \langle v \rangle^{2\gamma} dv \leq 16 \|b\|_\infty \|\langle \cdot \rangle^{\frac{\gamma}{2}} f\|_1^{1+\frac{2\gamma}{3}} \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2^{2-\frac{2\gamma}{3}}. \quad (7.38)$$

Proof. First, by Cauchy-Schwarz inequality, we have

$$\int_{\mathbb{R}^3} \mathcal{Q}_{\gamma,b}^+(f,f) f(v) \langle v \rangle^{2\gamma} dv \leq \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2 \left\| \langle \cdot \rangle^{\frac{\gamma}{2}} \mathcal{Q}_{\gamma,b}^+(f,f) \right\|_2.$$

Now notice that for any $(v, v_*, \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2$ we have $\langle v \rangle^{\frac{\gamma}{2}} \leq \langle v' \rangle^{\frac{\gamma}{2}} \langle v_*' \rangle^{\frac{\gamma}{2}}$, where we recall the notation (7.3) for v' and v_*' . From this we deduce that for any $v \in \mathbb{R}^3$, we have

$$\langle v \rangle^{\frac{\gamma}{2}} \mathcal{Q}_{\gamma,b}^+(f,f)(v) \leq \mathcal{Q}_{\gamma,b}^+(\langle \cdot \rangle^{\frac{\gamma}{2}} f, \langle \cdot \rangle^{\frac{\gamma}{2}} f)(v).$$

Lastly, we use the gain of integrability property (7.35) to obtain that

$$\left\| \mathcal{Q}_{\gamma,b}^+(\langle \cdot \rangle^{\frac{\gamma}{2}} f, \langle \cdot \rangle^{\frac{\gamma}{2}} f) \right\|_2 \leq 16 \|b\|_\infty \|\langle \cdot \rangle^{\frac{\gamma}{2}} f\|_1^{1+\frac{2\gamma}{3}} \|\langle \cdot \rangle^{\frac{\gamma}{2}} f\|_2^{1-\frac{2\gamma}{3}}.$$

Since $\|\langle \cdot \rangle^{\frac{\gamma}{2}} f\|_2 \leq \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2$ and $1 - \frac{2\gamma}{3} \geq 0$, we indeed obtain (7.38). \square

We consider in the next result an estimate for $\mathcal{Q}_{\gamma,b}^+$, similar to Young's convolution inequality, under the mere cutoff assumption (7.4b):

Proposition 7.9. *Consider an angular kernel b satisfying the cutoff assumption (7.4b) and $\gamma \in (0, 1]$. Then for any $f \in L_{3\gamma}^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, we have*

$$\int_{\mathbb{R}^3} \mathcal{Q}_{\gamma,b}^+(f, f) f(v) \langle v \rangle^{2\gamma} dv \leq 2^{\frac{3}{4}} \|b\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2^2. \quad (7.39)$$

Proof. We follow the same steps as in the proof of the previous Proposition 7.8 and recall that

$$\int_{\mathbb{R}^3} \mathcal{Q}_{\gamma,b}^+(f, f) f(v) \langle v \rangle^{2\gamma} dv \leq \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2 \left\| \langle \cdot \rangle^{\frac{\gamma}{2}} \mathcal{Q}_{\gamma,b}^+(f, f) \right\|_2.$$

Second, notice that for any $(v, v_*, \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2$ it holds that

$$|v - v_*|^\gamma = |v' - v'_*|^\gamma \leq \langle v' \rangle^\gamma \langle v'_* \rangle^\gamma,$$

and $\langle v \rangle^{\frac{\gamma}{2}} \leq \langle v' \rangle^{\frac{\gamma}{2}} \langle v'_* \rangle^{\frac{\gamma}{2}}$, where we recall the notation (7.3) for v' and v'_* . Then, for any $v \in \mathbb{R}^3$,

$$\langle v \rangle^{\frac{\gamma}{2}} \mathcal{Q}_{\gamma,b}^+(f, f)(v) \leq \langle v \rangle^{\frac{\gamma}{2}} \mathcal{Q}_{0,b}^+(\langle \cdot \rangle^\gamma f, \langle \cdot \rangle^\gamma f)(v) \leq \mathcal{Q}_{0,b}^+(\langle \cdot \rangle^{\frac{3\gamma}{2}} f, \langle \cdot \rangle^{\frac{3\gamma}{2}} f)(v).$$

Since (7.33) in Proposition 7.5 gives

$$\left\| \mathcal{Q}_{0,b}^+(\langle \cdot \rangle^{\frac{3\gamma}{2}} f, \langle \cdot \rangle^{\frac{3\gamma}{2}} f) \right\|_2 \leq 2^{\frac{3}{4}} \|b\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2,$$

we can conclude to (7.39). \square

Finally, we provide the following proposition, which is a straightforward consequence of [8, Corollary 35].

Proposition 7.10. *Consider angular kernels b_S and b_R satisfying the cutoff assumption (7.4b) and such that b_S vanishes in the vicinity of $\{-1, 1\}$. Then for any $\gamma \in (0, 1]$ and $f \in L_{2\gamma}^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, we have*

$$\left\| \mathcal{Q}_{\gamma,b_S}^+(f, f) \right\|_\infty \leq C_{b_S}(2, 2) \|\langle \cdot \rangle^\gamma f\|_2^2, \quad (7.40)$$

where $C_{b_S}(2, 2)$ is defined by (7.32), and for any $v \in \mathbb{R}^3$,

$$\mathcal{Q}_{\gamma,b_R}^+(f, f)(v) \leq 4 \|b_R\|_1 \|f\|_1 \|f\|_\infty \langle v \rangle^\gamma. \quad (7.41)$$

Proof. The only difference with [8, Corollary 35] is that we explicit the constant $4 \|b_R\|_1$ in (7.41) and that we have added up the two last equations of [8, Corollary 35, (7.29)]. The 4 is not explicitly given in [8, Corollary 35] but can be obtained by noting that the constant is there given by $2^{\frac{7}{2}} (C_{b_R^+}(\infty, 1) + C_{b_R^-}(1, \infty))$ (where b_R^+ and b_R^- are defined there), that one can obtain from (7.32), with

$$C_{b_R^+}(\infty, 1) \leq 2^{\frac{3}{2}} \|b_R^+\|_1, \quad C_{b_R^-}(1, \infty) \leq 2^{\frac{3}{2}} \|b_R^-\|_1,$$

hence allowing to bound the constant by $2^{\frac{\gamma+3}{2}} \|b_R\|_1$. We then conclude as $\gamma \leq 1$. \square

7.2.3.2 Estimates on $\Gamma_{\gamma,b}$

In this subsection, we make use of the estimates on $\mathcal{Q}_{\gamma,b}^+$ obtained in the previous subsection as well as Lemma 7.4 to simply obtain crucial estimates on $\Gamma_{\gamma,b}$.

Propositions 7.11–7.12 and 7.13–7.14 are the analogues to Propositions 7.8–7.9 and 7.10 for $\Gamma_{\gamma,b}$.

Proposition 7.11. *Consider a bounded angular kernel $b \in L^\infty((-1, 1))$. Then for any $\gamma \in (0, 1]$ and $0 \leq f \in L_{3\gamma}^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, we have*

$$\int_{\mathbb{R}^3} \frac{f(v)}{\|f\|_\infty} \Gamma_{\gamma,b}(f, f) f(v) \langle v \rangle^{2\gamma} dv \leq 32 \|b\|_\infty \|\langle \cdot \rangle^\gamma f\|_1^{1+\frac{2\gamma}{3}} \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2^{2-\frac{2\gamma}{3}}. \quad (7.42)$$

Proof. First, notice that applying the Cauchy-Schwarz inequality yields

$$\int_{\mathbb{R}^3} \frac{f(v)}{\|f\|_\infty} \Gamma_{\gamma,b}(f, f) f(v) \langle v \rangle^{2\gamma} dv \leq \|f\|_\infty^{-1} \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2 \left\| \langle \cdot \rangle^{\frac{\gamma}{2}} f \Gamma_{\gamma,b}(f, f) \right\|_2. \quad (7.43)$$

Clearly, by Riesz representation theorem,

$$\left\| \langle \cdot \rangle^{\frac{\gamma}{2}} f \Gamma_{\gamma,b}(f, f) \right\|_2 = \sup_{\|g\|_2=1} \int_{\mathbb{R}^3} g(v) \Gamma_{\gamma,b}(f, f) f(v) \langle v \rangle^{\frac{\gamma}{2}} dv.$$

Applying Lemma 7.4, this gives

$$\begin{aligned} \left\| \langle \cdot \rangle^{\frac{\gamma}{2}} f \Gamma_{\gamma,b}(f, f) \right\|_2 &= \sup_{\|g\|_2=1} \int_{\mathbb{R}^3} f(v) \left\{ \mathcal{Q}_{\gamma,b}^+(\langle \cdot \rangle^{\frac{\gamma}{2}} fg, f) + \mathcal{Q}_{\gamma,b}^+(f, \langle \cdot \rangle^{\frac{\gamma}{2}} fg) \right\} dv \\ &\leq \|f\|_2 \sup_{\|g\|_2=1} \left\{ \left\| \mathcal{Q}_{\gamma,b}^+(\langle \cdot \rangle^{\frac{\gamma}{2}} fg, f) \right\|_2 + \left\| \mathcal{Q}_{\gamma,b}^+(f, \langle \cdot \rangle^{\frac{\gamma}{2}} fg) \right\|_2 \right\}. \end{aligned}$$

where we used Cauchy-Schwarz inequality for the last estimate. Using the gain of integrability property (7.35) in Proposition 7.7, we deduce that

$$\left\| \langle \cdot \rangle^{\frac{\gamma}{2}} f \Gamma_{\gamma,b}(f, f) \right\|_2 \leq \|f\|_2 \sup_{\|g\|_2=1} \left\{ 32 \|b\|_\infty \left\| \langle \cdot \rangle^{\frac{\gamma}{2}} fg \right\|_1 \|f\|_1^{\frac{2\gamma}{3}} \|f\|_2^{1-\frac{2\gamma}{3}} \right\}.$$

Using again Cauchy-Schwarz inequality, we obtain

$$\begin{aligned} \left\| \langle \cdot \rangle^{\frac{\gamma}{2}} f \Gamma_{\gamma,b}(f, f) \right\|_2 &\leq \|f\|_2 \sup_{\|g\|_2=1} \left\{ 32 \|b\|_\infty \left\| \langle \cdot \rangle^{\frac{\gamma}{2}} f \right\|_2 \|g\|_2 \|f\|_1^{\frac{2\gamma}{3}} \|f\|_2^{1-\frac{2\gamma}{3}} \right\} \\ &= 32 \|b\|_\infty \|f\|_1^{\frac{2\gamma}{3}} \left\| \langle \cdot \rangle^{\frac{\gamma}{2}} f \right\|_2 \|f\|_2^{2-\frac{2\gamma}{3}}. \end{aligned}$$

Recalling (7.43), we then conclude that

$$\int_{\mathbb{R}^3} \frac{f(v)}{\|f\|_\infty} \Gamma_{\gamma,b}(f, f) f(v) \langle v \rangle^{2\gamma} dv \leq 32 \|b\|_\infty \|f\|_\infty^{-1} \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2 \|f\|_1^{\frac{2\gamma}{3}} \left\| \langle \cdot \rangle^{\frac{\gamma}{2}} f \right\|_2 \|f\|_2^{2-\frac{2\gamma}{3}}.$$

The result comes after noticing that

$$\|f\|_2 \leq \|f\|_1^{\frac{1}{2}} \|f\|_\infty^{\frac{1}{2}}, \quad \|\langle \cdot \rangle^{\frac{\gamma}{2}} f\|_2 \leq \|\langle \cdot \rangle^\gamma f\|_1^{\frac{1}{2}} \|f\|_\infty^{\frac{1}{2}},$$

while $\|f\|_1 \leq \|\langle \cdot \rangle^\gamma f\|_1$ and $\|f\|_2 \leq \left\| \langle \cdot \rangle^{\frac{3\gamma}{2}} f \right\|_2$. \square

For b satisfying the cutoff assumption (7.4b), we have the following version of Young's convolution inequality

Proposition 7.12. *Consider $\gamma \in (0, 1]$, an angular kernel b satisfying the cutoff assumption (7.4b) and $f \in L^1_2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. Then*

$$\int_{\mathbb{R}^3} \frac{f}{\|f\|_\infty} \Gamma_{\gamma,b}(f, f) f(v) \langle v \rangle^{2\gamma} \mathbf{d}v \leq 2\|b\|_1 \|\langle \cdot \rangle^\gamma f\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2^2. \quad (7.44)$$

