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Andrea Bondesan

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THÈSE DE DOCTORAT

Spécialité : **Mathématiques Appliquées**

présentée par

**Andrea BONDESAN**

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# Asymptotique diffusive de l'équation de Boltzmann pour les mélanges gazeux, étude mathématique et numérique

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*À ma famille. Sans son soutien,  
cette thèse n'existerait pas.*



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# Asymptotique diffusive de l'équation de Boltzmann pour les mélanges gazeux, étude mathématique et numérique

**Résumé.** Cette thèse est consacrée à plusieurs études reliant l'équation de Boltzmann pour les mélanges gazeux aux équations de Maxwell-Stefan décrivant la diffusion gazeuse. Notre analyse est construite sur une linéarisation de la solution de l'équation cinétique autour d'un état maxwellien local ayant des vitesses différentes pour chaque espèce du mélange, mais de l'ordre du paramètre d'échelle qui prescrit l'asymptotique diffusive. Dans une première partie, nous montrons que l'opérateur de Boltzmann linéarisé autour d'une telle maxwellienne, ne constituant pourtant pas un état d'équilibre pour le gaz, satisfait une propriété de quasi-stabilité de son trou spectral : le trou spectral obtenu en linéarisant l'opérateur de collision autour d'un état d'équilibre global est préservé à une correction du même ordre que le paramètre d'échelle. Ainsi, nous sommes ensuite en mesure de prouver que le système de Maxwell-Stefan peut être dérivé rigoureusement à partir de l'équation de Boltzmann multi-espèce. Cette dérivation est obtenue en montrant existence et unicité des solutions perturbatives des modèles cinétique et macroscopique, grâce en particulier à des estimations d'hypocoercivité. Dans une deuxième partie du manuscrit, par le biais de la méthode des moments, nous construisons un schéma numérique capable de décrire le comportement des solutions aux différentes échelles de l'asymptotique diffusive. Pour ce schéma, nous prouvons un résultat d'existence et de positivité des solutions, et un caractère préservant l'asymptotique est montré à travers plusieurs tests numériques.

**Mots-clés :** Théorie cinétique ; Équation de Boltzmann ; Mélanges gazeux ; Équation de Maxwell-Stefan ; Diffusion croisée ; Limites hydrodynamiques ; Hypocoercivité ; Schéma préservant l'asymptotique.



# Diffusive asymptotics of the Boltzmann equation for gaseous mixtures, mathematical and numerical study

**Abstract.** This thesis is devoted to several studies which aim at investigating the link between the Boltzmann equation for gaseous mixtures and the Maxwell-Stefan equations, modelling purely diffusive phenomena inside a gas. Our analysis is built on a linearization of the solution of the kinetic equation around a local Maxwellian state characterized by different bulk velocities for each species of the mixture, but having the same order of magnitude of the scaling parameter which prescribes the diffusive asymptotic. In a first part, we start by showing that the Boltzmann operator linearized around such a Maxwellian, which does not constitute an equilibrium for the gas, exhibits a quasi-stability property on its spectral gap : the spectral gap known to exist for the collision operator linearized a global equilibrium state is preserved up to a correction which is of the same order of the scaling parameter. Thanks to this feature and *via* the derivation of suitable hypocoercivity estimates, we are then able to prove that the Maxwell-Stefan system can be rigorously obtained from the Boltzmann multi-species equation, by showing that the solutions of the kinetic and macroscopic models exist uniquely in a perturbative sense. In a second part of the manuscript, using the moment method, we design a numerical scheme which captures the correct behaviour of the solutions at different scales of the diffusive asymptotic. We prove that our scheme possesses at least one solution with positive concentrations, and we show numerically that it is asymptotic preserving in the vanishing limit of the scaling parameter.

**Keywords:** Kinetic theory; Boltzmann equation; Gaseous mixtures; Maxwell-Stefan model; Cross-diffusion; Hydrodynamic limit; Hypocoercivity; Asymptotic preserving scheme.





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# Chapitre 1

## Introduction

Ce manuscrit est dédié à l'étude mathématique et numérique de l'équation de Boltzmann multi-espèce et de son asymptotique diffusive vers les équations de Maxwell-Stefan. L'équation de Boltzmann est le plus ancien des modèles de la théorie cinétique. Elle permet de décrire l'évolution d'un gaz raréfié et, plus généralement, de tout système formé d'un grand nombre de particules. Ses applications sont nombreuses et lui valent l'importance et l'intérêt portés à son étude aujourd'hui. Nous pouvons citer par exemple ses diverses utilisations en physique et en ingénierie, pour modéliser les plasmas, les semi-conducteurs, le transfert radiatif ou le transport de neutrons à l'intérieur d'un réacteur nucléaire ; mais elle est appliquée aussi en biologie et en médecine, pour décrire le mouvement de grands ensembles d'animaux ou d'agglomérats de cellules, ainsi que dans de multiples autres domaines comme l'économie, ou l'étude du comportement humain (mouvement de foule, trafic routier, etc.).

Les équations de la théorie cinétique s'insèrent parmi les trois types de description physique dont on dispose pour étudier l'évolution d'un gaz : *microscopique*, *mésoscopique* et *macroscopique*.

### Différents types de description

Un gaz (ou un fluide) peut être modélisé par un système constitué d'un grand nombre de particules de même masse (petite)  $m$  qui interagissent à l'intérieur d'un domaine spatial  $\Omega \in \mathbb{R}^3$ , chacune caractérisée par une vitesse de déplacement  $v \in \mathbb{R}^3$ . En fonction de l'échelle d'observation du système, on a accès à plusieurs descriptions possibles.

Une première approximation est fournie par la mécanique classique : on représente l'évolution d'un système de particules non chargées et sujettes à la seule action d'une force extérieure à l'aide des équations de Newton. Selon ses lois fondamentales du mouvement (énoncées dans l'ouvrage *Philosophiae naturalis principia mathematica* [165] en 1687), en connaissant la position initiale de chaque particule, la dynamique du système est décrite par  $6n$  équations différentielles ordinaires du premier ordre, couplées. C'est ce qu'on appelle la description microscopique, où l'on s'intéresse à l'ensemble des trajectoires des particules. Même si une telle description est très détaillée, elle présente des inconvénients majeurs. D'un côté, la résolution analytique et numérique des équations de Newton est inaccessible dans des cas réalistes (il suffit de penser qu'une mole de gaz contient environ  $10^{23}$  particules). D'autre part, connaître l'évolution des positions et des vitesses de chaque particule ne nous permet pas d'obtenir une information sur les observables physiques intéressantes (quantité de matière, vitesse d'ensemble et température du système).

Une approche alternative consiste à analyser l'évolution de ces mêmes quantités observables, à travers l'application des lois de conservation de la mécanique classique à des élé-

ments infinitésimaux de volume d'un fluide, plutôt qu'à chaque particule séparément. C'est l'idée derrière la description macroscopique : un fluide est vu comme un milieu continu, où le simple élément microscopique ne joue plus un rôle prééminent sur le mouvement du système global. Parmi les équations macroscopiques (ou hydrodynamiques) les plus importantes figurent les équations d'Euler, modélisant un fluide non visqueux, et les équations de Navier-Stokes, modélisant un fluide visqueux. Le fait de négliger complètement la dynamique moléculaire peut constituer un désavantage. Ainsi, aucune dérivation des paramètres physiques importants du système, tels que les coefficients de transport, n'est possible à partir des modèles hydrodynamiques.

Entre ces deux descriptions se situe la théorie cinétique des gaz, qui décrit un niveau intermédiaire, ou mésoscopique. À la base des modèles mésoscopiques (entre autres, les équations de Boltzmann, Landau, Vlasov-Fokker-Planck, etc.) se trouve l'idée que la position et la vitesse d'une particule ne sont déterminées que de façon approchée. L'évolution du gaz est alors décrite par une densité<sup>1</sup> de probabilité  $F = F(t, x, v)$  qui trace la position et la vitesse moyennes d'une particule. Autrement dit, la quantité  $F(t, x, v)dx dv$  donne le nombre de particules à l'intérieur de la boule  $B(x, dx)$  de centre  $x$  et rayon infinitésimal  $dx$ , avec vitesse dans  $B(v, dv)$  et à un instant de temps  $t$  fixé. Dans cette approche le nombre de degrés de liberté du système est considérablement réduit par rapport à la description microscopique, puisque nous ne nous préoccupons plus de localiser précisément position et vitesse de chaque particule, mais plutôt de tenir compte de son déplacement « typique ». Toutefois, ce choix de modélisation permet aussi de préserver l'information qui provient des interactions moléculaires, contrairement à la description macroscopique. De plus, il est possible d'interpréter les observables physiques précédemment évoquées en terme d'observables probabilistes sur la densité  $F$  (masse, espérance et variance). Ainsi, nous pouvons reconstruire les quantités macroscopiques locales en temps et en espace,

$$\begin{aligned} c(t, x) &= \int_{\mathbb{R}^3} F(t, x, v) dv, \\ u(t, x) &= \frac{1}{c(t, x)} \int_{\mathbb{R}^3} v F(t, x, v) dv, \\ \theta(t, x) &= \frac{1}{3K_B c(t, x)} \int_{\mathbb{R}^3} |v - u(t, x)|^2 F(t, x, v) dv, \end{aligned} \tag{1.0.1}$$

qui correspondent respectivement au nombre de particules, à la vitesse d'ensemble et à la température du gaz (où  $K_B$  désigne la constante de Boltzmann). Enfin, soulignons que les équations cinétiques permettent également de décrire l'évolution des gaz qui ne sont pas à l'équilibre thermodynamique<sup>2</sup>, hypothèse qui est revanche nécessaire afin d'établir les modèles hydrodynamiques.

La description mésoscopique semble alors fournir un cadre très général, et ses multiples avantages nous incitent à focaliser notre intérêt sur la théorie cinétique des gaz. Parmi ses nombreux modèles, nous choisissons le premier à avoir été introduit : l'équation de Boltzmann.

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1. Dans la suite, on parlera plutôt de « fonction de distribution », pour éviter toute confusion avec le concept de densité en physique.

2. L'hypothèse d'équilibre thermodynamique correspond à demander que la distribution des vitesses des particules à l'intérieur de tout volume infinitésimal soit donnée par une gaussienne.

## 1.1 Présentation des modèles utilisés

L'idée que toute la matière soit caractérisée par une structure atomique sous-jacente indivisible remonte aux théories atomistes de l'Inde et de la Grèce antiques. Néanmoins, il faut attendre le début du XVIII<sup>e</sup> siècle pour observer une première formalisation scientifique du principe qu'une quantité macroscopique (comme la pression exercée par un gaz) peut être interprétée en terme d'action microscopique des particules (les collisions). Grâce aux idées de Daniel Bernoulli, en 1738, on voit la naissance de la théorie cinétique des gaz. Les nombreuses contributions successives dans ce nouveau domaine de recherche culminent avec les travaux de James Clerk Maxwell en 1866 [153, 154] et de Ludwig Boltzmann en 1872 [28, 29] qui sont reconnus comme les fondateurs de la théorie cinétique moderne. En particulier, Boltzmann fut le premier à compléter la dérivation formelle de l'équation qui porte aujourd'hui son nom.

### Hypothèses sur la physique des collisions

Dans cette thèse, nous considérerons toujours des gaz parfaits, inertes et monoatomiques, confinés dans le tore  $\mathbb{T}^3$  et non soumis à l'action de forces extérieures. Physiquement, cela veut dire que les particules interagissent seulement à travers des collisions microscopiques<sup>3</sup>, que leur taille est négligeable par rapport à la distance intermoléculaire moyenne, et que l'état de chaque particule est complètement décrit par sa position  $x$  et sa vitesse  $v$ . En particulier, le gaz est composé d'atomes qui ne possèdent pas de degrés de liberté internes de rotation et de vibration propres à une molécule. Enfin, le choix du tore est une simplification typique dans les études mathématiques de l'équation de Boltzmann car elle permet de gérer un domaine d'espace borné mais sans les complications d'un bord.

Les hypothèses qui décrivent la physique des collisions et qui ont permis à Boltzmann d'établir heuristiquement son équation sont les suivantes.

- Le gaz est assez raréfié pour considérer des collisions purement binaires et négliger les interactions faisant intervenir plus de deux particules.
- Toute collision est localisée en temps et en espace, ce qui implique que les interactions entre particules se produisent dans des échelles de temps et d'espace négligeables par rapport aux échelles d'observation macroscopiques.
- Les collisions sont élastiques et préservent donc la quantité de mouvement et l'énergie cinétique au niveau microscopique.
- La dynamique de la collision est réversible en temps : lors d'une collision, la probabilité que les vitesses des deux particules  $(v', v'_*)$  soient échangées en  $(v, v_*)$  est égale à la probabilité d'observer la transformation inverse  $(v, v_*) \mapsto (v', v'_*)$ .
- Les vitesses de deux particules en collision ne sont pas corrélées avant leur interaction, mais seulement après le contact. Il s'agit du « Stosszahlansatz » de Boltzmann, ou hypothèse de *chaos moléculaire* du gaz : le processus de collision contient une asymétrie passé-futur qui permet d'augmenter les corrélations entre particules au cours du temps.

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3. Ici, une collision est un processus physique d'interaction selon lequel les trajectoires de deux particules suffisamment proches sont fortement déviées en un temps très court.

### 1.1.1 L'équation de Boltzmann pour un gaz seul

Considérons un gaz parfait, inerte, monoatomique et mono-espèce de masse atomique  $m$ , qui vérifie les hypothèses présentées précédemment. Puisque les collisions se produisent de manière élastique, quand deux particules de vitesses respectives  $(v', v'_*)$  entrent en contact, leurs nouvelles vitesses  $(v, v_*)$  doivent respecter les lois de conservation

$$v + v_* = v' + v'_*, \quad |v|^2 + |v_*|^2 = |v'|^2 + |v'_*|^2, \quad (1.1.1)$$

qui permettent de fixer 4 parmi les 6 degrés de liberté de  $(v, v_*)$ . Ainsi, les vitesses pré-collisionnelles  $(v', v'_*)$  peuvent s'exprimer en fonction des vitesses post-collisionnelles  $(v, v_*)$  selon les relations

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

où  $\sigma \in \mathbb{S}^2$  est un paramètre qui tient compte des deux degrés de liberté restants.

L'évolution du gaz est alors décrite par une fonction de distribution  $F = F(t, x, v)$  satisfaisant l'équation, posée sur  $\mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ ,

$$\partial_t F + v \cdot \nabla_x F = Q(F, F). \quad (1.1.2)$$

Le terme de gauche est l'opérateur linéaire de transport libre. Il traduit l'idée intuitive qu'en l'absence d'interactions, les particules se déplacent en ligne droite à vitesse constante selon les lois de Newton. La physique des collisions est complètement décrite par  $Q$ , un opérateur bilinéaire en  $F$  et local en  $(t, x)$ , agissant uniquement sur la variable  $v$  et qui a la forme

$$Q(F, F)(v) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} B(|v - v_*|, \cos \vartheta) (F' F'^* - F F^*) dv_* d\sigma,$$

avec la notation classique  $F' = F(t, x, v')$ ,  $F'^* = F(t, x, v'_*)$ ,  $F^* = F(t, x, v_*)$ . Le noyau de collision  $B$  est une fonction positive qui dépend seulement du module de la vitesse relative  $v - v_*$  et de l'angle de déviation  $\vartheta \in [0, \pi]$  entre  $v - v_*$  et  $\sigma \in \mathbb{S}^2$ . Il contient les informations sur la nature des interactions microscopiques et son choix (crucial pour l'étude mathématique) sera détaillé dans la suite.

L'équation (1.1.2) a permis à Boltzmann de démontrer en 1872 un résultat fondamental, le théorème  $H$ , qui fournit pour la première fois un cadre à la théorie du retour à l'équilibre thermodynamique et une justification mathématique (seulement à un niveau formel) du principe de croissance de l'entropie physique<sup>4</sup>. Afin de pouvoir énoncer les différents aspects du théorème, nous commençons par présenter deux formulations faibles de l'opérateur de collision ainsi que leurs conséquences directes.

En utilisant les changements de variable standard  $(v, v_*) \mapsto (v', v'_*)$  et  $(v, v_*) \mapsto (v_*, v)$ , on peut dériver [57, 190] les formulations faibles

$$\begin{aligned} \int_{\mathbb{R}^3} Q(F, F)(v) \psi(v) dv &= \\ \frac{1}{2} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B(|v - v_*|, \cos \vartheta) F F^* (\psi' + \psi'^* - \psi - \psi^*) dv dv_* d\sigma, \end{aligned} \quad (1.1.3)$$

$$\begin{aligned} \int_{\mathbb{R}^3} Q(F, F)(v) \psi(v) dv &= \\ -\frac{1}{4} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B(|v - v_*|, \cos \vartheta) (F' F'^* - F F^*) (\psi' + \psi'^* - \psi - \psi^*) dv dv_* d\sigma. \end{aligned} \quad (1.1.4)$$

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4. Introduite en 1865 par Rudolf Clausius, dans le contexte du deuxième principe de la thermodynamique classique.

valables pour toute fonction test  $\psi : \mathbb{R}^3 \rightarrow \mathbb{R}$  telle que les intégrales de gauche sont bien définies. Grâce aux lois de conservation microscopiques, il est en particulier possible de montrer à partir de (1.1.3) [59] que l'égalité<sup>5</sup>

$$\int_{\mathbb{R}^3} Q(F, F)(v)\psi(v)dv = 0 \quad (1.1.5)$$

est vérifiée si et seulement si  $\psi$  est un invariant de collision, soit

$$\psi \in \text{Vect} (1, v_1, v_2, v_3, |v|^2). \quad (1.1.6)$$

De plus, avec le choix  $\psi(v) = \ln F(v)$ , on voit facilement que (1.1.4) nous donne aussi l'inégalité

$$\int_{\mathbb{R}^3} Q(F, F)(v) \ln F(v)dv \leq 0. \quad (1.1.7)$$

### Production d'entropie et retour à l'équilibre thermodynamique

Ces deux dernières propriétés permettent de prouver le théorème  $H$  de Boltzmann. Celui-ci affirme que la fonctionnelle de production d'entropie

$$S(F) = \int_{\mathbb{R}^3} Q(F, F)(v) \ln F(v)dv,$$

s'annule si et seulement si  $F$  a la forme d'une distribution de Maxwell locale  $M_{(c,u,\theta)}$  donnée, pour tout  $t \in \mathbb{R}_+$ ,  $x \in \mathbb{T}^3$  et  $v \in \mathbb{R}^3$ , par

$$M_{(c,u,\theta)}(t, x, v) = \frac{c(t, x)}{(2\pi K_B \theta(t, x))^{3/2}} \exp \left\{ -\frac{|v - u(t, x)|^2}{2K_B \theta(t, x)} \right\}, \quad (1.1.8)$$

où les quantités macroscopiques locales  $c$ ,  $u$  et  $\theta$  sont définies par les relations (1.0.1). De plus, cette condition est aussi équivalente à demander que  $Q(F, F) = 0$ .

Les conséquences de ce résultat sont cruciales. Tout d'abord, il nous dit que les seuls états d'équilibre possibles du gaz sont représentés par les maxwelliennes locales (1.1.8). Ceci permet donc de cibler les « bonnes » distributions autour desquelles construire une théorie de retour à l'équilibre thermodynamique. En second lieu, dans le cadre du confinement dans un tore que l'on considère, la combinaison de cette propriété avec l'action de l'opérateur de transport libre nous montre plus précisément qu'il existe un unique état d'équilibre global du gaz satisfaisant simultanément les équations

$$Q(F, F)(x, v) = 0 \quad \text{et} \quad v \cdot \nabla_x F(x, v) = 0, \quad \forall x \in \mathbb{T}^3, \forall v \in \mathbb{R}^3.$$

Cet équilibre a la forme d'une distribution de Maxwell globale  $\mu$  donné par

$$\mu(v) = \frac{c_\infty}{(2\pi K_B \theta_\infty)^{3/2}} \exp \left\{ -\frac{|v - u_\infty|^2}{2K_B \theta_\infty} \right\}, \quad v \in \mathbb{R}^3, \quad (1.1.9)$$

où les observables globales  $c_\infty$ ,  $u_\infty$  et  $\theta_\infty$ , qui sont le nombre de particules, la vitesse d'ensemble et la température du gaz, s'écrivent

$$c_\infty = \int_{\mathbb{T}^3 \times \mathbb{R}^3} \mu(v) dx dv, \quad u_\infty = \frac{1}{c_\infty} \int_{\mathbb{T}^3 \times \mathbb{R}^3} v \mu(v) dx dv,$$

$$\theta_\infty = \frac{1}{3K_B c_\infty} \int_{\mathbb{T}^3 \times \mathbb{R}^3} |v - u_\infty|^2 \mu(v) dx dv,$$

---

5. Cette égalité donne les lois de conservation de la masse, de la quantité de mouvement et de l'énergie macroscopiques.



grâce aux propriétés de conservation de l'opérateur de collision (1.1.5). Enfin, si nous introduisons la fonctionnelle d'entropie  $H$  associée à une solution  $F$

$$H(F) = \int_{\mathbb{T}^3 \times \mathbb{R}^3} F \ln F dx dv,$$

en multipliant l'équation (1.1.2) par  $\ln F$  et en l'intégrant en  $(x, v)$ , l'utilisation de (1.1.7) montre formellement que  $H$  est liée à  $S$  par la relation

$$\frac{d}{dt} H(F) = \int_{\mathbb{T}^3} S(F) dx \leq 0.$$

Grâce au théorème  $H$ , l'inégalité précédente implique que l'entropie décroît au cours du temps jusqu'à atteindre un état maxwellien local ou global (qui maximise la production d'entropie). Cela signifie donc que l'équation de Boltzmann contient un mécanisme intrinsèque de retour à l'équilibre thermodynamique local (ou global).

**Remarque 1.1.1.** *Il est intéressant de noter que la fonctionnelle  $H$  considérée par Boltzmann est l'opposée de l'entropie physique. La dernière inégalité appliquée à  $-H$  fournit alors une justification mathématique du deuxième principe de la thermodynamique. De plus, elle permet de montrer l'irréversibilité temporelle de l'équation de Boltzmann, puisque le changement de variable  $(t, x, v) \mapsto (-t, x, -v)$  entraînerait une décroissance de l'entropie physique*

$$\frac{d}{dt} H(F) = - \int_{\mathbb{T}^3} S(F) dx \geq 0.$$

Nous présentons maintenant le modèle cinétique de mélanges gazeux qui est au cœur de cette thèse : l'équation de Boltzmann multi-espèce. Notre objectif est de mettre en évidence les différences significatives avec le cadre mono-espèce. Pour ce faire, nous suivons les mêmes étapes vues pour l'équation de Boltzmann classique.

### 1.1.2 Un modèle cinétique pour les mélanges

Nous nous intéressons au comportement d'un mélange constitué de  $N \geq 2$  gaz parfaits, inertes et monoatomiques, dont chaque espèce  $\mathcal{E}_i$ ,  $1 \leq i \leq N$ , est caractérisée par des particules de masse atomique  $m_i$ . Dans ce cadre, les lois de conservation microscopiques doivent être modifiées pour inclure les interactions élastiques entre particules de masse différente. Ainsi, quand deux particules d'espèces respectives  $\mathcal{E}_i$  et  $\mathcal{E}_j$  entrent en collision avec des vitesses  $(v', v'_*)$  et repartent avec de nouvelles vitesses  $(v, v_*)$ , la quantité de mouvement et l'énergie cinétique du processus sont préservées selon les relations

$$m_i v + m_j v_* = m_i v' + m_j v'_*, \quad m_i |v|^2 + m_j |v_*|^2 = m_i |v'|^2 + m_j |v'_*|^2. \quad (1.1.10)$$

Ces relations permettent alors de déduire que les vitesses pre-collisionnelles  $(v', v'_*)$  s'écrivent en terme des vitesses post-collisionnelles  $(v, v_*)$  comme

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

où  $\sigma \in \mathbb{S}^2$  représente les deux degrés de liberté permis par les lois de conservation. On observe donc une asymétrie entre les masses des espèces, qui a des implications significatives pour l'étude des propriétés du modèle.

L'évolution du mélange gazeux peut alors être décrite à l'aide d'un système d'équations de Boltzmann couplées [70, 39, 37] qui s'écrivent, pour chaque  $1 \leq i \leq N$ ,

$$\partial_t F_i(t, x, v) + v \cdot \nabla_x F_i(t, x, v) = Q_i(\mathbf{F}, \mathbf{F})(t, x, v), \quad t \geq 0, \quad x \in \mathbb{T}^3, \quad v \in \mathbb{R}^3 \quad (1.1.11)$$

Ici  $\mathbf{F} = (F_1, \dots, F_N)$  désigne la fonction de distribution des particules du mélange gazeux global, tandis que chaque composante  $F_i = F_i(t, x, v)$  représente la fonction de distribution spécifique à l'espèce  $\mathcal{E}_i$ . Par la suite, la notation en caractères gras indiquera tout vecteur et toute fonction vectorielle dont les composantes font référence aux différentes espèces du mélange (les composantes seront alors indiquées par les caractères correspondants indexés). Par exemple,  $\mathbf{W}$  dénote le vecteur ou la fonction vectorielle  $(W_1, \dots, W_N)$ . Pour simplifier les calculs, nous utiliserons également la convention que toute multiplication entre vecteurs et fonctions vectorielles à  $N$  composantes est à effectuer terme à terme, soit, par exemple,  $\mathbf{w}\mathbf{W} = (w_1 W_1, \dots, w_N W_N)$  et  $\mathbf{W}^q = (W_1^q, \dots, W_N^q)$ , pour tout  $q \in \mathbb{Q}$ .

L'opérateur de Boltzmann multi-espèce  $\mathbf{Q}(\mathbf{F}, \mathbf{F}) = (Q_1(\mathbf{F}, \mathbf{F}), \dots, Q_N(\mathbf{F}, \mathbf{F}))$  contient la physique des collisions. Il s'agit d'un opérateur quadratique en  $\mathbf{F}$ , local en temps et en espace, dont chaque composante  $Q_i(\mathbf{F}, \mathbf{F})$  est donnée, pour tout  $v \in \mathbb{R}^3$ , par

$$\begin{aligned} Q_i(\mathbf{F}, \mathbf{F})(v) &= \sum_{j=1}^N Q_{ij}(F_i, F_j) \\ &= \sum_{j=1}^N \int_{\mathbb{R}^3 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) (F_i' F_j'^* - F_i F_j^*) dv_* d\sigma, \end{aligned} \quad (1.1.12)$$

et chaque section efficace de collision  $B_{ij}$  contient les informations sur les collisions croisées entre les espèces  $\mathcal{E}_i$  et  $\mathcal{E}_j$ . Notons en particulier que les interactions entre particules d'une même espèce  $\mathcal{E}_i$  sont modélisées par le terme  $Q_{ii}(F_i, F_i)$  qui n'est rien d'autre que l'opérateur de Boltzmann mono-espèce. Ceci implique que nous pouvons finalement présenter d'une façon unifiée les hypothèses sur la structure des noyaux de collisions (le cas mono-espèce étant inclus avec  $B_{ii}$ ). Précisément, chaque  $B_{ij}$  vérifie les propriétés suivantes.

(H1) Il satisfait une propriété de symétrie par rapport aux indices d'espèce  $i$  et  $j$

$$B_{ij}(|v - v_*|, \cos \vartheta) = B_{ji}(|v - v_*|, \cos \vartheta), \quad \forall v, v_* \in \mathbb{R}^3, \quad \forall \vartheta \in [0, \pi].$$

(H2) Il s'écrit sous une forme de produit d'une partie cinétique  $\Phi_{ij} \geq 0$  et d'une partie angulaire  $b_{ij} \geq 0$

$$B_{ij}(|v - v_*|, \cos \vartheta) = \Phi_{ij}(|v - v_*|) b_{ij}(\cos \vartheta), \quad \forall v, v_* \in \mathbb{R}^3, \quad \forall \vartheta \in [0, \pi].$$

(H3) La partie cinétique correspond à des potentiels durs ou de Maxwell ( $\gamma = 0$ ), *i.e.*

$$\Phi_{ij}(|v - v_*|) = C_{ij}^\Phi |v - v_*|^\gamma, \quad C_{ij}^\Phi > 0, \quad \gamma \in [0, 1], \quad \forall v, v_* \in \mathbb{R}^3.$$

(H4) La partie angulaire satisfait une forme forte de la condition de troncature angulaire de Grad [105]. En particulier, il existe une constante  $C > 0$  telle que

$$0 < b_{ij}(\cos \vartheta) \leq C |\sin \vartheta| |\cos \vartheta| \quad \text{et} \quad b'_{ij}(\cos \vartheta) \leq C, \quad \forall \vartheta \in [0, \pi].$$

Enfin, nous supposons que la condition suivante est vérifiée pour tout  $1 \leq i \leq N$  :

$$\inf_{\sigma_1, \sigma_2 \in \mathbb{S}^2} \int_{\mathbb{S}^2} \min\{b_{ii}(\sigma_1 \cdot \sigma_3), b_{ii}(\sigma_2 \cdot \sigma_3)\} d\sigma_3 > 0.$$

Les propriétés de symétrie des sections efficaces, combinées avec les mêmes changements de variable  $(v, v_*) \mapsto (v', v'_*)$  et  $(v, v_*) \mapsto (v_*, v)$  utilisés précédemment, nous permettent alors de dériver les nouvelles formulations faibles, pour tous  $1 \leq i, j \leq N$ ,

$$\int_{\mathbb{R}^3} Q_{ij}(F_i, F_j)(v) \psi_i(v) dv = \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) F_i F_j^* (\psi'_i - \psi_i) dv dv_* d\sigma, \quad (1.1.13)$$

$$\begin{aligned} \int_{\mathbb{R}^3} Q_{ij}(F_i, F_j)(v) \psi_i(v) dv + \int_{\mathbb{R}^3} Q_{ji}(F_j, F_i)(v) \psi_j(v) dv = \\ -\frac{1}{2} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) (F'_i F'_j - F_i F_j^*) (\psi'_i + \psi'_j - \psi_i - \psi_j^*) dv dv_* d\sigma, \end{aligned} \quad (1.1.14)$$

pour toute fonction test  $\boldsymbol{\psi} = (\psi_1, \dots, \psi_N) : \mathbb{R}^3 \rightarrow \mathbb{R}^N$  telle que les intégrales à gauche sont bien définies. La relation (1.1.14) nous permet de constater pour la première fois l'effet des interactions entre différentes espèces : nous ne pouvons pas espérer déduire des propriétés de conservation, autre que la masse, impliquant chaque espèce séparément. Plus précisément, (1.1.13) et (1.1.14) nous disent que l'égalité

$$\sum_{i=1}^N \int_{\mathbb{R}^3} Q_i(\mathbf{F}, \mathbf{F})(v) \psi_i(v) dv = 0 \quad (1.1.15)$$

est vérifiée si et seulement si  $\boldsymbol{\psi}$  est un invariant de collision pour le mélange, notamment

$$\boldsymbol{\psi} \in \text{Vect}(\mathbf{e}^{(1)}, \dots, \mathbf{e}^{(N)}, v_1 \mathbf{m}, v_2 \mathbf{m}, v_3 \mathbf{m}, |v|^2 \mathbf{m}), \quad (1.1.16)$$

où  $\mathbf{e}^{(i)} = (\delta_{ij})_{1 \leq j \leq N}$  for  $1 \leq i \leq N$ , et  $\mathbf{m} = (m_1, \dots, m_N)$ .

Enfin, avec le choix  $\boldsymbol{\psi}(v) = \left( \ln \frac{F_1(v)}{m_1^3}, \dots, \ln \frac{F_N(v)}{m_N^3} \right)$ , la relation (1.1.14) induit aussi l'inégalité

$$\sum_{i=1}^N \int_{\mathbb{R}^3} Q_i(\mathbf{F}, \mathbf{F})(v) \ln \frac{F_i(v)}{m_i^3} dv \leq 0. \quad (1.1.17)$$

### Théorème H pour mélanges et nouveaux équilibres

La version multi-espèce du théorème H [70] nous dit que les distributions  $\mathbf{F} = (F_1, \dots, F_N)$  vérifiant, pour tous  $1 \leq i, j \leq N$ ,

$$Q_{ij}(F_i, F_j)(v) = 0, \quad \forall v \in \mathbb{R}^3, \quad (1.1.18)$$

sont les mêmes qui annulent la fonctionnelle

$$S(\mathbf{F}) = \sum_{i=1}^N \int_{\mathbb{R}^3} Q_i(\mathbf{F}, \mathbf{F})(v) \ln \frac{F_i(v)}{m_i^3} dv.$$

De plus, toutes ces solutions  $\mathbf{F}$  ont la forme d'une distribution de Maxwell locale donnée, pour tout  $t \in \mathbb{R}_+$ ,  $x \in \mathbb{T}^3$  et  $v \in \mathbb{R}^3$ , par

$$F_i(t, x, v) = c_i(t, x) \left( \frac{m_i}{2\pi K_B \theta(t, x)} \right)^{3/2} \exp \left\{ -m_i \frac{|v - u(t, x)|^2}{2K_B \theta(t, x)} \right\}, \quad 1 \leq i \leq N, \quad (1.1.19)$$

où les quantités  $(c_i)_{1 \leq i \leq N}$ ,  $u$  et  $\theta$  représentent les observables physiques locales du mélange.

Nous pouvons alors dériver les états d'équilibre globaux, c'est-à-dire toutes les distributions (1.1.19) qui annulent l'opérateur de transport,  $v \cdot \nabla_x \mathbf{F} = 0$ . Celles-ci auront la forme d'une maxwellienne globale  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_N)$  donnée pour tout  $1 \leq i \leq N$  par

$$\mu_i(v) = c_{i,\infty} \left( \frac{m_i}{2\pi K_B \theta_\infty} \right)^{3/2} \exp \left\{ -m_i \frac{|v - u_\infty|^2}{2K_B \theta_\infty} \right\}, \quad v \in \mathbb{R}^3, \quad (1.1.20)$$

où les observables

$$c_{i,\infty} = \int_{\mathbb{R}^3} \mu_i(v) dv, \quad 1 \leq i \leq N,$$

$$\rho_\infty u_\infty = \sum_{i=1}^N \int_{\mathbb{R}^3} m_i v \mu_i(v) dv, \quad \frac{3}{2} K_B \rho_\infty \theta_\infty = \sum_{i=1}^N \int_{\mathbb{R}^3} \frac{m_i}{2} |v - u_\infty|^2 \mu_i(v) dv,$$

sont préservées pour tout temps  $t \geq 0$  grâce aux propriétés de conservation de l'opérateur de collision  $\mathbf{Q}$ . Ici,  $c_{i,\infty}$  représente le nombre total de particules de l'espèce  $\mathcal{E}_i$  et on a aussi défini la masse totale du mélange  $\rho_\infty = \sum_{i=1}^N m_i c_{i,\infty}$ , sa quantité de mouvement totale  $\rho_\infty u_\infty$  et son énergie totale  $\frac{3}{2} K_B \rho_\infty \theta_\infty$ . Notons que les états d'équilibre (locaux et globaux) sont caractérisés par une vitesse d'ensemble et une température communes à toutes les espèces. On en déduit en particulier qu'une maxwellienne locale  $\mathbf{M} = (M_1, \dots, M_N)$  construite à partir de valeurs arbitraires  $c_i \in \mathbb{R}$ ,  $u_i \in \mathbb{R}^3$ ,  $\theta_i \in \mathbb{R}$ ,  $1 \leq i \leq N$ , et ayant la forme

$$M_i(v) = c_i \left( \frac{m_i}{2\pi K_B \theta_i} \right)^{3/2} \exp \left\{ -m_i \frac{|v - u_i|^2}{2K_B \theta_i} \right\}, \quad v \in \mathbb{R}^3,$$

ne sera pas un état d'équilibre pour le mélange, ni solution des équations (1.1.18). C'est une caractéristique remarquable du modèle qui diversifie considérablement le panorama des états d'équilibre par rapport à l'équation de Boltzmann mono-espèce. Nous verrons pourtant dans la suite que ces états maxwelliens locaux de non-équilibre seront l'outil fondamental à la base de notre étude.