Proof. We first note that, since $|v - v_*|^\gamma \leq \langle v \rangle^\gamma \langle v_* \rangle^\gamma$, where we recall that $\langle v \rangle = (1 + |v|^2)^{\frac{1}{2}}$, we have

$$\begin{aligned} \int_{\mathbb{R}^3} \frac{f}{\|f\|_\infty} \Gamma_{\gamma,b}(f, f) f(v) \langle v \rangle^{2\gamma} \mathbf{d}v &\leq \|f\|_\infty^{-1} \int_{\mathbb{R}^3} \Gamma_{0,b}(\langle \cdot \rangle^\gamma f, f) f^2(v) \langle v \rangle^{3\gamma} \mathbf{d}v \\ &\leq \|f\|_\infty^{-1} \|\Gamma_{0,b}(\langle \cdot \rangle^\gamma f, f)\|_\infty \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2^2. \end{aligned} \quad (7.45)$$

As before, thanks to Riesz representation theorem together with Lemma 7.4, we have

$$\begin{aligned} \|\Gamma_{0,b}(\langle \cdot \rangle^\gamma f, f)\|_\infty &= \sup_{\|g\|_1=1} \int_{\mathbb{R}^3} g(v) \Gamma_{0,b}(\langle \cdot \rangle^\gamma f, f) \mathbf{d}v \\ &= \sup_{\|g\|_1=1} \int_{\mathbb{R}^3} f(v) \left(\mathcal{Q}_{0,b}^+(g, \langle \cdot \rangle^\gamma f) + \mathcal{Q}_{0,b}^+(\langle \cdot \rangle^\gamma f, g) \right) \mathbf{d}v. \end{aligned}$$

Clearly, this implies that

$$\|\Gamma_{0,b}(\langle \cdot \rangle^\gamma f, f)\|_\infty \leq \|f\|_\infty \sup_{\|g\|_1=1} \left(\|\mathcal{Q}_{0,b}^+(g, \langle \cdot \rangle^\gamma f)\|_1 + \|\mathcal{Q}_{0,b}^+(\langle \cdot \rangle^\gamma f, g)\|_1 \right).$$

We apply Young's inequality (7.31) from Proposition 7.5 with $(p, q, r) = (1, 1, 1)$ to deduce that

$$\|\Gamma_{0,b}(\langle \cdot \rangle^\gamma f, f)\|_\infty \leq \|f\|_\infty \sup_{\|g\|_1=1} (2\|b\|_1 \|g\|_1 \|\langle \cdot \rangle^\gamma f\|_1) = 2\|b\|_1 \|f\|_\infty \|\langle \cdot \rangle^\gamma f\|_1.$$

Combining this estimate with (7.45) yields (7.44). \square

Proposition 7.13. *Consider an angular kernel b satisfying the cutoff assumption (7.4b) and such that b vanishes in the vicinity of $\{-1, 1\}$. Then for any $\gamma \in (0, 1]$ and $f \in L^2_\gamma(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, we have for any $v \in \mathbb{R}^3$,*

$$\frac{f(v)}{\|f\|_\infty} \Gamma_{\gamma,b}(f, f)(v) \leq (C_b(1, 2) + C_b(2, 1)) \|\langle \cdot \rangle^\gamma f\|_2 \|f\|_2 \langle v \rangle^\gamma, \quad (7.46)$$

where $C_b(1, 2)$ and $C_b(2, 1)$ are defined in (7.32).

Proof. For $g \in L^2(\mathbb{R}^3)$, writing the L^∞ norm in weak form yields

$$\|\Gamma_{0,b}(g, f)\|_\infty = \sup_{\|h\|_1=1} \int_{\mathbb{R}^3} h(v) \Gamma_{0,b}(g, f)(v) \mathbf{d}v.$$

Applying Lemma 7.4, the above right-hand-side becomes

$$\sup_{\|h\|_1=1} \int_{\mathbb{R}^3} f(v) \left\{ \mathcal{Q}_{0,b}^+(h,g)(v) + \mathcal{Q}_{0,b}^+(g,h)(v) \right\} \mathrm{d}v,$$

which, by a Cauchy-Schwarz argument, is lower than

$$\|f\|_2 \sup_{\|h\|_1=1} \left(\|\mathcal{Q}_{0,b}^+(h,g)\|_2 + \|\mathcal{Q}_{0,b}^+(g,h)\|_2 \right).$$

We apply Young's inequality (7.31) from Proposition 7.5 respectively with $(p,q,r) = (1,2,2)$ and $(p,q,r) = (2,1,2)$ to obtain that the above term is lower than

$$\|f\|_2 \sup_{\|h\|_1=1} (C_b(1,2) + C_b(2,1)) \|g\|_2 \|h\|_1,$$

so that

$$\|\Gamma_{0,b}(g,f)\|_\infty \leq (C_b(1,2) + C_b(2,1)) \|g\|_2 \|f\|_2.$$

Finally, we recall that, for any $(v, v_*, \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2$, we have $|v - v_*|^\gamma \leq \langle v \rangle^\gamma \langle v_* \rangle^\gamma$, so that

$$\Gamma_{\gamma,b}(g,f)(v) \leq \Gamma_{0,b}(\langle \cdot \rangle^\gamma g, f)(v) \langle v \rangle^\gamma,$$

ending the proof, after noticing that $\frac{f(v)}{\|f\|_\infty} \leq 1$. \square

Proposition 7.14. *Consider an angular kernel b satisfying the cutoff assumption (7.4b). Then for any $\gamma \in (0, 1]$ and $f \in L_\gamma^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, we have for any $v \in \mathbb{R}^3$,*

$$\frac{f(v)}{\|f\|_\infty} \Gamma_{\gamma,b}(f,f)(v) \leq 2 \|b\|_1 \|f\|_{L_\gamma^1} f(v) \langle v \rangle^\gamma. \quad (7.47)$$

Proof. For $g \in L^1(\mathbb{R}^3)$, we showed in the first lines of the proof of the previous proposition that

$$\|\Gamma_{0,b}(g,f)\|_\infty \leq \sup_{\|h\|_1=1} \int_{\mathbb{R}^3} f(v) \left\{ \mathcal{Q}_{0,b}^+(h,g)(v) + \mathcal{Q}_{0,b}^+(g,h)(v) \right\} \mathrm{d}v.$$

Therefore,

$$\|\Gamma_{0,b}(g,f)\|_\infty \leq \|f\|_\infty \sup_{\|h\|_1=1} \left(\|\mathcal{Q}_{0,b}^+(h,g)\|_1 + \|\mathcal{Q}_{0,b}^+(g,h)\|_1 \right).$$

We apply Young's inequality (7.31) from Proposition 7.5 with $(p,q,r) = (1,1,1)$ to obtain that

$$\|\Gamma_{0,b}(g,f)\|_\infty \leq 2 \|b\|_1 \|g\|_1 \|f\|_\infty.$$

Finally, we recall that, for any $(v, v_*, \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2$, we have $|v - v_*|^\gamma \leq \langle v \rangle^\gamma \langle v_* \rangle^\gamma$, so that

$$\Gamma_{\gamma,b}(g,f)(v) \leq \Gamma_{0,b}(\langle \cdot \rangle^\gamma g, f)(v) \langle v \rangle^\gamma,$$

ending the proof. \square

7.2.3.3 Estimate on $\mathcal{Q}_{\gamma,b}^-$

Lastly, we use a standard lower-bound estimate on the loss operator $\mathcal{Q}_{\gamma,b}^-$.

Proposition 7.15. *Consider $\gamma \in (0, 1]$ and an angular kernel b satisfying the cutoff assumption (7.4b). Then for any $0 \leq f \in L^1_3(\mathbb{R}^3)$, there exists an explicit constant $\mathbf{c}_{\gamma, f} > 0$ depending on γ and on f only through its L^1 and L^1_2 norms and an upper-bound on its L^1_3 norm, such that*

$$\int_{\mathbb{R}^3} \mathcal{Q}_{\gamma, b}^-(f, f) f(v) \langle v \rangle^{2\gamma} dv \geq \mathbf{c}_{\gamma, f} \|b\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f\|_2^2. \quad (7.48)$$

Proof. First note that the loss operator may be written as, for any $v \in \mathbb{R}^3$,

$$\mathcal{Q}_{\gamma, b}^-(f, f)(v) = f(v) \|b\|_1 (f * |\cdot|^\gamma)(v).$$

Then [8, Lemma 8] provides the existence of an explicit $\mathbf{c}_{\gamma, f} > 0$ depending on γ and on f only through $\|f\|_1$, $\|f\|_{L^1_2}$ and an upper bound on $\|f\|_{L^1_3}$ such that for any $v \in \mathbb{R}^3$,

$$(f * |\cdot|^\gamma)(v) \geq \mathbf{c}_{\gamma, f} \langle v \rangle^\gamma. \quad (7.49)$$

Combining those two fact, it then comes that

$$\int_{\mathbb{R}^3} \mathcal{Q}_{\gamma, b}^-(f, f) f(v) \langle v \rangle^{2\gamma} dv \geq \mathbf{c}_{\gamma, f} \|b\|_1 \int_{\mathbb{R}^3} f(v)^2 \langle v \rangle^{3\gamma} dv,$$

concluding the proof. \square

7.2.4 Derivation of L^2_γ bounds

In this subsection, we provide, in Proposition 7.16, a uniform-in-time and uniform-in- ε L^2_γ bound on the solutions to (7.1). We only recall that, according to the results in Appendix 7.B, assuming that $f^{\text{in}} \in L^1_3(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, for any $0 < \varepsilon \leq \|f^{\text{in}}\|_\infty^{-1}$, the unique solution f^ε to **(BFD Eq.)** is such that

$$\sup_{t \geq 0} \|f^\varepsilon(t, \cdot)\|_{L^1_3} \leq \mathbf{C}_{1,3}, \quad (7.50)$$

with $\mathbf{C}_{1,3} > 0$ explicit and depending only on γ , b , ϱ^{in} , u^{in} , E^{in} and an upper-bound on $\|f^{\text{in}}\|_{L^1_3}$ - in particular, not on ε .

We now have all the tools we need to obtain the following proposition.

Proposition 7.16. (L^2_γ bound.) *Consider a collision kernel B of the form (7.4) with $\gamma \in (0, 1]$. Given an initial datum $0 \leq f^{\text{in}} \in L^1_3(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, there exists an explicit constant $\mathbf{C}_{2,\gamma}$ depending only on γ , b , ϱ^{in} , u^{in} , E^{in} and upper-bounds on $\|f^{\text{in}}\|_{L^1_3}$ and $\|f^{\text{in}}\|_\infty$ such that for any $\varepsilon \in (0, \|f^{\text{in}}\|_\infty^{-1}]$, the unique solution f^ε to (7.1) satisfies*

$$\sup_{t \geq 0} \|f^\varepsilon(t)\|_{L^2_\gamma} \leq \mathbf{C}_{2,\gamma}. \quad (7.51)$$

Proof. For the sake of clarity, since we are working here with fixed ε and fixed initial datum, we simply denote in the following $f(t) \equiv f^\varepsilon(t, \cdot)$ for any $t \geq 0$ as the unique solution to

$$\partial_t f(t)(v) = \mathcal{Q}_{\gamma, b}^\varepsilon(f(t), f(t))(v), \quad f(t=0) = f^{\text{in}}.$$

Using Proposition 7.29 we get, as pointed out in Remark 7.6 together with the definition of $\tilde{\mathcal{Q}}_{\gamma, b}$ (see Eq. (7.28)), we deduce that, for any $t \geq 0$,

$$\partial_t f(t) \leq \tilde{\mathcal{Q}}_{\gamma, b}(f(t), f(t)) = \mathcal{Q}_{\gamma, b}^+(f(t), f(t)) + \frac{f(t)}{\|f(t)\|_\infty} \Gamma_{\gamma, b}(f(t), f(t)) - \mathcal{Q}_{\gamma, b}^-(f(t), f(t)).$$

Multiplying both sides by $f(t)(v)\langle v \rangle^{2\gamma}$ and integrating on $v \in \mathbb{R}^3$, it comes that

$$\frac{1}{2} \frac{d}{dt} \|f(t)\|_{L^\gamma}^2 \leq \int_{\mathbb{R}^3} \left(\mathcal{Q}_{\gamma,b}^+(f(t), f(t))(v) + \frac{f(t)(v)}{\|f(t)\|_\infty} \Gamma_{\gamma,b}(f(t), f(t))(v) - \mathcal{Q}_{\gamma,b}^-(f(t), f(t))(v) \right) f(t)(v) \langle v \rangle^{2\gamma} dv.$$

In the rest of the proof, we follow the ideas developed in [8, Section 7] (see also [10]) and split the kernel b into $b = b^\infty + b^1$, with $b^\infty \in L^\infty((-1, 1))$. Since $b \mapsto \mathcal{Q}_{\gamma,b}^+$ and $b \mapsto \Gamma_{\gamma,b}$ are linear applications, we can split the above right-hand-side as

$$\frac{1}{2} \frac{d}{dt} \|f(t)\|_{L^\gamma}^2 \leq \int_{\mathbb{R}^3} \mathcal{Q}_{\gamma,b^\infty}^+(f(t), f(t))(v) f(t)(v) \langle v \rangle^{2\gamma} dv \quad (7.52)$$

$$+ \int_{\mathbb{R}^3} \mathcal{Q}_{\gamma,b^1}^+(f(t), f(t))(v) f(t)(v) \langle v \rangle^{2\gamma} dv \quad (7.53)$$

$$+ \int_{\mathbb{R}^3} \frac{f(t)(v)}{\|f(t)\|_\infty} \Gamma_{\gamma,b^\infty}(f(t), f(t))(v) f(t)(v) \langle v \rangle^{2\gamma} dv \quad (7.54)$$

$$+ \int_{\mathbb{R}^3} \frac{f(t)(v)}{\|f(t)\|_\infty} \Gamma_{\gamma,b^1}(f(t), f(t))(v) f(t)(v) \langle v \rangle^{2\gamma} dv \quad (7.55)$$

$$- \int_{\mathbb{R}^3} \mathcal{Q}_{\gamma,b}^-(f(t), f(t))(v) f(t)(v) \langle v \rangle^{2\gamma} dv. \quad (7.56)$$

All of these terms have been studied and bounded from above in Subsection 7.2.3. Namely:

- Equation (7.38) in Proposition 7.8 allows to bound from above (7.52)
- Equation (7.39) in Proposition 7.9 allows to bound from above (7.53)
- Equation (7.42) in Proposition 7.11 allows to bound from above (7.54)
- Equation (7.44) in Proposition 7.12 allows to bound from above (7.55)
- Equation (7.48) in Proposition 7.15 allows to bound from above (7.56).

Putting everything together, (7.52)–(7.56) implies

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|f(t)\|_{L^\gamma}^2 + \mathbf{c}_{\gamma,f(t)} \|b\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^2 &\leq 16 \|b^\infty\|_\infty \|\langle \cdot \rangle^{\frac{\gamma}{2}} f(t)\|_1^{1+\frac{2\gamma}{3}} \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^{2-\frac{2\gamma}{3}} \\ &\quad + 2^{\frac{3}{4}} \|b^1\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^2 \\ &\quad + 32 \|b^\infty\|_\infty \|\langle \cdot \rangle^\gamma f(t)\|_1^{1+\frac{2\gamma}{3}} \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_1^{2-\frac{2\gamma}{3}} \\ &\quad + 2 \|b^1\|_1 \|\langle \cdot \rangle^\gamma f(t)\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^2. \end{aligned}$$

We observe now that $2^{\frac{3}{4}} \leq 2$ and, since $\gamma \in (0, 1]$,

$$\|\langle \cdot \rangle^{\frac{\gamma}{2}} f(t)\|_1 \leq \|\langle \cdot \rangle^\gamma f(t)\|_1 \leq \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_1 \leq \|f(t)\|_{L_2^1} = \|f^{\text{in}}\|_{L_2^1},$$

since mass and energy are conserved during the evolution, we deduce that

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|f(t)\|_{L^\gamma}^2 + \mathbf{c}_{\gamma,f(t)} \|b\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^2 &\leq 48 \|b^\infty\|_\infty \|f^{\text{in}}\|_{L_2^1}^{1+\frac{2\gamma}{3}} \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^{2-\frac{2\gamma}{3}} \\ &\quad + 4 \|b^1\|_1 \|f^{\text{in}}\|_{L_2^1} \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^2. \quad (7.57) \end{aligned}$$

We now recall that $\mathbf{c}_{\gamma, f(t)}$, coming from Proposition 7.15 only depends on $f(t)$ through $\|f\|_1$, $\|f\|_{L^1_2}$ and an upper bound on $\|f\|_{L^1_3}$. Using now (7.50), we conclude to the existence of a constant $\tilde{\mathbf{c}}_{\gamma, f^{\text{in}}} > 0$ that depends only on γ and f^{in} , which is *explicit and independent of ε* , such that for any $t \geq 0$, we have $\mathbf{c}_{\gamma, f(t)} \geq \tilde{\mathbf{c}}_{\gamma, f^{\text{in}}}$. Therefore, (7.57) may be recast into

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|f(t)\|_{L^2_\gamma}^2 + \tilde{\mathbf{c}}_{\gamma, f^{\text{in}}} \|b\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^2 &\leq 48 \|b^\infty\|_\infty \left\| f^{\text{in}} \right\|_{L^1_2}^{1+\frac{2\gamma}{3}} \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^{2-\frac{2\gamma}{3}} \\ &\quad + 4 \|b^1\|_1 \|f^{\text{in}}\|_{L^1_2} \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^2. \end{aligned}$$

We can choose $b^\infty \in L^\infty((-1, 1))$ such that

$$\|b^1\|_1 = \|b - b^\infty\|_1 \leq \frac{\tilde{\mathbf{c}}_{\gamma, f^{\text{in}}} \|b\|_1}{8 \|f^{\text{in}}\|_{L^1_2}}.$$

For such a choice of b^∞ , we set $\frac{1}{2} A_1 = 48 \|f^{\text{in}}\|_{L^1_2}^{1+\frac{2\gamma}{3}} \|b^\infty\|_\infty$ and deduce that

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|f(t)\|_{L^2_\gamma}^2 + \tilde{\mathbf{c}}_{\gamma, f^{\text{in}}} \|b\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^2 &\leq \\ \frac{1}{2} A_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^{2-\frac{2\gamma}{3}} + \frac{1}{2} \tilde{\mathbf{c}}_{\gamma, f^{\text{in}}} \|b\|_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^2, \end{aligned}$$

that is

$$\frac{d}{dt} \|f(t)\|_{L^2_\gamma}^2 \leq A_1 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^{2-\frac{2\gamma}{3}} - 2A_2 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^2, \quad (7.58)$$

where we denoted $A_2 := \frac{1}{2} \tilde{\mathbf{c}}_{\gamma, f^{\text{in}}} \|b\|_1$. Notice that $A_1 \geq 0$ and $A_2 > 0$ *do not depend on time, nor on ε* . A study of $X \mapsto A_1 X^{2-\frac{2\gamma}{3}} - A_2 X^2$ leads to, for any $X \geq 0$,

$$A_1 X^{2-\frac{2\gamma}{3}} - A_2 X^2 \leq \left(\frac{\frac{2\gamma}{3}}{2^{\frac{3}{2\gamma}} (2 - \frac{2\gamma}{3})^{1-\frac{3}{\gamma}}} \right) \times \frac{A_1^{\frac{3}{\gamma}}}{A_2^{\frac{3}{\gamma}-1}},$$

The term inside the parentheses on the right-hand side is actually increasing in γ , thus can be bounded by its value at $\gamma = 1$, and we conclude that for any $X \geq 0$,

$$A_1 X^{2-\frac{2\gamma}{3}} - A_2 X^2 \leq \frac{4}{27} \times \frac{A_1^{\frac{3}{\gamma}}}{A_2^{\frac{3}{\gamma}-1}} =: A_3.$$

Noticing that $\|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2 \geq \|f(t)\|_{L^2_\gamma}$, this leads us to

$$\frac{d}{dt} \|f(t)\|_{L^2_\gamma}^2 \leq A_3 - A_2 \|\langle \cdot \rangle^{\frac{3\gamma}{2}} f(t)\|_2^2 \leq A_3 - A_2 \|f(t)\|_{L^2_\gamma}^2, \quad \forall t \geq 0.$$

A straightforward ODE integration and the fact that $f(t=0) = f^{\text{in}}$ then yields, for any $t \geq 0$,

$$\|f(t)\|_{L^2_\gamma}^2 \leq \max \left(\|f^{\text{in}}\|_{L^2_\gamma}^2, \frac{A_3}{A_2} \right).$$

We conclude by taking the supremum in time. Finally, note that $\|f^{\text{in}}\|_{L_\gamma^2}^2$ is bounded by $\|f^{\text{in}}\|_{L_2^1} \|f^{\text{in}}\|_\infty$, and $\frac{A_3}{A_2}$ is *explicit* and depends only on γ, b and f^{in} through its L^1 and L_2^1 norms and an upper-bound on its L_3^1 norm - in particular, *not on* ε . \square

7.2.5 Conclusion to the proof of Theorem 7.3

We assume that the assumptions of Theorem 7.3 are in force and adopt the notations introduced therein. We provide in this subsection the conclusion of the proof of this Theorem. As in the proof of Proposition 7.16, we denote in the following $f(t) \equiv f^\varepsilon(t, \cdot)$ for any $t \geq 0$ to avoid ambiguity and for clarity, and we have for any $v \in \mathbb{R}^3$,

$$\partial_t f(t)(v) \leq \mathcal{Q}_{\gamma,b}^+(f(t), f(t))(v) + \frac{f(t)(v)}{\|f(t)\|_\infty} \Gamma_{\gamma,b}(f(t), f(t))(v) - \mathcal{Q}_{\gamma,b}^-(f(t), f(t))(v), \quad t \geq 0.$$

Following the ideas of [8, Subsection 7.3], we split $b = b_S + b_R$ with b_S vanishing in the vicinity of $\{-1, 1\}$. Since $\mathcal{Q}_{\gamma,b}^+$ and $\Gamma_{\gamma,b}$ depend *linearly* on the kernel b , we observe that, for any $(t, v) \in \mathbb{R}_+ \times \mathbb{R}^3$,

$$\begin{aligned} \partial_t f(t)(v) + \mathcal{Q}_{\gamma,b}^-(f(t), f(t))(v) &\leq \mathcal{Q}_{\gamma,b_S}^+(f(t), f(t))(v) + \mathcal{Q}_{\gamma,b_R}^+(f(t), f(t))(v) \\ &\quad + \frac{f(t)(v)}{\|f(t)\|_\infty} \Gamma_{\gamma,b_S}(f(t), f(t))(v) \\ &\quad + \frac{f(t)(v)}{\|f(t)\|_\infty} \Gamma_{\gamma,b_R}(f(t), f(t))(v). \end{aligned} \quad (7.59)$$

Here again, all the above terms have been studied and estimated in Subsection 7.2.3. Namely, Equation (7.40) in Proposition 7.10 allows to bound $\mathcal{Q}_{\gamma,b_S}^+$ from above, Equation (7.41) in Proposition 7.10 allows to estimate $\mathcal{Q}_{\gamma,b_R}^+$ while (7.46) and (7.47) provide the estimates for Γ_{γ,b_S} and Γ_{γ,b_R} respectively. Finally, $\mathcal{Q}_{\gamma,b}^-$ is bounded from below thanks to (7.49). With all these estimates, (7.59) becomes

$$\begin{aligned} \partial_t f(t)(v) + \mathbf{c}_{\gamma,f(t)} \|b\|_1 f(t)(v) \langle v \rangle^\gamma &\leq C_{b_S}(2, 2) \|f(t)\|_{L_\gamma^2}^2 \\ &\quad + 4 \|b_R\|_1 \|f(t)\|_1 \|f(t)\|_\infty \langle v \rangle^\gamma \\ &\quad + (C_{b_S}(1, 2) + C_{b_S}(2, 1)) \langle v \rangle^\gamma \|f(t)\|_{L_\gamma^2} \|f(t)\|_2 \\ &\quad + 2 \|b_R\|_1 \|f(t)\|_{L_\gamma^1} f(t)(v) \langle v \rangle^\gamma. \end{aligned}$$

As already explained in the lines following (7.57), there exists an explicit $\tilde{\mathbf{c}}_{\gamma, f^{\text{in}}} > 0$ depending only on γ and f^{in} such that for any $t \geq 0$, $\mathbf{c}_{\gamma, f(t)} \geq \tilde{\mathbf{c}}_{\gamma, f^{\text{in}}}$. Moreover we have for any $t \geq 0$ that

$$\|f(t)\|_1 \leq \|f(t)\|_{L_\gamma^1} \leq \|f(t)\|_{L_2^1} = \|f^{\text{in}}\|_{L_2^1}.$$