Pour conclure, nous pouvons à nouveau définir la fonctionnelle d'entropie associée à la solution  $\mathbf{F}$

$$H(\mathbf{F}) = \sum_{i=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} F_i \log \frac{F_i}{m_i^3} dx dv,$$

et l'équation (1.1.11) montre formellement que  $H$  est liée à la fonctionnelle de production d'entropie  $S$  par la relation

$$\frac{d}{dt} H(\mathbf{F}) = \int_{\mathbb{T}^3} S(\mathbf{F}) dx \leq 0,$$

et l'on peut ainsi déterminer un mécanisme de retour à l'équilibre similaire à celui vu précédemment.

## 1.2 Méthodologie et origine des problèmes étudiés

Les résultats établis par Boltzmann ont été fortement critiqués à l'époque. En effet, il paraissait douteux<sup>6</sup> de pouvoir obtenir un comportement irréversible (conséquence de la

6. Nous rappelons notamment les paradoxes formulés par Loschmidt et par Zermelo, qui furent infirmés par Boltzmann même.

décroissance de la fonctionnelle d'entropie) à partir des dynamiques réversibles des équations de Newton. Néanmoins, ces nouvelles théories ont réussi à s'imposer rapidement dans la communauté mathématique, en particulier grâce aux contributions de Hilbert. L'une des questions cruciales concernait la dérivation des équations d'Euler et de Navier-Stokes à partir des équations de la mécanique classique. L'histoire de cette problématique remonte au début du XX<sup>e</sup> siècle quand Hilbert la posa [119] pour la première fois au Congrès International des Mathématiciens qui eut lieu à Paris en 1900. L'idée de Hilbert était d'utiliser l'équation de Boltzmann pour connecter les deux descriptions, microscopique et macroscopique. Nous savons aujourd'hui que la bonne échelle pour établir l'équation de Boltzmann à partir d'un système de particules gouverné par les lois de Newton est la limite de Boltzmann-Grad [105]. Sa dérivation rigoureuse a été obtenue dans le cadre des sphères dures par Lanford en 1964 [143], pour des temps très courts, et a été ensuite étendue à des intervalles de temps arbitrairement grands dans la série de travaux [128, 129, 130]. En revanche, le passage du niveau mésoscopique au macroscopique est étroitement lié à la problématique du retour à l'équilibre thermodynamique, condition nécessaire afin d'établir les modèles fluides. Pour assurer la validité de ce phénomène, nous sommes d'abord amenés à développer une théorie rigoureuse de relaxation vers l'état d'équilibre global du gaz.

### 1.2.1 Théorie quantitative du retour à l'équilibre thermodynamique

L'objectif de la théorie quantitative du retour à l'équilibre thermodynamique consiste à étudier le comportement d'une solution en temps grand, afin de montrer qu'elle converge asymptotiquement vers la maxwellienne globale (1.1.9) qui lui est associée. De plus, elle vise à déterminer explicitement la vitesse de cette convergence pour quantifier le temps du retour à l'équilibre. Une telle estimation est cruciale car l'hypothèse de chaos moléculaire, à la base de la dérivation du modèle de Boltzmann, est raisonnable seulement en temps fini. Plus précisément, elle suppose que chaque particule constituant le gaz n'est corrélée à une autre particule qu'après leur collision. Cela implique que la validité de l'équation de Boltzmann est limitée à un ordre de  $\mathcal{N}_A \sim 10^{23}$  (le nombre d'Avogadro) unités de temps, l'instant au bout duquel chaque particule aura collisionné avec une fraction non négligeable des autres particules. Il est donc nécessaire de s'assurer que l'équilibre est atteint bien avant ce temps critique.

Une réponse satisfaisante à cette difficulté n'a été découverte que récemment, dans le cadre de l'équation de Boltzmann mono-espèce. En effet, nous pouvons faire remonter aux années 1930 le premier résultat de retour à l'équilibre, établi par Carleman [51] pour les solutions spatialement homogènes et pour des noyaux de collision de type sphères dures ( $\gamma = 1$ ) avec troncature angulaire<sup>7</sup>. Cependant, cet article et les travaux dans sa lignée utilisent une méthode basée sur la compacité de l'opérateur de collision et ils sont donc non constructifs. C'est seulement dans les années 1990 que l'on observe un renouveau des techniques, avec la naissance de la *méthode d'entropie*. L'idée à la base de cette approche [7, 192] est de quantifier la production d'entropie du système à l'aide d'une inégalité du type

$$S(F) \leq -\Theta(H(F|\mu)),$$

où  $H(F|\mu) = H(F) - H(\mu) \geq 0$  désigne l'entropie relative par rapport à l'équilibre global (1.1.9) et  $\Theta$  est une fonction strictement positive sur  $\mathbb{R}_+$ . Formellement, on peut déduire

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7. Plus précisément, Carleman a montré l'existence d'au moins une solution dans l'espace physique  $L^1$  et sa convergence vers l'équilibre global, sans déterminer le type de convergence. Nous soulignons que ce résultat a été ensuite amélioré à la fin des années 1980 par Arkeryd [6], qui a réussi à obtenir pour la première fois un taux de convergence exponentiel (mais toujours non explicite).

du théorème  $H$  et de cette inégalité l'estimation

$$\frac{d}{dt}H(F|\mu) \leq -\Theta(H(F|\mu)),$$

permettant d'obtenir la convergence explicite de  $F$  vers  $\mu$ , en ayant assez d'informations sur la forme de  $\Theta$ . Après les travaux de Carlen et Carvalho [53, 54] qui ont initié la méthode, les articles fondamentaux [185, 191] ont pu montrer que, pour tout  $\delta > 0$  et sous certaines hypothèses naturelles sur la régularité et la décroissance de la solution  $F$ , il existe une constante explicite  $C_{\delta,F} > 0$  telle que

$$S(F) \leq -C_{\delta,F}H(F|\mu)^{1+\delta}.$$

À partir de ce résultat, au début des années 2000, Desvillettes et Villani [71] obtiennent finalement un retour à l'équilibre pour l'équation de Boltzmann non homogène, dans des espaces de Sobolev infiniment réguliers et à poids polynomiaux. De plus, la vitesse de cette convergence est explicite, d'ordre  $\mathcal{O}(t^{-1/\delta})$  pour tout  $\delta > 0$ .

Malheureusement, la théorie non linéaire ne fournit pas la bonne échelle de temps physique pour la convergence vers l'équilibre, *i.e.* le taux de retour exponentiel prévu par les résultats non constructifs d'Arkeryd [6]. Néanmoins, elle assure qu'une solution suffisamment régulière de l'équation de Boltzmann (1.1.2) se trouvera dans un voisinage de l'équilibre global  $\mu$  qui lui est associé, au bout d'un certain temps fini. L'idée est alors de considérer des solutions qui sont proches de  $\mu$ , en un sens à préciser. C'est le point de départ de la théorie perturbative des solutions, qui permet de compléter le cadre de la problématique du retour quantitatif à l'équilibre thermodynamique.

## Théorie perturbative des solutions

La théorie perturbative a été initiée par Hilbert [120] et ensuite largement développée par Carleman [51] et Grad [105, 106]. Elle suppose de pouvoir décomposer toute solution de l'équation de Boltzmann (1.1.2) en une somme  $F = \mu + f$ , et elle étudie les variations  $f$  autour de l'état stationnaire  $\mu$ . Puisque ce dernier dépend seulement de la variable  $v$ , et puisque le théorème  $H$  implique  $Q(\mu, \mu) = 0$ , l'évolution de  $f = f(t, x, v)$  est modélisée par l'équation

$$\partial_t f + v \cdot \nabla_x f = L(f) + Q(f, f) \quad \text{sur } \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3, \quad (1.2.1)$$

où nous avons défini l'opérateur de Boltzmann linéarisé autour de l'équilibre global

$$\begin{aligned} L(f) &= Q(\mu, f) + Q(f, \mu) \\ &= \int_{\mathbb{R}^3 \times \mathbb{S}^2} B(|v - v_*|, \cos \vartheta) (\mu' f'^* + \mu'^* f' - \mu f^* - \mu^* f) dv_* d\sigma. \end{aligned}$$

Si nous introduisons l'espace à poids  $L^2(\mathbb{R}^3, \mu^{-\frac{1}{2}})$  défini par son produit scalaire et sa norme

$$\langle f, g \rangle_{L_v^2(\mu^{-\frac{1}{2}})} = \int_{\mathbb{R}^3} f g \mu^{-1} dv, \quad \|f\|_{L_v^2(\mu^{-\frac{1}{2}})}^2 = \langle f, f \rangle_{L_v^2(\mu^{-\frac{1}{2}})},$$

les propriétés de conservation microscopiques (1.1.1) et les mêmes changements de variable utilisés pour dériver les formulations faibles de  $Q$  nous donnent la relation fondamentale

$$\begin{aligned} \langle L(f), f \rangle_{L_v^2(\mu^{-\frac{1}{2}})} &= -\frac{1}{4} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B(|v - v_*|, \cos \vartheta) \\ &\quad \times \left( \frac{f'}{\mu'} + \frac{f'^*}{\mu'^*} - \frac{f}{\mu} - \frac{f^*}{\mu^*} \right)^2 \mu \mu^* dv dv_* d\sigma \leq 0. \end{aligned}$$

Celle-ci nous permet de déduire que  $L$  est un opérateur auto-adjoint et négatif dans l'espace  $L^2(\mathbb{R}^3, \mu^{-\frac{1}{2}})$ . De plus, nous pouvons l'utiliser pour dériver une version linéarisée du théorème  $H$  en définissant la fonctionnelle de production d'entropie linéaire<sup>8</sup>, ou forme de Dirichlet,

$$S_L(f) = \langle L(f), f \rangle_{L_v^2(\mu^{-\frac{1}{2}})} = \int_{\mathbb{R}^3} L(f) f \mu^{-1} dv.$$

La formulation faible de  $L$  nous dit en particulier que  $S_L(f) = 0$  si et seulement si  $f \in \ker L$ , c'est-à-dire  $f \in \text{Vect}(\mu, v_1\mu, v_2\mu, v_3\mu, |v|^2\mu)$ .

Dans ce cadre perturbatif des solutions, l'étude du problème de Cauchy pour l'équation (1.2.1) et la quantification du retour à l'équilibre thermodynamique se réduisent alors à une étude de stabilité du spectre de l'opérateur  $L - v \cdot \nabla_x$ . Dans les années 1960, Grad [107, 108] réussit à prouver avec une approche non constructive l'existence d'un trou spectral en vitesse pour l'opérateur linéarisé  $L$  (avec potentiels durs et troncature angulaire). On peut réinterpréter son résultat comme une estimation de coercivité sur la forme de Dirichlet  $S(L)$ . Plus précisément, il est possible de montrer [57, 59] que

$$\langle L(f), f \rangle_{L_v^2(\mu^{-\frac{1}{2}})} \leq -\lambda_L \|f - \pi_L(f)\|_{L_v^2(\mu^{-\frac{1}{2}})}^2, \quad \forall f \in L^2(\mathbb{R}^3, \mu^{-\frac{1}{2}}), \quad (1.2.2)$$

où  $\pi_L$  est la projection orthogonale sur  $\ker L$  et  $\lambda_L > 0$  est la plus petite des valeurs propres du spectre essentiel de  $-L$ , *i.e.* le trou spectral de  $L$ . Ceci a permis à Ukai [186, 187] d'établir unicité et existence globale en temps de la solution (sous forme perturbée) pour l'équation de Boltzmann non homogène et de montrer pour la première fois la convergence exponentielle de cette solution vers l'équilibre  $\mu$ . En utilisant une décomposition de l'équation (1.2.1) en modes de Fourier, il vise à obtenir des estimations de décroissance sur le semi-groupe engendré par l'opérateur  $L - v \cdot \nabla_x$ , afin de contrôler le reste  $Q$  et montrer la stabilité non linéaire autour de  $\mu$ . Malheureusement, puisque le taux du retour à l'équilibre dépend du trou spectral  $\lambda_L$ , la stratégie de cette approche s'appuie sur les méthodes non constructives de Grad et ne fournit donc aucune information explicite sur la vitesse de convergence (pensons par exemple à l'influence que pourraient avoir la donnée initiale ou les paramètres du modèle).

Toutefois, durant les mêmes années, Wang Chang *et al.* [194], puis Bobylev [26, 27] obtiennent une diagonalisation complète de l'opérateur linéarisé dans le cas des molécules maxwelliennes, ce qui leur permet de dériver une estimation explicite de  $\lambda_L$ . Au début des années 2000, ces résultats ouvrent la voie à une série d'articles [11, 159, 163] qui arrivent enfin à quantifier le trou spectral de  $L$  pour des noyaux de collision très généraux (dont le cas des potentiels durs avec troncature angulaire).

Parallèlement, l'émergence de la méthode d'entropie donne un nouvel élan au développement de la théorie perturbative. L'idée consiste à adapter les techniques de quantification de la production d'entropie non linéaire au cas linéaire, où l'on a accès à une décroissance exponentielle le long du semi-groupe de  $L$ . Nous citons les deux axes de recherche qui nous concernent de plus près. Dans les travaux de Guo *et al.* [113, 114, 181, 116, 46], basés sur une décomposition micro-macro de la perturbation  $f$ , un contrôle explicite de la partie fluide  $\pi_L(f)$  par la partie microscopique  $f - \pi_L(f)$  est obtenu dans des normes de Sobolev à poids contenant des dérivées temporelles. Cela permet de déduire les estimations d'énergie non linéaires nécessaires à récupérer la stabilité autour de l'équilibre global. Par ailleurs, la série de travaux [118, 193, 161, 117, 78, 80, 79, 40] s'insère dans le cadre de la théorie

8. Notons que la fonctionnelle d'entropie linéaire est simplement donnée par  $H_L(f) = \|f\|_{L_v^2(\mu^{-\frac{1}{2}})}^2$ .

de l'hypocoercivité. Cette approche vise à étudier certaines équations cinétiques caractérisées par l'effet combiné d'un opérateur anti-symétrique et conservatif avec un opérateur dissipatif et dégénéré, *i.e.* possédant un noyau qui inclut strictement l'espace des équilibres globaux de l'équation. Le but est alors de comprendre quel type de propriétés structurelles les deux opérateurs doivent satisfaire afin d'obtenir une dissipativité globale et la relaxation vers l'équilibre. Pour l'équation de Boltzmann (1.2.1), la problématique revient à analyser le couplage non trivial de l'opérateur de transport  $v \cdot \nabla_x$  et de l'opérateur linéarisé  $L$ . En utilisant le commutateur  $[v \cdot \nabla_x, \nabla_v] = -\nabla_x$ , Mouhot et Neumann [161] montrent alors qu'il est possible de construire une fonctionnelle d'entropie modifiée (par rapport à la fonctionnelle standard  $H_L$ ) qui fournit la convergence exponentielle et explicite vers  $\mu$ .

Ces nombreuses contributions offrent un cadre satisfaisant à l'étude du retour à l'équilibre thermodynamique, et la théorie perturbative des solutions s'est imposée en tant que complément essentiel à la méthode non linéaire précédemment évoquée, puisqu'elle a finalement permis de récupérer (et de quantifier) le résultat non constructif obtenu par Arkeryd [6]. De plus, les techniques développées par la théorie linéaire se sont également avérées d'importance cruciale afin d'établir les limites hydrodynamiques de l'équation de Boltzmann. Cela constitue alors la suite naturelle de notre présentation.

## 1.2.2 Limites hydrodynamiques de l'équation de Boltzmann

Considérons l'équation de Boltzmann non homogène mono-espèce. Afin de lier les régimes mésoscopique et macroscopique, la première étape consiste à se placer dans les bonnes échelles d'observation. Une possibilité est d'introduire un paramètre de scaling<sup>9</sup>  $\varepsilon > 0$  et d'opérer les changements de variable  $t' = \varepsilon^{r+1}t$  et  $x' = \varepsilon x$  dans (1.1.2), en fonction du taux de compressibilité<sup>10</sup> du fluide  $0 \leq r \leq 1$ . En continuant à nommer les variables rééchelonnées  $(t, x)$ , nous sommes amenés à étudier le problème adimensionné pour les distributions  $F^\varepsilon = F^\varepsilon(t, x, v)$

$$\varepsilon^r \partial_t F^\varepsilon + v \cdot \nabla_x F^\varepsilon = \frac{1}{\varepsilon} Q(F^\varepsilon, F^\varepsilon) \quad \text{sur } \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3. \quad (1.2.3)$$

Puisque la description macroscopique est légitime uniquement dans un régime physique où les collisions entre particules sont très fréquentes<sup>11</sup>, nous pouvons observer que toute limite hydrodynamique n'est dérivable que sous l'hypothèse  $\varepsilon \rightarrow 0$ . D'un point de vue formel, cela équivaut à imposer la relaxation vers un équilibre thermodynamique local où  $Q(F^\varepsilon, F^\varepsilon) = 0$ , condition qui est vérifiée par les seules distributions  $M_{(c,u,\theta)}$  de la forme (1.1.8).

Un exemple simple qui montre le lien entre l'équation de Boltzmann (1.2.3) et les équations fluides est donné par la limite d'Euler compressible, qui correspond au choix de scaling  $r = 0$ . En effet, si on multiplie les deux côtés de l'équation adimensionnée par les invariants de collision (1.1.6) et si on intègre en  $v$ , les propriétés de conservation (1.1.5) de  $Q$  nous donnent les relations

$$\partial_t \int_{\mathbb{R}^3} F^\varepsilon \psi(v) dv + \nabla_x \cdot \int_{\mathbb{R}^3} v F^\varepsilon \psi(v) dv = 0, \quad \psi(v) = 1, v_1, v_2, v_3, |v|^2, \quad (1.2.4)$$

9. C'est le nombre de Knudsen  $\text{Kn} = \frac{l}{L}$ , une grandeur adimensionnelle qui mesure le régime d'écoulement d'un fluide. Il est donné par le rapport entre le libre parcours moyen  $l$  d'un atome à l'intérieur du fluide et une longueur caractéristique  $L$  de l'échelle d'observation macroscopique.

10. La quantité  $\varepsilon^r$  correspond au nombre de Mach  $\text{Ma} = \frac{u_0}{c}$ , une grandeur adimensionnelle qui mesure la compressibilité d'un fluide. Il est donné par le rapport entre la vitesse locale  $u_0$  du fluide et la vitesse de son  $c$  à l'intérieur de ce même fluide.

11. En effet, physiquement le facteur  $1/\varepsilon$  représente le nombre moyen de collisions subies par une particule du gaz au cours d'une unité de temps macroscopique.



qui constituent les bilans de masse, de quantité de mouvement et d'énergie associé à (1.2.3). Sous l'hypothèse que  $\varepsilon \rightarrow 0$ , on peut alors choisir en première approximation  $F^\varepsilon = M_{(c,u,\theta)}$ . Un calcul direct des premiers moments permet de réécrire le système en terme des quantités  $c$ ,  $u$  et  $\theta$ , soit

$$\begin{cases} \partial_t c + \nabla_x \cdot (cu) = 0, \\ \partial_t(cu) + \nabla_x \cdot (cu \otimes u) + \nabla_x p = 0, \\ \partial_t E + \nabla_x \cdot ((E + p)u) = 0, \\ p = cK_B\theta, \quad E = \frac{1}{2}c(|u|^2 + 3K_B\theta), \end{cases} \quad (1.2.5)$$

où  $p$  et  $E$  représentent la pression et l'énergie totale du gaz. Ces équations constituent le système d'Euler compressible, dont la fermeture est garantie par la loi d'état des gaz parfaits  $p = cK_B\theta$ .

Comment généraliser alors cet exemple, ainsi que l'hypothèse  $F^\varepsilon = M_{(c,u,\theta)}$ , pour établir une approche plus rigoureuse à la dérivation des limites hydrodynamiques de l'équation de Boltzmann? Cette problématique possède plus d'un siècle d'histoire et a posé d'importantes difficultés à la fois d'un point de vue théorique et numérique. Nous évoquerons uniquement les résultats qui sont en lien direct avec les travaux présents dans ce manuscrit, mais le lecteur intéressé peut se référer aux articles de revue récents [189, 100, 176, 101, 75, 123] pour une description plus détaillée.

Essentiellement, nous pouvons classer les méthodes développées en deux groupes principaux : la méthode basée sur la théorie perturbative des solutions et la méthode des moments. Les techniques qui font partie de la première catégorie sont les plus anciennes et sont nées des travaux de Hilbert [120] et de Chapman et Enskog [84, 61]. Leurs idées sont très similaires et consistent à chercher une solution de l'équation de Boltzmann (1.2.3) sous forme d'une somme formelle infinie

$$F^\varepsilon(t, x, v) = f_0(t, x, v) + \sum_{n \geq 1} \varepsilon^n f_n(t, x, v).$$

Suivant la méthode de Hilbert, les  $f_n$  sont déterminées à partir d'équations obtenues en identifiant les coefficients des différentes puissance de  $\varepsilon$ , tandis que la méthode de Chapman-Enskog explicite les  $f_n$  en les faisant dépendre de  $v$  et des quantités fluides  $c$ ,  $u$  et  $\theta$  (voir [106, 57]). En revanche, la méthode des moments a été initiée par Grad [105, 106], puis étendue à un cadre mathématique plus général par Levermore [147]. Elle consiste à déterminer une hiérarchie d'équations satisfaites par les moments successifs de la solution  $F^\varepsilon$ , c'est-à-dire par les quantités  $\int_{\mathbb{R}^3} F^\varepsilon(t, x, v) v_1^{\alpha_1} v_2^{\alpha_2} v_3^{\alpha_3} dv$ . La fermeture du système est ensuite obtenue en utilisant un argument de minimisation de la fonctionnelle d'entropie. La limite d'Euler compressible (1.2.5) vue précédemment en est un exemple. Il est possible de montrer que la hiérarchie d'équations (1.2.4) peut être fermée en résolvant le problème de minimisation de l'entropie

$$\min \left\{ H(F^\varepsilon) = \int_{\mathbb{R}^3} F^\varepsilon \log F^\varepsilon dv, \quad F^\varepsilon(t, x, v) \geq 0, \right. \\ \left. \int_{\mathbb{R}^3} F^\varepsilon(t, x, v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = \begin{pmatrix} c \\ cu \\ c(|u|^2 + 3K_B\theta) \end{pmatrix} \right\},$$

qui a précisément comme unique solution la maxwellienne locale  $F^\varepsilon = M_{(c,u,\theta)}$ .

Que ce soit par un développement de Hilbert/Chapman-Enskog ou par un calcul des moments à la Grad, sous la condition  $\varepsilon \rightarrow 0$ , il est alors possible d'établir formellement

- les équations d'Euler compressible (1.2.5) quand  $r = 0$  ;
- toujours dans le cas  $r = 0$ , les équations de Navier-Stokes compressible asymptotique, avec un terme de viscosité<sup>12</sup> en  $\mathcal{O}(\varepsilon)$  ;
- les équations d'Euler incompressible, pour les valeurs  $0 < r < 1$  du taux de compressibilité ;
- les équations de Navier-Stokes incompressible, dans le cas  $r = 1$  (limite diffusive de l'équation de Boltzmann).

Ces premières dérivations formelles ont ensuite été rendues rigoureuse par divers auteurs dans un cadre perturbatif autour d'un équilibre local  $M_{(c,u,\theta)}$  pour les limites compressibles [166, 48, 9, 49, 85, 8], ou d'un équilibre global  $\mu$  pour les limites incompressibles [83, 66, 15, 86]. En particulier, nous portons notre attention sur l'article [66] qui sert d'inspiration à une partie du travail de cette thèse. En utilisant une approche similaire à celle de Cafisch [48] pour la dérivation des équations d'Euler compressible, les auteurs montrent la convergence de l'équation de Boltzmann (1.2.3) vers les équations de Navier-Stokes incompressible, dans la limite diffusive  $r = 1$  et  $\varepsilon \rightarrow 0$ . Plus précisément, ils prouvent que toute solution  $F^\varepsilon$  assez régulière de

$$\varepsilon \partial_t F^\varepsilon + v \cdot \nabla_x F^\varepsilon = \frac{1}{\varepsilon} Q(F^\varepsilon, F^\varepsilon) \quad \text{sur } \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3,$$

se stabilise (à un ordre  $\varepsilon^2$  près) autour d'un équilibre local  $M^\varepsilon = M_{(\bar{c}, \varepsilon u(t,x), \bar{\theta})}$  qui est caractérisé par une densité  $\bar{c}$  et une température  $\bar{\theta}$  constantes, et par une faible vitesse d'ensemble d'ordre  $\varepsilon$ . La quantité locale  $u(t, x)$  est alors une solution régulière des équations de Navier-Stokes incompressible

$$\begin{cases} \bar{c} \partial_t u + \bar{c} u \cdot \nabla_x u + \nabla_x p = \nu \Delta_x u, \\ \nabla_x \cdot u = 0, \end{cases}$$

où la pression  $p$  et le coefficient de viscosité  $\nu$  sont explicitement calculés en fonction de  $\bar{c}$ ,  $u$  et  $\bar{\theta}$ . Notons que la distribution  $M^\varepsilon$  va tendre vers  $M_{(\bar{c}, 0, \bar{\theta})}$  qui est l'équilibre thermodynamique prévu par les limites diffusives. L'originalité de cette approche consiste à intégrer la fluctuation autour de l'équilibre global  $M_{(\bar{c}, 0, \bar{\theta})}$  directement dans la vitesse macroscopique de la maxwellienne locale  $M^\varepsilon$ .

Malheureusement, les solutions de l'équation de Boltzmann qui sont construites par ces méthodes n'existent que localement en temps, puisqu'elles dépendent de la régularité de la solution du système hydrodynamique limite. C'est au début des années 1990 que les travaux fondateurs de Bardos, Golse et Levermore [12, 13, 14] ouvrent la voie aux résultats d'existence globale, qui se servent de techniques développées par la théorie du retour à l'équilibre. La méthode d'entropie est adaptée au cadre perturbatif par Golse et Saint-Raymond [102, 103] qui montrent la convergence rigoureuse des solutions faibles à la DiPerna et Lions [76] pour l'équation de Boltzmann (vues comme des fluctuations autour d'un équilibre global) vers les solutions faibles à la Leray [146] pour les équations de Navier-Stokes incompressible. Une décomposition micro-macro de la solution de (1.2.3) et la méthode d'énergie non linéaire [113, 114] sont utilisées dans [195, 124, 125, 149, 81] pour

12. Nous rappelons que la viscosité du régime limite est déterminée par le nombre de Reynolds  $\text{Re} = \frac{VL}{\nu}$ , une grandeur adimensionnelle donnée par le rapport entre une vitesse  $V$  et une longueur  $L$  caractéristiques du fluide, et sa viscosité cinématique  $\nu$ . La relation de von Karman  $\text{Re} = \frac{\text{Ma}}{\text{Kn}}$  permet alors de déduire l'ordre du terme de viscosité qui apparaît dans le système de Navier-Stokes compressible.

dériver la stabilité autour des équations d'Euler et Navier-Stokes compressibles. De façon similaire, dans [115], ces techniques sont combinées avec un développement asymptotique à la Caflisch afin de montrer la relaxation vers le système de Navier-Stokes incompressible. Enfin, le formalisme hypocoercif de [161] est adapté dans [43] au cadre de la limite diffusivité  $r = 1$  de l'équation de Boltzmann pour des noyaux de collision de type potentiels durs. La solution de (1.2.3) est écrite sous forme perturbée autour de l'équilibre global comme  $F^\varepsilon = \mu + \varepsilon f^\varepsilon$  et les fluctuations  $f^\varepsilon = f^\varepsilon(t, x, v)$  vérifient l'équation linéarisée

$$\partial_t f^\varepsilon + \frac{1}{\varepsilon} v \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon^2} L(f^\varepsilon) + \frac{1}{\varepsilon} Q(f^\varepsilon, f^\varepsilon) \quad \text{sur } \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3, \quad (1.2.6)$$

qui est la contrepartie adimensionnée de (1.2.1). En utilisant les estimations de trou spectral explicites de [159] et le retour négatif dominant du terme  $\varepsilon^{-2} L(f^\varepsilon)$ , l'auteur construit une fonctionnelle d'entropie linéaire modifiée (avec des coefficients dépendant du paramètre  $\varepsilon$ ) qui donne la convergence exponentielle et explicite de  $F^\varepsilon$  vers  $\mu$ , dans des espaces de Sobolev infiniment réguliers. De plus, il est possible de montrer que la suite  $(f^\varepsilon)_{0 < \varepsilon \leq 1}$  converge faiblement vers une fonction  $f$  ayant la forme

$$f(t, x, v) = \left( c(t, x) + v \cdot u(t, x) + \frac{1}{2} (|v|^2 - 3) \theta(t, x) \right) \mu(v),$$

dont les quantités macroscopiques associées sont solutions faibles au sens de Leray du système de Navier-Stokes incompressible

$$\begin{cases} \partial_t u + u \cdot \nabla_x u + \nabla_x p = \nu \Delta_x u, \\ \nabla_x \cdot u = 0, \\ \partial_t \theta + u \cdot \nabla_x \theta = \kappa \nabla_x \theta, \end{cases}$$

avec la relation de Boussinesq  $\nabla_x (c + \theta) = 0$ . En particulier, les coefficients de viscosité  $\nu$  et de conductivité thermique  $\kappa$  sont déterminés en fonction de l'opérateur linéarisé  $L$ .

## Étude numérique des limites hydrodynamiques

Parallèlement aux contributions en analyse mathématique, nous observons l'émergence de nouvelles méthodes numériques pour simuler la transition entre les régimes mésoscopique et macroscopique de l'équation (1.2.3). Quand le paramètre  $\varepsilon$  est très proche de 0, il est légitime de prendre comme solution une maxwellienne locale  $M_{(c,u,\theta)}$  dont les quantités observables satisfont un certain système d'équations fluides qui peut être résolu numériquement avec des méthodes classiques [183, 98, 99]. De façon similaire, quand  $\varepsilon \sim 1$ , la difficulté numérique consiste essentiellement à construire un algorithme pour discrétiser l'opérateur de collision [167, 90, 169, 162]. En revanche, pour des valeurs intermédiaires du nombre de Knudsen, la description macroscopique n'est pas assez précise et les méthodes numériques développées pour l'équation de Boltzmann n'arrivent pas à gérer efficacement la raideur du terme non linéaire  $\varepsilon^{-1} Q(F^\varepsilon, F^\varepsilon)$ . Considérer des situations où  $\varepsilon \ll 1$  impose en particulier une contrainte sur les paramètres de discrétisation, qui doivent être réduits proportionnellement à  $\varepsilon$ . Ce choix entraîne l'émergence de phénomènes de diffusion numérique indésirables et l'explosion des temps de calcul dans la limite  $\varepsilon \rightarrow 0$ . Une méthode standard pourrait alors échouer à approcher correctement le problème étudié quand le libre parcours moyen des particules devient très petit.

Un schéma numérique capable de capturer à la fois les solutions physiques d'un modèle mathématique qui décrit un régime raréfié et les solutions de ses contreparties en

régime macroscopique en gardant les paramètres de discrétisation de temps et d'espace uniformes est qualifié de préservant l'asymptotique (*asymptotic preserving*, AP). Cette approche remonte au début des années 1990 et, depuis, elle a été largement utilisée pour traiter des nombreux problèmes d'asymptotique pour les modèles cinétiques et hyperboliques [64, 131, 50, 134, 104, 168, 132, 67]. En particulier, la littérature autour des schémas AP simulant le passage de l'équation de Boltzmann (1.2.3) aux équations hydrodynamiques est très vaste et se focalise principalement sur le cadre des scalings  $r = 0$  et  $r = 1$ . Plusieurs techniques se sont avérées efficaces pour simuler les limites d'Euler et de Navier-Stokes compressibles ( $r = 0$ ) dans un contexte très général (noyaux de collision de type potentiels durs avec troncature angulaire). Nous évoquons entre autres :

- les résultats utilisant une méthode de splitting pour l'équation de Boltzmann, qui permet de gérer l'opérateur de transport et le terme raide  $Q/\varepsilon$  séparément [91, 72]. La solution de (1.2.3) est approchée sur un intervalle de temps  $[t^n, t^n + \Delta t]$  en deux étapes

$$\frac{F^{n+\frac{1}{2}} - F^n}{\Delta t} = \frac{1}{\varepsilon} Q(F, F), \quad \text{puis} \quad \frac{F^{n+1} - F^{n+\frac{1}{2}}}{\Delta t} + v \cdot \nabla_x F = 0,$$

où nous avons défini la valeur numérique  $F^{n+\frac{1}{2}} \simeq F(t^n + \frac{\Delta t}{2})$ , et les opérateurs de collision et de transport sont discrétisés de façon explicite ou implicite selon la nécessité ;

- les travaux basés sur un développement de type Chapman-Enskog de la solution pour expliciter le système fluide limite. La décomposition micro-macro permet en particulier d'obtenir un système d'équations de transport couplées qui sont discrétisées de façon semi-implicite et sans splitting en temps [17, 144, 93] ;
- les schémas numériques IMEX basés sur une discrétisation implicite de l'opérateur de collision et explicite de l'opérateur de transport

$$\frac{F^{n+1} - F^n}{\Delta t} + v \cdot \nabla_x F^n = \frac{1}{\varepsilon} Q(F^{n+1}, F^{n+1}).$$

Puisque la raideur du problème est résolue, la difficulté se réduit à trouver une technique efficace pour l'inversion de l'opérateur  $Q$ . On peut en particulier citer les méthodes de Runge-Kutta [73, 74] et la méthode proposée par Filbet et Jin [89] qui consiste à pénaliser  $Q$  par un opérateur BGK linéaire  $P(F) = \beta(M_{(c,u,\theta)} - F)$ , où le coefficient  $\beta$  est choisi de sorte que  $Q \sim P$ . Comme le terme  $\varepsilon^{-1}(Q - P)$  est moins raide et  $P$  peut être inversé explicitement, la discrétisation de l'opérateur de collision est finalement donnée par

$$\frac{Q(F^n, F^n) - P(F^n)}{\varepsilon} + \frac{P(F^{n+1})}{\varepsilon}.$$

En revanche, pour l'asymptotique vers Navier-Stokes incompressible ( $r = 1$ ) les résultats sont encore partiels puisque la présence du facteur d'amplification  $\varepsilon^{-1}$  devant le terme de transport produit une nouvelle raideur le long des caractéristiques et entraîne l'impossibilité de découpler l'action des opérateurs  $Q$  et  $v \cdot \nabla_x$ . Par conséquent, les méthodes de splitting et les schémas IMEX ne sont plus applicables dans le cadre non linéaire de la limite de diffusion, tout comme la méthode micro-macro qui nécessiterait une discrétisation implicite de  $Q$  et donc des temps de calcul trop prohibitifs. Cependant, quand on se restreint au cas

d'opérateurs de collision linéaires, les résultats sont très variés. Nous citons par exemple les méthodes de décomposition de la solution en parties paire et impaire en vitesse [140, 135, 32], qui donnent un système d'équations de transport couplées où la raideur reste concentrée uniquement sur le terme de source, ainsi que les travaux qui utilisent la méthode micro-macro déjà évoquée [145, 144]. Enfin, nous rappelons également l'adaptation de la méthode des moments dans [55], où le système hydrodynamique limite peut être isolé de l'équation cinétique, permettant ainsi d'utiliser un *splitting* en temps qui élimine la raideur du terme de transport.

### 1.2.3 Le cadre multi-espèce : positionnement du problème

Une question naturelle qui se pose est de comprendre dans quelle mesure il est possible de généraliser les résultats théoriques et numériques que nous avons présentés au cadre des mélanges, pour le modèle (1.1.11). Il se trouve qu'une telle extension est difficile à établir, en raison de la structure de l'opérateur de collision multi-espèce (1.1.12). En effet, les interactions croisées entre particules de masses atomiques différentes jouent un rôle déterminant sur la dynamique du système, qui se traduit par une perte des propriétés de symétrie dans l'opérateur  $\mathbf{Q}$ . En conséquence, l'adaptation des méthodes développées dans le cadre mono-espèce est souvent complexe, voire parfois irréalisable. C'est pourquoi divers modèles cinétiques pour les mélanges ont été proposés à partir des années 1960 [179, 158, 111, 95, 41], mais leur analyse mathématique et numérique constitue un domaine de recherche actif, où les résultats sont encore partiels. Depuis le début des années 2000, plusieurs auteurs se sont notamment intéressés à l'étude du retour à l'équilibre thermodynamique et des limites fluides pour l'équation de Boltzmann multi-espèce. Que ce soit pour des gaz inertes ou réactifs, monoatomiques ou polyatomiques, cela a permis d'obtenir les extensions du théorème  $H$  [4, 70, 24, 47] et la dérivation des systèmes d'Euler et de Navier-Stokes (compressibles et incompressibles) pour les mélanges [16, 23, 70, 24, 77, 25, 22, 20, 18, 19, 10]. Toutefois, ces contributions sont valides uniquement à un niveau formel<sup>13</sup>.

Les seuls résultats rigoureux à notre connaissance viennent de la théorie perturbative des solutions. Celle-ci a été récemment étendue<sup>14</sup> avec succès, d'abord dans [65] pour des mélanges formés d'espèces avec même masse atomique ( $m_i = m_j$  pour tout  $1 \leq i, j \leq N$ ), puis par Briant et Daus [45] dans le cadre général d'espèces avec masses différentes  $m_i \neq m_j$ . Si l'on suppose pouvoir écrire la solution de (1.1.11) sous la forme  $\mathbf{F} = \boldsymbol{\mu} + \mathbf{f}$ , la perturbation  $\mathbf{f} = \mathbf{f}(t, x, v)$  satisfait l'équation

$$\partial_t \mathbf{f} + v \cdot \nabla_x \mathbf{f} = \mathbf{L}(\mathbf{f}) + \mathbf{Q}(\mathbf{f}, \mathbf{f}) \quad \text{sur } \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3, \quad (1.2.7)$$

où l'opérateur de collision  $\mathbf{L} = (L_1, \dots, L_N)$  linéarisé à partir de (1.1.12) est donné pour tout  $1 \leq i \leq N$  par

$$L_i(\mathbf{f}) = Q_i(\boldsymbol{\mu}, \mathbf{f}) + Q_i(\mathbf{f}, \boldsymbol{\mu}). \quad (1.2.8)$$

Cet opérateur possède un trou spectral explicite  $\lambda_{\mathbf{L}} > 0$  [45] dans l'espace

$$L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}) = \left\{ \mathbf{f} : \mathbb{R}^3 \rightarrow \mathbb{R}^N \text{ mesurable} : \|\mathbf{f}\|_{L^2_v(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 = \sum_{i=1}^N \int_{\mathbb{R}^3} f_i^2 \mu_i^{-1} dv < +\infty \right\},$$

13. Dans [16] les auteurs fournissent des justifications semi-rigoureuses à la dérivation des systèmes de Vlasov-Euler compressible et de Vlasov-Navier-Stokes incompressible, mais ils considèrent le cadre très simplifié d'un mélange avec seulement deux espèces.

14. Dans le cadre de mélanges de gaz inertes et monoatomiques et pour des noyaux de collision de type potentiels durs.

qui fournit une estimation de coercivité pour  $\mathbf{L}$  équivalente à (1.2.2). Il est alors possible de quantifier l'apport négatif du semi-groupe engendré par l'opérateur linéarisé le long des caractéristiques. Une adaptation des méthodes de Guo [112, 115] et une nouvelle représentation de Carleman pour  $\mathbf{L}$  permettent enfin d'obtenir l'unicité et l'existence globale de la solution sous forme perturbée, ainsi qu'une convergence exponentielle (avec un taux explicite qui dépend de  $\lambda_{\mathbf{L}}$ ) de  $\mathbf{F}$  vers  $\boldsymbol{\mu}$  dans des espaces  $L_x^\infty L_v^1(1 + |v|^k)$  à poids polynomiaux.

La dérivation rigoureuse des modèles hydrodynamiques pour les mélanges à partir de l'équation de Boltzmann multi-espèce reste en revanche un problème ouvert. Comme nous l'avons précédemment évoqué, il s'agit d'une question d'importance cruciale afin de justifier mathématiquement la cohérence des différentes échelles physiques de description (mésoscopique et macroscopique) et d'en comprendre les régimes de validité. Motivés par l'absence d'un tel résultat et par les avancements récents de la théorie perturbative, nous nous proposons d'apporter quelques nouvelles contributions dans cette direction. Plus précisément, ce travail vise d'une part à établir rigoureusement la limite de diffusion pour l'équation de Boltzmann multi-espèce vers le modèle macroscopique de diffusion de Maxwell-Stefan et de l'autre à étudier numériquement cette asymptotique. Le point de départ de notre étude est la série d'articles récents [39, 127, 35]. Nous en décrivons les passages clés afin de fixer le cadre de la thèse.

## Le modèle de diffusion de Maxwell-Stefan

On s'intéresse à la modélisation d'un mélange de  $N \geq 2$  gaz parfaits, inertes et monoatomiques, qui interagissent dans le tore  $\mathbb{T}^3$  selon un processus isotherme et isobare, caractérisé par des dynamiques purement diffusives (aucun effet de convection n'est présent). Puisque la température  $T > 0$  du milieu est supposée constante, nous pouvons décrire l'état physique de chaque espèce  $\mathcal{E}_i$ ,  $1 \leq i \leq N$ , à travers les observables macroscopiques qui sont le nombre de particules  $c_i = c_i(t, x)$  présentes en  $x \in \mathbb{T}^3$  à l'instant  $t \geq 0$  et le flux  $\mathcal{F}_i = \mathcal{F}_i(t, x)$  associé. Nous nous attendons alors à ce que l'évolution du système soit complètement déterminée par les conservations de masse et de quantité de mouvement de chaque espèce. D'un côté, la conservation de la masse est donnée sous la forme d'une équations de continuité, pour tout  $1 \leq i \leq N$ ,

$$\partial_t c_i + \nabla_x \cdot \mathcal{F}_i = 0 \quad \text{sur } \mathbb{R}_+ \times \mathbb{T}^3. \quad (1.2.9)$$

Par ailleurs, si nous définissons également le nombre total de particules  $c = \sum_i c_i$  et la fraction molaire  $n_i = c_i/c$  de chaque espèce  $\mathcal{E}_i$ , la conservation de la quantité de mouvement fournit des conditions pour relier les gradients de concentration  $(\nabla_x n_i)_{1 \leq i \leq N}$  aux flux  $(\mathcal{F}_i)_{1 \leq i \leq N}$ . En particulier, ces relations modélisent la diffusion à l'intérieur du mélange.

Dans le cas d'un milieu binaire ( $N = 2$ ), la loi de Fick [88] fournit une description satisfaisante. Classiquement, elle traduit l'idée que les particules diffusent des régions à plus forte concentration vers les régions à plus faible concentration. Le transfert de matière se réduit alors à une dépendance linéaire entre  $\nabla_x n_i$  et  $\mathcal{F}_i$ . Plus précisément, nous avons les équations

$$\mathcal{F}_1 = -cD\nabla_x n_1, \quad \mathcal{F}_2 = -cD\nabla_x n_2, \quad \text{sur } \mathbb{R}_+ \times \mathbb{T}^3,$$

où  $D > 0$  est le coefficient de diffusion entre les deux espèces considérées. En revanche, pour des milieux multi-espèces à  $N \geq 3$  composantes, une telle description n'est plus valable en général. Nous citons en particulier l'expérience de Duncan et Toor [82] pour un mélange gazeux ternaire, où l'on observe l'apparition de phénomènes de *diffusion remontante* (les particules diffusent vers des régions à plus forte concentration).

Cette expérience a mis en évidence les équations de Maxwell-Stefan [141], qui s'écrivent, pour tout  $1 \leq i \leq N$ ,

$$-c \nabla_x n_i = \frac{1}{c} \sum_{j \neq i} \frac{c_j \mathcal{F}_i - c_i \mathcal{F}_j}{D_{ij}} \quad \text{sur } \mathbb{R}_+ \times \mathbb{T}^3, \quad (1.2.10)$$

où les coefficients  $D_{ij} = D_{ji} > 0$  décrivent la diffusion binaire entre les espèces  $\mathcal{E}_i$  et  $\mathcal{E}_j$ . Introduites indépendamment par Maxwell [153] pour les gaz peu denses et par Stefan [180] pour les liquides, ces équations se voient aujourd'hui appliquées dans de multiples domaines. En chimie physique par exemple, pour modéliser la diffusion des polluants dans l'air (les particules fines, les oxydes d'azote, le dioxyde de soufre, etc.) et le mécanisme de leur interaction avec le processus respiratoire; mais aussi en médecine, pour décrire les échanges gazeux dans les générations plus profondes du poumon humain, afin d'étudier l'impact de certains aérosols thérapeutiques sur les pathologies respiratoires appartenant à la catégorie des bronchopneumopathies chroniques obstructives [184, 60, 34]. À côté de leur utilité applicative, les équations de Maxwell-Stefan suscitent aussi un grand intérêt académique, puisque l'étude mathématique de ce genre de modèles (dits de *diffusion croisée*) est particulièrement complexe [62, 68, 137], à cause des dépendances non linéaires entre les quantités en jeu. Commençons par analyser le lien des équations de Maxwell-Stefan avec le modèle cinétique de Boltzmann multi-espèce, puis nous décrirons les résultats principaux connus sur ce modèle macroscopique.

### La limite diffusive de Boltzmann mélanges vers Maxwell-Stefan

Considérons le système d'équations de Boltzmann (1.1.11), adimensionné avec un scaling diffusif<sup>15</sup>  $(t, x) \mapsto (t/\varepsilon^2, x/\varepsilon)$ . Pour tout  $\varepsilon \in (0, 1]$ , l'évolution du mélange gazeux est alors décrite par une fonction de distribution  $\mathbf{F}^\varepsilon = (F_1^\varepsilon, \dots, F_N^\varepsilon)$  dont les composantes vérifient, pour tout  $1 \leq i \leq N$ ,

$$\varepsilon \partial_t F_i^\varepsilon + v \cdot \nabla_x F_i^\varepsilon = \frac{1}{\varepsilon} \sum_{i=1}^N Q_{ij}(F_i^\varepsilon, F_j^\varepsilon) \quad \text{sur } \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3. \quad (1.2.11)$$

Par le biais de la méthode des moments de Grad, la première dérivation formelle du modèle de Maxwell-Stefan (1.2.9)–(1.2.10) à partir des équations (1.2.11) a été obtenue dans [39] pour des noyaux de collision de type molécules de Maxwell. Ce résultat a ensuite été étendu dans [127] à des sections efficaces analytiques et généralisé dans [35] à des noyaux de collision vérifiant uniquement des propriétés d'invariance galiléenne et la troncature angulaire de Grad. L'idée majeure de tous ces travaux consiste à introduire l'ansatz suivant. Il existe deux fonctions  $c_i^\varepsilon : \mathbb{R}_+ \times \mathbb{T}^3 \rightarrow \mathbb{R}$  et  $u_i^\varepsilon : \mathbb{R}_+ \times \mathbb{T}^3 \rightarrow \mathbb{R}^3$ , restant  $\mathcal{O}(1)$  quand  $\varepsilon$  tend vers 0, telles que  $\mathbf{F}^\varepsilon$  s'écrit sous forme d'une maxwellienne locale  $\mathbf{M}^\varepsilon$  donnée, composante par composante, par

$$M_i^\varepsilon(t, x, v) = c_i^\varepsilon(t, x) \left( \frac{m_i}{2\pi K_B T} \right)^{3/2} \exp \left\{ -m_i \frac{|v - \varepsilon u_i^\varepsilon(t, x)|^2}{2K_B T} \right\}, \quad t \geq 0, \quad x \in \mathbb{T}^3, \quad v \in \mathbb{R}^3, \quad (1.2.12)$$

où  $m_i$  représente la masse atomique de l'espèce  $\mathcal{E}_i$  et  $T > 0$  est la température uniforme (en espace) et constante (en temps) du milieu considéré. Il est important de souligner que, contrairement au cas mono-espèce, les distributions (1.2.12) ne constituent pas un état

15. Cela correspond à choisir le paramètre de compressibilité  $r = 1$ . Physiquement, les nombres de Mach et de Knudsen sont alors du même ordre de grandeur  $\text{Ma} = \text{Kn} = \varepsilon \ll 1$ .

d'équilibre dynamique pour le mélange gazeux, puisque les vitesses macroscopiques diffèrent d'une espèce à l'autre. Toutefois, d'un point de vue formel, les quantités  $(\varepsilon u_i^\varepsilon)_{1 \leq i \leq N}$  restent proches de zéro si  $\varepsilon \ll 1$ , ce qui implique que  $\mathbf{M}^\varepsilon$  est censée converger, quand  $\varepsilon$  tend vers 0, vers un état d'équilibre global ayant une vitesse macroscopique nulle. Cet aspect est crucial dans la suite de notre analyse.

Dans ce contexte, si nous intégrons par rapport à  $v \in \mathbb{R}^3$  les équations (1.2.11) contre les fonctions test

$$\varphi_i(v) = \mathbf{e}^{(i)}, \quad \psi_i(v) = v \mathbf{m}^{(i)}, \quad \phi(v) = \frac{1}{2}|v|^2 \mathbf{m}, \quad 1 \leq i \leq N,$$

nous obtenons les  $2N + 1$  équations qui traduisent les bilans de masse et de quantité de mouvement de chaque espèce  $\mathcal{E}_i$ ,  $1 \leq i \leq N$ , et le bilan de l'énergie totale du système. L'application des propriétés de conservation des opérateurs de collision mono-espèce et bi-espèce et un calcul direct des premiers moments de  $\mathbf{M}^\varepsilon$  nous donnent alors, pour tout  $1 \leq i \leq N$ , la hiérarchie d'équations

$$\begin{aligned} \partial_t c_i^\varepsilon + \nabla_x \cdot (c_i^\varepsilon u_i^\varepsilon) &= 0, \\ \varepsilon^2 \frac{m_i}{K_B T} \left[ \partial_t (c_i^\varepsilon u_i^\varepsilon) + \nabla_x (c_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon) \right] + \nabla_x c_i^\varepsilon &= \frac{1}{\varepsilon K_B T} \sum_{j \neq i} \int_{\mathbb{R}^3} m_i v Q_{ij}(F_i^\varepsilon, F_j^\varepsilon) dv, \end{aligned} \quad (1.2.13)$$

$$3\partial_t c^\varepsilon + 5\nabla_x \cdot (c^\varepsilon u^\varepsilon) + \varepsilon^2 \sum_{i=1}^N \left[ \frac{m_i}{K_B T} \partial_t (c_i^\varepsilon |u_i^\varepsilon|^2) + \nabla_x \cdot (c_i^\varepsilon u_i^\varepsilon |u_i^\varepsilon|^2) \right] = 0,$$

en notant  $c^\varepsilon u^\varepsilon = \sum_i c_i^\varepsilon u_i^\varepsilon$ . Sous l'hypothèse que pour tout  $1 \leq i \leq N$ ,  $c_i^\varepsilon$  tend vers  $c_i$  et  $u_i^\varepsilon$  vers  $u_i$ , le terme intégral converge [35]

$$\frac{1}{\varepsilon K_B T} \sum_{j \neq i} \int_{\mathbb{R}^3} m_i v Q_{ij}(F_i^\varepsilon, F_j^\varepsilon) dv \xrightarrow{\varepsilon \rightarrow 0} - \sum_{j \neq i} c_i c_j \frac{u_i - u_j}{\Delta_{ij}}, \quad 1 \leq i \leq N,$$

où les coefficients  $\Delta_{ij}$  sont positifs, forment une matrice symétrique, et peuvent être explicitement calculés en fonction des masses atomiques  $m_i$ , des sections efficaces  $B_{ij}$  et des constantes  $K_B$  et  $T$ . Ainsi, il est possible de montrer que le système (1.2.13) converge formellement, pour tout  $1 \leq i \leq N$  et pour tout  $t \in \mathbb{R}_+$  et  $x \in \mathbb{T}^3$ , vers

$$\partial_t c_i + \nabla_x \cdot (c_i u_i) = 0, \quad (1.2.14)$$

$$-\nabla_x c_i = \sum_{j \neq i} \frac{c_i c_j u_i - c_i c_j u_j}{\Delta_{ij}}, \quad (1.2.15)$$

$$\partial_t \left( \sum_{i=1}^N c_i \right) = 0, \quad \nabla_x \cdot \left( \sum_{i=1}^N c_i u_i \right) = 0. \quad (1.2.16)$$

En sommant sur  $i$  les équations (1.2.15), on obtient la relation

$$\nabla_x \left( \sum_{i=1}^N c_i(t, x) \right) = 0, \quad t \geq 0, \quad x \in \mathbb{T}^3,$$

qui, combinée à (1.2.16), permet de déduire que le nombre total  $c$  de particules du mélange reste uniforme en espace et constant en temps. En définissant alors  $D_{ij} = \Delta_{ij}/c$  et les flux  $\mathcal{F}_i = c_i u_i$ , pour tout  $1 \leq i \leq N$ , nous récupérons enfin les équations de continuité



(1.2.9) et les équations de Maxwell-Stefan (1.2.10), couplées avec la condition d'incompressibilité (1.2.16).

Comprendre la méthode sous-jacente à la dérivation formelle des limites hydrodynamiques est fondamental pour cibler une bonne stratégie de preuve rigoureuse de la convergence. Par exemple, dans le cadre mono-espèce, les méthodes de Hilbert et de Chapman-Enskog suggéraient d'étudier les systèmes macroscopiques d'Euler compressible et de Navier-Stokes incompressible comme étant des perturbations de l'équation de Boltzmann autour d'un état d'équilibre local  $M_{(c,u,\theta)}$  (pour Euler) ou global  $\mu$  (pour Navier-Stokes). Voyons comment la même idée s'applique dans ce cadre multi-espèce.

### 1.3 Résultats obtenus

On souhaite prouver rigoureusement la convergence et étudier le comportement numérique des solutions  $\mathbf{F}^\varepsilon$  de l'équation de Boltzmann multi-espèce adimensionnée

$$\partial_t \mathbf{F}^\varepsilon + \frac{1}{\varepsilon} v \cdot \nabla_x \mathbf{F}^\varepsilon = \frac{1}{\varepsilon^2} \mathbf{Q}(\mathbf{F}^\varepsilon, \mathbf{F}^\varepsilon) \quad \text{sur } \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3, \quad (1.3.1)$$

vers les solutions du système de Maxwell-Stefan (1.2.14)–(1.2.16). En s'inspirant de l'approche formelle que nous avons présentée, on élabore deux stratégies différentes pour l'étude théorique et pour celle numérique.

#### Étude théorique

L'étude de la convergence rigoureuse est l'objet des chapitres 2 et 3. Elle est réalisée dans le cadre des sections efficaces  $B_{ij}$  vérifiant les hypothèses (H1)–(H4), *i.e.* de type potentiels durs ( $\gamma \in [0, 1]$ ) avec troncature angulaire de Grad. Notre analyse repose sur le développement d'une théorie perturbative des solutions  $\mathbf{F}^\varepsilon$  autour de la maxwellienne locale  $\mathbf{M}^\varepsilon$ , donnée par (1.2.12). Plus précisément, nous supposons pouvoir écrire toute solution de (1.3.1) sous la forme  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}$ , en fonction du paramètre  $\varepsilon \in (0, 1]$ . La perturbation  $\mathbf{f} = (f_1, \dots, f_N)$ , qui dépend bien sûr de  $\varepsilon$ , est alors solution de l'équation de Boltzmann perturbée

$$\partial_t \mathbf{f} + \frac{1}{\varepsilon} v \cdot \nabla_x \mathbf{f} = \frac{1}{\varepsilon^2} \mathbf{L}^\varepsilon(\mathbf{f}) + \frac{1}{\varepsilon} \mathbf{Q}(\mathbf{f}, \mathbf{f}) + \mathbf{S}^\varepsilon \quad \text{sur } \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3. \quad (1.3.2)$$

Ici, nous avons défini  $\mathbf{L}^\varepsilon = (L_1^\varepsilon, \dots, L_N^\varepsilon)$ , l'opérateur de collision linéarisé autour de la maxwellienne locale  $\mathbf{M}^\varepsilon$ , qui est donné par

$$L_i^\varepsilon(\mathbf{f}) = \sum_{j=1}^N \left( Q_{ij}(M_i^\varepsilon, f_j) + Q_{ij}(f_i, M_j^\varepsilon) \right), \quad 1 \leq i \leq N, \quad (1.3.3)$$

et le terme source<sup>16</sup>

$$\mathbf{S}^\varepsilon = -\frac{1}{\varepsilon} \partial_t \mathbf{M}^\varepsilon - \frac{1}{\varepsilon^2} v \cdot \nabla_x \mathbf{M}^\varepsilon + \frac{1}{\varepsilon^3} \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon), \quad (1.3.4)$$

qui donne la « distance » entre le système de Maxwell-Stefan et la partie fluide de l'équation de Boltzmann (1.3.2). Les difficultés de l'étude théorique résident alors dans le traitement de  $\mathbf{L}^\varepsilon$  et de  $\mathbf{S}^\varepsilon$ , qui constituent la nouveauté principale de notre travail.

16. Notons en particulier qu'un aspect central de notre analyse est précisément la présence du terme non linéaire  $\mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon)$ , qui ne s'annule pas puisque  $\mathbf{M}^\varepsilon$  n'est pas un état d'équilibre du mélange.

Nous avons vu que la convergence rigoureuse de l'équation de Boltzmann mono-espèce vers les modèles hydrodynamiques a été systématiquement obtenue en montrant l'existence d'un trou spectral pour l'opérateur linéarisé, qui donnait un retour négatif capable de contrôler le reste bilinéaire. La même approche a été adaptée au cadre multi-espèce dans [45], où le retour négatif de l'opérateur  $\mathbf{L}$  est utilisé pour prouver la relaxation vers l'équilibre thermodynamique. Malheureusement, tandis que  $\mathbf{L}$  est linéarisé près de l'équilibre global  $\boldsymbol{\mu}$ ,  $\mathbf{L}^\varepsilon$  vient d'une linéarisation autour d'un état maxwellien qui n'est pas un équilibre pour le mélange. Cela engendre une série de problèmes (à commencer par la perte des propriétés de symétrie, puisque l'opérateur n'est plus auto-adjoint) qui rendent inaccessible l'analyse du spectre de  $\mathbf{L}^\varepsilon$  avec les méthodes classiques. Par ailleurs, même si nous parvenions à une estimation de trou spectral explicite pour  $\varepsilon^{-2}\mathbf{L}^\varepsilon(\mathbf{f})$ , permettant de gérer le terme  $\varepsilon^{-1}\mathbf{Q}(\mathbf{f}, \mathbf{f})$ , son ordre de grandeur resterait *a priori* inférieur à celui du terme source, d'ordre  $\mathcal{O}(\varepsilon^{-3})$ . Puisque les comportements de  $\mathbf{L}^\varepsilon$  et de  $\mathbf{S}^\varepsilon$  dépendent de la structure de  $\mathbf{M}^\varepsilon$ , son choix est alors crucial pour établir un contrôle sur ces deux termes.

Voici notre idée de départ. D'un point de vue heuristique, la maxwellienne locale  $\mathbf{M}^\varepsilon$  devrait converger vers  $\boldsymbol{\mu}$  quand  $\varepsilon$  tend vers 0. En d'autres termes, en réécrivant  $\mathbf{M}^\varepsilon$  sous la forme d'une perturbation de l'équilibre global comme  $\mathbf{M}^\varepsilon = \boldsymbol{\mu} + (\mathbf{M}^\varepsilon - \boldsymbol{\mu})$ , on voudrait avoir que  $\mathbf{M}^\varepsilon - \boldsymbol{\mu} = \mathcal{O}(\varepsilon)$ . La stratégie consiste alors à choisir intelligemment les quantités macroscopiques  $(c_i^\varepsilon, u_i^\varepsilon)_{1 \leq i \leq N}$  de sorte à pouvoir comparer l'ordre de grandeur de  $\mathbf{M}^\varepsilon$  avec celui de  $\boldsymbol{\mu}$ , et à obtenir une estimation rigoureuse de la pénalisation. Nous verrons alors qu'une telle estimation fournira les contrôles  $\mathbf{L}^\varepsilon(\mathbf{f}) = \mathbf{L}(\mathbf{f}) + \mathcal{O}(\varepsilon)$  et  $\mathbf{S}^\varepsilon = \mathcal{O}(\varepsilon^{-1})$ , qui permettent de se ramener au trou spectral de l'opérateur  $\mathbf{L}$  et d'en exploiter le retour négatif dominant<sup>17</sup>.

Pour mettre en place cette stratégie, il faut d'abord fixer la forme des maxwelliennes  $\boldsymbol{\mu}$  et  $\mathbf{M}^\varepsilon$ . À une translation et une homothétie du système de coordonnées près, nous pouvons supposer sans perte de généralité  $u_\infty = 0$  et  $K_B\theta_\infty = 1$ . Sous cette hypothèse, l'unique état d'équilibre global du mélange  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_N)$  est alors défini, pour tout  $1 \leq i \leq N$ , par les distributions

$$\mu_i(v) = c_{i,\infty} \left( \frac{m_i}{2\pi} \right)^{3/2} e^{-m_i \frac{|v|^2}{2}}, \quad v \in \mathbb{R}^3, \quad (1.3.5)$$

Notons en particulier que le fait de prendre une vitesse  $u_\infty$  nulle est en accord avec la limite diffusive de l'équation de Boltzmann, qui prévoit précisément l'absence d'effets convectifs quand le nombre de Mach tend vers 0.

Pour la maxwellienne locale  $\mathbf{M}^\varepsilon$ , nous opérons en revanche deux choix différents, un pour chaque chapitre, qui sont expliqués dans les sections qui suivent.

### 1.3.1 Stabilité du trou spectral pour l'opérateur de Boltzmann linéarisé autour de l'état $\mathbf{M}^\varepsilon$

Le deuxième chapitre vise à quantifier explicitement l'apport négatif fourni par  $\mathbf{L}^\varepsilon$ . Classiquement, ce type d'analyse a toujours été relié à l'étude du spectre de l'opérateur linéarisé en question. À ce propos, rappelons que l'inégalité de coercivité (1.2.2) pour le linéarisé mono-espèce  $L$  a été prouvée par les méthodes non constructives<sup>18</sup> de Carleman et Grad [52, 106, 108], puis par les quantifications explicites plus récentes [194, 26, 27, 11, 159, 163]. Des résultats similaires ont été ensuite obtenus pour l'opérateur linéarisé multi-espèce dans [65, 45], où les auteurs montrent l'existence d'une constante explicitement calculable  $\lambda_{\mathbf{L}} > 0$

17. En effet, ce retour négatif sera d'ordre  $\mathcal{O}(\varepsilon^{-2})$ .

18. Basées sur l'application du théorème de Weyl à  $L$ , écrit comme une perturbation compacte d'un opérateur multiplicatif dont le spectre est simple à déterminer [139].

telle que la fonctionnelle de production d'entropie linéaire (ou forme de Dirichlet) associée à  $\mathbf{L}$  vérifie la majoration

$$\langle \mathbf{L}(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq -\lambda_{\mathbf{L}} \|\mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2, \quad \forall \mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}), \quad (1.3.6)$$

où  $\pi_{\mathbf{L}}$  est la projection orthogonale sur  $\ker \mathbf{L}$ ,  $\gamma \in [0, 1]$  est donné par (H3), et où nous avons noté  $\langle v \rangle = (1 + |v|^2)^{1/2}$ , fonction qui émerge également dans les estimations de coercivité pour Boltzmann mono-espèce [159].

Afin d'établir une estimation de coercivité pour  $\mathbf{L}^\varepsilon$  analogue à (1.3.6), des difficultés majeures se présentent, puisque la maxwellienne  $\mathbf{M}^\varepsilon$  utilisée pour la linéarisation ne constitue plus un état d'équilibre pour le mélange : sa structure ne permet pas la symétrie, caractéristique<sup>19</sup> des opérateurs linéarisés mono-espèce et bi-espèce. En particulier, notons que pour des vitesses  $v - \varepsilon u_i$  et  $v_* - \varepsilon u_j$ , les lois de conservation microscopiques (1.1.10) ne sont plus valables si  $u_i \neq u_j$ , ce qui implique en général  $M_i^{\varepsilon'} M_j^{\varepsilon' *} \neq M_i^\varepsilon M_j^{\varepsilon *}$ . En raison de cette asymétrie intrinsèque, l'opérateur  $\mathbf{L}^\varepsilon$  ne vérifie aucun caractère auto-adjoint, et donc les résultats que nous avons évoqués ne peuvent pas s'appliquer de manière directe. De plus, il semble très compliqué de décrire la forme de l'espace  $\ker \mathbf{L}^\varepsilon$ , et donc de définir de façon pertinente la projection orthogonale  $\pi_{\mathbf{L}^\varepsilon}$  sur  $\ker \mathbf{L}^\varepsilon$  indéfinie dans notre cas. Par conséquent, nous sommes amenés à développer une approche alternative.

Notre idée est de relier les opérateurs  $\mathbf{L}^\varepsilon$  et  $\mathbf{L}$ , pour dériver une majoration de la fonctionnelle de production d'entropie associée à  $\mathbf{L}^\varepsilon$  à partir de l'estimation de coercivité (1.3.6). Plus précisément, on écrit  $\mathbf{L}^\varepsilon$  comme une somme  $\mathbf{L}^\varepsilon = \mathbf{L} + (\mathbf{L}^\varepsilon - \mathbf{L})$  et on montre que le retour négatif (1.3.6) vérifié par la forme de Dirichlet de  $\mathbf{L}$  est préservé par la forme de Dirichlet de  $\mathbf{L}^\varepsilon$ , modulo l'apparition de deux nouvelles quantités d'ordre  $\varepsilon$  qui tiennent compte du terme  $\mathbf{L}^\varepsilon - \mathbf{L}$ . Nous voyons alors l'importance du choix des maxwelliennes  $\boldsymbol{\mu}$  et  $\mathbf{M}^\varepsilon$ , dont la différence apparaît explicitement dans ce terme de pénalisation. Dans le chapitre 2, nous supposons que la forme de  $\mathbf{M}^\varepsilon = (M_1^\varepsilon, \dots, M_N^\varepsilon)$  est donnée, pour tout  $1 \leq i \leq N$ , par

$$M_i^\varepsilon(t, x, v) = c_{i,\infty} \left( \frac{m_i}{2\pi} \right)^{3/2} \exp \left\{ -m_i \frac{|v - \varepsilon u_i(t, x)|^2}{2} \right\}, \quad t \geq 0, \quad x \in \mathbb{T}^3, \quad v \in \mathbb{R}^3. \quad (1.3.7)$$

Cela permet de faire correspondre les nombres de particules de  $\mathbf{M}^\varepsilon$  et celles de l'équilibre global (1.3.5).

La propriété de stabilité que nous démontrons est décrite par le théorème suivant.

**Théorème 1.3.1.** *Soient  $B_{ij}$  des sections efficaces satisfaisant les conditions (H1)–(H4), et soit  $\lambda_{\mathbf{L}} > 0$  le trou spectral dans  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  de l'opérateur  $\mathbf{L}$ , linéarisé autour de l'équilibre global (1.3.5). Il existe une constante  $C > 0$  telle que, pour tout  $\varepsilon > 0$ , l'opérateur  $\mathbf{L}^\varepsilon$ , linéarisé autour de l'état maxwellien (1.3.7), vérifie l'estimation a priori suivante. Pour presque tout  $t \geq 0$  et  $x \in \mathbb{T}^3$ , et pour toute  $\mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ ,*

$$\begin{aligned} \langle \mathbf{L}^\varepsilon(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} &\leq - \left( \lambda_{\mathbf{L}} - C\varepsilon \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i(t, x)| \mathcal{R}_{\varepsilon,i} \right\} \right) \|\mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + C\varepsilon \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i(t, x)| \mathcal{R}_{\varepsilon,i} \right\} \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2, \end{aligned} \quad (1.3.8)$$

19. Les propriétés de symétrie classiques de  $L$  (et de sa contrepartie multi-espèce), linéarisé autour d'un état d'équilibre local  $M_{(c,u,\theta)}$  ou global  $\mu$ , entraînent l'applicabilité des lois de conservation microscopiques (1.1.1). Leur conséquence immédiate est alors la validité des relations  $M'_{(c,u,\theta)} M_{(c,u,\theta)}^* = M_{(c,u,\theta)} M_{(c,u,\theta)}^*$  et  $\mu' \mu^* = \mu \mu^*$ , qui permettent d'obtenir le caractère auto-adjoint de l'opérateur.

où  $\pi_{\mathbf{L}}$  est la projection orthogonale sur  $\ker \mathbf{L}$  dans  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , et

$$\mathcal{R}_{\varepsilon,i} = 1 + \varepsilon |u_i(t, x)| \exp \left\{ \frac{4m_i}{1-\delta} \varepsilon^2 |u_i(t, x)|^2 \right\},$$

pour un  $\delta \in (0, 1)$  choisi indépendamment de  $\varepsilon$ . La constante  $C$  est explicite et dépend uniquement de  $N$ , des masses atomiques  $(m_i)_{1 \leq i \leq N}$ , des sections efficaces  $(B_{ij})_{1 \leq i, j \leq N}$  et du paramètre  $\delta \in (0, 1)$ . En particulier, elle est indépendante de  $\varepsilon$  et des quantités macroscopiques  $(c_{i,\infty}, u_i)_{1 \leq i \leq N}$ .

La preuve de ce résultat est menée en plusieurs étapes, que nous décrivons ici de façon schématique. Tout d'abord, à travers la pénalisation  $\mathbf{L}^\varepsilon - \mathbf{L}$ , on peut lier la fonctionnelle de production d'entropie de  $\mathbf{L}^\varepsilon$  à celle de  $\mathbf{L}$ , en réécrivant

$$\langle \mathbf{L}^\varepsilon(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \langle \mathbf{L}(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} + \langle \mathbf{L}^\varepsilon(\mathbf{f}) - \mathbf{L}(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})}.$$

Le premier terme est trivialement contrôlé avec la majoration (1.3.6), tandis que le deuxième demande une analyse plus approfondie et produit les deux contributions d'ordre  $\varepsilon$  qui figurent dans l'inégalité (1.3.8). Un calcul direct donne l'estimation initiale

$$\langle \mathbf{L}^\varepsilon(\mathbf{f}) - \mathbf{L}(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \mathcal{T}^\varepsilon(\mathbf{f}),$$

où chaque terme dans  $\mathcal{T}^\varepsilon(\mathbf{f})$  contient un facteur de type  $|M_i^\varepsilon - \mu_i|$ , dépendant des vitesses microscopiques  $v', v'_*, v$  ou  $v_*$ .