Moreover remarking that $\|f(t)\|_2 \leq \|f(t)\|_{L_\gamma^2}$, $f(t)(v) \leq \|f(t)\|_\infty$ and $1 \leq \langle v \rangle^\gamma$, we then obtain

$$\begin{aligned} \partial_t f(t, v) &\leq (C_{b_S}(2, 2) + C_{b_S}(1, 2) + C_{b_S}(2, 1)) \|f(t)\|_{L_\gamma^2}^2 \langle v \rangle^\gamma \\ &\quad + 6 \|b_R\|_1 \|f^{\text{in}}\|_{L_2^1} \|f(t)\|_\infty \langle v \rangle^\gamma - \tilde{\mathbf{c}}_{\gamma, f^{\text{in}}} \|b\|_1 f(t)(v) \langle v \rangle^\gamma. \end{aligned}$$

We now apply Proposition 7.16, providing the uniform-in-time L_γ^2 bound

$$\sup_{t \geq 0} \|f(t)\|_{L_\gamma^2}^2 \leq \mathbf{C}_{2,\gamma}^2.$$

We choose the kernel b_S close enough (in the L^1 sense) to b , to ensure that

$$\|b_R\|_1 \leq \frac{\tilde{\mathbf{c}}_{\gamma, f^{\text{in}}} \|b\|_1}{12 \|f^{\text{in}}\|_{L_2^1}}.$$

In this event, we obtain that for any $(t, v) \in \mathbb{R}_+ \times \mathbb{R}^3$ we have

$$\partial_t f(t, v) \leq A'_1 \langle v \rangle^\gamma + A_2 \|f(t)\|_\infty \langle v \rangle^\gamma - 2A_2 f(t)(v) \langle v \rangle^\gamma,$$

where

$$A'_1 = (C_{b_S}(2, 2) + C_{b_S}(1, 2) + C_{b_S}(2, 1)) \mathbf{C}_{2,\gamma}^2 \quad \text{and} \quad A_2 = \frac{1}{2} \tilde{\mathbf{c}}_{\gamma, f^{\text{in}}} \|b\|_1$$

are explicit and depend only on γ , b and f^{in} through its L^1 and L_2^1 norms and upper-bounds on its L_3^1 and L^∞ norms - in particular, neither on time t nor on ε . Fixing $t > 0$, we then have for any $s \in [0, t]$ that, at fixed $v \in \mathbb{R}^3$,

$$\partial_s f(s, v) + 2A_2 f(s, v) \langle v \rangle^\gamma \leq (A'_1 + A_2 \sup_{0 \leq t' \leq t} \|f(t')\|_\infty) \langle v \rangle^\gamma.$$

Multiplying the above inequation by $e^{-2A_2 \langle v \rangle^\gamma s}$ and integrating for $s \in [0, t]$, while keeping v fixed, yields, as the right-hand-side does not depend on s ,

$$f(t, v) \leq f^{\text{in}}(v) e^{-2A_2 \langle v \rangle^\gamma t} + \left(\frac{A'_1}{2A_2} + \frac{1}{2} \sup_{0 \leq t' \leq t} \|f(t')\|_\infty \right) (1 - e^{-2A_2 \langle v \rangle^\gamma t}).$$

In particular,

$$f(t, v) \leq \max \left(\|f^{\text{in}}\|_\infty, \frac{A'_1}{2A_2} + \frac{1}{2} \sup_{0 \leq t' \leq t} \|f(t')\|_\infty \right).$$

As a consequence

$$\sup_{0 \leq t' \leq t} \|f(t')\|_\infty \leq \max \left(\|f^{\text{in}}\|_\infty, \frac{A'_1}{2A_2} + \frac{1}{2} \sup_{0 \leq t' \leq t} \|f(t')\|_\infty \right),$$

and, since $\sup_{0 \leq t' \leq t} \|f(t')\|_\infty \leq \varepsilon^{-1} < +\infty$, we easily deduce the bound

$$\sup_{0 \leq t' \leq t} \|f(t')\|_\infty \leq \max \left(\|f^{\text{in}}\|_\infty, \frac{A'_1}{A_2} \right).$$

Theorem 7.3 follows as the right-hand side does not depend on time t , and $\frac{A'_1}{A_2}$ is explicit and depends only on γ , b and f^{in} through its L^1 and L_2^1 norms and upper-bounds on its L_3^1 and L^∞ norms - in particular, not on ε .

7.3 Explicit rate of convergence to equilibrium: proof of Theorem 7.4

To deduce from the above result the proof of Theorem 7.4, it remains to obtain some suitable conditions on the initial datum f^{in} ensuring that the solution f^ε to (7.1) belongs to the class \mathcal{C}_ε as described in the introduction. In particular, we first need to prove the existence of pointwise lower bounds of exponential type. This is the object of the next section which, once again, fully exploits known results for the classical Boltzmann equation as well as a comparison principle between $\mathcal{Q}_B^\varepsilon$ and \mathcal{Q}_B ,

7.3.1 Maxwellian pointwise lower bound

The following Proposition 7.17 is the equivalent to [143, Theorem 1.1] for the fermionic case, the latter being stated for the classical Boltzmann equation.

Proposition 7.17. *Consider the assumptions of Theorem 7.3 along with the same notations. Then for any $\kappa_0 \in (0, 1)$, $\varepsilon \in (0, (1 - \kappa_0)\mathbf{C}_\infty^{-1}]$ and positive time $t_0 > 0$, there exist two positive constants K_0 and A_0 depending only on t_0 , κ_0 , γ , b and f^{in} only through its L^1 and L^1_2 norms and an upper bound on its entropy, such that the solution f^ε to (7.1) is such that, for all $t \geq t_0$,*

$$f^\varepsilon(t, v) \geq K_0 e^{-A_0 |v|^2}, \quad v \in \mathbb{R}^3. \quad (7.60)$$

Remark 7.8. *We insist on the fact that, as in the previous results, the positive constants K_0, A_0 in (7.60) do not depend on ε .*

Proof. We do not provide a full proof of this result since it is, actually, exactly the same proof as the one valid for the classical Boltzmann equation. Indeed, the key point here is that the solution f^ε satisfies

$$\partial_t f^\varepsilon(t, v) \geq \kappa_0^2 \mathcal{Q}_{\gamma, b}^+(f^\varepsilon(t), f^\varepsilon(t))(v) - \mathcal{Q}_{\gamma, b}^-(f^\varepsilon(t), f^\varepsilon(t))(v) \quad \forall (t, v) \in \mathbb{R}_+ \times \mathbb{R}^3. \quad (7.61)$$

This is easily seen recalling the splittings (7.24a)–(7.25b) and observing that, under the assumption $\kappa_0 \leq 1 - \varepsilon f \leq 1$, it holds

$$\mathcal{Q}_{\gamma, b}^{\varepsilon, +}(f, f) \geq \kappa_0^2 \mathcal{Q}_{\gamma, b}^+(f, f), \quad \mathcal{Q}_{\gamma, b}^{\varepsilon, -}(f, f) \leq \mathcal{Q}_{\gamma, b}^-(f, f).$$

Since $\partial_t f^\varepsilon = \mathcal{Q}_{\gamma, b}^{\varepsilon, +}(f, f) - \mathcal{Q}_{\gamma, b}^{\varepsilon, -}(f, f)$, we deduce readily from Corollary 7.2 that f^ε satisfies (7.61). With this, one sees that f^ε is a “supersolution” (in the sense of (7.61)) of an equation very similar to the classical Boltzmann equation, the only difference being that the $\mathcal{Q}_{\gamma, b}^+$ operator is multiplied by κ_0^2 . This allows to resume the whole proof of [143, Theorem 1.1] (the fact that we are dealing with “supersolution” and not solution to (7.61) plays no role since we consider lower bounds for f^ε). We notice that, although the conservation of mass and energy and the decrease of the entropy are not embedded in (7.61), they do hold as f^ε solves (7.1) and this allows to copycat the proof of [143, Theorem 1.1]. \square

7.3.2 Conclusion to the proof of Theorem 7.4

In this last Subsection, we provide the core of the proof of Theorem 7.4 and conclude. We recall that we assume here that B is a collision kernel of the form (7.4) with $\gamma \in (0, 1]$ and an angular kernel b satisfying the cutoff assumption (7.4b). We fix an initial datum $0 \leq f^{\text{in}} \in L^1_3(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$.

According to Theorem 7.3 (more precisely Corollary 7.2), there is an explicit $\mathbf{C}_\infty > 0$ such that for any $\kappa_0 \in (0, 1)$ and $\varepsilon \in (0, (1 - \kappa_0)\mathbf{C}_\infty^{-1}]$, the associated solution f^ε to (7.1) with $f^\varepsilon(t = 0) = f^{\text{in}}$ is such that

$$1 - \varepsilon f^\varepsilon(t, v) \geq \kappa_0 \quad (t, v) \in \mathbb{R}_+ \times \mathbb{R}^3. \quad (7.62)$$

From now on, we fix κ_0 and ε such that (7.62) holds true and denote for simplicity $f(t) \equiv f^\varepsilon(t, \cdot)$.

We arbitrarily choose a positive time $t_0 > 0$ (one could for instance take $t_0 = 1$). Using the result of [123, Theorem 2. (I)], we deduce that, for any $s > 2$, there exists an explicit constant $\mathbf{C}_{1,s} > 0$ (depending on $s, B, \|f^{\text{in}}\|_1, \|f^{\text{in}}\|_{L^1_2}$ and t_0 but not ε) such that

$$\sup_{t \geq t_0} \|f(t)\|_{L^1_s} \leq \mathbf{C}_{1,s}. \quad (7.63)$$

Moreover, a simple interpolation together with Theorem 7.3 yields

$$\sup_{t \geq 0} \|f(t)\|_p \leq \|f^{\text{in}}\|_1^{\frac{1}{p}} \mathbf{C}_\infty^{1-\frac{1}{p}} \quad \forall p > 1. \quad (7.64)$$

Moreover, we recall the notation (it is not a norm), for any measurable $h : \mathbb{R}^3 \mapsto \mathbb{R}_+$ and $s \geq 0$,

$$\|h\|_{L^1_s \log L} = \int_{\mathbb{R}^3} \langle v \rangle^s h(v) |\log h(v)| \, dv.$$

When $h \in L^1_{s+1}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, the above can be bounded as follows,

$$\|h\|_{L^1_s \log L} \leq \log^+ (\|h\|_\infty) \|h\|_{L^1_s} + \|h\|_{L^1_{s+1}} + \int_{\mathbb{R}^3} e^{-\langle v \rangle} \langle v \rangle^{s+1} \, dv.$$

Therefore, combining the above (with $h = f(t)$) with (7.63) and the L^∞ bound on f , it holds that

$$\sup_{t \geq t_0} \|f(t)\|_{L^1_s \log L} \leq \log^+ (\mathbf{C}_\infty) \mathbf{C}_{1,s} + \mathbf{C}_{1,s+1} + \int_{\mathbb{R}^3} e^{-\langle v \rangle} \langle v \rangle^{s+1} \, dv. \quad (7.65)$$

Equations (7.64) and (7.65) can be reformulated as the fact that, for all $p > 1$ and $s \geq 0$, there exist explicit $\mathbf{C}_p > 0$ and $\mathbf{C}_s^{\log} > 0$ such that

$$\sup_{t \geq t_0} \|f(t)\|_p \leq \mathbf{C}_p, \quad \text{and} \quad \sup_{t \geq t_0} \|f(t)\|_{L^1_s \log L} \leq \mathbf{C}_s^{\log}. \quad (7.66)$$

In particular, both \mathbf{C}_p and \mathbf{C}_s^{\log} only depend on γ, b and f^{in} through its L^1 and L^1_2 norms and upper-bounds on its L^1_3 and L^∞ norms, and respectively on p and s . Moreover, from Proposition 7.17, there exist $K_0 > 0$ and $A_0 > 0$ depending only on t_0, κ_0, γ, b and f^{in} through its L^1 and L^1_2 norms and an upper bound on its entropy, such that for any $(t, v) \in [t_0, +\infty) \times \mathbb{R}^3$, we have

$$f(t, v) \geq K_0 e^{-A_0 |v|^2}. \quad (7.67)$$

Let us now define, for any $t \geq 0$

$$g(t) := \varphi_\varepsilon(f(t)) = \frac{f(t)}{1 - \varepsilon f(t)}.$$

Since, for any $t \in \mathbb{R}_+$, $0 \leq f(t) \in L^1_2(\mathbb{R}^3)$ and $1 - \varepsilon f \geq \kappa_0$, we also have $0 \leq g(t) \in L^1_2(\mathbb{R}^3)$, as well as, from (7.62)–(7.66), that for any $p > 1$ and $s \geq 0$, it holds that

$$\sup_{t \geq t_0} \|g(t)\|_p \leq \kappa_0^{-1} \mathbf{C}_p, \quad \text{and} \quad \sup_{t \geq t_0} \|g(t)\|_{L^1_s \log L} \leq \kappa_0^{-1} \mathbf{C}_s^{\log} + \kappa_0^{-1} \log(\kappa_0^{-1}) \mathbf{C}_{1,s}. \quad (7.68)$$

Moreover, since $g \geq f$, Equation (7.67) implies

$$g(t, v) \geq K_0 e^{-A_0 |v|^2}, \quad \forall t \geq t_0, \quad v \in \mathbb{R}^3.$$

We are now able to apply the functional inequality in Theorem 7.2 to the function $g(t)$, for $t \geq t_0$, which, with the choices

$$\beta_- = 0, \quad \beta_+ = \gamma, \quad p = 3, \quad s = 4 + \frac{4}{\gamma}, \quad \text{and} \quad q_0 = 2 \quad \text{so that } \alpha = 1 + \gamma,$$

provides the existence of a positive constant $\mathbf{A}_0 > 0$ such that

$$\mathcal{D}_0(g(t)) \geq \mathbf{A}_0 \mathcal{H}_0 \left(g(t) | \mathcal{M}_0^{g(t)} \right)^{1+\gamma}. \quad (7.69)$$

We point out that the positive constant \mathbf{A}_0 can be defined as $\mathbf{A}_0 = \inf_{t \geq t_0} \mathbf{A}(t)$ where, according to Theorem 7.2, $\mathbf{A}(t)$ is depending on A_0, K_0 , upper and lower bounds to $\|g(t)\|_1$ and $\|g(t)\|_{L^2}$, and upper bounds to $\|g(t)\|_3, \|g(t)\|_{L^{s+2}}$ and $\|g(t)\|_{L^s \log L}$. This shows in particular that the positive constant \mathbf{A}_0 depends only on $t_0, \varrho^{\text{in}}, u^{\text{in}}, E^{\text{in}}, \kappa_0, K_0, A_0, \mathbf{C}_3, \mathbf{C}_s^{\log}$ and $\mathbf{C}_{1,s+2}$.