Le premier passage clé consiste alors à s'assurer que la maxwellienne locale  $\mathbf{M}^\varepsilon$  reste proche (en norme euclidienne) de l'équilibre global  $\boldsymbol{\mu}$ . Grâce aux choix (1.3.7) et (1.3.5) que nous avons faits, les nombres de particules des deux maxwelliennes sont donnés par le même état stationnaire constant  $(c_{i,\infty})_{1 \leq i \leq N}$ . Cela nous permet de factoriser par ces quantités communes et de comparer les vitesses macroscopiques figurant dans les exposants respectifs. En particulier, on est capable de montrer que pour presque tout  $t \geq 0$ ,  $x \in \mathbb{T}^3$  et pour tout paramètre arbitraire  $\delta \in (0, 1)$ , il existe une constante explicite  $C_\delta > 0$  (indépendante de  $\varepsilon$  et des observables  $c_{i,\infty}$  et  $u_i$ ) telle que, pour tout  $\varepsilon > 0$  et pour tout  $1 \leq i \leq N$ ,

$$|M_i^\varepsilon(v) - \mu_i(v)| \leq C_\delta \varepsilon c_{i,\infty}^{1-\delta} |u_i(t, x)| \mathcal{R}_{\varepsilon,i} \mu_i^\delta(v), \quad \forall v \in \mathbb{R}^3,$$

avec le reste  $\mathcal{R}_{\varepsilon,i}$  défini précédemment. Cette inégalité permet ensuite de borner  $\mathcal{T}^\varepsilon(\mathbf{f})$  par une quantité positive en  $\mathcal{O}(\varepsilon)$ .

Cependant, l'étude de certains termes de  $\mathcal{T}^\varepsilon(\mathbf{f})$  comporte quelques complications. Afin de contrôler efficacement ces termes intégraux, on doit écrire explicitement leurs noyaux via une représentation de Carleman récemment établie dans [45] pour l'opérateur de Boltzmann multi-espèce. On observe ici une conséquence directe de l'interaction croisée entre les diverses espèces du mélange : les noyaux intégraux peuvent être majorés ponctuellement par des maxwelliennes [45, Lemma 5.1], ayant chacune un taux de décroissance qui varie en fonction des différentes masses atomiques  $m_i$  et des différentes vitesses macroscopiques  $\varepsilon u_i$ , et qui dépend linéairement du paramètre  $\delta \in (0, 1)$ . Notre preuve réside ensuite sur la dérivation d'un contrôle  $L_v^1$  précis des noyaux, obtenu en choisissant le paramètre  $\delta \sim 1$  (indépendamment de  $\varepsilon$ ), de façon à récupérer une estimation uniforme des différents poids exponentiels. Ce contrôle  $L_v^1$  se traduit en un contrôle  $L_v^2$  sur les termes intégraux posant problèmes dans  $\mathcal{T}^\varepsilon(\mathbf{f})$ . En particulier, nous sommes en mesure d'établir la majoration

$$\langle \mathbf{L}^\varepsilon(\mathbf{f}) - \mathbf{L}(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq C \varepsilon \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i(t, x)| \mathcal{R}_{\varepsilon,i} \right\} \|\mathbf{f}\|_{L_v^2(\langle v \rangle^{\frac{3}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2,$$

valide pour tout  $\mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ . On conclut immédiatement en utilisant la décomposition  $\mathbf{f} = (\mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f})) + \pi_{\mathbf{L}}(\mathbf{f})$  dans (1.3.8).

### 1.3.2 Étude rigoureuse de la limite diffusive de l'équation de Boltzmann multi-espèce vers le modèle de Maxwell-Stefan

Dans le troisième chapitre nous montrons comment dériver rigoureusement le système de Maxwell-Stefan (1.2.14)–(1.2.16) dans la limite diffusive  $\varepsilon \rightarrow 0$  de l'équation de Boltzmann perturbée (1.3.2).

Tout d'abord, nous reprenons la forme de la maxwellienne locale (1.2.12). Plus précisément, nous demandons que :

- Dans la limite  $\varepsilon \rightarrow 0$ ,  $\mathbf{M}^\varepsilon$  se rapproche de l'équilibre global du mélange  $\boldsymbol{\mu}$  défini par (1.3.5). Il s'agit d'une hypothèse naturelle qui sert à garantir la stabilité des solutions  $\mathbf{F}^\varepsilon$  autour de l'équilibre global prescrit par la limite de diffusion ;
- La distance entre ces deux états maxwelliens reste de l'ordre du paramètre  $\varepsilon \in (0, 1]$ , soit  $\mathbf{M}^\varepsilon - \boldsymbol{\mu} = \mathcal{O}(\varepsilon)$ . C'est une hypothèse technique minimale qui est nécessaire afin d'exploiter le résultat du deuxième chapitre et déduire le retour négatif de l'opérateur  $\mathbf{L}^\varepsilon$  ;
- Les quantités macroscopiques  $(c_i^\varepsilon, u_i^\varepsilon)_{1 \leq i \leq N}$  associées à la maxwellienne  $\mathbf{M}^\varepsilon$  soient solutions du système de Maxwell-Stefan (1.2.14)–(1.2.16). Cette hypothèse consiste à inclure toute l'information du modèle hydrodynamique limite directement dans la maxwellienne  $\mathbf{M}^\varepsilon$ .

Afin de respecter ces trois conditions, notre idée est de considérer des solutions  $(c_i^\varepsilon, u_i^\varepsilon)_{1 \leq i \leq N}$  du modèle limite, perturbées (à un ordre  $\varepsilon$  près) autour d'un équilibre macroscopique. En remarquant que tout état stationnaire du système (1.2.14)–(1.2.16) est donné par  $(\bar{c}_i, \bar{u})_{1 \leq i \leq N}$ , où  $\bar{c}_i \in \mathbb{R}$  pour tout  $1 \leq i \leq N$ , et la fonction  $\bar{u} : \mathbb{R}_+ \times \mathbb{T}^3 \rightarrow \mathbb{R}$  (commune à toutes les espèces du mélange) vérifie la condition d'incompressibilité  $\nabla_x \cdot \bar{u} = 0$ , nous opérons le choix suivant. La maxwellienne locale  $\mathbf{M}^\varepsilon = (M_1^\varepsilon, \dots, M_N^\varepsilon)$  est donnée, pour tout  $1 \leq i \leq N$ , par

$$M_i^\varepsilon(t, x, v) = c_i(t, x) \left( \frac{m_i}{2\pi} \right)^{3/2} \exp \left\{ -m_i \frac{|v - \varepsilon u_i(t, x)|^2}{2} \right\}, \quad t \geq 0, \quad x \in \mathbb{T}^3, \quad v \in \mathbb{R}^3, \quad (1.3.9)$$

où nous avons défini les quantités macroscopiques comme étant des solutions du système de Maxwell-Stefan (1.2.14)–(1.2.16), perturbées autour de l'état stationnaire  $(c_{i,\infty}, \bar{u})_{1 \leq i \leq N}$ , soit

$$\begin{cases} c_i(t, x) = c_{i,\infty} + \varepsilon \tilde{c}_i(t, x), \\ u_i(t, x) = \bar{u}(t, x) + \varepsilon \tilde{u}_i(t, x), \quad \nabla_x \cdot \bar{u} = 0, \end{cases} \quad (1.3.10)$$

pour tout  $1 \leq i \leq N$  et pour tout  $t \geq 0$ ,  $x \in \mathbb{T}^3$ . À partir de ce choix, notre stratégie s'articule en deux étapes.

**Remarque 1.3.1.** *Il est important de noter que même si les états stationnaires de (1.2.14)–(1.2.16) incluent tout vecteur constant  $\bar{\mathbf{c}} \in \mathbb{R}^N$ , le seul compatible (au sens des trois conditions évoquées) avec l'équilibre global  $\boldsymbol{\mu}$  est celui qui vérifie  $\bar{\mathbf{c}} = \mathbf{c}_\infty$ .*

Le premier résultat présenté concerne l'existence et l'unicité des solutions (au sens perturbatif) du système macroscopique limite (1.2.14)–(1.2.16), et fournit une quantification de leur convergence exponentielle vers l'équilibre macroscopique  $(c_{i,\infty}, \bar{u})_{1 \leq i \leq N}$  qui définit la perturbation. L'étude mathématique du modèle de Maxwell-Stefan pose d'importantes difficultés, qui viennent de la nature fortement non linéaire du problème et de la non-inversibilité de la relation flux-gradients de concentration, caractéristique des équations

(1.2.15). En effet, en sommant ces  $N$  équations entre elles, on obtient une dépendance linéaire qui donne  $\nabla_x (\sum_i c_i) = 0$ . On a donc accès uniquement à  $N - 1$  relations sur les flux, ce qui implique la nécessité d'introduire une condition supplémentaire qui permette de fermer le système. L'hypothèse classiquement utilisée dans la littérature consiste à considérer la situation de *diffusion équimolaire* dans le mélange gazeux, caractérisée par

$$\sum_{i=1}^N \mathcal{F}_i(t, x) = 0, \quad t \geq 0, \quad x \in \mathbb{T}^3. \quad (1.3.11)$$

À partir de cette condition, le problème d'existence (locale ou globale), d'unicité et de retour à l'équilibre macroscopique pour les équations (1.2.14)–(1.2.15) a été analysé sous différentes formes dans de nombreux travaux [96, 33, 38, 138, 152, 63, 177]. Nous proposons ici une approche alternative non basée sur l'hypothèse (1.3.11), mais exploitant la condition d'incompressibilité (1.2.16). Le prix à payer est la perte de l'existence et de l'unicité au sens fort des solutions : l'existence globale et l'unicité que nous démontrons sont à entendre uniquement au sens perturbatif. Cependant, on souligne que notre résultat décrit toutes les solutions possibles dans le régime perturbatif autour d'un état stationnaire  $(\bar{c}_i, \bar{u})_{1 \leq i \leq N}$  tel que  $\bar{c}_i > 0$  pour tout  $1 \leq i \leq N$  et la vitesse  $\bar{u} : \mathbb{R}_+ \times \mathbb{T}^3 \rightarrow \mathbb{R}^3$  vérifie  $\nabla_x \cdot \bar{u} = 0$  (le cas particulier  $\bar{c} = \mathbf{c}_\infty$  étant donc inclus). Nous en présentons alors la forme plus générale, valable pour un  $\bar{c} \in (\mathbb{R}_+^*)^N$  quelconque.

**Théorème 1.3.2.** *Soit  $s > 3$  un entier, et supposons que  $\bar{u} \in L^\infty(\mathbb{R}_+; H^s(\mathbb{T}^3))$ . Il existe trois constantes  $\delta_{MS}, \lambda_{MS}, C_{MS} > 0$  telles que, pour tout  $\varepsilon \in (0, 1]$  et pour toute donnée initiale bien préparée  $(\bar{c} + \varepsilon \tilde{\mathbf{c}}^{\text{in}}, \bar{\mathbf{u}} + \varepsilon \tilde{\mathbf{u}}^{\text{in}})$ , vérifiant  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{u}}^{\text{in}}) \in H^s(\mathbb{T}^3) \times H^{s-1}(\mathbb{T}^3)$  et les estimations*

$$\|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s} \leq \delta_{MS}, \quad \|\bar{\mathbf{u}}\|_{L_t^\infty H_x^s} \leq \delta_{MS},$$

*il existe une unique solution  $(\bar{c} + \varepsilon \tilde{\mathbf{c}}, \bar{\mathbf{u}} + \varepsilon \tilde{\mathbf{u}})$  du système de Maxwell-Stefan (1.2.14)–(1.2.16), telle que  $(\tilde{\mathbf{c}}, \tilde{\mathbf{u}}) \in L^\infty(\mathbb{R}_+; H^s(\mathbb{T}^3)) \times L^\infty(\mathbb{R}_+; H^{s-1}(\mathbb{T}^3))$  et  $(\tilde{\mathbf{c}}, \tilde{\mathbf{u}})|_{t=0} = (\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{u}}^{\text{in}})$ . De plus, cette solution vérifie, pour tout  $1 \leq i \leq N$  et pour presque tout  $(t, x) \in \mathbb{R}_+ \times \mathbb{T}^3$ , les propriétés*

$$\bar{c}_i + \varepsilon \tilde{c}_i(t, x) > 0, \quad \sum_{i=1}^N \tilde{c}_i(t, x) = 0, \quad \sum_{i=1}^N c_i(t, x) \tilde{u}_i(t, x) = 0,$$

*et les estimations*

$$\begin{aligned} \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{c}^{-\frac{1}{2}})} &\leq e^{-\lambda_{MS} t} \|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s(\bar{c}^{-\frac{1}{2}})}, \\ \|\tilde{\mathbf{u}}\|_{H_x^{s-1}} &\leq C_{MS} e^{-\lambda_{MS} t} \|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s(\bar{c}^{-\frac{1}{2}})}. \end{aligned}$$

*Les constantes  $\delta_{MS}, \lambda_{MS}$  et  $C_{MS}$  sont explicites et dépendent uniquement du nombre d'espèces  $N$ , de  $s$ , de  $(\bar{c}_i)_{1 \leq i \leq N}$  et des quantités  $\Delta_{ij}$ .*

La preuve du théorème s'inspire des méthodes micro-macro développées en théorie cinétique perturbative [113, 114]. Par le biais de l'opérateur non injectif

$$A(\mathbf{c}) = \left( \frac{c_i c_j}{\Delta_{ij}} - \delta_{ij} \sum_{k=1}^N \frac{c_i c_k}{\Delta_{ik}} \right)_{1 \leq i, j \leq N}, \quad (1.3.12)$$

qui permet d'écrire les équations de Maxwell-Stefan (1.2.15) sous forme matricielle et qui a pour noyau l'espace  $\ker A = \text{Vect}(\mathbf{1})$ , on introduit la décomposition

$$\mathbf{u} = \pi_A(\mathbf{u}) + \mathbf{U},$$

où  $\pi_A$  est la projection orthogonale sur  $\ker A$  et  $\mathbf{U}$  dénote la composante normale dans l'espace  $(\ker A)^\perp$ . Soit  $\mathbf{1}$  le vecteur dont les  $N$  composantes sont égales à 1, et définissons pour tout  $\mathbf{w}, \mathbf{W} \in \mathbb{R}^N$  le produit scalaire  $\langle \mathbf{w}, \mathbf{W} \rangle_N = \sum_i w_i W_i$ . Il est possible de montrer que  $(\mathbf{c}, \mathbf{u}) \in H^s(\mathbb{T}^3) \times H^{s-1}(\mathbb{T}^3)$  est solution du système de Maxwell-Stefan (1.2.14)–(1.2.16) si et seulement si le couple  $(\mathbf{c}, \mathbf{U})$ , est solution du système

$$\partial_t \mathbf{c} + \nabla_x \cdot \left( \mathbf{c} \mathbf{U} - \mathbf{c} \frac{\langle \mathbf{c}, \mathbf{U} \rangle_N}{\langle \mathbf{c}, \mathbf{1} \rangle_N} \mathbf{1} \right) + \bar{\mathbf{u}} \cdot \nabla_x \mathbf{c} = 0, \quad (1.3.13)$$

$$\nabla_x \mathbf{c} = A(\mathbf{c}) \mathbf{U}, \quad (1.3.14)$$

et la forme complète de  $\mathbf{u}$  est récupérée en posant

$$\pi_A(\mathbf{u}) = \bar{\mathbf{u}} - \frac{\langle \mathbf{c}, \mathbf{U} \rangle_N}{\langle \mathbf{c}, \mathbf{1} \rangle_N} \mathbf{1}. \quad (1.3.15)$$

Cette approche ramène alors l'étude pour des solutions  $(\mathbf{c}, \mathbf{u})$  du système de Maxwell-Stefan (1.2.14)–(1.2.16) à l'analyse du système équivalent (1.3.13)–(1.3.15) dont les solutions impliquent uniquement  $\mathbf{c}$  et la partie orthogonale de  $\mathbf{u}$ , ce qui évite les problématiques liées à l'inversion de la matrice  $A$  et la nécessité de recourir à la théorie de Perron-Frobenius pour calculer sa pseudo-inverse, comme dans [97, 33, 138, 36]. L'obtention d'estimations *a priori* pour  $(\mathbf{c}, \mathbf{u})$ , à partir du système (1.3.13)–(1.3.15), permet de déduire l'existence et l'unicité voulues.

En particulier, on obtient l'existence globale et l'unicité des quantités macroscopiques (1.3.10), autour d'une vitesse incompressible  $\bar{\mathbf{u}}$  vérifiant les hypothèses du théorème. Par conséquent, la maxwellienne  $\mathbf{M}^\varepsilon$  donnée par (1.3.9) reste bien définie globalement en temps, ce qui légitime le cadre perturbatif des solutions  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}$  auquel on s'intéresse. Le deuxième résultat que nous présentons étudie le problème de Cauchy pour la perturbation  $\mathbf{f}$ . Notre méthode s'inspire du formalisme hypocoercif des travaux [161, 43] et se base sur l'introduction d'une fonctionnelle de Lyapunov dépendant du paramètre d'échelle  $\varepsilon$  et construite à partir de la norme de Sobolev standard de  $H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , à laquelle on ajoute les contributions associées au commutateur  $[v \cdot \nabla_x, \nabla_v] = -\nabla_x$ . Avec cette norme de Sobolev modifiée, que nous notons  $\|\cdot\|_{\mathcal{H}_\varepsilon^s}$ , il est alors possible de dériver des estimations *a priori* pour  $\mathbf{f}$ , permettant d'en montrer l'existence globale et l'unicité.

Introduisons l'opérateur  $\mathbf{T}^\varepsilon = \varepsilon^{-2} \mathbf{L} - \varepsilon^{-1} v \cdot \nabla_x$  et la projection orthogonale  $\pi_{\mathbf{T}^\varepsilon}$  associée (celle-ci est bien définie, puisque l'on considère l'opérateur  $\mathbf{L}$ , et non  $\mathbf{L}^\varepsilon$ ). Le théorème qui établit la convergence rigoureuse de l'équation de Boltzmann multi-espèce vers le modèle de Maxwell-Stefan (1.2.14)–(1.2.16) est le suivant.

**Théorème 1.3.3.** *Soient  $B_{ij}$  des sections efficaces satisfaisant les conditions (H1)–(H4), et considérons la maxwellienne locale  $\mathbf{M}^\varepsilon$  donnée par (1.3.9)–(1.3.10). Il existe  $s_0 \in \mathbb{N}^*$  et deux constantes  $\bar{\delta}_{MS} > 0$ ,  $\varepsilon_0 \in (0, 1]$  tels que, pour tout entier  $s \geq s_0$ , il existe  $\delta_B > 0$  tel que, pour tout  $\varepsilon \in (0, \varepsilon_0]$ , pour tout  $\delta_{MS} \in [0, \bar{\delta}_{MS}]$  et pour toute donnée initiale  $\mathbf{f}^{\text{in}}$  dans  $H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  satisfaisant*

$$\|\mathbf{f}^{\text{in}}\|_{\mathcal{H}_\varepsilon^s} \leq \delta_B, \quad \|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \mathcal{O}(\delta_{MS}), \quad (1.3.16)$$

il existe une unique  $\mathbf{f} \in C^0\left(\mathbb{R}_+; H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})\right)$  telle que  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}$  est l'unique solution faible de l'équation de Boltzmann multi-espèce (1.3.2). En particulier, si initialement  $\mathbf{F}^{\varepsilon, \text{in}} = \mathbf{M}^{\varepsilon, \text{in}} + \varepsilon \mathbf{f}^{\text{in}} \geq 0$ , alors  $\mathbf{F}^\varepsilon \geq 0$  p.p. sur  $\mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ . De plus,  $\mathbf{F}^\varepsilon$  vérifie pour tout  $t \geq 0$  la propriété de stabilité

$$\|\mathbf{F}^\varepsilon - \mathbf{M}^\varepsilon\|_{\mathcal{H}_\varepsilon} \leq \varepsilon \delta_B, \quad \forall \varepsilon \in (0, \varepsilon_0].$$

La constante  $\delta_B$  est explicite et indépendante des paramètres  $\delta_{MS}$  et  $\varepsilon$ .

La stratégie pour démontrer ce résultat consiste essentiellement à exhiber les propriétés d'hypocoercivité de l'équation de Boltzmann (1.3.2) pour la norme  $\|\cdot\|_{\mathcal{H}_\varepsilon}$ , suivant la présentation des hypothèses structurelles de [161, 43]. Nous sommes en mesure de prouver que les estimations *a priori* obtenues dans [43] peuvent être récupérées dans ce cadre multi-espèce, corrigées par des termes d'ordre  $\varepsilon$  ou  $\delta_{MS}$ , comme nous l'avons vu pour le cas du trou spectral de  $\mathbf{L}^\varepsilon$ . Notons toutefois qu'il ne s'agit pas d'une simple adaptation des calculs, et que le traitement de l'opérateur linéarisé  $\mathbf{L}^\varepsilon$  et du terme source  $\mathbf{S}^\varepsilon$  est très technique. D'un côté, les méthodes développées dans le deuxième chapitre sont revisitées ici afin d'obtenir le contrôle nécessaire sur le terme  $\nabla_v \mathbf{K}^\varepsilon$ , où  $\mathbf{K}^\varepsilon$  est la partie compacte de l'opérateur  $\mathbf{L}^\varepsilon$ . En particulier, nous dérivons une représentation de Carleman de  $\mathbf{K}^\varepsilon$  qui est complètement explicite, en transformant les inégalités ponctuelles de [45] sur les noyaux intégraux de l'opérateur linéarisé, en des égalités ponctuelles. Cette analyse est en effet cruciale pour pouvoir appliquer l'opérateur de dérivation en vitesse avant d'en établir la borne. Par suite, nous montrons que les majorations obtenues sur les quantités macroscopiques  $(\mathbf{c}, \mathbf{u})$  sont suffisantes afin de contrôler le terme source  $\mathbf{S}^\varepsilon$ . Nous soulignons également que, à la différence de [161, 43], nous ne disposons plus d'une inégalité de Poincaré exacte pour la projection orthogonale  $\pi_{\mathbf{L}^\varepsilon}$ , puisque nous considérons un régime perturbatif autour d'un état maxwellien local qui n'est pas un équilibre, où les perturbations  $\mathbf{f}$  doivent respecter une propriété similaire à la condition de compatibilité initiale  $\|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \mathcal{O}(\delta_{MS})$ . Cet inconvénient sera résolu en notant encore une fois que l'inégalité de Poincaré est applicable, modulo l'apparition d'un reste qui est précisément d'ordre  $\delta_{MS}$ . Plus généralement, nous mettons en lumière l'importance de ce paramètre qui prescrit l'ordre de grandeur des quantités macroscopiques  $(\mathbf{c}, \mathbf{u})$  et qui représente la vraie clé de notre étude, permettant d'établir une estimation d'énergie pour  $\mathbf{f}$  qui est uniforme en temps et qui fournit enfin l'existence globale et l'unicité de la perturbation.

**Remarque 1.3.2.** *L'approche que nous utilisons peut être vue comme une extension au cadre multi-espèce des techniques développées dans [48, 66], dont l'idée consiste précisément à montrer une propriété de stabilité des solutions de l'équation de Boltzmann autour d'un état maxwellien local qui contient toute la physique du modèle hydrodynamique limite. Toutefois, notre méthode comporte certaines améliorations importantes. En premier lieu, elle permet de traiter des perturbations autour d'un état maxwellien qui n'est pas un équilibre du gaz. En outre, puisque l'existence des quantités macroscopiques  $(c_i, u_i)_{1 \leq i \leq N}$  qui définissent  $\mathbf{M}^\varepsilon$  est garantie pour tout  $t \geq 0$ , la solution  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}$  existe globalement en temps. Enfin, les résultats dans [48, 66] sont construits sur un développement de Hilbert ou de Chapman-Enskog de la solution, où le reste du développement est supposé égal à 0 initialement. Cette hypothèse peut en particulier conduire à des solutions  $\mathbf{F}^\varepsilon$  négatives. L'apparition de tels effets non physiques est en revanche empêchée dans notre étude, puisque l'on demande uniquement que la donnée initiale  $\mathbf{F}^{\varepsilon, \text{in}}$  partage les mêmes quantités macroscopiques de la maxwellienne  $\mathbf{M}^{\varepsilon, \text{in}}$  à un ordre  $\delta_{MS}$  près, comme prescrit par (1.3.16). En particulier, nous verrons que celle-ci s'agit d'une condition de compatibilité qui est naturellement préservée à tout temps  $t \geq 0$  par l'équation de Boltzmann.*



## Étude numérique

L'étude numérique de la limite diffusive pour l'équation de Boltzmann (1.3.1) est l'objet du chapitre 4. Nous nous contentons d'analyser le cadre unidimensionnel en espace, et  $v$  désigne maintenant la première coordonnée du vecteur vitesse variable. En d'autres termes, on considère un modèle intégré dans les deux autres coordonnées de la vitesse. De plus, nous considérons des sections efficaces  $B_{ik}$  de type molécules maxwelliennes avec  $b_{ik} : [-1, 1] \rightarrow \mathbb{R}_+$  paire, pour tout  $1 \leq i, k \leq N$ . Soulignons en particulier que l'extension des nos résultats en dimension supérieure d'espace et pour une forme plus générale des noyaux de collision n'est pour le moment pas claire. Enfin, dans cette partie nous travaillons uniquement sur des mélanges gazeux évoluant à l'intérieur d'un ouvert borné  $\Omega$  de  $\mathbb{R}$ , et non plus dans  $\mathbb{T}^3$ . Cette hypothèse est principalement motivée par le fait que l'on vise à simuler des expériences physiques (telles que l'expérience de Duncan et Toor [82] que nous avons mentionnée) où le confinement spatial est nécessaire afin d'observer les effets de diffusion croisée. Dans ce contexte, on veut construire un schéma numérique approchant la solution du système d'équations de Boltzmann (1.3.1), écrites ici pour  $1 \leq i \leq N$ ,

$$\varepsilon \partial_t F_i^\varepsilon + v \partial_x F_i^\varepsilon = \frac{1}{\varepsilon} Q_i(\mathbf{F}^\varepsilon, \mathbf{F}^\varepsilon) \quad \text{sur } \mathbb{R}_+ \times \Omega \times \mathbb{R}, \quad (1.3.17)$$

et permettant de capturer (en faisant varier le paramètre  $\varepsilon$  pour des paramètres de discrétisation fixés) à la fois les solutions cinétiques  $\mathbf{F}^\varepsilon$  et les solutions du modèle macroscopique limite (1.2.9)–(1.2.10), où l'on impose, pour tout  $t \geq 0$  et pour tout  $1 \leq i \leq N$ , les conditions au bord  $\mathcal{F}_i|_{\partial\Omega} = 0$ .

Plusieurs approches semblent envisageables. Par exemple, les méthodes de décomposition micro-macro et de pénalisation ont été récemment étendues dans [136, 133] au cas de l'équation de Boltzmann multi-espèce, pour les limites d'Euler et de Navier-Stokes compressibles ( $r = 0$ ). Toutefois, nous avons déjà vu que dans le cas de la limite diffusive ces techniques s'appliquent uniquement à des opérateurs de Boltzmann linéaires et ne peuvent pas fournir une réponse satisfaisante à notre problème.

L'approche que nous utilisons consiste plutôt à reproduire les calculs formels de [39], en appliquant la méthode des moments. Plus précisément, nous supposons que les composantes de  $\mathbf{F}^\varepsilon = (F_1^\varepsilon, \dots, F_N^\varepsilon)$  ont, pour tout  $1 \leq i \leq N$ , la forme

$$F_i^\varepsilon(t, x, v) = c_i^\varepsilon(t, x) \left( \frac{m_i}{2\pi K_B T} \right)^{1/2} \exp \left\{ -m_i \frac{(v - \varepsilon u_i^\varepsilon(t, x))^2}{2K_B T} \right\}, \quad t \geq 0, \quad x \in \Omega, \quad v \in \mathbb{R}, \quad (1.3.18)$$

et nous dérivons les bilans de masse et de quantité de mouvement qui gouvernent l'évolution des concentrations  $c_i^\varepsilon$  et des flux  $\mathcal{F}_i^\varepsilon$ , définis par les relations  $\mathcal{F}_i^\varepsilon = c_i^\varepsilon u_i^\varepsilon$ . Le système macroscopique que l'on cherche est obtenu à partir de l'ansatz (1.3.18) en intégrant en  $v$  les équations (1.3.17) contre les vecteurs  $\mathbf{m}$  et  $v\mathbf{m}$ , et est donné, pour tout  $1 \leq i \leq N$ , par

$$\begin{cases} \partial_t c_i^\varepsilon + \partial_x \mathcal{F}_i^\varepsilon = 0, \\ \varepsilon^2 m_i \partial_t \mathcal{F}_i^\varepsilon + \varepsilon^2 m_i \partial_x (c_i^\varepsilon (u_i^\varepsilon)^2) + K_B T \partial_x c_i^\varepsilon = \sum_{k \neq i} \mu_{ik} \tilde{B}_{ik} (c_i^\varepsilon \mathcal{F}_k^\varepsilon - c_k^\varepsilon \mathcal{F}_i^\varepsilon), \end{cases} \quad (1.3.19)$$

où  $\mu_{ik} = \frac{2m_i m_k}{m_i + m_k}$  est la masse réduite associée aux espèces  $\mathcal{E}_i$  et  $\mathcal{E}_k$ , et nous avons dénoté  $\tilde{B}_{ik} = \frac{1}{2} \|b_{ik}\|_{L^1(-1,1)}$ . Le système est ensuite complété avec les conditions initiales et de bord supplémentaires

$$\begin{aligned} c_i^\varepsilon(0, \cdot) &= c_i^{\text{in}} \geq 0 \quad \text{et} \quad \mathcal{F}_i^\varepsilon(0, \cdot) = \mathcal{F}_i^{\text{in}} \quad \text{dans } \Omega, \\ \mathcal{F}_i^\varepsilon(t, \cdot)|_{\partial\Omega} &= 0, \quad t \geq 0, \end{aligned} \quad (1.3.20)$$

pour tout  $1 \leq i \leq N$ .

**Remarque 1.3.3.** *Notons que cette approche ne se base pas sur une perturbation exacte de la solution, de type  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}$ . Toutefois, contrairement à l'étude analytique où la perturbation  $\mathbf{f}$  était nécessaire afin de rendre rigoureuse l'expansion autour de l'état maxwellien (1.3.9), dans ce cadre numérique une telle correction est prise en compte par la forme générale des quantités fluides  $(c_i^\varepsilon, u_i^\varepsilon)_{1 \leq i \leq N}$ , qui ne sont plus fixées comme étant des solutions des équations limites (1.2.9)–(1.2.10), mais vérifient le système (1.3.19), modélisant un régime intermédiaire entre les descriptions macroscopique et mésoscopique. Ceci est en accord avec l'idée de la méthode des moments, selon laquelle la hiérarchie d'équations qui donne les bilans des moments successifs de la solution fournit une bonne approximation à la fois des régimes gouvernés par l'équation de Boltzmann et de ceux gouvernés par les modèles hydrodynamiques.*

### 1.3.3 Un schéma numérique pour la limite de diffusion de l'équation de Boltzmann multi-espèce vers le modèle de Maxwell-Stefan

Considérons un pas de temps  $\Delta t > 0$  et un pas d'espace  $\Delta x > 0$  qui donne la subdivision en  $J + 1$  points  $(x_j)_{0 \leq j \leq J}$  du domaine  $\Omega$ , avec  $x_j = j\Delta x$ . Pour les concentrations et les flux nous utilisons une discrétisation à mailles décalées en espace : pour tout  $n \geq 0$ , pour tout  $0 \leq j \leq J$  et pour tout  $1 \leq i \leq N$ ,  $c_{i,j}^n \simeq c_i^\varepsilon(t^n, x_j)$  et  $\mathcal{F}_{i,j+\frac{1}{2}}^n \simeq \mathcal{F}_i^\varepsilon\left(t^n, x_{j+\frac{1}{2}}\right)$  représentent les approximations numériques respectives, où l'on a noté  $x_{j+\frac{1}{2}} = (j + \frac{1}{2})\Delta x$ . En introduisant le rapport  $\lambda = \Delta t/\Delta x$ , le schéma numérique que nous proposons s'écrit, pour tout  $1 \leq i \leq N$ ,

$$\begin{cases} c_{i,j}^{n+1} + \lambda \left( \mathcal{F}_{i,j+\frac{1}{2}}^{n+1} - \mathcal{F}_{i,j-\frac{1}{2}}^{n+1} \right) = c_{i,j}^n, & 0 \leq j \leq J, \\ \left( -\Delta t \sum_{k \neq i} \mu_{ik} \tilde{B}_{ik} c_{k,j+\frac{1}{2}}^{n+1} - \varepsilon^2 m_i \right) \mathcal{F}_{i,j+\frac{1}{2}}^{n+1} + \Delta t c_{i,j+\frac{1}{2}}^{n+1} \sum_{k \neq i} \mu_{ik} \tilde{B}_{ik} \mathcal{F}_{k,j+\frac{1}{2}}^{n+1} \\ = K_B T \lambda \left( c_{i,j+1}^{n+1} - c_{i,j}^{n+1} \right) + \varepsilon^2 m_i \lambda R_{i,j+\frac{1}{2}}^n - \varepsilon^2 m_i \mathcal{F}_{i,j+\frac{1}{2}}^n, & 0 \leq j \leq J-1, \end{cases} \quad (1.3.21)$$

où  $R_{i,j+\frac{1}{2}}^n$  est la discrétisation du terme non linéaire  $\partial_x(c_i^\varepsilon(u_i^\varepsilon)^2)$  et les valeurs des concentrations aux points milieux des mailles principales sont données par

$$c_{i,j+\frac{1}{2}}^{n+1} = \min \left\{ c_{i,j}^{n+1}, c_{i,j+1}^{n+1} \right\}. \quad (1.3.22)$$

Enfin, le système discret est fermé avec les conditions au bord

$$\mathcal{F}_{i,-\frac{1}{2}}^{n+1} = \mathcal{F}_{i,J+\frac{1}{2}}^{n+1} = 0, \quad 1 \leq i \leq N. \quad (1.3.23)$$

Dans ce chapitre, nous obtenons trois résultats principaux. Le premier donne la conservation de la masse de chaque espèce  $\mathcal{E}_i$  du mélange : en sommant sur  $j$  les équations de continuité du système discret (1.3.21) et en utilisant les conditions limites (1.3.23), il est immédiat de voir que, pour tout  $1 \leq i \leq N$ , nous avons

$$\sum_{j=0}^J c_{i,j}^{n+1} = \sum_{j=0}^J c_{i,j}^n, \quad \forall n \geq 0. \quad (1.3.24)$$

On récupère ensuite une borne inférieure sur les  $(\mathbf{c}_j^n)_{0 \leq j \leq J}$ , obtenue en supposant pouvoir contrôler les termes source  $\mathbf{S}_{j+\frac{1}{2}}^n = (m_i \lambda R_{i,j+\frac{1}{2}}^n - m_i F_{i,j+\frac{1}{2}}^n)_{1 \leq i \leq N}$  uniformément par rapport à  $\varepsilon$ . Plus précisément, sous l'hypothèse que

$$\varepsilon^2 \max_{1 \leq i \leq N} \max_{n \geq 0} \max_{0 \leq j \leq J-1} \left| \mathcal{S}_{i,j+\frac{1}{2}}^n \right| \xrightarrow{\varepsilon \rightarrow 0} 0, \quad (1.3.25)$$

le résultat donnant la positivité des concentrations est le suivant.

**Proposition 1.3.4.** *Pour tout  $\varepsilon \in (0, 1]$ , soit  $(c_{i,j}^n)_{0 \leq j \leq J}$ ,  $(\mathcal{F}_{i,j+\frac{1}{2}}^n)_{0 \leq j \leq J-1}$  une solution du schéma numérique (1.3.21)–(1.3.23), définie pour tout  $1 \leq i \leq N$  et  $n \geq 0$ . Si la donnée initiale  $(c_{i,j}^{\text{in}})_{0 \leq j \leq J}$  associée est positive, pour tout  $1 \leq i \leq N$ , et la condition (1.3.25) est satisfaite, alors, pour tout  $\varepsilon$  suffisamment petit,  $c_{i,j}^n \geq 0$  pour tout  $1 \leq i \leq N$ ,  $0 \leq j \leq J$  et  $n \geq 0$ .*

La preuve se base sur la méthode proposée dans [3] et est obtenue par récurrence sur l'indice de temps  $n \geq 0$ . On suppose  $c_{i,j}^n \geq 0$  pour tout  $i, j$  et on montre que les  $c_{i,j}^{n+1}$  vérifient la même propriété. Pour cela, on exploite la structure spécifique du système (1.3.21), pouvant se réécrire sous forme vectorielle par le biais de la matrice

$$\left[ A_{j+\frac{1}{2}}^{n+1} \right]_{ik} = \begin{cases} -\Delta t \mu_{ik} \tilde{B}_{ik} c_{i,j+\frac{1}{2}}^{n+1} & \text{si } i \neq k, \\ \Delta t \sum_{\ell \neq i} \mu_{i\ell} \tilde{B}_{i\ell} c_{\ell,j+\frac{1}{2}}^{n+1} + \varepsilon^2 m_i & \text{si } i = k, \end{cases} \quad (1.3.26)$$

contrepartie discrète de la matrice de Maxwell-Stefan (1.3.12). Grâce à la présence des termes diagonaux  $\varepsilon^2 m_i$ , il est immédiat de montrer que  $A$  est toujours inversible si les quantités  $c_{i,j+\frac{1}{2}}^{n+1}$  sont positives, puisqu'il s'agit d'une matrice à diagonale strictement dominante pour tout  $\varepsilon > 0$ . Afin d'en assurer l'inversibilité, l'idée initiale de notre stratégie consiste à introduire un autre système discret où nous remplaçons les  $c_{i,j+\frac{1}{2}}^{n+1}$  à l'intérieur de la matrice (1.3.26) par leurs parties positives  $[c_{i,j+\frac{1}{2}}^{n+1}]^+$ . Dans ce problème auxiliaire, nous pouvons exprimer les flux en terme des concentrations et dériver l'équation vectorielle

$$\begin{aligned} & \sum_{j=0}^J \left\langle \frac{\mathbf{c}_j^{n+1} - \mathbf{c}_j^n}{\lambda}, [\mathbf{c}_j^{n+1}]^- \right\rangle_N \\ & + \sum_{j=0}^J \left\langle \left( A_{j+\frac{1}{2}}^{n+1} \right)^{-1} \left( K_B T \lambda (\mathbf{c}_{j+1}^{n+1} - \mathbf{c}_j^{n+1}) + \varepsilon^2 \mathbf{S}_{j+\frac{1}{2}}^n \right), ([\mathbf{c}_{j+1}^{n+1}]^- - [\mathbf{c}_j^{n+1}]^-) \right\rangle_N = 0, \end{aligned}$$

où figurent uniquement les concentrations et les termes de source définis précédemment. En particulier, la deuxième somme est caractérisée par la présence de deux types de termes s'écrivant, pour tout  $1 \leq i, k \leq N$  avec  $k \neq i$ ,

$$\begin{aligned} T_{ik} &= \left[ \left( A_{j+\frac{1}{2}}^{n+1} \right)^{-1} \right]_{ik} \left( K_B T \lambda (c_{k,j+1}^{n+1} - c_{k,j}^{n+1}) + \varepsilon^2 S_{k,j+\frac{1}{2}}^n \right) ([c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^-), \\ T_{ii} &= \left[ \left( A_{j+\frac{1}{2}}^{n+1} \right)^{-1} \right]_{ii} \left( K_B T \lambda (c_{i,j+1}^{n+1} - c_{i,j}^{n+1}) + \varepsilon^2 S_{i,j+\frac{1}{2}}^n \right) ([c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^-). \end{aligned}$$

D'un côté, on a que  $T_{ik} = 0$  puisqu'il contient un facteur  $[c_{i,j+\frac{1}{2}}^{n+1}]^+ ([c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^-)$ , s'annulant à cause du choix de discrétisation (1.3.22). De même, grâce à l'hypothèse (1.3.25),

les  $T_{ii}$  sont négatifs pour tout  $\varepsilon$  suffisamment petit, puisque les termes diagonaux de la matrice  $A^{-1}$  sont toujours positifs et  $(a-b)(a^- - b^-) \leq 0$  pour tout  $a, b \in \mathbb{R}$ . On déduit ainsi la validité de la relation

$$\sum_{i=1}^N \sum_{j=0}^J \left| \left[ c_{i,j}^{n+1} \right]^- \right|^2 \leq 0,$$

qui donne  $\left[ c_{i,j}^{n+1} \right]^- = 0$ , et donc  $c_{i,j}^n \geq 0$  pour tout  $n \geq 0$ . En conclusion, puisque les concentrations sont positives, la solution  $(c_{i,j}^n)_{0 \leq j \leq J}$ ,  $(\mathcal{F}_{i,j+\frac{1}{2}}^n)_{0 \leq j \leq J-1}$  du système auxiliaire est également solution du système (1.3.21).

En particulier, en combinant la conservation de la masse et la positivité des concentrations, nous dérivons une estimation  $\ell^1$  *a priori* sur  $(\mathbf{c}_j^n)_{0 \leq j \leq J}$  qui permet de prouver notre dernier résultat.

**Théorème 1.3.4.** *Pour tout  $\varepsilon > 0$  suffisamment petit et pour tout vecteur  $(c_{i,j}^{\text{in}})_{i,j}$  positif, il existe au moins une solution  $(c_{i,j}^n)_{0 \leq j \leq J}$ ,  $(\mathcal{F}_{i,j+\frac{1}{2}}^n)_{0 \leq j \leq J-1}$  du schéma numérique (1.3.21)–(1.3.23), qui est définie pour tout  $1 \leq i \leq N$  et  $n \geq 0$ , et qui possède comme donnée initiale  $(c_{i,j}^{\text{in}})_{i,j}$ . En particulier,  $c_{i,j}^n \geq 0$  pour tout  $1 \leq i \leq N$ ,  $0 \leq j \leq J$  et  $n \geq 0$ .*

L'idée de la preuve consiste à introduire un deuxième schéma auxiliaire, obtenu à partir du système (1.3.21) en remplaçant les concentrations inconnues par leurs parties positives. Par suite, on définit les vecteurs  $y_1^{n+1} \in (\mathbb{R}_+)^{N(J+1)}$  et  $y_2^{n+1} \in \mathbb{R}^{NJ}$  qui contiennent respectivement les valeurs des concentrations  $([c_j^{n+1}]^+)_{0 \leq j \leq J}$  et des flux  $(\mathcal{F}_{j+\frac{1}{2}}^{n+1})_{0 \leq j \leq J-1}$ , et on écrit le nouveau schéma sous forme de système linéaire

$$\mathbb{S}^\varepsilon (y_1^{n+1}) y^{n+1} = b^n, \quad y^{n+1} = (y_1^{n+1}, y_2^{n+1})^\top, \quad (1.3.27)$$

où  $b^n$  dénote le vecteur des termes connus du système discret, et  $\mathbb{S}^\varepsilon(y_1^{n+1})$  est une matrice par blocs  $2 \times 2$  qui dépend uniquement de  $\varepsilon$ , des quantités  $[c_{i,j}^{n+1}]^+$  et des paramètres du problème. Par le biais du complément de Schur, on montre que  $\mathbb{S}^\varepsilon(y_1^{n+1})$  est inversible pour tout  $\varepsilon > 0$  et qu'il est possible de déterminer explicitement la structure de son inverse. Le système linéaire (1.3.27) peut donc être inversé pour tout  $\varepsilon > 0$ , et réécrit

$$\begin{cases} y_1^{n+1} = f(y_1^{n+1}), \\ y_2^{n+1} = g(y_1^{n+1}), \end{cases}$$

où  $f$  et  $g$  sont données par des produits et sommes des blocs de  $\mathbb{S}^\varepsilon(y_1^{n+1})$ , et de leurs inverses. Ainsi, on arrive à découpler les dépendances non linéaires entre flux et concentrations, ce qui permet d'établir la formulation de point fixe  $y_1^{n+1} = f(y_1^{n+1})$  impliquant les seules quantités  $[c_{i,j}^{n+1}]^+$ . Nous sommes en particulier en mesure de prouver que la fonction  $f : (\mathbb{R}_+)^{N(J+1)} \rightarrow (\mathbb{R}_+)^{N(J+1)}$  est continue et compacte, et que l'ensemble

$$E = \left\{ y_1^{n+1} \in (\mathbb{R}_+)^{N(J+1)} \mid \exists \xi \in [0, 1] \text{ tel que } y_1^{n+1} = \xi f(y_1^{n+1}) \right\}$$

est borné dans norme  $\ell^1$  de  $\mathbb{R}^{N(J+1)}$ , grâce aux estimations *a priori* que nous avons précédemment dérivées sur  $y_1^{n+1}$ . Pour tout  $\varepsilon > 0$ , le théorème de point fixe de Schaefer [87] donne alors l'existence d'une solution pour l'équation  $y_1^{n+1} = f(y_1^{n+1})$ , et la valeur des flux  $y_2^{n+1}$  est déterminée par la relation  $y_2^{n+1} = g(y_1^{n+1})$ . En appliquant enfin la proposition 1.3.4, pour  $\varepsilon$  suffisamment petit la solution que nous avons trouvée fournit également

une solution  $(c_{i,j}^n)_{0 \leq j \leq J}$ ,  $(\mathcal{F}_{i,j+\frac{1}{2}}^n)_{0 \leq j \leq J-1}$  du schéma numérique original (1.3.21)–(1.3.23), telle que  $c_{i,j}^n \geq 0$  pour tout  $1 \leq i \leq N$ ,  $0 \leq j \leq J$  et  $n \geq 0$ .

Pour conclure, à cause de la nature non linéaire du système discret (1.3.21) qui complexifie grandement son analyse théorique, plusieurs questions restent ouvertes. D'une part, le caractère bien posé du schéma est encore partiel, puisque nous n'avons pas obtenu de résultat d'unicité. D'autre part, il est immédiat de vérifier que le schéma numérique (1.3.21)–(1.3.23) est consistant à l'ordre 1 avec le modèle continu (1.3.19)–(1.3.20) pour tout  $\varepsilon \geq 0$ , mais pour le moment nous n'avons pas de propriété de stabilité donnant une condition CFL indépendante de  $\varepsilon$ . Par conséquent, les informations que nous possédons ne sont pas suffisantes pour prouver que le schéma préserve l'asymptotique du problème. Toutefois, nous soulignons qu'au moins d'un point de vue numérique, notre schéma révèle effectivement un caractère AP, qui dérive probablement de la discrétisation implicite en temps que nous avons choisie.

## Chapitre 2

# Stability of the spectral gap for the Boltzmann multi-species operator linearized around non-equilibrium Maxwell distributions

Ce chapitre fait l'objet de la publication [30],  
en collaboration avec Laurent Boudin, Marc Briant et B erence Grec.

### 2.1 Introduction

The study of the convergence to the equilibrium for the Boltzmann equation has a long history (see the reviews [57, 59, 190, 188]) and is at the core of the kinetic theory of gases. In the mono-species setting, the Boltzmann equation models the behaviour of a dilute gas composed of a large number of identical and monatomic particles which are supposed to only interact via microscopic binary collisions. It describes the time evolution of the gas distribution function  $F = F(t, x, v)$  and reads, on  $\mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ ,

$$\partial_t F + v \cdot \nabla_x F = Q(F, F). \quad (2.1.1)$$

Without going into any details on the structure of the Boltzmann operator  $Q$  for the moment, let us just mention that it is a quadratic operator which contains all the information about the collision process, prescribing how the microscopic interactions between particles take place. In particular, one of its main features is that it satisfies the celebrated  $H$ -theorem, which states that the entropy functional  $H(F) = \int_{\mathbb{R}^3} F \log F dv$  decreases with respect to time and the gas reaches an equilibrium state whenever  $Q(F, F) = 0$ , namely when  $F$  has the form of a local Maxwellian distribution

$$M(t, x, v) = \frac{c(t, x)}{(2\pi K_B \theta(t, x))^{3/2}} \exp \left\{ -\frac{|v - u(t, x)|^2}{2K_B \theta(t, x)} \right\}, \quad t \geq 0, \quad x \in \mathbb{T}^3, \quad v \in \mathbb{R}^3,$$

where  $K_B$  is the Boltzmann constant. Consequently, taking into account the influence of the transport operator in the left-hand side of (2.1.1), the  $H$ -theorem suggests that, for large time asymptotics, the solutions of the Boltzmann equation should converge towards a global equilibrium having the form of a uniform (in time and space) Maxwellian distribution  $M_\infty(v) = c_\infty / (2\pi K_B \theta_\infty)^{3/2} \exp \left\{ -\frac{|v - u_\infty|^2}{2K_B \theta_\infty} \right\}$ , with  $c_\infty, \theta_\infty > 0$  and  $u_\infty \in \mathbb{R}^3$ . Here,

the quantities  $c_\infty$ ,  $u_\infty$  and  $\theta_\infty$  respectively represent the number of particles, macroscopic velocity and temperature of the gas, and their values are prescribed by the initial datum. For the sake of simplicity, up to a translation and a dilation of the coordinate system, it is always possible to choose  $M_\infty$  as being the global Maxwellian distribution

$$\mu(v) = \frac{c_\infty}{(2\pi)^{3/2}} e^{-\frac{|v|^2}{2}}, \quad v \in \mathbb{R}^3.$$

Starting from an initial datum close enough to  $\mu$ , one could expect that the solutions to the Boltzmann equation remain in a neighbourhood of the equilibrium and eventually converge to it in the large time asymptotic. A common strategy to tackle the problem of convergence towards the equilibrium is then to perform studies near the global Maxwellian distribution by investigating the behaviour of a small perturbation  $f$  around  $\mu$ , *i.e.*  $F = \mu + f$ .

This theory was initiated by Hilbert [121] and later on further developed by Carleman [52] and Grad [106]. In the perturbative regime around the global equilibrium  $\mu$ , the Boltzmann operator  $Q$  can be rewritten as  $Q(F, F) = \{Q(\mu, f) + Q(f, \mu)\} + Q(f, f)$ , since  $Q(\mu, \mu) = 0$ . Because  $f$  is supposed to remain small, the dominant term in the previous relation is the so-called linearized Boltzmann operator

$$L(f) = Q(\mu, f) + Q(f, \mu).$$

The question which naturally arises concerns its spectral properties. In fact, as done in the nonlinear case for  $Q$ , it is possible to prove a linearized version of the  $H$ -theorem which asserts that the entropy production functional (or Dirichlet form)  $D(f) = \int_{\mathbb{R}^3} L(f) f \mu^{-1} dv$  is nonpositive and satisfies in particular the following fundamental coercivity estimate [52, 106, 108, 57, 59, 11]:

$$D(f) \leq -\lambda_L \|f - \pi_L(f)\|_{L_v^2(\mu^{-\frac{1}{2}})}^2, \quad \forall f \in L^2(\mathbb{R}^3, \mu^{-\frac{1}{2}}), \quad (2.1.2)$$

where  $L^2(\mathbb{R}^3, \mu^{-\frac{1}{2}}) = \left\{ f : \mathbb{R}^3 \rightarrow \mathbb{R} \text{ measurable} : \|f\|_{L_v^2(\mu^{-\frac{1}{2}})}^2 = \int_{\mathbb{R}^3} f^2 \mu^{-1} dv < +\infty \right\}$ .

Here,  $\pi_L$  is the orthogonal projection onto  $\ker L$  (the space of the equilibrium states of  $L$ ), and  $\lambda_L > 0$  can be taken to be the smallest nonzero eigenvalue of  $-L$ , *i.e.* the spectral gap of the linearized Boltzmann operator.

Consequently, in a purely linear setting where  $\partial_t f + v \cdot \nabla_x f = L(f)$ , the above inequality allows to formally deduce that the associated linearized entropy functional  $\int_{\mathbb{R}^3} f^2 \mu^{-1} dv$  is monotonically decreasing with respect to time, and the gas reaches an equilibrium state whenever  $L(f) = 0$ . Proving that  $L$  satisfies (2.1.2) provides a powerful tool in estimating the asymptotic behaviour of solutions of the Boltzmann equation close to the equilibrium, since it allows to derive a quantitative information about the rate of relaxation of  $F$  towards  $\mu$ .

The existence of a spectral gap  $\lambda_L$  for  $L$  has been known for long and many results have been proved in this regard over the past sixty years, starting with Carleman and Grad themselves [52, 106, 108] in the case of Maxwellian, hard-potential and hard-sphere collision kernels with cutoff. The idea behind these methods is to apply Weyl's theorem to  $L$ , written as a compact perturbation of a multiplicative operator, and they are thus non-constructive. Consequently, a major inconvenience of this strategy is that it does not provide any information about the width of the spectral gap, or its dependence on the initial datum and on the physical quantities appearing in the problem (in particular its sensitivity to perturbations of the collision kernel).

The derivation of explicit estimates for the spectral gap of the linearized Boltzmann operator is fundamental to construct a quantitative theory near the equilibrium and to

obtain explicit convergence rates to the equilibrium. In fact, when proving that solutions to the Boltzmann equation in the perturbative regime have an exponential trend of relaxation of order  $\mathcal{O}(e^{-t/\tau})$  towards the equilibrium [160, 161], one can use the information provided by (2.1.2) in order to link the rate  $1/\tau$  to the spectral gap  $\lambda_L$  and recover an explicit convergence speed. This feature has been of great importance in the kinetic theory of gases, starting from the studies of Boltzmann himself. Indeed, one expects that the approximation provided by the chaos molecular assumption is legitimate for a time of order at most  $O(N_A)$ , where  $N_A = 10^{23}$  is the Avogadro's number. By this time, each particle will have collided with a nonnegligible fraction of the other atoms and thus the validity of the Boltzmann equation should break down (see the discussion in [190, Chapter 1, Section 2.5]). It is therefore crucial to obtain constructive quantitative informations on the time scale of the convergence, in order to show that this time scale is much smaller than the time scale of validity of the model.

In the mono-species setting, the first outcome about explicit estimates for the spectral gap  $\lambda_L$  has been obtained by Bobylev in [26, 27] for the case of Maxwell molecules, using Fourier methods to obtain a complete and explicit diagonalization of  $L$ . More recently, a systematic derivation of explicit coercivity estimates for the linearized collision operator has been established [11, 159, 163] for a wide class of collision kernels (including cutoff hard-potential and hard-sphere).

Starting from these results, in the past few years, the question of convergence towards the equilibrium has also been addressed in the case of multi-species kinetic models. Many Boltzmann-like equations describing the time evolution of a mixture of different gases can be found in the literature. To mention a few of them, we can refer to [179, 111, 158] for the first kinetic models for mixtures, to [95, 4, 47] for some BGK-type models, and to [174, 179, 41, 175, 70] for multi-species kinetic models where also chemical reactions are taken into account. Moreover, we recall the recent works [37, 65, 45, 44], where some of these models are mathematically investigated.

In this work, we focus on the multi-species setting. The equation we consider [70, 39, 35] can be seen as the counterpart of (2.1.1) in the case of gaseous mixtures, and shall be presented in detail in the next section. We only recall here that it models a mixture of  $N$  different ideal and monatomic gases, prescribing the time evolution of the multi-component gas distribution function  $\mathbf{F} = (F_1, \dots, F_N)$ . It reads, on  $\mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ ,

$$\partial_t \mathbf{F} + v \cdot \nabla_x \mathbf{F} = \mathbf{Q}(\mathbf{F}, \mathbf{F}). \quad (2.1.3)$$

Note that we consider the torus  $\mathbb{T}^3$  as spatial domain of the above equation. This choice is made only for a convenience when we shall describe the *a priori* conservation laws holding for (2.1.3). However, since the present chapter aims at establishing spectral properties that are local in time and space, our main theorems would still hold if  $x$  belonged to the whole space or to any bounded domain  $\Omega \subset \mathbb{R}^3$ .

As in the mono-species framework, it is possible to prove [70] a multi-species version of the  $H$ -theorem for the Boltzmann operator  $\mathbf{Q}$ , which suggests in this case that the global equilibrium of the mixture can be taken, after rescaling of the coordinate system, to be the global Maxwellian distribution  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_N)$ , with

$$\mu_i(v) = c_{i,\infty} \left( \frac{m_i}{2\pi} \right)^{3/2} e^{-m_i \frac{|v|^2}{2}}, \quad v \in \mathbb{R}^3,$$

for any  $1 \leq i \leq N$ . Here, we have denoted by  $(m_i)_{1 \leq i \leq N}$  and  $(c_{i,\infty})_{1 \leq i \leq N} \in \mathbb{R}^N$  the atomic masses and numbers of particles of each species in the gaseous mixture.



In order to investigate the convergence of solutions of (2.1.3) towards the equilibrium  $\boldsymbol{\mu}$ , we can study the behaviour of a small perturbation  $\mathbf{f} = (f_1, \dots, f_N)$  around  $\boldsymbol{\mu}$ . This approach raises the same kind of questions explained in our earlier discussion on the mono-species setting. In particular, the analysis of the large time asymptotic relaxation for solutions of the Boltzmann multi-species equation shall eventually lead to deal again with the problem of explicitly quantifying the rate of convergence to the equilibrium.

The study of explicit coercivity estimates for the linearized Boltzmann multi-species operator  $\mathbf{L}(\mathbf{f}) = \mathbf{Q}(\boldsymbol{\mu}, \mathbf{f}) + \mathbf{Q}(\mathbf{f}, \boldsymbol{\mu})$  has been very recently tackled, and the existence of a spectral gap for this operator has been shown in [65] for mixtures where the atomic masses of the different species are the same ( $m_i = m_j$  for any  $1 \leq i, j \leq N$ ), and in [45], in the general case of species with different atomic masses. Both results are valid for Maxwellian, hard-potential and hard-sphere collision kernels with cutoff.

Multicomponent mixtures exhibit some physical phenomena which are not usual in the mono-species case. For instance, if we focus on gaseous diffusion, Fick's law or Maxwell-Stefan's equations for a gaseous mixture imply specific movements of each component inside the mixture, which cannot happen for one sole gas: it is a so-called cross-diffusion effect, see for instance [97, 38]. Inspired by [39, 35], where the moment method is used, we here investigate a new perturbative setting around local Maxwellian distributions  $\mathbf{M}^\varepsilon = (M_1^\varepsilon, \dots, M_N^\varepsilon)$  with small macroscopic velocities of order  $\varepsilon$ , different for each species of the mixture. More precisely, for any  $1 \leq i \leq N$ , we can write  $M_i^\varepsilon$  as

$$M_i^\varepsilon(t, x, v) = c_{i,\infty} \left( \frac{m_i}{2\pi} \right)^{3/2} \exp \left\{ -m_i \frac{|v - \varepsilon u_i(t, x)|^2}{2} \right\}, \quad t \geq 0, \quad x \in \mathbb{T}^3, \quad v \in \mathbb{R}^3. \quad (2.1.4)$$

We note in particular that the parameter  $\varepsilon$  only translates the smallness of the macroscopic velocities of the different species, and not the order of the perturbation around  $\mathbf{M}^\varepsilon$ . We furthermore emphasize that these local Maxwellians describe mixtures where all the species share a common temperature, set to 1 here. Recent derivations [35] show that in this setting the multi-species Boltzmann equation formally converges to the Maxwell-Stefan system of equations that is widely used in physics to model fluid mixtures without chemical reactions. Allowing non-identical temperatures in the form  $1 + \varepsilon \theta_i(t, x)$  should not bring further difficulties to obtain equivalent results to our main theorems but physically this would mean that we are looking at the next order expansion of the Boltzmann equation.

We shall see that these Maxwellians are not a local equilibrium for the mixture, whereas they were in the mono-species setting. This feature induces additional difficulties if one wants to analyze the spectrum of the linearized operator  $\mathbf{L}^\varepsilon(\mathbf{f}) = \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{f}) + \mathbf{Q}(\mathbf{f}, \mathbf{M}^\varepsilon)$ , because  $\mathbf{L}^\varepsilon$  does not satisfy any self-adjointness property and it appears problematic to determine the space of equilibrium states  $\ker \mathbf{L}^\varepsilon$ . Consequently, we did not manage to give a detailed description of the spectrum of  $\mathbf{L}^\varepsilon$  and show explicit spectral gap estimates, using the same methods developed in [65, 45].

Instead of trying to recover a full spectral gap property, our idea is to establish an explicit estimate for an upper bound of the entropy production functional associated to  $\mathbf{L}^\varepsilon$ . More precisely, we prove that the estimate known to exist for the Dirichlet form of  $\mathbf{L}$  [65, 45] remains valid for the Dirichlet form of  $\mathbf{L}^\varepsilon$ , up to a correction term of order  $\varepsilon$ . The strategy exploits the fact that the non-equilibrium state  $\mathbf{M}^\varepsilon$  is close to the global equilibrium  $\boldsymbol{\mu}$  up to a factor of order  $\varepsilon$ , and the same property holds for  $\mathbf{L}^\varepsilon$  and  $\mathbf{L}$ . Specifically, we analyze the structure of the operator  $\mathbf{L}^\varepsilon - \mathbf{L}$ , showing that it can be seen as the sum of a multiplicative operator and an integral one. To deal with the latter, we exhibit its kernel structure by writing down a Carleman representation and deduce useful pointwise estimates. The core of the proof then relies on a mixing effect (see Lemma 2.4.6) in the exponential decay rates

among the cross-interactions between species: each species has a different atomic mass  $m_i$  and a different macroscopic velocity  $\varepsilon u_i$  which interplay inside the perturbation. We thus need to carefully treat the Maxwellian weights by deriving accurate  $L^1$  controls in the velocity variable. In the end, the operator  $\mathbf{L}^\varepsilon - \mathbf{L}$  is bounded from above by a positive quantity of order  $\varepsilon$ , producing the correction term in the estimate of the Dirichlet form of  $\mathbf{L}^\varepsilon$ .

The work is organized as follows. We first recall the multi-species model and give a detailed description of its main features, introducing the linearizations of the Boltzmann multi-species operator which we intend to study. Next, we recall the fundamental properties of the linearized Boltzmann multi-species operator and state our main result. The last section is dedicated to the proof of this result.

## 2.2 A kinetic model for mixtures

The evolution of a dilute gas composed of  $N \geq 2$  different species of chemically non-reacting monoatomic particles having atomic masses  $(m_i)_{1 \leq i \leq N}$  can be modelled by the following equations of Boltzmann type, for any  $1 \leq i \leq N$ ,

$$\partial_t F_i(t, x, v) + v \cdot \nabla_x F_i(t, x, v) = Q_i(\mathbf{F}, \mathbf{F})(t, x, v), \quad t \geq 0, \quad x \in \mathbb{T}^3, \quad v \in \mathbb{R}^3, \quad (2.2.1)$$

The vector  $\mathbf{F} = (F_1, \dots, F_N)$  denotes the unknown vector-valued distribution function describing the mixture and each  $F_i$  is the distribution function corresponding to the  $i$ -th species, which depends on time  $t$ , position  $x$  and velocity  $v$ . Henceforth, vectors and vector-valued functions will be denoted by bold letters, while the corresponding indexed letters will indicate their components. For example,  $\mathbf{W}$  represents the vector or vector-valued function  $(W_1, \dots, W_N)$ .

The Boltzmann multi-species operator  $\mathbf{Q}(\mathbf{F}, \mathbf{F}) = (Q_1(\mathbf{F}, \mathbf{F}), \dots, Q_N(\mathbf{F}, \mathbf{F}))$  describes the way the mixture molecules interact. The operator only acts on the velocity variable and it is defined component-wise, for any  $1 \leq i \leq N$  and any  $v \in \mathbb{R}^3$ , by

$$Q_i(\mathbf{F}, \mathbf{F})(v) = \sum_{j=1}^N Q_{ij}(F_i, F_j)(v) = \sum_{j=1}^N \int_{\mathbb{R}^3 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) (F_i' F_j'^* - F_i F_j^*) dv_* d\sigma.$$

In the previous equality, we used the standard shorthand notations  $F_i' = F_i(v')$ ,  $F_i = F_i(v)$  and  $F_j'^* = F_j(v'_*)$ ,  $F_j^* = F_j(v_*)$ . The pre-collisional velocities  $v'$  and  $v'_*$  are given in terms of the post-collisional velocities  $v$  and  $v_*$  by the elastic collision rules

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

where  $\sigma \in \mathbb{S}^2$  is a parameter whose existence is ensured by the conservation of microscopic momentum and kinetic energy

$$m_i v' + m_j v'_* = m_i v + m_j v_*, \quad \frac{1}{2} m_i |v'|^2 + \frac{1}{2} m_j |v'_*|^2 = \frac{1}{2} m_i |v|^2 + \frac{1}{2} m_j |v_*|^2. \quad (2.2.2)$$

The collisional cross-sections  $B_{ij}$  are nonnegative functions of  $|v - v_*|$  and the cosine of the deviation angle  $\vartheta \in [0, \pi]$  between  $v - v_*$  and  $\sigma \in \mathbb{S}^2$ . They encode all the information about the microscopic interactions between molecules in the mixture, and their choice is essential when studying the properties of the Boltzmann operator. In this work, we focus on cutoff Maxwellian, hard-potential and hard-sphere collision kernels. Namely, let us make the following assumptions on each  $B_{ij}$ ,  $i$  and  $j$  being fixed.

(H1) It satisfies a symmetry property with respect to the interchange of the species indices  $i$  and  $j$

$$B_{ij}(|v - v_*|, \cos \vartheta) = B_{ji}(|v - v_*|, \cos \vartheta), \quad \forall v, v_* \in \mathbb{R}^3, \forall \vartheta \in [0, \pi].$$

(H2) It decomposes into the product of a kinetic part  $\Phi_{ij} \geq 0$  and an angular part  $b_{ij} \geq 0$ , namely

$$B_{ij}(|v - v_*|, \cos \vartheta) = \Phi_{ij}(|v - v_*|)b_{ij}(\cos \vartheta), \quad \forall v, v_* \in \mathbb{R}^3, \forall \vartheta \in [0, \pi].$$

(H3) The kinetic part has the form of hard or Maxwellian ( $\gamma = 0$ ) potential, *i.e.*

$$\Phi_{ij}(|v - v_*|) = C_{ij}^\Phi |v - v_*|^\gamma, \quad C_{ij}^\Phi > 0, \quad \gamma \in [0, 1], \quad \forall v, v_* \in \mathbb{R}^3.$$

(H4) For the angular part, we consider a strong form of Grad's angular cutoff [105]. We assume that there exists a constant  $C > 0$  such that

$$0 < b_{ij}(\cos \vartheta) \leq C |\sin \vartheta| |\cos \vartheta| \quad \text{and} \quad b'_{ij}(\cos \vartheta) \leq C, \quad \forall \vartheta \in [0, \pi].$$

Furthermore, we assume that for any  $1 \leq i \leq N$

$$\inf_{\sigma_1, \sigma_2 \in \mathbb{S}^2} \int_{\mathbb{S}^2} \min\{b_{ii}(\sigma_1 \cdot \sigma_3), b_{ii}(\sigma_2 \cdot \sigma_3)\} d\sigma_3 > 0.$$

Let us discuss the hypotheses we made. We first emphasize that these are standard assumptions on collision kernels for multi-species equations [65, 45] but also in the mono-species case [11, 159] to obtain spectral properties for the linear operator. Assumption (H1) conveys the idea that collisions are micro-reversible. We use (H2) for the sake of clarity (even though it is common in a lot of physical models) and one could dismiss it at the price of technicalities. Assumption (H3) holds for collision kernels coming from interaction potentials which behave like power-laws. At last, the positivity assumption in (H4) is satisfied by most physical models and is required to obtain a spectral gap in the mono-species case [11, 159] and was thus a prerequisite for having a spectral gap in the multi-species case [45].

From now on, let us use the following notations. Consider a positive measurable vector-valued function  $\mathbf{W} = (W_1, \dots, W_N) : \mathbb{R}^3 \rightarrow (\mathbb{R}_+^*)^N$  in the variable  $v$ . For any  $1 \leq i \leq N$ , we define the weighted Hilbert space  $L^2(\mathbb{R}^3, W_i)$  by introducing the scalar product and norm

$$\langle f_i, g_i \rangle_{L^2_v(W_i)} = \int_{\mathbb{R}^3} f_i g_i W_i^2 dv, \quad \|f_i\|_{L^2_v(W_i)}^2 = \langle f_i, f_i \rangle_{L^2_v(W_i)}, \quad \forall f_i, g_i \in L^2(\mathbb{R}^3, W_i).$$

With this definition, we say that  $\mathbf{f} = (f_1, \dots, f_N) : \mathbb{R}^3 \rightarrow \mathbb{R}^N \in L^2(\mathbb{R}^3, \mathbf{W})$  if and only if  $f_i : \mathbb{R}^3 \rightarrow \mathbb{R} \in L^2(\mathbb{R}^3, W_i)$ , and we associate to  $L^2(\mathbb{R}^3, \mathbf{W})$  the natural scalar product and norm

$$\langle \mathbf{f}, \mathbf{g} \rangle_{L^2_v(\mathbf{W})} = \sum_{i=1}^N \langle f_i, g_i \rangle_{L^2_v(W_i)}, \quad \|\mathbf{f}\|_{L^2_v(\mathbf{W})} = \left( \sum_{i=1}^N \|f_i\|_{L^2_v(W_i)}^2 \right)^{1/2}.$$

Moreover, for the sake of simplicity, we define the shorthand notation

$$\langle v \rangle = \left( 1 + |v|^2 \right)^{1/2},$$

not to be confused with the usual Euclidean scalar product  $\langle \cdot, \cdot \rangle$  in  $\mathbb{R}^3$ , also used in the upcoming computations.