We now apply Proposition 7.1 to get that

$$\mathcal{H}_\varepsilon(f(t) | \mathcal{M}_\varepsilon^{f(t)}) \leq \mathcal{H}_0 \left(g(t) | \mathcal{M}_0^{g(t)} \right) \quad \text{and} \quad \mathcal{D}_\varepsilon(f(t)) \geq \kappa_0^4 \mathcal{D}_0(g(t)),$$

which, combined with (7.69) yields

$$\mathcal{D}_\varepsilon(f(t)) \geq \kappa_0^4 \mathbf{A}_0 \mathcal{H}_\varepsilon(f(t) | \mathcal{M}_\varepsilon^{f(t)})^{1+\gamma}. \quad (7.70)$$

Now notice that for any $t \geq 0$, we have, since f solves **(BFD Eq.)**,

$$\mathcal{M}_\varepsilon^{f(t)} = \mathcal{M}_\varepsilon^{f^{\text{in}}}.$$

According to the entropy identity (7.77) (see Theorem 7.6), for all $t \geq 0$, we have

$$\frac{d}{dt} \mathcal{H}_\varepsilon(f(t) | \mathcal{M}_\varepsilon^{f^{\text{in}}}) = \frac{d}{dt} \mathcal{H}_\varepsilon(f(t)) = -\mathcal{D}_\varepsilon(f(t)).$$

In particular, according to (7.70),

$$\frac{d}{dt} \mathcal{H}_\varepsilon(f(t) | \mathcal{M}_\varepsilon^{f^{\text{in}}}) \leq -\kappa_0^4 \mathbf{A}_0 \mathcal{H}_\varepsilon(f(t) | \mathcal{M}_\varepsilon^{f^{\text{in}}})^{1+\gamma}, \quad \forall t \geq t_0.$$

Integrating this inequality on the interval $[t_0, t]$ and using, as the entropy decreases with time, that

$$\mathcal{H}_\varepsilon \left(f(t_0) | \mathcal{M}_\varepsilon^{f^{\text{in}}} \right) \leq \mathcal{H}_\varepsilon \left(f^{\text{in}} | \mathcal{M}_\varepsilon^{f^{\text{in}}} \right),$$

we easily deduce that

$$\mathcal{H}_\varepsilon(f(t) | \mathcal{M}_\varepsilon^{f^{\text{in}}}) \leq \left(\mathcal{H}_\varepsilon(f^{\text{in}} | \mathcal{M}_\varepsilon^{f^{\text{in}}})^{-\gamma} + \gamma \kappa_0^4 \mathbf{A}_0 (t - t_0) \right)^{-\frac{1}{\gamma}}, \quad \forall t \geq t_0.$$

Finally, using again that the mapping $t \mapsto \mathcal{H}_\varepsilon(f(t) | \mathcal{M}_\varepsilon^{f^{\text{in}}})$ is nonincreasing, we deduce that for all $t \geq 0$,

it holds that

$$\mathcal{H}_\varepsilon(f(t)|\mathcal{M}_\varepsilon^{f^{\text{in}}}) \leq \mathbf{B} (1 + (t - t_0)_+)^{-\frac{1}{\gamma}},$$

with

$$\mathbf{B} = \max \left(\mathcal{H}_\varepsilon(f^{\text{in}}|\mathcal{M}_\varepsilon^{f^{\text{in}}}), (\gamma \kappa_0^4 \mathbf{A}_0)^{-\frac{1}{\gamma}} \right).$$

The latter then implies (7.22) for all $\varepsilon \in (0, (1 - \kappa_0) \mathbf{C}_\infty^{-1}]$, with $\mathbf{C}_\mathcal{H} = (1 + t_0)^{\frac{1}{\gamma}} \mathbf{B}$.

While for (7.22), one could take $\varepsilon^{\text{in}} = (1 - \kappa_0) \mathbf{C}_\infty^{-1}$, we choose for the following

$$\varepsilon^{\text{in}} = \min \left((1 - \kappa_0) \mathbf{C}_\infty^{-1}, \varepsilon_{\text{sat}}^\dagger \right),$$

where $\varepsilon_{\text{sat}}^\dagger$ is defined in Lemma 7.20 in Appendix 7.C, is explicit and (as we apply the lemma to $f = f^{\text{in}}$) depends only on ϱ^{in} and E^{in} (it is approximately $0.06 \varepsilon_{\text{sat}}$).

We finally show (7.23) for all $\varepsilon \in (0, \varepsilon^{\text{in}}]$. We make use of the weighted L^p Csiszàr-Kullback-Pinsker inequality recalled in Proposition 7.19 in Appendix 7.B, with $p = 1$ and $\varpi = \langle \cdot \rangle^k$ for some $k \geq 0$, giving for any $t \geq 0$, as $\mathcal{M}_\varepsilon^{f(t)} = \mathcal{M}_\varepsilon^{f^{\text{in}}}$,

$$\left\| f(t) - \mathcal{M}_\varepsilon^{f^{\text{in}}} \right\|_{L_k^1}^2 \leq 2 \max \left(\left\| \mathcal{M}_\varepsilon^{f^{\text{in}}} \right\|_{L_{2k}^1}, \|f(t)\|_{L_{2k}^1} \right) \mathcal{H}_\varepsilon \left(f(t) | \mathcal{M}_\varepsilon^{f^{\text{in}}} \right).$$

Since $\varepsilon \leq \varepsilon_{\text{sat}}^\dagger$, Lemma 7.20 in Appendix 7.C provides the existence of $\mathbf{C}_{\mathcal{M},1,2k}$, explicit and depending only on ϱ^{in} and E^{in} (in particular, not on ε) such that $\left\| \mathcal{M}_\varepsilon^{f^{\text{in}}} \right\|_{L_{2k}^1} \leq \mathbf{C}_{\mathcal{M},1,2k}$. Then, letting

$$\mathbf{C}_{\mathcal{H},1,k} = \sqrt{2 \max(\mathbf{C}_{\mathcal{M},1,2k}, \mathbf{C}_{1,2k})} \mathbf{C}_\mathcal{H}, \quad (7.71)$$

we obtain, using the proven (7.22),

$$\left\| f(t) - \mathcal{M}_\varepsilon^{f^{\text{in}}} \right\|_{L_k^1} \leq \mathbf{C}_{\mathcal{H},1,k} (1 + t)^{-\frac{1}{2\gamma}}. \quad (7.72)$$

Finally, let $p > 1$. As

$$\| \cdot \|_{L_k^p} \leq \| \cdot \|_\infty^{1-\frac{1}{p}} \| \cdot \|_{L_{pk}^1}^{\frac{1}{p}},$$

and since, as $\varepsilon \leq \varepsilon_{\text{sat}}^\dagger$, Lemma 7.20 in Appendix 7.C provides the existence of $\mathbf{C}_{\mathcal{M},\infty}$, explicit and depending only on ϱ^{in} and E^{in} (in particular, not on ε) such that $\left\| \mathcal{M}_\varepsilon^{f^{\text{in}}} \right\|_\infty \leq \mathbf{C}_{\mathcal{M},\infty}$, we deduce (7.23) from (7.72), with

$$\mathbf{C}_{\mathcal{H},p,k} = \max(\mathbf{C}_{\mathcal{M},\infty}, \mathbf{C}_\infty)^{1-\frac{1}{p}} \mathbf{C}_{\mathcal{H},1,pk}^{\frac{1}{p}},$$

where we used the fact that $\|f(t) - \mathcal{M}_\varepsilon^{f^{\text{in}}}\|_\infty \leq \max(\left\| \mathcal{M}_\varepsilon^{f^{\text{in}}} \right\|_\infty, \|f(t)\|_\infty)$, which holds as both $f(t)$ and $\mathcal{M}_\varepsilon^{f^{\text{in}}}$ are nonnegative.

Since every presented constant is explicit and depends only (at most) on γ , b , ϱ^{in} , u^{in} , E^{in} and upper-bounds to $\|f^{\text{in}}\|_{L_3^1}$ and $\|f^{\text{in}}\|_\infty$, in particular not on ε , the proof of Theorem 7.4 is complete.

7.A More physically relevant models

We briefly discuss here the possibility of recovering the results established in the core of the text when dealing with more realistic collision kernels. We begin with briefly recalling some facts about such physically relevant kernels.

7.A.1 Quantum collision kernels

While collision kernels B are fully explicit for classical particles, the situation is much more involved for quantum (pseudo)-particles. In this case, **(BFD Eq.)** has been derived from the Schrödinger equation in the weak-coupling regime and the derived kernel B takes the form

$$B(v, v_*, \sigma) = |z| \left[\widehat{\phi} \left(\left| z \sin \left(\frac{\theta}{2} \right) \right| \right) - \widehat{\phi} \left(\left| z \cos \left(\frac{\theta}{2} \right) \right| \right) \right]^2, \quad z = v - v_*, \cos \theta = \frac{z}{|z|} \cdot \sigma, \quad (7.73)$$

and where $\widehat{\phi}$ is the (generalized) Fourier transform of the particle interaction potential $\phi = \phi(|x|)$, $x \in \mathbb{R}^3$. As in [119], we make the general assumption on B :

Assumption 7.1. *The collision kernel $B(v, v_*, \sigma) = B(|v - v_*|, \sigma) = B(|v - v_*|, \cos \theta)$ is assumed to be such that*

$$|z|^\gamma \Phi_*(|z|) b_*(\cos \theta) \leq B(|z|, \cos \theta) = B(v, v_*, \sigma) \leq (1 + |z|)^\gamma b^*(\cos \theta)$$

for $\gamma \in (0, 1]$ and some Borel even functions $b_*(\cdot), b^*(\cdot)$ defined on $(-1, 1)$ and a Borel function $\Phi_* : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ such that

$$0 < b_*(\cos \theta) \leq b^*(\cos \theta), \quad \theta \in (-\pi, \pi); \quad \int_0^\pi b^*(\cos \theta) \sin \theta d\theta < \infty \quad (7.74)$$

and

$$\Phi_*(r) > 0 \quad \forall r > 0, \quad \inf_{r \geq 1} \Phi_*(r) \geq 1, \quad \sup_{r \geq 0} \Phi_*(r) < \infty. \quad (7.75)$$

Example 7.1. *It has been observed in [119, Appendix A] that, for potential interactions of the type*

$$\phi(x) = |x|^{-\alpha}, \quad 0 < \alpha < 3$$

the kernel B defined by (7.73) is such that

$$B(z, \sigma) = |z|^\gamma b(\cos \theta), \quad \gamma = 2\alpha - 5$$

with

$$b(\cos \theta) = C_\alpha \left((1 - \cos \theta)^{-\beta} - (1 + \cos \theta)^\beta \right)^2, \quad \beta = \frac{3 - \alpha}{2}$$

for some positive constant C_α . One can check that b actually meets the cutoff assumption (7.4b). In particular, it satisfies Assumption 7.1 as soon as $\alpha \in (\frac{5}{2}, 3)$. Notice that such a kernel is of the form of kernels studied in the core of our work here.