Let us now recall the main properties of  $\mathbf{Q}$ , which can be found in [59, 70, 39, 65, 45]. Using the symmetries of the collision operator combined with classical changes of variables  $(v, v_*) \mapsto (v', v'_*)$  and  $(v, v_*) \mapsto (v_*, v)$ , we can obtain the weak formulations of  $Q_{ij}(F_i, F_j)$

$$\begin{aligned} \int_{\mathbb{R}^3} Q_{ij}(F_i, F_j)(v) \psi_i(v) dv &= \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) F_i F_j^* (\psi'_i - \psi_i) dv dv_* d\sigma, \\ \int_{\mathbb{R}^3} Q_{ij}(F_i, F_j)(v) \psi_i(v) dv + \int_{\mathbb{R}^3} Q_{ji}(F_j, F_i)(v) \psi_j(v) dv &= \\ &= -\frac{1}{2} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) (F'_i F'_j{}^* - F_i F_j^*) (\psi'_i + \psi'_j{}^* - \psi_i - \psi_j^*) dv dv_* d\sigma, \end{aligned}$$

for any vector-valued function  $\boldsymbol{\psi} = (\psi_1, \dots, \psi_N) : \mathbb{R}^3 \rightarrow \mathbb{R}^N$  such that the integrals on the left-hand side of the above equalities are well-defined. These relations allow to deduce the conservation properties of the Boltzmann multi-species operator. More precisely, the equality

$$\sum_{i=1}^N \int_{\mathbb{R}^3} Q_i(\mathbf{F}, \mathbf{F})(v) \psi_i(v) dv = 0$$

holds if and only if  $\boldsymbol{\psi}$  is a collision invariant of the mixture, namely

$$\boldsymbol{\psi} \in \text{Span}(\mathbf{e}^{(1)}, \dots, \mathbf{e}^{(N)}, v_1 \mathbf{m}, v_2 \mathbf{m}, v_3 \mathbf{m}, |v|^2 \mathbf{m}),$$

where  $\mathbf{e}^{(i)} = (\delta_{ij})_{1 \leq j \leq N}$  for  $1 \leq i \leq N$ , and  $\mathbf{m} = (m_1, \dots, m_N)$ . In particular, from (2.2.1) and the conservation properties of  $\mathbf{Q}$ , we immediately get that the quantities

$$\begin{aligned} c_{i,\infty} &= \int_{\mathbb{T}^3 \times \mathbb{R}^3} F_i(t, x, v) dx dv, \quad 1 \leq i \leq N, \\ \rho_\infty u_\infty &= \sum_{i=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} m_i v F_i dx dv, \quad \frac{3}{2} K_B \rho_\infty \theta_\infty = \sum_{i=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} \frac{m_i}{2} |v - u_\infty|^2 F_i dx dv, \end{aligned} \tag{2.2.3}$$

are preserved for any time  $t \geq 0$ . Here,  $c_{i,\infty}$  stands for the total number of particles of the  $i$ -th species, and we have also defined the total mass of the mixture  $\rho_\infty = \sum_{i=1}^N m_i c_{i,\infty}$ , its total momentum  $\rho_\infty u_\infty$  and its total energy  $\frac{3}{2} K_B \rho_\infty \theta_\infty$ .

Moreover, the operator  $\mathbf{Q}$  satisfies a multi-species version of the  $H$ -theorem, see [70, Proposition 1]. It states, in particular, that the only solutions of the equation  $\mathbf{Q}(\mathbf{F}, \mathbf{F}) = 0$  are distribution functions  $\mathbf{F} = (F_1, \dots, F_N)$  such that their components take the form of local Maxwellians with a common macroscopic velocity, *i.e.* for any  $1 \leq i \leq N$  and any  $(t, x, v) \in \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ ,

$$F_i(t, x, v) = c_{i,\text{loc}}(t, x) \left( \frac{m_i}{2\pi K_B \theta_{\text{loc}}(t, x)} \right)^{3/2} \exp \left\{ -m_i \frac{|v - u_{\text{loc}}(t, x)|^2}{2K_B \theta_{\text{loc}}(t, x)} \right\}. \tag{2.2.4}$$

Here, we have defined the following local quantities:

$$\begin{aligned} c_{i,\text{loc}}(t, x) &= \int_{\mathbb{R}^3} F_i(t, x, v) dv, \quad 1 \leq i \leq N, \\ \rho_{\text{loc}}(t, x) &= \sum_{i=1}^N m_i c_{i,\text{loc}}(t, x), \\ u_{\text{loc}}(t, x) &= \frac{1}{\rho_{\text{loc}}(t, x)} \sum_{i=1}^N \int_{\mathbb{R}^3} m_i v F_i(t, x, v) dv, \\ \theta_{\text{loc}}(t, x) &= \frac{1}{3K_B \rho_{\text{loc}}(t, x)} \sum_{i=1}^N \int_{\mathbb{R}^3} m_i |v - u_{\text{loc}}(t, x)|^2 F_i(t, x, v) dv. \end{aligned}$$

It is worth noting that the local Maxwellian distributions (2.2.4) constitute a local equilibrium for the mixture, since  $\mathbf{Q}(\mathbf{F}, \mathbf{F}) = 0$ . This is not the case for the local Maxwellians  $M_i^\varepsilon$  introduced in (2.1.4), which in contrary form a non-equilibrium state for the mixture because of the different macroscopic velocities  $\varepsilon u_i$ .

In particular, since we work in  $\mathbb{T}^3$ , we can use the fact that the quantities (2.2.3) are conserved with respect to time, to deduce that the only global equilibrium of the mixture, *i.e.* the unique stationary solution  $\mathbf{F} = (F_1, \dots, F_N)$  to (2.2.1), is given for any  $1 \leq i \leq N$  by the global Maxwellians

$$F_i(v) = c_{i,\infty} \left( \frac{m_i}{2\pi K_B \theta_\infty} \right)^{3/2} \exp \left\{ -m_i \frac{|v - u_\infty|^2}{2K_B \theta_\infty} \right\}, \quad v \in \mathbb{R}^3.$$

Up to a translation and a dilation of the coordinate system, we can assume that  $u_\infty = 0$  and  $K_B \theta_\infty = 1$ , so that the only global equilibrium  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_N)$  becomes

$$\mu_i(v) = c_{i,\infty} \left( \frac{m_i}{2\pi} \right)^{3/2} e^{-m_i \frac{|v|^2}{2}}, \quad v \in \mathbb{R}^3, \quad (2.2.5)$$

for any  $1 \leq i \leq N$ . In what follows, we shall always work in the weighted Hilbert space  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , where we use the notation  $\boldsymbol{\mu}^{-\frac{1}{2}} = (\mu_1^{-\frac{1}{2}}, \dots, \mu_N^{-\frac{1}{2}})$ .

As already mentioned in the introduction, in order to study the Cauchy problem (2.2.1) and the convergence of the solution to equilibrium, it is common [70, 37, 65, 45] to consider a perturbative regime where each distribution function  $F_i$  is close to the global equilibrium given by (2.2.5). More precisely, when writing  $F_i(t, x, v) = \mu_i(v) + f_i(t, x, v)$  for any  $1 \leq i \leq N$ , where  $f_i$  is a small perturbation of the global equilibrium  $\mu_i$ , equations (2.2.1) can be rewritten in the form of the following perturbed multi-species Boltzmann system, set on  $\mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ ,

$$\partial_t \mathbf{f} + v \cdot \nabla_x \mathbf{f} = \mathbf{L}(\mathbf{f}) + \mathbf{Q}(\mathbf{f}, \mathbf{f}).$$

The linearized Boltzmann multi-species operator is given by  $\mathbf{L} = (L_1, \dots, L_N)$ , with

$$L_i(\mathbf{f}) = \sum_{j=1}^N L_{ij}(f_i, f_j) = \sum_{j=1}^N \left( Q_{ij}(\mu_i, f_j) + Q_{ij}(f_i, \mu_j) \right), \quad (2.2.6)$$

for any  $1 \leq i \leq N$ , and its main properties will be recalled in the next section. This operator has been intensively studied in the past few years, and the main results about his

kernel and his spectral properties have been obtained in [65] in the case of species having the same masses  $m_i = m_j$  and in [45] in the general case of species with different masses.

In this work, we consider a new perturbative regime around the local Maxwellian distributions  $\mathbf{M}^\varepsilon = (M_1^\varepsilon, \dots, M_N^\varepsilon)$ , given for any  $1 \leq i \leq N$  by

$$M_i^\varepsilon(t, x, v) = c_{i,\infty} \left(\frac{m_i}{2\pi}\right)^{3/2} \exp\left\{-m_i \frac{|v - \varepsilon u_i(t, x)|^2}{2}\right\}, \quad t \geq 0, \quad x \in \mathbb{T}^3, \quad v \in \mathbb{R}^3, \quad (2.2.7)$$

with small macroscopic velocities depending on the parameter  $\varepsilon \ll 1$ . We again stress the fact that the distribution functions  $M_i^\varepsilon$  are local in time and space like the Maxwellians given in (2.2.4), but they are not a local equilibrium for the Boltzmann operator  $\mathbf{Q} = (Q_1, \dots, Q_N)$ . In fact, the macroscopic velocities are different for each species of the mixture (since  $u_i \neq u_j$  for  $i \neq j$ ), implying that  $\mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon)$  is not zero anymore. Nevertheless, it is also important to note that the macroscopic velocities we consider are small (of order  $\varepsilon$ ), and this requirement is crucial to recover our result, since it shall be used to show that  $\mathbf{M}^\varepsilon$  is close to  $\boldsymbol{\mu}$  up to an order  $\varepsilon$ . Thus, even if  $\mathbf{M}^\varepsilon$  is a non-equilibrium state, it is still not far away from the global equilibrium of the mixture.

If we now assume that each distribution function  $F_i$  is close to a local Maxwellian of type (2.2.7), namely  $F_i(t, x, v) = M_i^\varepsilon(t, x, v) + f_i(t, x, v)$  for all  $1 \leq i \leq N$ , with  $\mathbf{f} = (f_1, \dots, f_N)$  being again a small perturbation, equations (2.2.1) posed on  $\mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$  can be rewritten as

$$\partial_t \mathbf{M}^\varepsilon + \partial_t \mathbf{f} + v \cdot \nabla_x \mathbf{M}^\varepsilon + v \cdot \nabla_x \mathbf{f} = \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon) + \mathbf{L}^\varepsilon(\mathbf{f}) + \mathbf{Q}(\mathbf{f}, \mathbf{f}). \quad (2.2.8)$$

The operator  $\mathbf{L}^\varepsilon = (L_1^\varepsilon, \dots, L_N^\varepsilon)$  is the Boltzmann multi-species operator linearized around the local Maxwellian distributions (2.2.7), and it is given by

$$L_i^\varepsilon(\mathbf{f}) = \sum_{j=1}^N L_{ij}^\varepsilon(f_i, f_j) = \sum_{j=1}^N \left( Q_{ij}(M_i^\varepsilon, f_j) + Q_{ij}(f_i, M_j^\varepsilon) \right), \quad (2.2.9)$$

for any  $1 \leq i \leq N$ .

Before going into details of our main result, we here note that, for velocities  $v - \varepsilon u_i$  and  $v_* - \varepsilon u_j$ , the microscopic conservation properties (2.2.2) do not hold anymore and consequently  $M_i^{\varepsilon'} M_j^{\varepsilon'*} \neq M_i^\varepsilon M_j^{\varepsilon*}$ . Therefore, the operator  $\mathbf{L}^\varepsilon$  exhibits no good self-adjointness properties and this peculiarity will force us to develop an alternative strategy to the one presented in [65] and [45] in order to investigate its spectral properties.

We also mention that looking at a perturbative regime around non-equilibrium Maxwellians  $M_i^\varepsilon$  to recover system (2.2.8) can be of particular interest in the investigation of the asymptotic approximation of solutions to the Maxwell-Stefan diffusion equations, in the spirit of [39, 35].

## 2.3 Main result

This section is dedicated to the presentation of our main theorem. Due to the choice of the linearization of  $\mathbf{Q}$  around  $\mathbf{M}^\varepsilon$ , the standard tools developed to perform the spectral analysis of  $\mathbf{L}$  are no more valid for the operator  $\mathbf{L}^\varepsilon$ . This issue will be overcome by connecting  $\mathbf{L}^\varepsilon$  to  $\mathbf{L}$ , in order to take advantage of the results known about the spectrum of  $\mathbf{L}$ . We are able to show that the Dirichlet form of  $\mathbf{L}^\varepsilon$  in the space  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  is upper-bounded by a negative term coming from the spectral gap of  $\mathbf{L}$  in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , plus a positive contribution of order  $\varepsilon$ , which takes into account the fact that we are working in a space where  $\mathbf{L}^\varepsilon$  is not self-adjoint.

We begin by recalling the fundamental result derived in [45] about the existence of a spectral gap for  $\mathbf{L}$  in the space  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ . To do this, we first present the structure of  $\ker \mathbf{L}$ .

The linearized Boltzmann multi-species operator  $\mathbf{L}$  defined by (2.2.6) is a closed self-adjoint operator in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , whose kernel can be described by means of an orthonormal basis  $(\boldsymbol{\phi}^{(k)})_{1 \leq k \leq N+4}$  in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , that is

$$\ker \mathbf{L} = \text{Span} \left( \boldsymbol{\phi}^{(1)}, \dots, \boldsymbol{\phi}^{(N+4)} \right),$$

where

$$\left\{ \begin{array}{l} \boldsymbol{\phi}^{(i)} = \frac{1}{\sqrt{c_{i,\infty}}} \mu_i \mathbf{e}^{(i)}, \quad 1 \leq i \leq N, \\ \boldsymbol{\phi}^{(N+\ell)} = \frac{v_\ell}{\left( \sum_{j=1}^N m_j c_{j,\infty} \right)^{1/2}} (m_i \mu_i)_{1 \leq i \leq N}, \quad 1 \leq \ell \leq 3, \\ \boldsymbol{\phi}^{(N+4)} = \frac{1}{\left( \sum_{j=1}^N c_{j,\infty} \right)^{1/2}} \left( \frac{m_i |v|^2 - 3}{\sqrt{6}} \mu_i \right)_{1 \leq i \leq N}. \end{array} \right.$$

Using this basis, for any  $\mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  we can define its orthogonal projection onto the space  $\ker \mathbf{L}$  in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  as

$$\pi_{\mathbf{L}}(\mathbf{f})(v) = \sum_{k=1}^{N+4} \langle \mathbf{f}, \boldsymbol{\phi}^{(k)} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \boldsymbol{\phi}^{(k)}(v).$$

Then, the linearized Boltzmann multi-species operator satisfies the following fundamental theorem, proved in [45].

**Theorem 2.3.1.** *Let the collision kernels  $B_{ij}$  satisfy assumptions (H1)–(H4). Then there exists an explicit constant  $\lambda_{\mathbf{L}} > 0$  such that, for all  $\mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ ,*

$$\langle \mathbf{L}(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq -\lambda_{\mathbf{L}} \|\mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{1}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2.$$

*The constant  $\lambda_{\mathbf{L}}$  only depends on  $N$ , the different masses  $(m_i)_{1 \leq i \leq N}$  and the collision kernels  $(B_{ij})_{1 \leq i, j \leq N}$ .*

In order to take advantage of this result, we choose to set our study in the global equilibrium weighted space  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ . Following the path of its proof, it appears that we strongly need the fact that the operator  $\mathbf{L}$  is self-adjoint in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , which is not the case for  $\mathbf{L}^\varepsilon$ . The lack of this property does not allow to directly apply the tools developed in [45] to show the existence of a spectral gap for  $\mathbf{L}^\varepsilon$ . In particular, one of the main issues we encountered is that we were not able to recover the form of  $\ker \mathbf{L}^\varepsilon$  in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , leaving the corresponding orthogonal projection  $\pi_{\mathbf{L}^\varepsilon}$  onto  $\ker \mathbf{L}^\varepsilon$  undefined. This led us to confront the problem from a different point of view.

The idea is to recover an estimate for the Dirichlet form of  $\mathbf{L}^\varepsilon$  in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , by finding a way to link the two operators and use what is known about the spectral properties of  $\mathbf{L}$  on this space. The price we have to pay is the appearance of two positive terms of order  $\varepsilon$  in the estimate. The first one is a correction to the spectral gap  $\lambda_{\mathbf{L}}$ , which comes from the choice of working with the orthogonal projection  $\pi_{\mathbf{L}}$  onto  $\ker \mathbf{L}$  in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , in place of  $\pi_{\mathbf{L}^\varepsilon}$ .

In fact, the Dirichlet form of  $\mathbf{L}^\varepsilon$  is taken with respect to the global equilibrium  $\boldsymbol{\mu}$  instead of a local Maxwellian  $\mathbf{M}^\varepsilon$ , and the correction to  $\lambda_{\mathbf{L}}$  translates the fact that  $\boldsymbol{\mu}$  and  $\mathbf{M}^\varepsilon$  are close in Euclidean norm, up to a factor of order  $\varepsilon$ . Moreover, a further consequence of our choice is that  $\pi_{\mathbf{L}}(\mathbf{f}) \notin \ker \mathbf{L}^\varepsilon$ , meaning that  $\mathbf{L}^\varepsilon(\pi_{\mathbf{L}}(\mathbf{f}))$  is not zero and has to be estimated, producing another contribution of order  $\varepsilon$ . The second term precisely takes into account this last feature.

Let us now state the main result that we shall prove.

**Theorem 2.3.2.** *Let the collision kernels  $B_{ij}$  satisfy assumptions (H1)–(H4), and consider  $\lambda_{\mathbf{L}} > 0$ , the spectral gap in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  of the operator  $\mathbf{L}$  defined by (2.2.6). There exists  $C > 0$  such that, for all  $\varepsilon > 0$ , the operator  $\mathbf{L}^\varepsilon$  defined by (2.2.9) satisfies the following a priori estimate. For almost every  $(t, x) \in \mathbb{R}_+ \times \mathbb{T}^3$ , and for any  $\mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ ,*

$$\begin{aligned} \langle \mathbf{L}^\varepsilon(\mathbf{f}), \mathbf{f} \rangle_{L^2_v(\boldsymbol{\mu}^{-\frac{1}{2}})} &\leq - \left( \lambda_{\mathbf{L}} - C\varepsilon \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i(t, x)| \mathcal{R}_{\varepsilon,i} \right\} \right) \|\mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f})\|_{L^2_v(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + C\varepsilon \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i(t, x)| \mathcal{R}_{\varepsilon,i} \right\} \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L^2_v(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2, \end{aligned} \quad (2.3.1)$$

where  $\pi_{\mathbf{L}}$  is the orthogonal projection onto  $\ker \mathbf{L}$  in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , and we have defined

$$\mathcal{R}_{\varepsilon,i} = 1 + \varepsilon |u_i(t, x)| \exp \left\{ \frac{4m_i}{1-\delta} \varepsilon^2 |u_i(t, x)|^2 \right\},$$

for some  $\delta \in (0, 1)$  independent of  $\varepsilon$  to be appropriately chosen.

The constant  $C$  is explicit and only depends on  $N$ , the different masses  $(m_i)_{1 \leq i \leq N}$ , the collision kernels  $(B_{ij})_{1 \leq i, j \leq N}$  and the parameter  $\delta \in (0, 1)$ . In particular, it does not depend on  $\varepsilon$ , the number of particles of the different species  $(c_{i,\infty})_{1 \leq i \leq N}$  and the macroscopic velocities  $(u_i)_{1 \leq i \leq N}$ .

This result provides an estimate which is local in space and time, meaning that  $(t, x)$  remains fixed. For the sake of simplicity, from now on we shall omit the explicit dependence of the macroscopic velocity  $u_i = u_i(t, x)$  on both variables.

As already mentioned, the main idea of the proof consists in linking  $\mathbf{L}^\varepsilon$  to  $\mathbf{L}$  in order to use the properties known on the linearized Boltzmann operator and apply Theorem 2.3.1. In view of this, we write  $\mathbf{L}^\varepsilon$  as a sum  $\mathbf{L}^\varepsilon = \mathbf{L} + (\mathbf{L}^\varepsilon - \mathbf{L})$  and we separately treat the two addends. The operator  $\mathbf{L}$  will be straightforwardly controlled using Theorem 2.3.1, producing the contribution  $\lambda_{\mathbf{L}}$  in the estimate of Theorem 2.3.2, and we shall need to prove that  $\mathbf{L}^\varepsilon - \mathbf{L}$  can be bounded and gives the remaining contributions of order  $\varepsilon$ .

In order to show the control on the penalty term, we first recover a bound of order  $\varepsilon$  for the differences  $M_i^\varepsilon - \mu_i$ , proving that even if the local Maxwellian distributions (2.2.7) constitute a non-equilibrium state for the Boltzmann multi-species operator, they are still very close to the global equilibrium  $\boldsymbol{\mu}$ . To take advantage of this property, the penalty term will be further split into two parts that we shall study independently. The first one will be a multiplicative operator that shall be easily controlled, while the second one will be an integral operator that shall be written under a kernel form (using the Carleman representation) and estimated pointwise with the strategy proposed in [45]. Here, we will encounter a major issue. In fact, we shall need to manage the complete lack of symmetry between cross-interacting species (different atomic mass  $m_i$  and macroscopic velocity  $\varepsilon u_i$  for each species of the mixture), which will lead to intricate mixing effects in the exponential decay rates of



the Maxwellian weights. To solve the difficulty we shall establish new accurate  $L^1$  controls in the velocity variable for the kernel operator. This will involve proving new technical lemmata, but will finally allow to close the estimate and recover our result.

## 2.4 Proof of Theorem 2.3.2

This section is devoted to the proof of our main result. In order to explain in a clear way the procedure, we divide the proof into several steps. We first split the operator  $\mathbf{L}^\varepsilon$  into the linearized Boltzmann operator  $\mathbf{L}$  plus a penalization term  $\mathbf{L}^\varepsilon - \mathbf{L}$ , and we study their associated Dirichlet forms. We then use Theorem 2.3.1 to bound the Dirichlet form of  $\mathbf{L}$ , while we note that the Dirichlet form of  $\mathbf{L}^\varepsilon - \mathbf{L}$  produces four terms. Each of these terms will be bounded separately in a dedicated step, proving that they produce a contribution of order  $\varepsilon$ . We shall finally collect all the estimates to recover Theorem 2.3.2 in the last step of the proof.

**Step 1 – Penalization of the operator  $\mathbf{L}^\varepsilon$ .** We consider the Dirichlet form of the operator  $\mathbf{L}^\varepsilon$  in the space  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , and we apply a splitting based on a penalization by the operator  $\mathbf{L}$ . More precisely, using Theorem 2.3.1 we successively get, for any  $\mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ ,

$$\begin{aligned} \langle \mathbf{L}^\varepsilon(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} &= \langle \mathbf{L}(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} + \langle \mathbf{L}^\varepsilon(\mathbf{f}) - \mathbf{L}(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &\leq -\lambda_{\mathbf{L}} \|\mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \langle \mathbf{L}^\varepsilon(\mathbf{f}) - \mathbf{L}(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})}, \end{aligned}$$

Then the penalty term writes

$$\langle \mathbf{L}^\varepsilon(\mathbf{f}) - \mathbf{L}(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \sum_{i,j} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) \Delta_{ij}^\varepsilon f_i \mu_i^{-1} dv dv_* d\sigma,$$

with the shorthand notation

$$\Delta_{ij}^\varepsilon := (M_i^{\varepsilon'} - \mu_i') f_j^* + (M_j^{\varepsilon' *} - \mu_j'^*) f_i' - (M_i^\varepsilon - \mu_i) f_j^* - (M_j^{\varepsilon *} - \mu_j^*) f_i.$$

By simply taking the modulus, we can bound from above  $\Delta_{ij}^\varepsilon$  in this way

$$\Delta_{ij}^\varepsilon \leq |M_i^{\varepsilon'} - \mu_i'| |f_j^*| + |M_j^{\varepsilon' *} - \mu_j'^*| |f_i'| + |M_i^\varepsilon - \mu_i| |f_j^*| + |M_j^{\varepsilon *} - \mu_j^*| |f_i|,$$

and to conclude the proof we shall need to control each of the four terms appearing in the inequality. For the sake of simplicity, we will separately consider the different terms, and we set

$$\mathcal{T}_1^\varepsilon(\mathbf{f}) = \sum_{i,j} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) |M_i^{\varepsilon'} - \mu_i'| |f_j^*| |f_i| \mu_i^{-1} dv dv_* d\sigma,$$

$$\mathcal{T}_2^\varepsilon(\mathbf{f}) = \sum_{i,j} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) |M_j^{\varepsilon' *} - \mu_j'^*| |f_i'| |f_i| \mu_i^{-1} dv dv_* d\sigma,$$

$$\mathcal{T}_3^\varepsilon(\mathbf{f}) = \sum_{i,j} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) |M_i^\varepsilon - \mu_i| |f_j^*| |f_i| \mu_i^{-1} dv dv_* d\sigma,$$

$$\mathcal{T}_4^\varepsilon(\mathbf{f}) = \sum_{i,j} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) |M_j^{\varepsilon *} - \mu_j^*| f_i^2 \mu_i^{-1} dv dv_* d\sigma.$$

**Step 2 – Preliminary lemmata.** In order to bound each component, we collect in this step two useful preliminary results. The first one yields an estimate which allows to compare the growth of the local Maxwellians given in (2.2.7) with the growth of the global Maxwellians (2.2.5).

**Lemma 2.4.1.** *Consider the local Maxwellian distribution  $\mathbf{M}^\varepsilon$  defined in (2.2.7) and the global equilibrium  $\boldsymbol{\mu}$  introduced in (2.2.5). For almost every  $(t, x) \in \mathbb{R}_+ \times \mathbb{T}^3$  and for all  $\delta \in (0, 1)$ , there exists an explicit constant  $C_\delta > 0$  (independent of  $\varepsilon$ , of the number of particles  $c_{i,\infty}$  and of the macroscopic velocities  $u_i$ ) such that, for all  $\varepsilon > 0$  and  $1 \leq i \leq N$ ,*

$$|M_i^\varepsilon(v) - \mu_i(v)| \leq C_\delta \varepsilon c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \mu_i^\delta(v), \quad \forall v \in \mathbb{R}^3, \quad (2.4.1)$$

recalling that we have defined for simplicity

$$\mathcal{R}_{\varepsilon,i} = 1 + \varepsilon |u_i| \exp \left\{ \frac{4m_i}{1-\delta} \varepsilon^2 |u_i|^2 \right\}.$$

*Proof.* Fix  $\delta \in (0, 1)$ . Noticing that  $M_i^\varepsilon(v) = \mu_i(v - \varepsilon u_i)$  and using Cauchy-Schwarz inequality, we obtain, for any  $v \in \mathbb{R}^3$ ,

$$\begin{aligned} |M_i^\varepsilon(v) - \mu_i(v)| &= \left| \int_0^1 m_i \langle v - s\varepsilon u_i, \varepsilon u_i \rangle \mu_i(v - s\varepsilon u_i) ds \right| \\ &\leq \varepsilon |u_i| \mu_i^\delta(v) \int_0^1 m_i |v - s\varepsilon u_i| \mu_i(v - s\varepsilon u_i) \mu_i^{-\delta}(v) ds. \end{aligned}$$

The product of the two Maxwellians inside the integral can be upper-estimated as

$$\mu_i(v - s\varepsilon u_i) \mu_i^{-\delta}(v) \leq c_{i,\infty}^{1-\delta} \left( \frac{m_i}{2\pi} \right)^{3(1-\delta)/2} \exp \left\{ -(1-\delta) \frac{m_i}{2} |v|^2 + s\varepsilon m_i |u_i| |v| \right\},$$

Consequently, the previous integral is bounded by

$$\begin{aligned} \int_0^1 m_i |v - s\varepsilon u_i| \mu_i(v - s\varepsilon u_i) \mu_i^{-\delta}(v) ds \\ \leq m_i c_{i,\infty}^{1-\delta} \left( \frac{m_i}{2\pi} \right)^{\frac{3(1-\delta)}{2}} \left( |v| + \varepsilon |u_i| \right) e^{-(1-\delta) \frac{m_i}{2} |v|^2 + \varepsilon m_i |u_i| |v|}. \end{aligned}$$

Starting from this last inequality, we distinguish two cases:

1. For  $|v| \geq \frac{4\varepsilon |u_i|}{1-\delta}$ , we have

$$\begin{aligned} \int_0^1 m_i |v - s\varepsilon u_i| \mu_i(v - s\varepsilon u_i) \mu_i^{-\delta}(v) ds \\ \leq m_i c_{i,\infty}^{1-\delta} \left( \frac{m_i}{2\pi} \right)^{\frac{3(1-\delta)}{2}} \frac{5-\delta}{4} |v| \exp \left\{ -(1-\delta) \frac{m_i}{4} |v|^2 \right\} \end{aligned}$$

which is clearly upper bounded since  $\delta \in (0, 1)$ .

2. For  $|v| < \frac{4\varepsilon |u_i|}{1-\delta}$ , we get

$$\begin{aligned} \int_0^1 m_i |v - s\varepsilon u_i| \mu_i(v - s\varepsilon u_i) \mu_i^{-\delta}(v) ds \\ \leq m_i c_{i,\infty}^{1-\delta} \left( \frac{m_i}{2\pi} \right)^{\frac{3(1-\delta)}{2}} \frac{5-\delta}{1-\delta} \varepsilon |u_i| \exp \left\{ \frac{4m_i}{1-\delta} \varepsilon^2 |u_i|^2 \right\}. \end{aligned}$$

For all  $v \in \mathbb{R}^3$ , we finally deduce the bound

$$\int_0^1 m_i |v - s\varepsilon u_i| \mu_i(v - s\varepsilon u_i) \mu_i^{-\delta}(v) ds \leq C_\delta \left( 1 + \varepsilon |u_i| \exp \left\{ \frac{4m_i}{1-\delta} \varepsilon^2 |u_i|^2 \right\} \right),$$

by simply taking

$$C_\delta = \max_{1 \leq i \leq N} m_i c_{i,\infty}^{1-\delta} \left( \frac{m_i}{2\pi} \right)^{\frac{3(1-\delta)}{2}} (5-\delta) \left( \sup_{|v| \in \mathbb{R}_+} \left( \frac{|v|}{4} e^{-(1-\delta)\frac{m_i}{4}|v|^2} \right) + \frac{1}{1-\delta} \right) > 0,$$

which concludes the proof.  $\square$

We also present a second important result that we shall use in the following. In that end, we first introduce an additional property of the linearized Boltzmann operator.

The operator  $\mathbf{L}$  can be written under the form

$$\mathbf{L} = \mathbf{K} - \boldsymbol{\nu},$$

where  $\mathbf{K} = (K_1, \dots, K_N)$  is a compact operator [37] defined, for any  $1 \leq i \leq N$  and any  $v \in \mathbb{R}^3$ , by

$$K_i(\mathbf{f})(v) = \sum_{j=1}^N \int_{\mathbb{R}^3 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) (\mu'_i f'_j{}^* + \mu'_j f'_i{}^* - \mu_i f_j^*) dv_* d\sigma, \quad (2.4.2)$$

and  $\boldsymbol{\nu} = (\nu_1, \dots, \nu_N)$  acts like a multiplicative operator, namely, for any  $1 \leq i \leq N$  and any  $v \in \mathbb{R}^3$ ,

$$\begin{aligned} \nu_i(\mathbf{f})(v) &= \sum_{j=1}^N \nu_{ij}(v) f_j(v), \\ \nu_{ij}(v) &= \int_{\mathbb{R}^3} B_{ij}(|v - v_*|, \cos \vartheta) \mu_j(v_*) dv_* d\sigma. \end{aligned} \quad (2.4.3)$$

It is well-known [57, 59, 190] that, under our assumptions on the collision kernels  $B_{ij}$ , each of the so-called collision frequencies  $\nu_{ij}$  satisfies the following lower and upper bounds. For all  $1 \leq i, j \leq N$ , there exist two explicit positive constants  $\bar{\nu}_{ij}, \tilde{\nu}_{ij} > 0$  such that

$$0 < \bar{\nu}_{ij} \leq \nu_{ij}(v) \leq \tilde{\nu}_{ij} (1 + |v|^\gamma), \quad \forall v \in \mathbb{R}^3. \quad (2.4.4)$$

The lemma we then recall has been proved in [45, Lemma 5.1] (see also [37]), and states that the operator  $\mathbf{K}$  can be written under a kernel form. The authors actually prove a more general result, showing that the full Boltzmann multi-species operator (and not only its linearized version) has a Carleman representation [52].

**Lemma 2.4.2.** *For any  $\mathbf{f} = (f_1, \dots, f_N) \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , the following Carleman representations hold:*

$$\begin{aligned} \int_{\mathbb{R}^3 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) f_i^* f_j^* dv_* d\sigma &= \\ C_{ij} \int_{\mathbb{R}^3} \left( \frac{1}{|v - v_*|} \int_{\tilde{E}_{vv_*}^{ij}} \frac{B_{ij} \left( v - V(u, v_*), \frac{v_* - u}{|u - v_*|} \right)}{|u - v_*|} f_i(u) d\tilde{E}(u) \right) f_j^* dv_*, \end{aligned}$$

$$\int_{\mathbb{R}^3 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) f'_i f'_j{}^* dv_* d\sigma =$$

$$C_{ji} \int_{\mathbb{R}^3} \left( \frac{1}{|v - v_*|} \int_{E_{vv_*}^{ij}} \frac{B_{ij}\left(v - V(v_*, u), \frac{u - v_*}{|u - v_*|}\right)}{|u - v_*|} f_i(u) dE(u) \right) f_j^* dv_*,$$

where we have defined  $V(u, v_*) = v_* + m_i m_j^{-1} u - m_i m_j^{-1} v$  and called  $C_{ij}, C_{ji} > 0$  some explicit constants which only depend on the masses  $m_i, m_j$ . Moreover, we have denoted by  $dE$  the Lebesgue measure on the hyperplane  $E_{vv_*}^{ij}$ , orthogonal to  $v - v_*$  and passing through

$$V_E(v, v_*) = \frac{m_i + m_j}{2m_j} v - \frac{m_i - m_j}{2m_j} v_*,$$

and by  $d\tilde{E}$  the Lebesgue measure on the space  $\tilde{E}_{vv_*}^{ij}$  which corresponds to the hyperplane  $E_{vv_*}^{ij}$ , whenever  $m_i = m_j$ , and to the sphere of radius

$$R_{vv_*} = \frac{m_j}{|m_i - m_j|} |v - v_*|$$

and centred at

$$O_{vv_*} = \frac{m_i}{m_i - m_j} v - \frac{m_j}{m_i - m_j} v_*,$$

whenever  $m_i \neq m_j$ .

Let us now pass to the actual estimate of the different terms  $\mathcal{T}_k^\varepsilon$ . For the sake of simplicity, we shall call  $C^{(k)}$  any constant bounding the corresponding term  $\mathcal{T}_k^\varepsilon$  independently of  $\varepsilon$  and  $u_i$ , but each of these constants will be explicit in the sense that all steps in our proofs are constructive and explicit computations of the constants could be extracted from them.

**Step 3 – Estimation of  $\mathcal{T}_4^\varepsilon$ .** Applying Lemma 2.4.1 for any fixed  $\delta \in (0, 1)$  and using the assumptions made on the collisional kernels, the term can be estimated as

$$\begin{aligned} \mathcal{T}_4^\varepsilon(\mathbf{f}) &= \sum_{i,j} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) |M_j^{\varepsilon*} - \mu_j^*| f_i^2 \mu_i^{-1} dv dv_* d\sigma \\ &\leq \varepsilon C_\delta \sum_{i,j} c_{j,\infty}^{1-\delta} |u_j| \mathcal{R}_{\varepsilon,j} \|b_{ij}\|_{L^1(\mathbb{S}^2)} \int_{\mathbb{R}^3} \left( \int_{\mathbb{R}^3} |v - v_*|^\gamma \mu_j^{*\delta} dv_* \right) f_i^2 \mu_i^{-1} dv \\ &\leq \varepsilon C_\delta \max_{1 \leq i,j \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \|b_{ij}\|_{L^1(\mathbb{S}^2)} \right\} \sum_{i,j} \int_{\mathbb{R}^3} \left( \int_{\mathbb{R}^3} |v - v_*|^\gamma \mu_j^{*\delta} dv_* \right) f_i^2 \mu_i^{-1} dv. \end{aligned}$$

Moreover, we notice that for all  $1 \leq j \leq N$ , the integral term

$$\nu_j^{(\delta)} = \int_{\mathbb{R}^3} |v - v_*|^\gamma \mu_j^{*\delta} dv_*$$

has the same form of the collision frequencies  $\nu_{ij}$  and it consequently satisfies an estimate similar to (2.4.4). Using the fact that  $(1 + |v|^\gamma) \sim \langle v \rangle^\gamma$ , there exist two strictly positive explicit constants  $\bar{\nu}_j^{(\delta)}, \tilde{\nu}_j^{(\delta)} > 0$  such that

$$0 < \bar{\nu}_j^{(\delta)} \leq \nu_j^{(\delta)}(v) \leq \tilde{\nu}_j^{(\delta)} \langle v \rangle^\gamma, \quad \forall v \in \mathbb{R}^3.$$

We finally deduce

$$\begin{aligned} \mathcal{T}_4^\varepsilon(\mathbf{f}) &\leq \varepsilon C_\delta \max_{1 \leq i, j \leq N} \left\{ c_{i, \infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon, i} \|b_{ij}\|_{L^1(\mathbb{S}^2)} \right\} \left( \sum_{j=1}^N \tilde{\nu}_j^{(\delta)} \right) \sum_{i=1}^N \int_{\mathbb{R}^3} \langle v \rangle^\gamma f_i^2 \mu_i^{-1} dv \\ &\leq \varepsilon C^{(4)} \max_{1 \leq i \leq N} \left\{ c_{i, \infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon, i} \right\} \|f\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2, \end{aligned} \quad (2.4.5)$$

with  $C^{(4)} = C_\delta \left( \sum_{j=1}^N \tilde{\nu}_j^{(\delta)} \right) \max_{1 \leq i, j \leq N} \|b_{ij}\|_{L^1(\mathbb{S}^2)}$ . The next constants  $C^{(k)}$  can be explicitly computed, but we shall not keep explicit estimates for the sake of clarity.