Example 7.2. *Choosing a potential of the form*

$$\phi(|x|) = \frac{1}{2^\beta \Gamma(\beta)} \int_0^\infty G_t(|x|) t^{\beta-1} \exp\left(-\frac{t}{2}\right) dt, \quad x \in \mathbb{R}^3, \quad 0 \leq \beta < \frac{1}{4}$$

where $\Gamma(\cdot)$ is the Gamma function and $G_t(|x|)$ is the heat kernel

$$G_t(|x|) = (2\pi t)^{-\frac{3}{2}} \exp\left(-\frac{|x|^2}{2t}\right), \quad x \in \mathbb{R}^3, t > 0$$

one can check that B defined by (7.73) is such that

$$B(z, \sigma) = \frac{4^\beta |z|}{(2 + |z|^2)^{2\beta}} \left((1 - a(|z|) \cos \theta)^{-\beta} - (1 + a(|z|) \cos \theta)^\beta \right)^2, \quad a(|z|) = \frac{|z|^2}{2 + |z|^2}.$$

It has been then observed in [119] that B satisfies then Assumptions 7.1 with $\gamma = 1 - 4\beta \in (0, 1)$,

$$\Phi_*(r) = \left(\frac{2r^2}{1+r^2} \right)^{2\beta+2}, \quad b_*(\cos \theta) = c_\beta \cos^2 \theta, \quad b^*(\cos \theta) = C_\beta \cos^2 \theta \sin^{-4\beta}(\theta)$$

for some positive constants $C_\beta, c_\beta > 0$.

Example 7.3. A general subclass of kernels B satisfying Assumptions 7.1 has been considered in [160] and corresponds to the choice $\gamma = 1$ and

$$\Phi_*(r) = 2 \frac{r^\beta}{1+r^\beta}, \quad \beta \geq 0,$$

and

$$b_*(\cos \theta) \geq \frac{1}{2} b_0 > 0, \quad b^*(\cos \theta) \leq b_1 < \infty.$$

This means in particular that

$$b_0 \frac{|v - v_*|^{\beta+1}}{1 + |v - v_*|^\beta} \leq B(v, v_*, \sigma) \leq b_1 |v - v_*|.$$

7.A.2 Main mathematical changes induced by quantum collision kernels

For simplicity of presentation, let us assume that the collision kernel is of a type generalizing the above example and assume that there exist $b_1 \geq b_0 > 0$ and $\gamma, \beta \in (0, 1)$ with $\gamma + \beta \in (0, 1)$ such that

$$b_0 \frac{|v - v_*|^{\beta+\gamma}}{1 + |v - v_*|^\beta} \leq B(v, v_*, \sigma) \leq b_1 |v - v_*|^\gamma, \quad v, v_*, \sigma \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2. \quad (7.76)$$

We briefly explain here what should be the main changes/obstacles for the derivation of the results obtained in the core of the paper for kernels of the type (7.4).

Notice that, for such collision kernels, as pointed out already in [119], the construction and properties of solutions as described in the above Appendix 7.B are easy to adapt (see the discussion hereafter).

We can check without too much difficulty that the whole set of results in Section 7.2 are still valid under the above assumption (7.76) culminating in the following version of Theorem 7.3

Theorem 7.5. Let $\gamma \in (0, 1]$ and $\beta \geq 0$ and let B be a collision kernel satisfying (7.76) with $b_1 \geq b_0 > 0$. For any $0 \leq f^{\text{in}} \in L^1_3(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, there exists an explicit $\mathbf{C}_\infty(B) > 0$, depending only on B and f^{in} only through its L^1 and L^2_3 norms and upper-bounds on its L^∞ and L^1_3 norms, such that for any $\varepsilon \in (0, \|f^{\text{in}}\|_\infty^{-1}]$, the unique solution f^ε to (7.1) associated to ε , the collision kernel defined by (7.4) and initial datum f^{in} satisfies

$$\sup_{t \geq 0} \|f^\varepsilon(t)\|_\infty \leq \mathbf{C}_\infty(B).$$

Indeed, the representation formula for \mathcal{Q}_B^+ allows again to define Γ_B as in (7.26) and, as in Section 7.2, we can define

$$\tilde{\mathcal{Q}}_B^+[f](g, h) := \mathcal{Q}_B^+(g, h) + \frac{f}{\|f\|_\infty} \Gamma_B(g, h),$$

and $\tilde{\mathcal{Q}}_B[f](g, h) := \tilde{\mathcal{Q}}_B^+[f](g, h) - \mathcal{Q}_B^-(g, h)$. With this, Proposition 7.3 and Lemma 7.4 still hold with obvious change of notations. Since the results in Section 7.2 are obtained through estimates involving somehow the weak form of \mathcal{Q}_B^+ , one checks easily that Proposition 7.7 (with $\|b\|_\infty$ replaced with b_1) can be deduced from Prop. 7.5. All the results, up to Prop. 7.14 remain then valid. The only change to be made lies in the proof of Proposition 7.15 but the proof of [10, Lemma 4] can be adapted to deduce the same result. All these results would yield Theorem 7.5.

Of course, the results recalled in the Introduction regarding the entropy production and entropy estimates remain valid for this class of collision kernel. The only result which does not seem to be directly deduced from existing results is the one in Section 7.3.1. Typically, it would be very interesting to check whether Proposition 7.17 (or a variant of it) still holds for collision kernels satisfying (7.76). Notice that the obstacle has nothing to do here with the quantum nature of the Boltzmann operator and one should rather check if the classical Boltzmann operator \mathcal{Q}_B^+ is satisfying the estimates derived in the original proof of [143]. It seems to us that the key point to be checked is the spreading properties of the collision operator \mathcal{Q}_B^+ when $B(v, v_*, \sigma) = b_0 \frac{|v-v_*|^{\beta+\gamma}}{1+|v-v_*|^\beta}$, namely, can we still prove that there exist $\eta > 0, r > 1$ such that

$$\mathcal{Q}_B^+(\mathbb{1}_{\mathcal{B}(v_0, \delta_0)}, \mathbb{1}_{\mathcal{B}(v_0, \delta_0)}) \geq \eta \mathbb{1}_{\mathcal{B}(v_0, r\delta_0)}$$

holds true for any $\delta_0 > 0, v_0 \in \mathbb{R}^3$? Here above, $\mathcal{B}(v, \delta)$ denotes the closed ball of \mathbb{R}^3 centered at $v \in \mathbb{R}^3$ with radius $\delta > 0$. Such a result, obtained usually through the Carleman representation of the gain part operator, allows to initiate the iterative procedure yielding the derivation of pointwise bounds. To keep the paper simple enough, we did not elaborate on this point but are confident that Proposition 7.17 is still true for general kernels B of the form (7.76). If this were the case, which is highly expected as, on a finite ball, the kernel B behaves like $|v - v_*|^{\gamma+\beta}$, for which we know the result holds, it would be straightforward then to resume the proof derived in Section 7.3.2 and obtain an analogue of Theorem 7.4.

7.B Known results about (BFD Eq.) and the Fermi-Dirac entropy

We collect in this section some known facts about (BFD Eq.) obtained in [123, 124] as well as some recent results regarding the relative Fermi-Dirac entropy obtained by the first author.

7.B.1 Cauchy problem and moment estimates

We briefly recall here the notion of solutions we consider in the present paper, the Cauchy result established in [123] as well as moment estimates.

We adopt the following framework and recall here that we always assume B to be a collision kernel satisfying (7.4).

Definition 7.2. Let $\varepsilon > 0$ and $0 \leq f^{\text{in}} \in L_2^1(\mathbb{R}^3)$ satisfying $1 - \varepsilon f^{\text{in}} \geq 0$. We say that a Lebesgue measurable function

$$f^\varepsilon : [0, \infty) \times \mathbb{R}^3 \rightarrow [0, \varepsilon^{-1}]$$

such that $\sup_{t \geq 0} \|f(t)\|_{L_2^1} < \infty$ is a weak solution to (BFD Eq.) if there is $\Lambda \in \mathbb{R}^3$ with zero Lebesgue

measure such that

$$\int_0^T dt \int_{\mathbb{R}^3 \times \mathbb{S}^2} B(v, v_*, \sigma) G^\pm(t, v, v_*, \sigma) dv_* d\sigma < \infty, \quad \forall 0 < T < \infty, \quad \forall v \in \mathbb{R}^3 \setminus \Lambda$$

where

$$G^+(t, v, v_*, \sigma) = [f' f'_* (1 - \varepsilon f)(1 - \varepsilon f_*)], \quad G^-(t, v, v_*, \sigma) = [f f_* (1 - \varepsilon f')(1 - \varepsilon f'_*)]$$

and

$$f^\varepsilon(t, v) = f^{\text{in}}(v) + \int_0^t \mathcal{Q}_B^\varepsilon(f^\varepsilon, f^\varepsilon)(\tau, v) d\tau, \quad t \geq 0.$$

For that class of solutions, existence of solutions have been established in [80, Theorem 1] and stability, uniqueness of solutions as well as the entropy identity have been established in [123, 124]:

Theorem 7.6. *Given $\varepsilon > 0$ and $0 \leq f^{\text{in}} \in L^1_2(\mathbb{R}^3)$ satisfying $1 - \varepsilon f^{\text{in}} \geq 0$, there exists a unique solution $f^\varepsilon = f^\varepsilon(t, v)$ to (7.1) in the sense of Definition 7.2. Moreover, such a solution satisfies the entropy identity*

$$\mathcal{H}_\varepsilon(f^\varepsilon(t)) = \mathcal{H}_\varepsilon(f^{\text{in}}) - \int_0^t \mathcal{D}_\varepsilon(f^\varepsilon(\tau)) d\tau, \quad \forall t \geq 0. \quad (7.77)$$

We also recall that moments are created for solutions to (7.1) associated to a collision kernel of the form (7.4) where we recall that $\gamma \in (0, 1]$:

Proposition 7.18. *Given $\varepsilon > 0$ and $0 \leq f^{\text{in}} \in L^1_2(\mathbb{R}^3)$ satisfying $1 - \varepsilon f^{\text{in}} \geq 0$, let $f^\varepsilon = f^\varepsilon(t, v)$ be the unique conservative solution to (7.1) in the sense of Definition 7.2. For any $s > 2$, one has*

$$\|f^\varepsilon(t)\|_{L^1_s} \leq \left[\frac{a_1}{1 - \exp(-a_2 t)} \right]^{\frac{s-2}{\gamma}}, \quad \forall t > 0$$

where $a_1 > 0, a_2 > 0$ are constants depending only on $B, \|f^{\text{in}}\|_1, \|f^{\text{in}}\|_{L^1_2}$ and not on ε . Moreover, given $s > 2$, there exists $C_B(f^{\text{in}}) > 0$ depending only on $B, \|f^{\text{in}}\|_1, \|f^{\text{in}}\|_{L^1_2}$ and $\|f^{\text{in}}\|_{L^1_s}$ but not on ε such that

$$\sup_{t \geq 0} \|f^\varepsilon(t)\|_{L^1_s} \leq C_B(f^{\text{in}}). \quad (7.78)$$

Remark 7.9. *Such a result is a simple consequence of [123, Theorem 2. (I)] where the creation of an L^1_s bound has been derived. We point out that, if one assumes the initial datum $f^{\text{in}} \in L^1_s(\mathbb{R}^3)$, then the uniform-in-time bound provided in (7.78) can be easily deduced from the equation just preceding [123, proof of Theorem 2, Equation (3.8)], which has a similar form as (7.58), and easily provides a short-time bound that satisfies the above-mentioned properties.*

Remark 7.10. *As explained in the Introduction of [119], the above properties (existence, uniqueness, moment estimates and entropy dissipation) of solutions to (7.1), obtained for collision kernel of the form (7.4) are easily extended to more general – and physically relevant – interaction kernels of the form described in Section 7.A. We refer to [119] as well as [105] for more details about this question.*

7.B.2 Csiszár-Kullback-Pinsker inequalities

We here state a recent improvement of the usual Csiszár-Kullback-Pinsker inequality (CKP inequality). We only recall here that the usual, original CKP inequality asserts that

$$\|f - \mathcal{M}_0^f\|_1^2 \leq 2 \|f\|_1 \mathcal{H}_0(f | \mathcal{M}_0^f)$$

for any $f \in L^1_2(\mathbb{R}^3)$ where \mathcal{M}_0^f is the Maxwellian state with the same mass, momentum and energy as f .

Such a result has been extended recently by the first author and generalized to Fermi-Dirac relative entropy yielding the following weighted L^p -version of the CKP inequality

Proposition 7.19. *For any $\varepsilon > 0$ and $0 \leq f \in L^1_2(\mathbb{R}^3) \setminus \{0\}$ satisfying (7.10) and such that $1 - \varepsilon f \geq 0$ and $r_E > \frac{2}{5}$, we have*

$$\|f - \mathcal{M}_\varepsilon^f\|_{L^1_2}^2 \leq 8 \|\mathcal{M}_\varepsilon\|_{L^1_4} \mathcal{H}_\varepsilon(f | \mathcal{M}_\varepsilon)$$

and, for any weight function $\varpi : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ and any $p \in [1, 2]$, it holds

$$\left\| \varpi (f - \mathcal{M}_\varepsilon^f) \right\|_p^2 \leq 2 \max \left(\left\| \varpi^2 \mathcal{M}_\varepsilon^f \right\|_{\frac{p}{2-p}}, \left\| \varpi^2 f \right\|_{\frac{p}{2-p}} \right) \mathcal{H}_\varepsilon(f | \mathcal{M}_\varepsilon^f),$$

where $\mathcal{M}_\varepsilon^f$ is the Fermi-Dirac distribution associated to f .

Remark 7.11. *Recall that, as observed in the Introduction, the assumption $r_E > \frac{2}{5}$ is equivalent to $\varepsilon < \varepsilon_{\text{sat}}$ where ε_{sat} is defined in (7.11) and this implies that $f \neq F_\varepsilon$ where F_ε is the saturated steady state defined in (7.9), and the existence of $\mathcal{M}_\varepsilon^f$. Of course, in the above result, for $p = 2$, we adopt the convention $\|\cdot\|_{\frac{p}{2-p}} = \|\cdot\|_\infty$.*

7.C Explicit and uniform-in- ε bounds for Fermi-Dirac statistics

In this last Appendix section, we provide, in the following Lemma 7.20, explicit uniform-in- ε bounds on the L^∞ and L^1_k , $k \geq 0$, norms of the Fermi-Dirac Statistics.

Lemma 7.20. *Consider a nonnegative $f \in L^1_2(\mathbb{R}^3)$, which density, average velocity and temperature we denote respectively by ϱ , u and E . We let*

$$\varepsilon_{\text{sat}}^\dagger := 2^{\frac{5}{2}} \cdot 3^{\frac{3}{2}} \cdot 5^{-\frac{5}{2}} \cdot \pi^{\frac{3}{2}} \varrho^{-1} E^{\frac{3}{2}}.$$

Then there exist $\mathbf{C}_{\mathcal{M}, \infty} > 0$ and, $\mathbf{C}_{\mathcal{M}, 1, k} > 0$, for any $k \geq 0$, which are explicit and depend only on ϱ , u and E , such that for any $\varepsilon \in (0, \varepsilon_{\text{sat}}^\dagger]$, we have

$$\|\mathcal{M}_\varepsilon^f\|_\infty \leq \mathbf{C}_{\mathcal{M}, \infty}, \tag{7.79}$$

and, for any $k \geq 0$,

$$\|\mathcal{M}_\varepsilon^f\|_{L^1_k} \leq \mathbf{C}_{\mathcal{M}, 1, k}. \tag{7.80}$$

Notice in particular that $\varepsilon_{\text{sat}}^\dagger = 2^{\frac{1}{2}} \cdot 3^{\frac{5}{2}} \cdot 5^{-4} \cdot \pi^{\frac{1}{2}} \varepsilon_{\text{sat}} \sim 0.06 \varepsilon_{\text{sat}}$.

Proof. For the sake of simplicity, we prove the lemma with the extra assumption $u = 0$ and briefly discuss the case $u \neq 0$ at the end of the proof. Let us recall the notation, for any $v \in \mathbb{R}^3$,

$$\mathcal{M}_\varepsilon^f(v) = \frac{e^{a_\varepsilon + b_\varepsilon |v|^2}}{1 + \varepsilon e^{a_\varepsilon + b_\varepsilon |v|^2}},$$

as well as

$$r_E := \frac{E}{\mathbf{T}(\varrho, \varepsilon)}, \quad \mathbf{T}(\varrho, \varepsilon) := \frac{1}{2} \left(\frac{3\varepsilon\varrho}{4\pi} \right)^{\frac{2}{3}}.$$

It is proven in [36, Proposition 18] that for any $\varepsilon \in (0, \varepsilon_{\text{sat}})$, as soon as

$$r_E \geq r^\dagger, \quad r^\dagger := \left(\frac{4}{\pi}\right)^{\frac{1}{3}} \left(\frac{5}{3}\right)^{\frac{5}{3}}, \quad (7.81)$$

we have

$$\varepsilon e^{a\varepsilon} \leq \frac{2}{3} \left(\frac{r_E}{r^\dagger}\right)^{-\frac{3}{2}}.$$

The above can be reformulated as

$$e^{a\varepsilon} \leq \frac{2}{3} r^\dagger^{\frac{3}{2}} E^{-\frac{3}{2}} \left(\frac{3\rho}{4\pi}\right),$$

which, by direct computation, gives in particular

$$e^{a\varepsilon} \leq \rho E^{-\frac{3}{2}}. \quad (7.82)$$

We notice that, letting

$$\varepsilon_{\text{sat}}^\dagger := 2^{\frac{5}{2}} \cdot 3^{\frac{3}{2}} \cdot 5^{-\frac{5}{2}} \cdot \pi^{\frac{3}{2}} \rho^{-1} E^{\frac{3}{2}}, \quad (7.83)$$

the condition (7.81) is equivalent to assuming $\varepsilon \in (0, \varepsilon_{\text{sat}}^\dagger]$. In this event, we have proven (7.79) with $\mathbf{C}_{\mathcal{M}, \infty} = \rho E^{-\frac{3}{2}}$, since

$$\|\mathcal{M}_\varepsilon^f\|_\infty \leq e^{a\varepsilon}.$$

Moving on to the proof of (7.80), and still assuming $\varepsilon \in (0, \varepsilon_{\text{sat}}^\dagger]$, we have by definition, for any $k \geq 0$,

$$\|\mathcal{M}_\varepsilon^f\|_{L_k^1} = \int_{\mathbb{R}^3} \mathcal{M}_\varepsilon^f(v) \langle v \rangle^k \mathbf{d}v,$$

so that

$$\|\mathcal{M}_\varepsilon^f\|_{L_k^1} \leq e^{a\varepsilon} \int_{\mathbb{R}^3} e^{b_\varepsilon |v|^2} \langle v \rangle^k \mathbf{d}v. \quad (7.84)$$

Passing to spherical coordinates $v \in \mathbb{R}^3 \setminus \{0\} \mapsto (r, \sigma) \in \mathbb{R}_+^* \times \mathbb{S}^2$ and then performing the change of variables $r \in \mathbb{R}_+^* \mapsto x = \sqrt{-b_\varepsilon} r \in \mathbb{R}_+^*$ (recall that b_ε is negative), we get

$$\|\mathcal{M}_\varepsilon^f\|_{L_k^1} \leq e^{a\varepsilon} |\mathbb{S}^2| \left(|b_\varepsilon|^{\frac{3}{2}} \min(1, |b_\varepsilon|)^k\right)^{-1} \int_{\mathbb{R}_+} e^{-x^2} x^2 (1+x^2)^{\frac{k}{2}} \mathbf{d}x, \quad (7.85)$$

where we used the fact that $1 + \left(\frac{x}{\sqrt{-b_\varepsilon}}\right)^2 \leq \min(1, |b_\varepsilon|)^{-1} (1+x^2)$. Letting

$$\mathbf{C}_{\mathcal{M}, 1, k}^0 = \rho E^{-\frac{3}{2}} 4\pi \int_{\mathbb{R}_+} e^{-x^2} x^2 (1+x^2)^{\frac{k}{2}} \mathbf{d}x,$$

which is explicit and has the same properties as $\mathbf{C}_{\mathcal{M}, \infty}$, Equation (7.85) yields, as we just proved $e^{a\varepsilon} \leq \rho E^{-\frac{3}{2}}$,

$$\|\mathcal{M}_\varepsilon^f\|_{L_k^1} \leq \mathbf{C}_{\mathcal{M}, 1, k}^0 \left(|b_\varepsilon|^{\frac{3}{2}} \min(1, |b_\varepsilon|)^k\right)^{-1}. \quad (7.86)$$

Let us now provide an explicit lower bound for $|b_\varepsilon|$. We follow a similar reasoning to the one of [36,

proof of Proposition 18] It is proven in [123, proof of Proposition 3] that, letting

$$I_s(\tau) := \int_0^\infty \frac{r^s}{1 + \tau e^{r^2}} dr, \quad P(\tau) := I_4(\tau) I_2(\tau)^{-5/3}, \quad \tau \in \mathbb{R}_+^*,$$

the function P is increasing from \mathbb{R}_+^* to $(\frac{3^{5/3}}{5}, +\infty)$, and we have

$$\left(\frac{\varepsilon}{4\pi}\right)^{2/3} P\left(\frac{1}{\varepsilon e^{a_\varepsilon}}\right) = \frac{3\rho E}{\rho^{5/3}}, \quad b_\varepsilon = -\left(\frac{4\pi}{\varepsilon\rho} I_2\left(\frac{1}{\varepsilon e^{a_\varepsilon}}\right)\right)^{\frac{2}{3}}. \quad (7.87)$$

As by definition of P , $I_2(\tau) = \left(\frac{I_4(\tau)}{P(\tau)}\right)^{\frac{3}{5}}$ for any $\tau \geq 0$, we deduce that, using both equations in (7.87),

$$|b_\varepsilon| = \left(\frac{4\pi}{\varepsilon\rho} \left\{ I_4\left(\frac{1}{\varepsilon e^{a_\varepsilon}}\right) \left(\frac{\varepsilon}{4\pi}\right)^{2/3} \frac{\rho^{5/3}}{3\rho E} \right\}^{\frac{3}{5}}\right)^{\frac{2}{3}},$$

which, raised to the power $\frac{5}{2}$, rewrites

$$|b_\varepsilon|^{\frac{5}{2}} = \left(\frac{4\pi}{3\varepsilon\rho E}\right) I_4\left(\frac{1}{\varepsilon e^{a_\varepsilon}}\right). \quad (7.88)$$

As it holds for any $r \geq 0$ and $\tau \geq 0$ that

$$\frac{1}{1 + \tau e^{r^2}} \geq \frac{e^{-r^2}}{1 + \tau},$$

we have for any $\tau \geq 0$ that

$$I_4(\tau) \geq \frac{1}{1 + \tau} \int_0^\infty r^4 e^{-r^2} dr = \frac{1}{1 + \tau} \cdot \frac{3}{8\sqrt{\pi}},$$

where the constant on the right-hand-side was computed from $\frac{1}{2}\Gamma\left(\frac{5}{2}\right)$, with Γ standing (here only) for the Gamma function. It thus comes that

$$I_4\left(\frac{1}{\varepsilon e^{a_\varepsilon}}\right) \geq \frac{3}{8\sqrt{\pi}} \frac{\varepsilon e^{a_\varepsilon}}{1 + \varepsilon e^{a_\varepsilon}}.$$

Since $\varepsilon \leq \varepsilon_{\text{sat}}^\dagger$, we can again make use of the result of [36, Proposition 18] (as, with their notation, $\gamma/\gamma^\dagger \geq 1$) to obtain that

$$\varepsilon e^{a_\varepsilon} \leq \frac{2}{3},$$

implying $1 + \varepsilon e^{a_\varepsilon} \leq 1 + \frac{2}{3} = \frac{5}{3}$, so that, also recalling (7.88), we have

$$|b_\varepsilon|^{\frac{5}{2}} \geq \left(\frac{4\pi}{3\rho E}\right) \frac{9}{8 \cdot 5\sqrt{\pi}} e^{a_\varepsilon}. \quad (7.89)$$

The last part of the proof consists in proving a lower bound for e^{a_ε} . We use a similar reasoning as

previously. As it holds for any $r \geq 0$ and $\tau \geq 0$ that

$$\frac{e^{-r^2}}{\tau} \geq \frac{1}{1 + \tau e^{r^2}} \geq \frac{e^{-r^2}}{1 + \tau},$$

we deduce that, for any $\tau \geq 0$,

$$P(\tau) \geq \frac{\tau^{\frac{5}{3}}}{1 + \tau} \cdot \frac{3 \cdot 2^{\frac{1}{3}}}{\pi^{\frac{1}{3}}},$$

where the constant on the right-hand-side comes from $\frac{1}{2}\Gamma\left(\frac{5}{2}\right)\left(\frac{1}{2}\Gamma\left(\frac{3}{2}\right)\right)^{-\frac{5}{3}}$. Setting $\tau = (\varepsilon e^{a\varepsilon})^{-1}$ in the previous inequality, and using (7.87), we obtain

$$\frac{3\rho E}{\rho^{5/3}} \left(\frac{4\pi}{\varepsilon}\right)^{2/3} \geq \frac{(\varepsilon e^{a\varepsilon})^{-\frac{2}{3}}}{1 + \varepsilon e^{a\varepsilon}} \cdot \frac{3 \cdot 2^{\frac{1}{3}}}{\pi^{\frac{1}{3}}}.$$