**Step 4 – Estimation of  $\mathcal{T}_3^\varepsilon$ .** Similarly, we can rewrite  $\mathcal{T}_3^\varepsilon$  in terms of  $\mathbf{h} = (h_1, \dots, h_N)$  with  $h_i = f_i \mu_i^{-\frac{1}{2}}$  for any  $1 \leq i \leq N$ , and obtain

$$\begin{aligned} \mathcal{T}_3^\varepsilon(\mathbf{f}) &= \sum_{i, j} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) |M_i^\varepsilon - \mu_i| \mu_i^{-\frac{1}{2}} \mu_j^{*\frac{1}{2}} |h_j^*| |h_i| dv dv_* d\sigma \\ &\leq \varepsilon C^{(3)} \max_{1 \leq i \leq N} \left\{ c_{i, \infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon, i} \right\} \sum_{i, j} \int_{\mathbb{R}^6} |v - v_*|^\gamma \mu_i^{\frac{2\delta-1}{2}} \mu_j^{*1/2} |h_j^*| |h_i| dv dv_*, \end{aligned}$$

where this time we have used Lemma 2.4.1 with  $\delta \in (1/2, 1)$ . Applying Young's inequality and Fubini's theorem allows to conclude that

$$\begin{aligned} \mathcal{T}_3^\varepsilon(\mathbf{f}) &\leq \varepsilon C^{(3)} \max_{1 \leq i \leq N} \left\{ c_{i, \infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon, i} \right\} \\ &\quad \sum_{i, j} \left( \int_{\mathbb{R}^6} |v - v_*|^\gamma \mu_i^{2\delta-1} h_j^{*2} dv dv_* + \int_{\mathbb{R}^6} |v - v_*|^\gamma \mu_j^* h_i^2 dv_* dv \right) \\ &\leq \varepsilon C^{(3)} \max_{1 \leq i \leq N} \left\{ c_{i, \infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon, i} \right\} \left( \sum_{j=1}^N \int_{\mathbb{R}^3} \langle v_* \rangle^\gamma f_j^{*2} \mu_j^{*-1} dv_* + \sum_{i=1}^N \int_{\mathbb{R}^3} \langle v \rangle^\gamma f_i^2 \mu_i^{-1} dv \right) \\ &\leq \varepsilon C^{(3)} \max_{1 \leq i \leq N} \left\{ c_{i, \infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon, i} \right\} \|\mathbf{f}\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2. \end{aligned} \quad (2.4.6)$$

**Step 5 – Estimation of  $\mathcal{T}_2^\varepsilon$ .** In order to estimate  $\mathcal{T}_2^\varepsilon$ , we first apply Lemma 2.4.1, like in the case of  $\mathcal{T}_4^\varepsilon$ , to bound the difference between the local and the global Maxwellians. We have

$$\begin{aligned} \mathcal{T}_2^\varepsilon(\mathbf{f}) &= \sum_{i, j} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) |M_j^{\varepsilon' *} - \mu_j^{*'}| |f_i'| |f_i| \mu_i^{-1} dv dv_* d\sigma \\ &\leq \varepsilon C^{(2)} \max_{1 \leq i \leq N} \left\{ c_{i, \infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon, i} \right\} \sum_{i, j} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) \mu_j^{*\delta} |f_i'| |f_i| \mu_i^{-1} dv dv_* d\sigma, \end{aligned}$$

for any  $\delta \in (0, 1)$ . Next, we write the previous integral in its kernel form using Lemma

2.4.2. That allows to get, for any  $1 \leq i, j \leq N$ ,

$$\begin{aligned} & \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) \mu_j'^{\delta} |f_i'| |f_i| \mu_i^{-1} \, dv dv_* d\sigma \\ &= C_{ji} \int_{\mathbb{R}^6} \left( \frac{1}{|v - v_*|} \int_{E_{vv_*}^{ij}} \frac{B_{ij} \left( v - V(v_*, u), \frac{u - v_*}{|u - v_*|} \right)}{|u - v_*|} \mu_j^\delta(u) \, dE(u) \right) |f_i'| |f_i| \mu_i^{-1} \, dv dv_* \\ &= C_{ji} \int_{\mathbb{R}^6} \left( \frac{1}{|v - v_*|} \int_{E_{vv_*}^{ij}} \frac{B_{ij} \left( v - V(v_*, u), \frac{u - v_*}{|u - v_*|} \right)}{|u - v_*|} \mu_j^\delta(u) \, dE(u) \right) \sqrt{\frac{\mu_i^*}{\mu_i}} |h_i^*| |h_i| \, dv dv_*. \end{aligned}$$

In order to estimate this integral, we use a result presented in [45, Lemma 5.1], in which the authors analyze the particular structure of the kernel form of the operator  $\mathbf{K}$  and they deduce explicit pointwise bounds on it. The strategy involves a careful treatment of the different exponential decay rates appearing in the Maxwellian weights. This feature is specific to the multi-species framework and is a direct consequence of the asymmetry in the cross-interactions between species of the mixture, where the different atomic masses lead to these intricate mixing effects. Their result is proved in the case of global equilibria  $\mu_i$ , but it also straightforwardly applies to any function of the form  $\mu_i^\delta$ , with  $\delta > 0$ . We omit the proof, since it exactly follows the same steps as in [45].

**Lemma 2.4.3.** *For any  $\delta \in (0, 1)$  and  $1 \leq i, j \leq N$ , let the operator  $I_{ji}^\delta$  be defined for  $v, v_* \in \mathbb{R}^3$  by*

$$I_{ji}^\delta(v, v_*) = \frac{C_{ji}}{|v - v_*|} \int_{E_{vv_*}^{ij}} \frac{B_{ij} \left( v - V(v_*, u), \frac{u - v_*}{|u - v_*|} \right)}{|u - v_*|} \mu_j^\delta(u) \, dE(u).$$

Then, there exist two explicit constants  $m, C_{ji}^\delta > 0$  such that

$$I_{ji}^\delta(v, v_*) \leq C_{ji}^\delta |v - v_*|^{\gamma-2} e^{-\delta m |v - v_*|^2 - \delta m \frac{|v|^2 - |v_*|^2}{|v - v_*|^2}} \left( \frac{\mu_i(v)}{\mu_i(v_*)} \right)^{\delta/2}, \quad \forall v, v_* \in \mathbb{R}^3.$$

The constant  $m$  only depends on the masses  $m_i, m_j$ , while the constant  $C_{ji}^\delta$  only depends on  $\delta$ , the masses  $m_i, m_j$  and the collisional kernel, and  $\gamma$  appears in (H3).

We here prove that this estimate allows us to recover an upper bound for  $I_{ij}^\delta$  in a weighted  $L_v^1$ -norm. We closely follow the proof presented in [112, Lemma 7].

**Lemma 2.4.4.** *There exists  $\bar{\delta} \in (0, 1)$  such that, for each  $\delta \in (\bar{\delta}, 1)$ , there exists a constant  $C_{ji}(\delta) > 0$  such that*

$$\int_{\mathbb{R}^3} I_{ji}^\delta(v, v_*) \sqrt{\frac{\mu_i(v_*)}{\mu_i(v)}} \, dv_* \leq C_{ji}(\delta), \quad \forall v \in \mathbb{R}^3,$$

$$\int_{\mathbb{R}^3} I_{ji}^\delta(v, v_*) \sqrt{\frac{\mu_i(v_*)}{\mu_i(v)}} \, dv \leq C_{ji}(\delta), \quad \forall v_* \in \mathbb{R}^3.$$

The constant  $C_{ji}(\delta)$  is explicit and only depends on the parameter  $\delta \in (\bar{\delta}, 1)$ , the atomic masses  $m_i, m_j$  and the collisional kernel  $B_{ij}$ .

*Proof.* We shall only prove the first inequality, since the second one can be showed in a similar way. Using the previous lemma, the term inside the integral can be bounded for all  $v, v_* \in \mathbb{R}^3$  by

$$I_{ji}^\delta(v, v_*) \sqrt{\frac{\mu_i(v_*)}{\mu_i(v)}} \leq C_{ji}^\delta |v - v_*|^{\gamma-2} e^{-\delta m |v - v_*|^2 - \delta m \frac{|v|^2 - |v_*|^2|^2}{|v - v_*|^2}} \left( \frac{\mu_i(v_*)}{\mu_i(v)} \right)^{\frac{1-\delta}{2}}.$$

After renaming  $\eta = v - v_*$  and  $v_* = v - \eta$  in the integral (for the second inequality we should set  $\eta = v_* - v$  and  $v = v_* - \eta$ ), direct algebraic manipulations on the total exponent in the last inequality yield

$$\begin{aligned} & -\delta m |\eta|^2 - \delta m \frac{||\eta|^2 - 2\langle \eta, v \rangle|^2}{|\eta|^2} - (1 - \delta) \frac{m_i}{4} (|v - \eta|^2 - |v|^2) \\ &= -2\delta m |\eta|^2 - 4\delta m \frac{\langle \eta, v \rangle^2}{|\eta|^2} + 4\delta m \langle \eta, v \rangle - (1 - \delta) \frac{m_i}{4} (|\eta|^2 - 2\langle \eta, v \rangle) \\ &= \left( -2\delta m - (1 - \delta) \frac{m_i}{4} \right) |\eta|^2 + \left( 4\delta m + (1 - \delta) \frac{m_i}{2} \right) \langle \eta, v \rangle - 4\delta m \frac{\langle \eta, v \rangle^2}{|\eta|^2}. \end{aligned}$$

The discriminant of the above quadratic form in  $|\eta|$  and  $\frac{\langle \eta, v \rangle}{|\eta|}$  can be computed and gives

$$\begin{aligned} \Delta(\delta) &= \left( 4\delta m + (1 - \delta) \frac{m_i}{2} \right)^2 - 8\delta m \left( 4\delta m + (1 - \delta) \frac{m_i}{2} \right) \\ &= \frac{m_i}{2} \left( 4\delta m + (1 - \delta) \frac{m_i}{2} \right) \left( 1 - \delta \left( 8 \frac{m}{m_i} + 1 \right) \right). \end{aligned}$$

If we now choose  $\bar{\delta} = \frac{m_i}{8m + m_i}$ , we clearly have that for all  $\delta \in (\bar{\delta}, 1)$ ,  $\Delta(\delta) < 0$  which implies that the quadratic form is negative definite. Consequently, for all  $\delta \in (\bar{\delta}, 1)$ , there exists a constant  $C(\delta) > 0$  such that

$$\begin{aligned} -\delta m |\eta|^2 - \delta m \frac{||\eta|^2 - 2\langle \eta, v \rangle|^2}{|\eta|^2} - (1 - \delta) \frac{m_i}{4} (|v - \eta|^2 - |v|^2) &\leq -C(\delta) \left( |\eta|^2 + \frac{\langle \eta, v \rangle^2}{|\eta|^2} \right) \\ &\leq -C(\delta) |\eta|^2. \end{aligned}$$

Using this last inequality, for each  $\delta \in (\bar{\delta}, 1)$  we deduce that

$$\begin{aligned} & \int_{\mathbb{R}^3} I_{ji}^\delta(v, v_*) \sqrt{\frac{\mu_i(v_*)}{\mu_i(v)}} dv_* \\ & \leq C_{ji}(\delta) \int_{\mathbb{R}^3} |\eta|^{\gamma-2} e^{-\delta m |\eta|^2 - \delta m \frac{||\eta|^2 - 2\langle \eta, v \rangle|^2}{|\eta|^2} - (1 - \delta) \frac{m_i}{4} (|v - \eta|^2 - |v|^2)} d\eta \\ & \leq C_{ji}(\delta) \int_{\mathbb{R}^3} |\eta|^{\gamma-2} e^{-C(\delta) |\eta|^2} d\eta \\ & \leq C_{ji}(\delta), \quad \forall v \in \mathbb{R}^3, \end{aligned}$$

since the integral is finite and in particular bounded by a constant only depending on  $\delta$ . This concludes the proof.  $\square$

Thanks to these results, we can now bound the term  $\mathcal{T}_2^\varepsilon$ . We choose  $\bar{\delta}_1 = \frac{m_i}{8m+m_i}$ . Then, for any  $\delta \in (\bar{\delta}_1, 1)$ , applying again Young's inequality, Fubini's theorem, and using the straightforward bound  $C_{ji}(\delta) \leq C_{ij}(\delta)(1 + |v|^\gamma)$  for any  $v \in \mathbb{R}^3$ , we have

$$\begin{aligned}
\mathcal{T}_2^\varepsilon(\mathbf{f}) &\leq \varepsilon C^{(2)} \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \sum_{i,j} \int_{\mathbb{R}^6} I_{ji}^\delta(v, v_*) \sqrt{\frac{\mu_i^*}{\mu_i}} |h_i^*| |h_i| dv dv_* \\
&\leq \varepsilon C^{(2)} \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \\
&\quad \sum_{i,j} \left( \int_{\mathbb{R}^6} I_{ji}^\delta(v, v_*) \sqrt{\frac{\mu_i^*}{\mu_i}} h_i^{*2} dv dv_* + \int_{\mathbb{R}^6} I_{ji}^\delta(v, v_*) \sqrt{\frac{\mu_i^*}{\mu_i}} h_i^2 dv dv_* \right) \\
&\leq \varepsilon C^{(2)} \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \\
&\quad \sum_{i,j} C_{ji}(\delta) \left( \int_{\mathbb{R}^3} (1 + |v_*|^\gamma) h_i^{*2} dv_* + \int_{\mathbb{R}^3} (1 + |v|^\gamma) h_i^2 dv \right) \\
&\leq \varepsilon C^{(2)} \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \|\mathbf{f}\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2. \tag{2.4.7}
\end{aligned}$$

**Step 6 – Estimation of  $\mathcal{T}_1^\varepsilon$ .** The estimate for the last term  $\mathcal{T}_1^\varepsilon$  is similar to the one for  $\mathcal{T}_2^\varepsilon$ , but more tricky. In fact, we shall deal with different masses  $m_i, m_j$ , which lead to an asymmetry in the Maxwellian weights inside the integral, namely the factor  $\sqrt{\frac{\mu_j(v_*)}{\mu_i(v)}}$  appearing in this case. As a consequence, a careful treatment of these weights is required to compare the different exponential decay rates. We first apply Lemma 2.4.1 to obtain, for all  $\delta \in (0, 1)$

$$\begin{aligned}
\mathcal{T}_1^\varepsilon(\mathbf{f}) &= \sum_{i,j} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) |M_i^{\varepsilon'} - \mu_i'| |f_j^{*'}| |f_i| \mu_i^{-1} dv dv_* d\sigma \\
&\leq \varepsilon C^{(1)} \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \sum_{i,j} \int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) \mu_i'^{\delta} |f_j^{*'}| |f_i| \mu_i^{-1} dv dv_* d\sigma,
\end{aligned}$$

with  $\delta$  actually ranging in a subinterval of  $(0, 1)$  as before, to be appropriately chosen later. Thanks to Lemma 2.4.2, we rewrite the integral under its kernel form as

$$\begin{aligned}
&\int_{\mathbb{R}^6 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) \mu_i'^{\delta} |f_j^{*'}| |f_i| \mu_i^{-1} dv dv_* d\sigma \\
&= C_{ij} \int_{\mathbb{R}^6} \left( \frac{1}{|v - v_*|} \int_{\tilde{E}_{vv_*}^{ij}} \frac{B_{ij}\left(v - V(u, v_*), \frac{v_* - u}{|u - v_*|}\right)}{|u - v_*|} \mu_i^\delta(u) d\tilde{E}(u) \right) |f_j^*| |f_i| \mu_i^{-1} dv dv_* \\
&= C_{ij} \int_{\mathbb{R}^6} \left( \frac{1}{|v - v_*|} \int_{\tilde{E}_{vv_*}^{ij}} \frac{B_{ij}\left(v - V(u, v_*), \frac{v_* - u}{|u - v_*|}\right)}{|u - v_*|} \mu_i^\delta(u) d\tilde{E}(u) \right) \sqrt{\frac{\mu_j^*}{\mu_i}} |h_j^*| |h_i| dv dv_*.
\end{aligned}$$

In the case  $m_i = m_j$ , the computations made for  $\mathcal{T}_2^\varepsilon$  apply in the same way, with the kernel operator satisfying the properties proved in the two lemmata of Step 5. We therefore suppose, from now on, that  $m_i \neq m_j$ . In this case, the equivalent result of Lemma 2.4.3 is the following.



**Lemma 2.4.5.** For any  $\delta \in (0, 1)$  and  $1 \leq i, j \leq N$ , let the operator  $I_{ij}^\delta$  be defined for  $v, v_* \in \mathbb{R}^3$  by

$$I_{ij}^\delta(v, v_*) = \frac{C_{ij}}{|v - v_*|} \int_{\tilde{E}_{vv_*}^{ij}} \frac{B_{ij}\left(v - V(u, v_*), \frac{v_* - u}{|u - v_*|}\right)}{|u - v_*|} \mu_i^\delta(u) \, d\tilde{E}(u).$$

Then, there exist two explicit constants  $\lambda, C_{ij}^\delta > 0$ , only depending on  $\delta$ , the masses  $m_i, m_j$  and the collisional kernel  $B_{ij}$ , such that, for any  $v, v_* \in \mathbb{R}^3$ ,

$$I_{ij}^\delta(v, v_*) \leq C_{ij}^\delta |v - v_*|^\gamma e^{-\delta\lambda|v - v_*|^2 - \delta\lambda \frac{|v|^2 - |v_*|^2|^2}{|v - v_*|^2} - \delta \frac{m_i + m_j}{16} |V^\perp|^2} \left( \frac{\mu_i(v)}{\mu_j(v_*)} \right)^{\delta/2},$$

where we have defined  $v + v_* = V^\parallel + V^\perp$ , with  $V^\parallel$  being the projection onto  $\text{Span}(v - v_*)$  and  $V^\perp$  orthogonal to  $\text{Span}(v - v_*)$ .

The proof still follows exactly the one presented in [45, Lemma 5.1] (see also the one presented in [37]), therefore it is omitted. On the other hand, we will see that the proof of the next result is a bit more intricate than the one of Lemma 2.4.4.

**Lemma 2.4.6.** There exists  $\bar{\delta} \in (0, 1)$  such that, for each  $\delta \in (\bar{\delta}, 1)$ , there exists a constant  $C_{ij}(\delta) > 0$  such that

$$\int_{\mathbb{R}^3} I_{ij}^\delta(v, v_*) \sqrt{\frac{\mu_j(v_*)}{\mu_i(v)}} \, dv_* \leq C_{ij}(\delta), \quad \forall v \in \mathbb{R}^3, \quad (2.4.8)$$

$$\int_{\mathbb{R}^3} I_{ij}^\delta(v, v_*) \sqrt{\frac{\mu_j(v_*)}{\mu_i(v)}} \, dv \leq C_{ij}(\delta), \quad \forall v_* \in \mathbb{R}^3. \quad (2.4.9)$$

The constant  $C_{ij}(\delta)$  is explicit and only depends on the parameter  $\delta \in (\bar{\delta}, 1)$ , the atomic masses  $m_i, m_j$  and the collisional kernel  $B_{ij}$ .

*Proof.* We begin by studying the term inside the integral of inequality (2.4.8). Using Lemma 2.4.5, we easily deduce that for all  $v, v_* \in \mathbb{R}^3$

$$I_{ij}^\delta(v, v_*) \sqrt{\frac{\mu_j(v_*)}{\mu_i(v)}} \leq C_{ij}^\delta |v - v_*|^\gamma e^{-\delta\lambda|v - v_*|^2 - \delta\lambda \frac{|v|^2 - |v_*|^2|^2}{|v - v_*|^2} - \delta \frac{m_i + m_j}{16} |V^\perp|^2} \left( \frac{\mu_j(v_*)}{\mu_i(v)} \right)^{\frac{1-\delta}{2}}, \quad (2.4.10)$$

recalling that we have defined  $v + v_* = V^\parallel + V^\perp$ , with  $V^\parallel$  being the projection onto the space  $\text{Span}(v - v_*)$  and  $V^\perp$  orthogonal to  $\text{Span}(v - v_*)$ .

We want to get rid of the asymmetry between the masses  $m_i$  and  $m_j$  in the Maxwellian weight  $\left( \frac{\mu_j(v_*)}{\mu_i(v)} \right)^{\frac{1-\delta}{2}}$ . Employing the decomposition  $v + v_* = V^\parallel + V^\perp$ , the following equality holds for any  $a, b \in \mathbb{R}$ :

$$\begin{aligned} |av - bv_*|^2 &= \left| \frac{a-b}{2}(v + v_*) + \frac{a+b}{2}(v - v_*) \right|^2 \\ &= \frac{(a-b)^2}{4} |V^\perp|^2 + \frac{(a-b)^2}{4} \frac{|v|^2 - |v_*|^2|^2}{|v - v_*|^2} \\ &\quad + \frac{(a-b)(a+b)}{2} (|v|^2 - |v_*|^2) + \frac{(a+b)^2}{4} |v - v_*|^2, \end{aligned}$$

since by definition

$$|V^\perp|^2 = \frac{\langle v + v_*, v - v_* \rangle^2}{|v - v_*|^2} = \frac{||v|^2 - |v_*|^2|^2}{|v - v_*|^2}.$$

Thus, taking  $(a, b) = (1, 0)$  and then  $(a, b) = (0, 1)$ , we immediately get

$$\begin{aligned} m_i|v|^2 - m_j|v_*|^2 &= \frac{m_i - m_j}{4}|V^\perp|^2 + \frac{m_i - m_j}{4} \frac{||v|^2 - |v_*|^2|^2}{|v - v_*|^2} \\ &\quad + \frac{m_i + m_j}{2}(|v|^2 - |v_*|^2) + \frac{m_i - m_j}{4}|v - v_*|^2 \end{aligned}$$

We can now apply this last equality in the study of the total exponent of (2.4.10). We first estimate

$$\begin{aligned} & -\delta\lambda|v - v_*|^2 - \delta\lambda \frac{||v|^2 - |v_*|^2|^2}{|v - v_*|^2} - \delta \frac{m_i + m_j}{16}|V^\perp|^2 + \frac{1 - \delta}{4}(m_i|v|^2 - m_j|v_*|^2) \\ &= \left( -\delta\lambda + (1 - \delta) \frac{m_i - m_j}{16} \right) \left( |v - v_*|^2 + \frac{||v|^2 - |v_*|^2|^2}{|v - v_*|^2} \right) \\ &\quad + (1 - \delta) \frac{m_i + m_j}{8}(|v|^2 - |v_*|^2) - \frac{m_i}{8} \left( \delta - \frac{m_i - m_j}{2m_i} \right) |V^\perp|^2 \\ &\leq \left( -\delta\lambda + (1 - \delta) \frac{m_i - m_j}{16} \right) \left( |v - v_*|^2 + \frac{||v|^2 - |v_*|^2|^2}{|v - v_*|^2} \right) \\ &\quad + (1 - \delta) \frac{m_i + m_j}{8}(|v|^2 - |v_*|^2), \end{aligned} \tag{2.4.11}$$

whenever  $\delta > \max \left\{ 0, \frac{m_i - m_j}{2m_i} \right\}$ .

As previously done, we inject  $\eta = v - v_*$  and  $v_* = v - \eta$  in the right-hand side of (3.2.6) and we obtain that the total exponent writes

$$\begin{aligned} & \left( -\delta\lambda + (1 - \delta) \frac{m_i - m_j}{16} \right) \left( |\eta|^2 + \frac{||\eta|^2 - 2\langle \eta, v \rangle|^2}{|\eta|^2} \right) \\ &\quad - (1 - \delta) \frac{m_i + m_j}{8}(|v - \eta|^2 - |v|^2) \\ &= \left( -2\delta\lambda - (1 - \delta) \frac{m_j}{4} \right) |\eta|^2 + \left( 4\delta\lambda + (1 - \delta) \frac{m_j}{2} \right) \langle \eta, v \rangle \\ &\quad + \left( -4\delta\lambda + (1 - \delta) \frac{m_i - m_j}{4} \right) \frac{\langle \eta, v \rangle^2}{|\eta|^2}. \end{aligned} \tag{2.4.12}$$

Computing the discriminant of the above quadratic form, we get

$$\begin{aligned} \Delta(\delta) &= \left( 4\delta\lambda + (1 - \delta) \frac{m_j}{2} \right)^2 + \left( 4\delta\lambda + (1 - \delta) \frac{m_j}{2} \right) \left( -8\delta\lambda + (1 - \delta) \frac{m_i - m_j}{2} \right) \\ &= \frac{m_i}{2} \left( 4\delta\lambda + (1 - \delta) \frac{m_j}{2} \right) \left( 1 - \delta \left( 8 \frac{\lambda}{m_i} + 1 \right) \right). \end{aligned}$$

Then we immediately check that if we choose  $\bar{\delta} = \max\left\{0, \frac{m_i - m_j}{2m_i}, \frac{m_i}{8\lambda + m_i}\right\}$ , inequality (3.2.6) and  $\Delta(\delta) < 0$  are both satisfied for any  $\delta \in (\bar{\delta}, 1)$ . This ensures that, for any  $\bar{\delta} < \delta < 1$ , the quadratic form (2.4.12) remains negative for any  $v \in \mathbb{R}^3$ . Consequently, we get that

$$\begin{aligned} & -\delta\lambda|\eta|^2 - \delta\lambda \frac{|\eta|^2 - 2\langle \eta, v \rangle|^2}{|\eta|^2} - \delta \frac{m_i + m_j}{16} |V^\perp|^2 - \frac{1-\delta}{4} (m_j|v-\eta|^2 - m_i|v|^2) \\ & \leq -C(\delta) \left( |\eta|^2 + \frac{\langle \eta, v \rangle^2}{|\eta|^2} \right) \\ & \leq -C(\delta)|\eta|^2, \end{aligned}$$

for some explicit constant  $C(\delta) > 0$  only depending on  $\delta$  and the masses  $m_i, m_j$ .

Proceeding as in the proof of Lemma 2.4.4, for each  $\delta \in (\bar{\delta}, 1)$  the integral in (2.4.8) can then be bounded as

$$\begin{aligned} & \int_{\mathbb{R}^3} I_{ij}^\delta(v, v_*) \sqrt{\frac{\mu_j(v_*)}{\mu_i(v)}} dv_* \\ & \leq C_{ij}(\delta) \int_{\mathbb{R}^3} |\eta|^\gamma e^{-\delta\lambda|\eta|^2 - \delta\lambda \frac{|\eta|^2 - 2\langle \eta, v \rangle|^2}{|\eta|^2} - \delta \frac{m_i + m_j}{16} |V^\perp|^2 - \frac{1-\delta}{4} (m_j|v-\eta|^2 - m_i|v|^2)} d\eta \\ & \leq C_{ij}(\delta) \int_{\mathbb{R}^3} |\eta|^{\gamma-2} e^{-C(\delta)|\eta|^2} d\eta \\ & \leq C_{ij}(\delta). \end{aligned}$$

Inequality (2.4.9) can be proved in the same way, by setting this time  $\eta = v_* - v$  and using  $v = v_* - \eta$ . This ends the proof.  $\square$

Young's inequality and Fubini's theorem allow to conclude that, taking  $\delta \in (\bar{\delta}_2, 1)$  with the choice  $\bar{\delta}_2 = \max_{1 \leq i, j \leq N} \left\{0, \frac{m_i - m_j}{2m_i}, \frac{m_i}{8\lambda + m_i}\right\}$ , the term  $\mathcal{T}_1^\varepsilon$  is bounded by

$$\begin{aligned} \mathcal{T}_1^\varepsilon(\mathbf{f}) & \leq \varepsilon C^{(1)} \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \sum_{i,j} \int_{\mathbb{R}^6} I_{ij}^\delta(v, v_*) \sqrt{\frac{\mu_j^*}{\mu_i}} |h_j^*| |h_i| dv dv_* \\ & \leq \varepsilon C^{(1)} \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \\ & \quad \sum_{i,j} \left( \int_{\mathbb{R}^6} I_{ij}^\delta(v, v_*) \sqrt{\frac{\mu_j^*}{\mu_i}} h_j^{*2} dv dv_* + \int_{\mathbb{R}^6} I_{ij}^\delta(v, v_*) \sqrt{\frac{\mu_j^*}{\mu_i}} h_i^2 dv_* dv \right) \\ & \leq \varepsilon C^{(1)} \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \\ & \quad \left( \sum_{j=1}^N \int_{\mathbb{R}^3} (1 + |v_*|^\gamma) h_j^{*2} dv_* + \sum_{i=1}^N \int_{\mathbb{R}^3} (1 + |v|^\gamma) h_i^2 dv \right) \\ & \leq \varepsilon C^{(1)} \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \|\mathbf{f}\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2. \end{aligned} \tag{2.4.13}$$

**Step 7 – End of the proof.** Choosing  $\bar{\delta} = \max\left\{\frac{1}{2}, \bar{\delta}_1, \bar{\delta}_2\right\}$ , estimates (2.4.5)–(2.4.7) and (2.4.13) are simultaneously verified, and we can gather them together to obtain, for all  $\mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ ,

$$\langle \mathbf{L}^\varepsilon(\mathbf{f}) - \mathbf{L}(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq C\varepsilon \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \|\mathbf{f}\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2,$$

with  $C = \max_{1 \leq k \leq 4} C^{(k)}$ .

To conclude, we simply observe that we can write  $\mathbf{f} = \mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f}) + \pi_{\mathbf{L}}(\mathbf{f})$  and then apply Young's inequality in this last estimate, to finally get

$$\begin{aligned} \langle \mathbf{L}^\varepsilon(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} &\leq - \left( \lambda_{\mathbf{L}} - C\varepsilon \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \right) \|\mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + C\varepsilon \max_{1 \leq i \leq N} \left\{ c_{i,\infty}^{1-\delta} |u_i| \mathcal{R}_{\varepsilon,i} \right\} \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2, \end{aligned}$$

for all  $\mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ .

The estimate holds for any  $\varepsilon > 0$  and Theorem 2.3.2 is then proved.



## Chapitre 3

# Stability of the Maxwell-Stefan system in the hydrodynamic limit of the Boltzmann multi-species equation

Ce chapitre est le fruit d'un travail en collaboration avec Marc Briant.

### 3.1 Introduction

The multi-species Boltzmann system is an extension of the standard Boltzmann mono-species equation, adapted to the case when the particles constituting the rarefied gas are of different kinds. More precisely, a gaseous mixture composed of  $N \geq 2$  species of chemically non-reacting monoatomic particles which are confined in the torus  $\mathbb{T}^3$ , can be modelled by means of a distribution function  $\mathbf{F} = (F_1, \dots, F_N)$ , where  $F_i = F_i(t, x, v)$  describes the evolution of the  $i$ -th species of the mixture and satisfies, for any  $1 \leq i \leq N$ , the Boltzmann-type equation

$$\partial_t F_i + v \cdot \nabla_x F_i = \frac{1}{\varepsilon} Q_i(\mathbf{F}, \mathbf{F}) \quad \text{on } \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3, \quad (3.1.1)$$

for some initial data

$$F_i(0, x, v) = F_i^{\text{in}}(x, v), \quad x \in \mathbb{T}^3, \quad v \in \mathbb{R}^3.$$

Here, the number  $\varepsilon > 0$  can be seen as the Knudsen number and the ratio  $1/\varepsilon$  then represents the average number of collisions undergone by a particle during a time unit. We also mention at this point that one can derive this type of equations from Newtonian mechanics at least formally in the case of single species [56, 59]. The rigorous derivation of the mono-species Boltzmann equation from Newtonian laws has by now only been proved locally in time, see [143, 129, 130] and, more recently, [92, 172].

Throughout the chapter,  $N$ -vectors (or vector-valued functions) will be denoted by bold letters, while the corresponding indexed letters will indicate their components. For example,  $\mathbf{W}$  represents the vector or vector-valued function  $(W_1, \dots, W_N)$ .

The Boltzmann operator  $\mathbf{Q} = (Q_1, \dots, Q_N)$  is given for any  $1 \leq i \leq N$  by

$$Q_i(\mathbf{F}, \mathbf{F}) = \sum_{j=1}^N Q_{ij}(F_i, F_j),$$

where  $Q_{ij}$  models the interactions between particles of either the same ( $i = j$ ) or of different ( $i \neq j$ ) species and is local in time and space. We focus on binary and elastic collisions, meaning that if two particles of different species, having respective atomic masses  $m_i$  and  $m_j$ , collide with velocities  $v'$  and  $v'_*$ , then their post-collisional velocities are respectively  $v$  and  $v_*$ , given by the conservation of momentum and kinetic energy

$$m_i v + m_j v_* = m_i v' + m_j v'_*, \quad \frac{1}{2} m_i |v|^2 + \frac{1}{2} m_j |v_*|^2 = \frac{1}{2} m_i |v'|^2 + \frac{1}{2} m_j |v'_*|^2. \quad (3.1.2)$$

We point out that, unlike the mono-species case where  $N = 1$ , we can see here an asymmetry in the role played by  $v$  and  $v_*$ , due to the different masses of the species. This issue will be of primary interest in our work. The bi-species collision operators then read, for any  $1 \leq i, j \leq N$ ,

$$Q_{ij}(F_i, F_j)(v) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) (F'_i F'_j - F_i F_j) dv_* d\sigma,$$

where the shorthand notations  $F'_i = F_i(v')$ ,  $F_i = F_i(v)$ ,  $F'_j = F_j(v'_*)$  and  $F_j = F_j(v_*)$  are used with the definitions

$$\begin{cases} v' = \frac{m_i v + m_j v_*}{m_i + m_j} + \frac{m_j}{m_i + m_j} |v - v_*| \sigma, \\ v'_* = \frac{m_i v + m_j v_*}{m_i + m_j} - \frac{m_i}{m_i + m_j} |v - v_*| \sigma, \end{cases} \quad \cos \vartheta = \frac{(v - v_*) \cdot \sigma}{|v - v_*|}.$$

In particular, the cross-sections  $B_{ij}$  model the physics of the binary collisions between particles. Here we shall focus on cutoff Maxwellian, hard-potential and hard-sphere collision kernels. Namely, let us make the following assumptions on each  $B_{ij}$ ,  $i$  and  $j$  being fixed.