Again, since $1 + \varepsilon e^{a\varepsilon} \leq \frac{5}{3}$, we thus have obtained, for any $\varepsilon \in (0, \varepsilon_{\text{sat}}^\dagger]$,

$$e^{a\varepsilon} \geq \left(\frac{3}{10\pi}\right)^{\frac{3}{2}} \rho E^{-\frac{3}{2}}.$$

Defining finally

$$\mathbf{C}_{\mathcal{M},1,k} = \mathbf{C}_{\mathcal{M},1,k}^0 \left(\mathbf{b}^{\frac{3}{2}} \min(1, \mathbf{b})^k\right)^{-1}, \quad \mathbf{b} = \frac{3}{10\pi^{\frac{3}{2}}} E^{-1},$$

this concludes the proof of (7.80). □

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Table des matières

Résumé	v
Remerciements	vii
Sommaire	ix
1 Introduction	5
1.1 Présentation de l'équation de Boltzmann	6
1.1.1 Construction de l'équation de Boltzmann	6
1.1.2 Conservations, entropie et équilibre thermodynamique	12
1.1.3 Méthodes entropiques pour un taux de relaxation vers l'équilibre	17
1.1.4 Théorie proche équilibre et opérateur de Boltzmann linéarisé	18
Quelques notations	21
1.2 Un cadre général de modèles de Boltzmann pour les gaz polyatomiques	22
1.2.1 Présentation du cadre général pour un gaz simple	22
1.2.2 Réduction de modèle : approches basées sur l'énergie	26
1.2.3 Extension aux mélanges avec réactions chimiques	31
1.3 Autour d'un modèle singulier : collisions résonantes et quasi-résonantes	37
1.3.1 Propriété de compacité du linéarisé pour un gaz polyatomique avec collisions résonantes	37
1.3.2 Un modèle de gaz polyatomique avec collisions quasi-résonantes	41
1.4 Méthodes entropiques et relaxation vers l'équilibre pour l'équation de Boltzmann-Fermi-Dirac	47
1.4.1 L'équation de Boltzmann-Fermi-Dirac	47
1.4.2 Transfert d'inégalités entropiques depuis le cas classique vers le cas quantique	51
1.4.3 Relaxation vers l'équilibre avec un taux algébrique explicite	56
I A general framework for Boltzmann models for polyatomic gases	63
Overview	65
2 A general framework for the kinetic modelling of polyatomic cases	67
2.1 Introduction	68
2.2 General setting and collision rules	70
2.3 Boltzmann model	73
2.3.1 Boltzmann collision operator	74
2.3.2 Note about degeneracy	76

2.3.3	Weak formulation	78
2.3.4	Collision invariants	80
2.4	H Theorem and collision equilibria	82
2.5	Euler limit	90
2.6	Equipartition Theorem	91
2.7	Models within the framework	93
2.7.1	Existing models	93
2.7.2	Combination of the continuous and discrete models	98
2.7.3	Building a model within the framework	99
2.8	Reduction to one real variable and comparison with Borgnakke-Larsen	103
2.9	Conclusions	108
	Acknowledgements	111
3	An internal state kinetic model for chemically reacting mixtures of monatomic and polyatomic gases	115
3.1	Introduction	117
3.2	Setting	118
3.3	Collision model	120
	Collision rules and transformation	121
3.4	The Boltzmann model	123
	Distribution function and kinetic equation	123
	Macroscopic quantities	123
3.4.1	Boltzmann operator	124
	Mechanical and chemical collision operators	126
3.4.2	Mechanical and global collision invariants	127
3.4.3	H-Theorem	130
3.5	Equilibrium	131
3.5.1	Mechanical equilibrium	132
3.5.2	Mechanical and chemical equilibrium	134
3.5.3	Rate of reaction	136
3.6	Euler limit	140
3.7	Example of a computation of the rate of reaction	143
3.8	Reduced models and energy of reaction	144
3.9	Example of a three species gas mixture undergoing one chemical reaction	145
	State-based model	146
	Corresponding energy-based model	146
	Quantities of interest	147
3.10	Conclusion	148
3.A	Auxiliary lemma	149
3.B	Physical and chemical quantities reminder	151
II	Around a singular polyatomic model: resonant and quasi-resonant collisions	157
	Overview	159

4 A compactness property of the linearized Boltzmann operator for a polyatomic gas undergoing resonant collisions	161
4.1 Introduction	162
4.2 Resonant collision model	163
Molecule model	164
Microscopic dynamics	164
Assumptions on the cross section	165
Kinetic operator, H theorem	167
4.3 Main result	168
4.4 Proof of the main result	168
4.4.1 Compactness of K_1	169
4.4.2 Compactness of K_2	170
4.4.3 Conclusion to the proof of Theorem 4.1	180
4.A Grad's proof revisited	180
4.A.1 Alternative change of variables	181
4.A.2 Study of the kernel form of K_2^m	183
4.B A technical lemma	189
5 A Boltzmann model for polyatomic gases undergoing quasi-resonant collisions	193
Introduction	194
5.1 A Boltzmann model with quasi-resonant collisions	194
5.1.1 Quasi-resonance by collision truncation	195
5.1.2 Quasi-resonant Boltzmann operator and H -theorem	197
5.1.3 Resonant asymptotics	199
5.2 Expected properties of the model, Landau-Teller equations	201
5.2.1 Expected properties	201
5.2.2 Derivation of Landau-Teller type equations	202
5.3 Numerical experiments	206
5.3.1 The DSMC method	206
5.3.2 Result of the experiment and discussion	210
5.A Technical lemmas	212
III On relaxation towards equilibrium for the Boltzmann-Fermi-Dirac equation	217
Overview	219
6 Extending Cercignani's conjecture results from Boltzmann to Boltzmann-Fermi-Dirac	221
6.1 Introduction	223
6.1.1 The Boltzmann-Fermi-Dirac operator	223
6.1.2 Macroscopic quantities and equilibrium distribution	225
6.1.3 Fermi-Dirac entropy	226
6.1.4 Entropy production	228
6.1.5 Trend to equilibrium and Cercignani's conjecture	228
6.2 Main results	230
6.2.1 Comparison of the Fermi-Dirac and Classical relative entropies	230
6.2.2 Entropy-entropy production inequalities for the Boltzmann-Fermi-Dirac (BFD) equation	230
6.2.3 About the Csiszár-Kullback-Pinsker inequality	231

6.2.4	Convergence towards equilibrium	233
6.3	Proof of Theorem 6.1 and Proposition 6.2	234
6.3.1	Key element of the proof	234
6.3.2	Continuity at zero	238
6.3.3	Final proof of Theorem 6.1	239
6.3.4	Final proof of Proposition 6.2	240
6.4	Proof of Corollary 6.3	243
6.4.1	Super quadratic kernels	243
6.4.2	General kernels	244
6.4.3	Inverse result	245
6.5	About the Landau-Fermi-Dirac equation	247
6.6	L^1 - L^2 weighted Csiszár-Kullback-Pinsker inequality	249
6.A	Similar results in the Bose-Einstein case	253
6.B	A general discussion about entropies and equilibria	255
6.C	Technical results	260
6.C.1	L^∞ bound for the Fermi-Dirac statistics	260
6.C.2	Regularity in ε of the coefficients of the Fermi-Dirac statistics	262
	Acknowledgements	265
7	Quantitative relaxation towards equilibrium for solutions to the Boltzmann-Fermi-Dirac equation with cutoff hard potentials	269
7.1	Introduction and main results	271
7.1.1	The Boltzmann-Fermi-Dirac equation	271
7.1.2	Notations	272
7.1.3	Relaxation to equilibrium	273
7.1.4	The role of relative entropy	275
7.1.5	Main results	278
7.1.6	Organization of the paper	280
7.2	Uniform-in- ε L^∞ bound: proof of Theorem 7.3	281
7.2.1	A link between the Fermi-Dirac and the classical cases	281
7.2.2	General estimates on $Q_{\gamma,b}^+$	283
7.2.3	Key estimates on $Q_{\gamma,b}^+$, $\Gamma_{\gamma,b}$ and $Q_{\gamma,b}^-$	285
7.2.4	Derivation of L_γ^2 bounds	290
7.2.5	Conclusion to the proof of Theorem 7.3	293
7.3	Explicit rate of convergence to equilibrium: proof of Theorem 7.4	295
7.3.1	Maxwellian pointwise lower bound	295
7.3.2	Conclusion to the proof of Theorem 7.4	295
7.A	More physically relevant models	299
7.A.1	Quantum collision kernels	299
7.A.2	Main mathematical changes induced by quantum collision kernels	300
7.B	Known results about (BFD Eq.) and the Fermi-Dirac entropy	301
7.B.1	Cauchy problem and moment estimates	301
7.B.2	Csiszár-Kullback-Pinsker inequalities	302
7.C	Explicit and uniform-in- ε bounds for Fermi-Dirac statistics	303
	Acknowledgments	306
	Table des matières	309
	Bibliographie	313

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CONTRIBUTIONS AUTOUR DE L'ÉQUATION DE BOLTZMANN ET CERTAINES DE SES VARIANTES

Résumé

Nous étudions certaines variantes de l'équation de Boltzmann, cette dernière décrivant via une approche classique les gaz raréfiés simples et monoatomiques à l'échelle mésoscopique. Dans un premier temps, nous proposons un cadre général de modélisation de Boltzmann des gaz polyatomiques, englobant une large classe de modèles pré-existants et permettant d'en construire de nouveaux. D'abord présenté pour un gaz simple, ce cadre est ensuite étendu aux mélanges gazeux, pour lesquels on autorise des réactions chimiques binaires. Dans un deuxième temps, nous nous intéressons à un type de gaz polyatomique singulier, au sein duquel les collisions sont résonantes. Nous prouvons une propriété de compacité pour l'opérateur linéarisé lié à ce modèle. Afin de rendre plus flexible le cadre résonant, nous proposons ensuite un formalisme de Boltzmann pour des collisions quasi-résonantes, étudions ses propriétés-clés et menons des expériences numériques pour étayer notre compréhension de celles-ci. Enfin, dans un troisième temps, nous nous tournons vers une équation de Boltzmann incluant le principe d'exclusion de Pauli, utile notamment pour la description de la distribution d'électrons dans les semi-conducteurs. Nous développons une méthode permettant de transférer certaines inégalités fonctionnelles, liées à l'entropie, connues dans le cas classique, vers ce cas quantique. Par suite, grâce à l'obtention de ces nouvelles inégalités, nous obtenons un taux explicite de relaxation à l'équilibre pour les solutions de l'équation de Boltzmann-Fermi-Dirac homogène pour les potentiels durs avec cut-off.

Mots clés : théorie cinétique, équation de Boltzmann, gaz polyatomiques, collisions résonantes, méthodes entropiques, équation de Nordheim, équation de Boltzmann-Fermi-Dirac

Abstract

We study some variants of the Boltzmann equation, the latter describing, via a classical approach, single and monatomic rarefied gases at the mesoscopic scale. First, we propose a general framework for Boltzmann modelling of polyatomic gases, encompassing a wide class of pre-existing models and allowing to build new ones. Primarily presented for a single gas, the framework is then extended to mixtures, within which we allow binary chemical reactions. Second, we focus on a singular type of polyatomic gas, the molecules of which undergo resonant collisions, and prove a compactness property of the linearized operator related to this model. In order to make the latter resonant framework more flexible, we then propose a Boltzmann formalism with quasi-resonant collisions, study its key properties and conduct numerical experiences to support our understanding of them. Third, we turn our attention towards a Boltzmann equation which includes Pauli's exclusion principle, notably used in the study of electron distributions in semi-conductors. We develop a method that allows to transfer some functional inequalities, related to entropy, which are known in the classical case, to this quantum case. As a consequence, we use these new inequalities to obtain an explicit rate of relaxation to equilibrium for solutions to the homogeneous Boltzmann-Fermi-Dirac equation with cut-off hard potentials.

Keywords: kinetic theory, Boltzmann equation, polyatomic gases, resonant collisions, entropy methods, Nordheim equation, Boltzmann-Fermi-Dirac equation