(H1) It satisfies a symmetry property with respect to the interchange of both species indices  $i$  and  $j$

$$B_{ij}(|v - v_*|, \cos \vartheta) = B_{ji}(|v - v_*|, \cos \vartheta), \quad \forall v, v_* \in \mathbb{R}^3, \quad \forall \vartheta \in [0, \pi].$$

(H2) It decomposes into the product of a kinetic part  $\Phi_{ij} \geq 0$  and an angular part  $b_{ij} \geq 0$ , namely

$$B_{ij}(|v - v_*|, \cos \vartheta) = \Phi_{ij}(|v - v_*|) b_{ij}(\cos \vartheta), \quad \forall v, v_* \in \mathbb{R}^3, \quad \forall \vartheta \in [0, \pi].$$

(H3) The kinetic part has the form of hard or Maxwellian ( $\gamma = 0$ ) potential, *i.e.*

$$\Phi_{ij}(|v - v_*|) = C_{ij}^\Phi |v - v_*|^\gamma, \quad C_{ij}^\Phi > 0, \quad \gamma \in [0, 1], \quad \forall v, v_* \in \mathbb{R}^3.$$

(H4) For the angular part, we consider a strong form of Grad's angular cutoff [105]. We assume that there exists a constant  $C > 0$  such that

$$0 < b_{ij}(\cos \vartheta) \leq C |\sin \vartheta| |\cos \vartheta| \quad \text{and} \quad b'_{ij}(\cos \vartheta) \leq C, \quad \forall \vartheta \in [0, \pi].$$

Furthermore, we assume that for any  $1 \leq i \leq N$

$$\inf_{\sigma_1, \sigma_2 \in \mathbb{S}^2} \int_{\mathbb{S}^2} \min\{b_{ii}(\sigma_1 \cdot \sigma_3), b_{ii}(\sigma_2 \cdot \sigma_3)\} d\sigma_3 > 0.$$

See Section 2.2 of Chapter 1 for a brief discussion about these hypotheses.

The first *a priori* laws one can extract [70, 65, 39] from (3.1.1) are the conservations, over time  $t \geq 0$ , of the quantities

$$\begin{aligned} c_{i,\infty} &= \int_{\mathbb{T}^3 \times \mathbb{R}^3} F_i(t, x, v) dx dv, \\ \rho_\infty u_\infty &= \sum_{i=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} m_i v F_i(t, x, v) dx dv, \\ \frac{3}{2} \rho_\infty \theta_\infty &= \sum_{i=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} \frac{m_i}{2} |v - u_\infty|^2 F_i(t, x, v) dx dv, \end{aligned} \quad (3.1.3)$$

where  $c_{i,\infty}$  stands for the number of particles of the  $i$ -th species, and we have denoted the total mass of the mixture  $\rho_\infty = \sum_{i=1}^N m_i c_{i,\infty}$ , its total momentum  $\rho_\infty u_\infty$  and its total energy  $\frac{3}{2} \rho_\infty \theta_\infty$ . The lack of symmetry mentioned before clearly appears here, since only the total momentum and energy of the gas are preserved, as opposed to a preservation of the momentum and energy of each single species.

The second important feature is that the operator  $\mathbf{Q} = (Q_1, \dots, Q_N)$  also satisfies a multi-species version of the classical  $H$ -theorem [70], from which one deduces that the only distribution functions satisfying  $\mathbf{Q}(\mathbf{F}, \mathbf{F}) = 0$  are given by the local Maxwellian vector  $(M_{(c_i, u, \theta)})_{1 \leq i \leq N}$ , having the specific form

$$M_{(c_i, u, \theta)}(t, x, v) = c_i(t, x) \left( \frac{m_i}{2\pi\theta(t, x)} \right)^{3/2} e^{-m_i \frac{|v - u(t, x)|^2}{2\theta(t, x)}}, \quad t \geq 0, \quad x \in \mathbb{T}^3, \quad v \in \mathbb{R}^3, \quad (3.1.4)$$

for some functions  $\mathbf{c} = (c_i)_{1 \leq i \leq N}$ ,  $u$  and  $\theta$ . These are the fluid quantities associated to  $\mathbf{M}$  and satisfy, for any  $(t, x) \in \mathbb{R}_+ \times \mathbb{T}^3$ , the relations

$$\begin{aligned} c_i(t, x) &= \int_{\mathbb{R}^3} M_{(c_i, u, \theta)}(t, x, v) dv, \quad 1 \leq i \leq N, \\ \sum_{i=1}^N m_i c_i(t, x) u(t, x) &= \sum_{i=1}^N \int_{\mathbb{R}^3} m_i v M_{(c_i, u, \theta)}(t, x, v) dv \\ \frac{3}{2} \sum_{i=1}^N m_i c_i(t, x) \theta(t, x) &= \sum_{i=1}^N \int_{\mathbb{R}^3} \frac{m_i}{2} |v - u(t, x)|^2 M_{(c_i, u, \theta)}(t, x, v) dv. \end{aligned}$$

In particular, we stress the fact that, as opposed to the case where only one gas is considered, in the multi-species framework not all local Maxwellian vectors are local equilibrium states for the mixture, since the relation  $\mathbf{Q}(\mathbf{F}, \mathbf{F}) = 0$  is satisfied if and only if the local bulk velocity  $u(t, x)$  and temperature  $\theta(t, x)$  are the same for each species.

Going further, since we work in  $\mathbb{T}^3$ , one can also prove that the only global equilibrium of the mixture, *i.e.* the unique stationary solution  $\mathbf{F}$  to (3.1.1), is given by the global Maxwellian vector  $(M_{(c_{i,\infty}, u_\infty, \theta_\infty)})_{1 \leq i \leq N}$  whose fluid quantities satisfy the relations (3.1.3). It is defined, for any  $1 \leq i \leq N$ , by

$$M_{(c_{i,\infty}, u_\infty, \theta_\infty)}(v) = c_{i,\infty} \left( \frac{m_i}{2\pi\theta_\infty} \right)^{3/2} e^{-m_i \frac{|v - u_\infty|^2}{2\theta_\infty}}, \quad v \in \mathbb{R}^3.$$



In particular, without loss of generality, in what follows we shall consider as unique global equilibrium of the mixture the  $N$ -vector  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_N)$ , defined componentwise as

$$\mu_i(v) = c_{i,\infty} \left( \frac{m_i}{2\pi} \right)^{3/2} e^{-m_i \frac{|v|^2}{2}}, \quad v \in \mathbb{R}^3, \quad (3.1.5)$$

and obtained by a translation and a dilation of the coordinate system, which allows to take  $u_\infty = 0$  and  $\theta_\infty = 1$ .

The Cauchy theory and the trend to equilibrium in a perturbative setting around the global Maxwellian state (3.1.5) has already been shown in  $L_x^\infty(\mathbb{T}^3; L_v^1(\mathbb{R}^3))$  with polynomial weights [45] and in  $L_{x,v}^\infty(\mathbb{T}^3 \times \mathbb{R}^3)$  with exponential and polynomial weights [44], for a fixed Knudsen number  $\varepsilon > 0$ . In the present work we are interested in studying the diffusion limit of equation (3.1.1). More precisely, we consider the following scaled version of (3.1.1), given for any  $1 \leq i \leq N$  by

$$\partial_t F_i^\varepsilon + \frac{1}{\varepsilon} v \cdot \nabla_x F_i^\varepsilon = \frac{1}{\varepsilon^2} Q_i(\mathbf{F}^\varepsilon, \mathbf{F}^\varepsilon) \quad \text{on } \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3, \quad (3.1.6)$$

and we investigate the behaviour of the fluid quantities  $c_i^\varepsilon$ ,  $u_i^\varepsilon$  and  $\theta_i^\varepsilon$  associated to each distribution  $F_i^\varepsilon$ , when  $\varepsilon > 0$  vanishes. A first formal derivation [39] showed, in the case where  $\mathbf{F}^\varepsilon = (M_{(c_i^\varepsilon, u_i^\varepsilon, \bar{\theta})})_{1 \leq i \leq N}$  is a local Maxwellian vector with constant temperature  $\bar{\theta} > 0$  and  $(c_i^\varepsilon, u_i^\varepsilon)_{1 \leq i \leq N}$  converge towards  $(c_i, u_i)_{1 \leq i \leq N}$ , that the limit macroscopic quantities are solutions to the incompressible Maxwell-Stefan system

$$\partial_t c_i + \nabla_x \cdot (c_i u_i) = 0, \quad (3.1.7)$$

$$-\nabla_x c_i = \sum_{j=1}^N c_i c_j \frac{u_i - u_j}{\Delta_{ij}}, \quad (3.1.8)$$

$$\partial_t \left( \sum_{i=1}^N c_i \right) = 0, \quad \nabla_x \cdot \left( \sum_{i=1}^N c_i u_i \right) = 0, \quad (3.1.9)$$

where  $\Delta_{ij}$  are symmetric (with respect to the species indices) positive constants only depending on  $\bar{\theta}$ , the masses  $(m_i)_{1 \leq i \leq N}$  and the collision kernels  $(B_{ij})_{1 \leq i, j \leq N}$ , and they are linked to the effective diffusion coefficients  $D_{ij}$  between species  $\mathcal{E}_i$  and  $\mathcal{E}_j$  through the relation  $D_{ij} = \Delta_{ij} / \sum_i c_i$ . Note that the incompressibility is to be understood in the whole and not for each species. At first sight, the structure of the limit equations looks rather different from the Navier-Stokes limit of the Boltzmann mono-species equation ( $N = 1$ ). However, as showed in [39], the momentum balance equation appears partly at order  $\varepsilon^2$  under the explicit form

$$\varepsilon^2 \frac{m_i}{\bar{\theta}} \left[ \partial_t (c_i^\varepsilon u_i^\varepsilon) + \nabla_x \cdot (c_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon) \right] + \nabla_x c_i^\varepsilon = \sum_{j=1}^N c_i^\varepsilon c_j^\varepsilon \frac{u_i^\varepsilon - u_j^\varepsilon}{\Delta_{ij}},$$

and we actually see the Navier-Stokes structure showing up, without viscous terms because the solution is supposed to be a local Maxwellian and therefore the interactions between the microscopic part and the fluid quantities are not taken into account.

In particular, the Maxwell-Stefan system (3.1.7)–(3.1.9) is of core importance in physics and biology, since it is used to model the evolution of diffusive phenomena in mixtures [153, 180, 184, 60, 34]. As such, its derivation from the kinetic equations is of great interest from both a mathematical and a physical point of view.

As already underlined, the problem at hand is reminiscent of the hydrodynamic limit of the mono-species Boltzmann equation, towards the incompressible Navier-Stokes system. Therefore, let us first give a brief description of the strategies which have been developed in this context. We emphasize that the list is not exhaustive, does not concern any other type of hydrodynamic limits (such as Euler equations or acoustics) and we refer to [176, 101] for more references and discussions.

The formal derivation of the Navier-Stokes limit from the mono-species Boltzmann equation came from a series of articles called the Bardos-Golse-Levermore (BGL) program [13, 14]. It has been made rigorous in various ways, always with the help of a Taylor expansion of the solution with respect to the parameter  $\varepsilon$  [109]. One could look at perturbative solutions around a global Maxwellian  $\mu(v) = c_\infty / (2\pi\theta_\infty)^{3/2} \exp\left\{-\frac{|v|^2}{2\theta_\infty}\right\}$ , that is to say solutions of the form  $F^\varepsilon = \mu + \varepsilon f^\varepsilon$ , and study their limit when  $\varepsilon$  tends to 0. This has been done by describing the spectrum of the linear operator  $L(f^\varepsilon) = \varepsilon^{-2}(Q(\mu, f^\varepsilon) + Q(f^\varepsilon, \mu))$  [83, 15], by directly tackling the Cauchy problem for  $f^\varepsilon$  in Sobolev spaces to get convergence results on the fluid quantities of  $f^\varepsilon$  in the setting of renormalised solutions [102, 103, 148], or by using hypocoercivity techniques [115, 43]. Another strategy is to investigate the stability of the Boltzmann equation not around a global equilibrium, but around a local Maxwellian whose fluid quantities solve the limit macroscopic system. In this spirit, De Masi, Esposito and Lebowitz [66] studied solutions of the form  $F^\varepsilon = M_{(c_\infty, \varepsilon u, \theta_\infty)} + \varepsilon f^\varepsilon$  where  $u = u(t, x)$  is a smooth solution of the perturbed incompressible Navier-Stokes equation, around the constant macroscopic equilibrium  $(c_\infty, 0, \theta_\infty)$ . The interest of this method, initiated by Caffisch [48] for the Euler limit of the Boltzmann equation, is that the main order term already encodes the limit system and one can thus study the fluid perturbations explicitly.

As we saw before, only a formal derivation of the Maxwell-Stefan system from the Boltzmann multi-species equation has been obtained [39] and, unlike the BGL program [14] for the mono-species case, the latter does not give any convergence of the fluid quantities given an *a priori* convergence in distribution. Note that other formal hydrodynamic limits have been also recently derived in a non-dissipative regime [16, 19, 10].

The strategy of studying close-to-global equilibrium solutions offers bounds (and thus compactness) in Sobolev spaces, but has to be transferred into a convergence of the nonlinear moments. We therefore chose to investigate the hydrodynamic limit of the multi-species Boltzmann equation in the spirit of [48, 66]. More precisely, we construct solutions in Sobolev spaces to the perturbed system (3.1.6) of the form  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}^\varepsilon$ , where the local Maxwellian state  $\mathbf{M}^\varepsilon = (M_1^\varepsilon, \dots, M_N^\varepsilon)$  is given for any  $1 \leq i \leq N$  by

$$M_i^\varepsilon(t, x, v) = c_i(t, x) \left(\frac{m_i}{2\pi\bar{\theta}}\right)^{3/2} \exp\left\{-m_i \frac{|v - \varepsilon u_i(t, x)|^2}{2\bar{\theta}}\right\}, \quad t \geq 0, x \in \mathbb{T}^3, v \in \mathbb{R}^3, \quad (3.1.10)$$

and its fluid quantities  $(c_i, u_i)_{1 \leq i \leq N}$  solves the Maxwell-Stefan system (3.1.7)–(3.1.8) with incompressibility condition (3.1.9). However, we differ from [66] in several ways. First of all, the local Maxwellian (3.1.10) is not an equilibrium state for the mixture, meaning in particular that the relation  $\mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon) = 0$  does not hold true in our setting. Secondly, even though we only deal with the case of a fixed temperature  $\bar{\theta}$ , we first do not ask  $c_i(t, x)$  to be constant, but we shall allow perturbations of a constant state. At last, we shall not use higher order fluid expansions, but we are able to develop a hypocoercivity strategy in the spirit of [161, 43], by separating the leading order of the limit Maxwell-Stefan components from the full microscopic and fluid part perturbations. The idea is indeed natural, remembering that the Maxwell-Stefan system is obtained when one only looks at

the interactions at the first order in  $\varepsilon$ . Moreover, the specific structure of the system links the masses and the momenta. We shall use this interplay to recover lower order controls.

We plug the perturbation  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}^\varepsilon$  into the rescaled Boltzmann system (3.1.6) and we obtain the perturbed equation

$$\partial_t \mathbf{f}^\varepsilon + \frac{1}{\varepsilon} v \cdot \nabla_x \mathbf{f}^\varepsilon = \frac{1}{\varepsilon^2} \mathbf{L}^\varepsilon(\mathbf{f}^\varepsilon) + \frac{1}{\varepsilon} \mathbf{Q}(\mathbf{f}^\varepsilon, \mathbf{f}^\varepsilon) + \mathbf{S}^\varepsilon, \quad (3.1.11)$$

where the linear operator  $\mathbf{L}^\varepsilon = (L_1^\varepsilon, \dots, L_N^\varepsilon)$  is given for any  $1 \leq i \leq N$  by

$$L_i^\varepsilon(\mathbf{f}^\varepsilon) = \sum_{j=1}^N \left( Q_{ij}(M_i^\varepsilon, f_j^\varepsilon) + Q_{ij}(f_i^\varepsilon, M_j^\varepsilon) \right), \quad (3.1.12)$$

and the source term  $\mathbf{S}^\varepsilon$  encodes the distance between the Maxwell-Stefan system and the fluid part of the perturbed Boltzmann equation, and is defined through the relation

$$\mathbf{S}^\varepsilon = \frac{1}{\varepsilon^3} \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon) - \frac{1}{\varepsilon} \partial_t \mathbf{M}^\varepsilon - \frac{1}{\varepsilon^2} v \cdot \nabla_x \mathbf{M}^\varepsilon. \quad (3.1.13)$$

The perturbative setting (3.1.11)–(3.1.13) is classical in the case of the Boltzmann mono-species equation. Usually, the strategy consists in proving that the linear operator  $\mathbf{L}^\varepsilon$  is self-adjoint in some space, with non-trivial null space, and features a spectral gap. In fact, the spectral gap allows to get strong negative feedback from the microscopic part (orthogonal to  $\ker \mathbf{L}^\varepsilon$ ) of the solution and therefore one is only left with finding a way to control the kernel part of the solution, in order to close the energy estimates. This can be achieved either by investigating the fluid equations [115, 45] or by using hypocoercive norms [161, 193, 43] which generates a complete negative return in higher Sobolev norms, *via* the commutator  $[v \cdot \nabla_x, \nabla_v] = -\nabla_x$ .

Unfortunately, the spectral gap core property essentially comes from the fact that, in the mono-species case, any local Maxwellian is a local equilibrium. As soon as  $N > 1$  we have seen that a local Maxwellian vector is an equilibrium of the system of equations (3.1.6) only if each component shares the same velocity (3.1.4). This is not the case for the local Maxwellian state (3.1.10) we consider, where each species evolves at its own speed  $\varepsilon u_i$ . Not only one loses the self-adjointness of the linear operator  $\mathbf{L}^\varepsilon$  in the usual  $L^2$  space weighted by the local Maxwellian  $\mathbf{M}^\varepsilon$ , but also the spectral gap property. However, we have shown in Chapter 2 that if one does not have a spectral gap, it is still possible to recover a negative return on the fluid part by adding an error term of order  $\varepsilon$ , as long as the velocities  $\varepsilon u_i$  remain small, of order  $\varepsilon$ . Our contribution aims at extending this perturbative result to the case of more general densities  $c_i(t, x)$ , in particular to the case of perturbative solutions to the Maxwell-Stefan system, where the loss of the spectral gap remains at a lower order of magnitude. We then construct a new modified Sobolev norm which allows to recover a coercivity property and to close the energy estimates on the nonlinear terms. This is an extension and an adaptation of the hypocoercivity methods developed in [161, 43], where fine controls over the  $\varepsilon$ -dependencies of the coefficients act to counter-balance the out-of-equilibrium property of our system, as well as the interactions with the nonconstant fluid quantities appearing in the weight. We emphasize again that this is achieved by looking at perturbative solutions to the Maxwell-Stefan system. Such a setting also appears in standard studies in the mono-species case, where one only recovers perturbative Leray solutions of the incompressible Navier-Stokes equation. Besides, the perturbative setting for the Maxwell-Stefan system proves itself to be exactly the one needed to control the problematic source term  $\mathbf{S}^\varepsilon$ . We emphasize here that the perturbative

setting we look at extends, to a nonconstant density and a non-zero momentum (even though the perturbations we consider are small), the previous results of Caffisch [48] and De Masi, Esposito and Lebowitz [66] in the mono-species case, and provides a hypocoercive approach to their framework.

In order to achieve our goal at the kinetic level, we also need to develop a complete Cauchy theory for the limit macroscopic model. In this regard, we point out that only few and recent mathematical results are known on the Maxwell-Stefan system [96, 33, 38, 138], and they are all based on the equimolar diffusion assumption

$$\sum_{i=1}^N c_i(t, x) u_i(t, x) = 0, \quad t \geq 0, \quad x \in \mathbb{T}^3. \quad (3.1.14)$$

This type of closure relation is usually required in order to ensure a good Cauchy theory for the Maxwell-Stefan system (3.1.7)–(3.1.8), since one cannot see the entire part of  $\mathbf{u}$  that evolves in the kernel of the right-hand side operator of (3.1.8). However, in the incompressible scenario that we look at, we do not need any closure assumption to recover relevant energy estimates. As we shall see, in this framework, we can derive an equivalent and orthogonal (with respect to the non-injective Maxwell-Stefan matrix) formulation of the Maxwell-Stefan system which is fully closed and exhibits a quasilinear parabolic structure. We however lose uniqueness in a strong sense, but we still get a complete description of all the possible solutions. Moreover, in order to construct  $\mathbf{M}^\varepsilon$  and, above all, to get enough control over the source term  $\mathbf{S}^\varepsilon$ , we derive uniform estimates in  $\varepsilon$  for perturbative solutions to the Maxwell-Stefan system, in higher Sobolev spaces. A use of an anisotropic norm allows us to raise a positivity property of the Maxwell-Stefan linear operator. We thus offer a new “hypocoercive” strategy inherited from the kinetic level, coupled with the pseudo-invertibility property existing between the densities  $(c_i)_{1 \leq i \leq N}$  and the orthogonal part of the velocities  $(u_i)_{1 \leq i \leq N}$ . At last, we underline that the perturbative setting we ask for the Maxwell-Stefan system is intrinsic to the hydrodynamic limits in a dissipative regime, as understood in the mono-species setting.

The rest of the chapter is thus dedicated to the proofs of our two main results. Section 3.2 is devoted to the study of the perturbative Cauchy theory for the Maxwell-Stefan system (3.1.7)–(3.1.9). We shall build global in time solutions  $(c_i, u_i)_{1 \leq i \leq N}$  which are unique in a perturbative sense, around any macroscopic equilibrium state of type  $(\bar{c}_i, \bar{u})_{1 \leq i \leq N}$ , where  $\bar{c}_i > 0$  is constant for any  $1 \leq i \leq N$  and the velocity  $\bar{u} : \mathbb{R}_+ \times \mathbb{T}^3 \rightarrow \mathbb{R}^3$  (common to all the species) satisfies the incompressibility condition  $\nabla_x \cdot \bar{u} = 0$ . Thanks to this result, we can then justify at the kinetic level the choice of the expansion  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}^\varepsilon$  around the local Maxwellian vector  $\mathbf{M}^\varepsilon$  given by (3.1.10). Starting from this, in Section 3.3, we establish global existence and uniqueness of the fluctuations  $\mathbf{f}^\varepsilon$ , which are solutions to the perturbed Boltzmann equation (3.1.11). The uniform in  $\varepsilon$  *a priori* estimates eventually allow us to state a convergence result which rigorously proves the derivation of the Maxwell-Stefan model (3.1.7)–(3.1.9) from the Boltzmann multi-species equation. In particular, our strategy exploits the hypocoercivity structure of (3.1.11), following the works [161, 43]. This consists in proving a series of *a priori* estimates satisfied by the multi-species operators  $\mathbf{L}^\varepsilon$  and  $\mathbf{Q}$ , and by the source term  $\mathbf{S}^\varepsilon$ . While in Section 3.3 we only introduce these fundamental results, all their technical proofs are collected in Section 3.4.

## Notations and conventions

For convenience, before going into details in our analysis, let us present here the main notations that we use throughout the chapter. Recalling that we denote  $\mathbf{W} = (W_1, \dots, W_N)$

any vector or vector-valued operator belonging to  $\mathbb{R}^N$ , we shall use the symbol  $\mathbf{1}$  to name the specific vector  $(1, \dots, 1)$ . Henceforth, the multiplication of  $N$ -vectors has to be understood in a component by component way, so that for any  $\mathbf{w}, \mathbf{W} \in \mathbb{R}^N$  and any  $q \in \mathbb{Q}$  we have

$$\mathbf{w}\mathbf{W} = (w_i W_i)_{1 \leq i \leq N}, \quad \mathbf{W}^r = (W_i^q)_{1 \leq i \leq N}.$$

Moreover, we introduce the Euclidean scalar product in  $\mathbb{R}^N$ , weighted by a vector  $\mathbf{W}$ , which is defined as

$$\langle \mathbf{f}, \mathbf{g} \rangle_{\mathbf{W}} = \sum_{i=1}^N f_i g_i W_i,$$

and induces the norm  $\|\mathbf{f}\|_{\mathbf{W}}^2 = \langle \mathbf{f}, \mathbf{f} \rangle_{\mathbf{W}}$ . In particular, when  $\mathbf{W} = \mathbf{1}$ , the index  $\mathbf{1}$  will be dropped in both the notations for the scalar product and the norm. At last, note that we shall also make use of the following shorthand notation

$$\langle v \rangle = \sqrt{1 + |v|^2},$$

not to be confused with the scalar product defined above.

The convention we choose for the functional spaces is to index the space by the name of the concerned variable. For  $p \in [1, +\infty]$  we have

$$L_t^p = L^p(0, +\infty), \quad L_x^p = L^p(\mathbb{T}^3), \quad L_v^p = L^p(\mathbb{R}^3).$$

Consider now some positive measurable vector-valued functions  $\mathbf{w} : \mathbb{T}^3 \rightarrow (\mathbb{R}_+^*)^N$  in the variable  $x$  and  $\mathbf{W} : \mathbb{R}^3 \rightarrow (\mathbb{R}_+^*)^N$  in the variable  $v$ . For any  $1 \leq i \leq N$ , we define the weighted Hilbert spaces  $L^2(\mathbb{T}^3, w_i)$  and  $L^2(\mathbb{R}^3, W_i)$  by introducing the respective scalar products and norms

$$\begin{aligned} \langle c_i, d_i \rangle_{L_x^2(w_i)} &= \int_{\mathbb{T}^3} c_i d_i w_i^2 dx, & \|c_i\|_{L_x^2(w_i)}^2 &= \langle c_i, c_i \rangle_{L_x^2(w_i)}, & \forall c_i, d_i &\in L^2(\mathbb{T}^3, w_i), \\ \langle f_i, g_i \rangle_{L_v^2(W_i)} &= \int_{\mathbb{R}^3} f_i g_i W_i^2 dv, & \|f_i\|_{L_v^2(W_i)}^2 &= \langle f_i, f_i \rangle_{L_v^2(W_i)}, & \forall f_i, g_i &\in L^2(\mathbb{R}^3, W_i). \end{aligned}$$

With these definitions, we say that  $\mathbf{c} : \mathbb{T}^3 \rightarrow \mathbb{R}^N$  belongs to  $L^2(\mathbb{T}^3, \mathbf{w})$  and that  $\mathbf{f} : \mathbb{R}^3 \rightarrow \mathbb{R}^N$  belongs to  $L^2(\mathbb{R}^3, \mathbf{W})$  if and only if  $c_i : \mathbb{T}^3 \rightarrow \mathbb{R} \in L^2(\mathbb{T}^3, w_i)$  and  $f_i : \mathbb{R}^3 \rightarrow \mathbb{R} \in L^2(\mathbb{R}^3, W_i)$  for any  $1 \leq i \leq N$ . The weighted Hilbert spaces  $L^2(\mathbb{T}^3, \mathbf{w})$  and  $L^2(\mathbb{R}^3, \mathbf{W})$  are therefore endowed with the induced scalar products and norms

$$\begin{aligned} \langle \mathbf{c}, \mathbf{d} \rangle_{L_x^2(\mathbf{w})} &= \sum_{i=1}^N \langle c_i, d_i \rangle_{L_x^2(w_i)}, & \|\mathbf{c}\|_{L_x^2(\mathbf{w})} &= \left( \sum_{i=1}^N \|c_i\|_{L_x^2(w_i)}^2 \right)^{1/2}, \\ \langle \mathbf{f}, \mathbf{g} \rangle_{L_v^2(\mathbf{W})} &= \sum_{i=1}^N \langle f_i, g_i \rangle_{L_v^2(W_i)}, & \|\mathbf{f}\|_{L_v^2(\mathbf{W})} &= \left( \sum_{i=1}^N \|f_i\|_{L_v^2(W_i)}^2 \right)^{1/2}, \end{aligned}$$

Note that in the specific case of positive measurable functions  $\mathbf{W} : \mathbb{R}^3 \rightarrow (\mathbb{R}_+^*)^N$  in the sole variable  $v$ , without risk of confusion we shall also consider the weighted Hilbert

space  $L^2(\mathbb{T}^3 \times \mathbb{R}^3, \mathbf{W})$ , defined similarly by the natural scalar product and norm

$$\langle \mathbf{f}, \mathbf{g} \rangle_{L^2_{x,v}(\mathbf{W})} = \sum_{i=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} f_i(x, v) g_i(x, v) W_i^2(v) dx dv,$$

$$\|\mathbf{f}\|_{L^2_{x,v}(\mathbf{W})}^2 = \sum_{i=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} f_i^2(x, v) W_i^2(v) dx dv,$$

for any  $\mathbf{f}, \mathbf{g} \in L^2(\mathbb{T}^3 \times \mathbb{R}^3, \mathbf{W})$ .

Finally, in the same way we can introduce the corresponding weighted Sobolev spaces. Consider two multi-indices  $\alpha, \beta \in \mathbb{N}^3$ , of lengths  $|\alpha| = \sum_{k=1}^3 \alpha_k$  and  $|\beta| = \sum_{k=1}^3 \beta_k$  respectively. We shall use the convention that  $\alpha$  always refers to  $x$ -derivatives while  $\beta$  refers to  $v$ -derivatives. Note in particular that we shall use the standard notation of the canonical basis in  $\mathbb{R}^3$  to name the specific multi-indices having one component equal to 1 and the others equal to 0, so for example  $e_1 = (1, 0, 0)$ .

For any  $s \in \mathbb{N}$  and any vector-valued functions  $\mathbf{c} \in H^s(\mathbb{T}^3, \mathbf{w})$  and  $\mathbf{f} \in H^s(\mathcal{S}, \mathbf{W})$ , where either  $\mathcal{S} = \mathbb{R}^3$  or  $\mathcal{S} = \mathbb{T}^3 \times \mathbb{R}^3$ , we define the norms

$$\|\mathbf{c}\|_{H^s_x(\mathbf{w})} = \left( \sum_{i=1}^N \sum_{|\alpha| \leq s} \|\partial_x^\alpha c_i\|_{L^2_x(w_i)}^2 \right)^{1/2},$$

$$\|\mathbf{f}\|_{H^s_v(\mathbf{W})} = \left( \sum_{i=1}^N \sum_{|\beta| \leq s} \|\partial_v^\beta f_i\|_{L^2_v(W_i)}^2 \right)^{1/2},$$

$$\|\mathbf{f}\|_{H^s_{x,v}(\mathbf{W})} = \left( \sum_{i=1}^N \sum_{|\alpha|+|\beta| \leq s} \|\partial_v^\beta \partial_x^\alpha f_i\|_{L^2_{x,v}(W_i)}^2 \right)^{1/2}.$$

## 3.2 Perturbative Cauchy theory for the Maxwell-Stefan model

We first deal with the study of the Maxwell-Stefan system (3.1.7)–(3.1.9). The Cauchy theory we build offers a complete description of all the perturbative solutions  $((c_i, u_i)_{1 \leq i \leq N})$  around a global macroscopic equilibrium state. We point out in particular that, because of the incompressibility condition (3.1.9), any macroscopic stationary state has the form  $(\bar{c}_i, \bar{u})_{1 \leq i \leq N}$ , where each  $\bar{c}_i$  is a positive constant and the velocity  $\bar{u} : \mathbb{R}_+ \times \mathbb{T}^3 \rightarrow \mathbb{R}^3$ , common to all the species, satisfies  $\nabla_x \cdot \bar{u}(t, x) = 0$  for any  $t \geq 0$  and  $x \in \mathbb{T}^3$ . For a sake of clarity, throughout the present section any perturbative vector-valued function  $\mathbf{w} = (w_1, \dots, w_N)$  shall be written under the specific form  $\mathbf{w} = \bar{\mathbf{w}} + \varepsilon \tilde{\mathbf{w}}$ , where the component  $\bar{\mathbf{w}}$  with the overbar symbol always refers to some (macroscopic) stationary state of the mixture and the component  $\tilde{\mathbf{w}}$  overlined by a tilde refers to the fluctuation around the corresponding equilibrium state. Moreover, note that for simplicity the specific quantity  $\bar{\mathbf{u}}$  will always denote an  $N$ -vector where all the components are given by a common incompressible velocity  $\bar{u}$ .

### 3.2.1 Statement of the result

The following theorem details the main results obtained in this section. We shall then provide below some useful remarks that will help in clarifying its essential points.

**Theorem 3.2.1.** *Let  $s > 3$  be an integer,  $\bar{u} : \mathbb{R}_+ \times \mathbb{T}^3 \rightarrow \mathbb{R}^3$  be in  $L^\infty(\mathbb{R}_+; H^s(\mathbb{T}^3))$  with  $\nabla_x \cdot \bar{u} = 0$ , and consider  $\bar{\mathbf{c}} > 0$ . There exist  $\delta_{MS}, C_{MS}, \lambda_{MS} > 0$  such that for all  $\varepsilon \in (0, 1]$  and for any initial datum  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{u}}^{\text{in}}) \in H^s(\mathbb{T}^3) \times H^{s-1}(\mathbb{T}^3)$  satisfying, for almost every  $x \in \mathbb{T}^3$  and for any  $1 \leq i \leq N$ ,*

$$(i) \text{ \textit{Mass compatibility:}} \quad \sum_{i=1}^N \tilde{c}_i^{\text{in}}(x) = 0 \quad \text{and} \quad \int_{\mathbb{T}^3} \tilde{c}_i^{\text{in}}(x) dx = 0,$$

$$(ii) \text{ \textit{Mass positivity:}} \quad \bar{c}_i + \varepsilon \tilde{c}_i^{\text{in}}(x) > 0,$$

$$(iii) \text{ \textit{Moment compatibility:}} \quad \nabla_x \tilde{c}_i^{\text{in}} = \sum_{j \neq i} \frac{c_i^{\text{in}} c_j^{\text{in}}}{\Delta_{ij}} (\tilde{u}_j^{\text{in}} - \tilde{u}_i^{\text{in}}),$$

$$(iv) \text{ \textit{Smallness assumptions:}} \quad \|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s} \leq \delta_{MS} \quad \text{and} \quad \|\bar{u}\|_{L_t^\infty H_x^s} \leq \delta_{MS},$$

there exists a unique weak solution

$$(\mathbf{c}, \mathbf{u}) = (\bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}, \bar{\mathbf{u}} + \varepsilon \tilde{\mathbf{u}})$$

in  $L^\infty(\mathbb{R}_+; H^s(\mathbb{T}^3)) \times L^\infty(\mathbb{R}_+; H^{s-1}(\mathbb{T}^3))$  to the incompressible Maxwell-Stefan system (3.1.7)–(3.1.9), such that initially  $(\mathbf{c}, \mathbf{u})|_{t=0} = (\bar{\mathbf{c}}^{\text{in}} + \varepsilon \tilde{\mathbf{c}}^{\text{in}}, \bar{\mathbf{u}} + \varepsilon \tilde{\mathbf{u}}^{\text{in}})$  a.e. in  $\mathbb{T}^3$ .

Moreover,  $\mathbf{c}$  is positive and the following equimolar diffusion-like relation holds a.e. on  $\mathbb{R}_+ \times \mathbb{T}^3$ :

$$\langle \mathbf{c}, \tilde{\mathbf{u}} \rangle = \sum_{i=1}^N c_i(t, x) \tilde{u}_i(t, x) = 0. \quad (3.2.1)$$

Finally, for almost every time  $t \geq 0$

$$\|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})} \leq e^{-\lambda_{MS} t} \|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})},$$

$$\|\tilde{\mathbf{u}}\|_{H_x^{s-1}} \leq C_{MS} e^{-\lambda_{MS} t} \|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}.$$

In particular, the constants  $\delta_{MS}, \lambda_{MS}$  and  $C_{MS}$  are constructive and only depend on  $s$ , the number of species  $N$ , the constant state  $\bar{\mathbf{c}}$  and the diffusion coefficients  $\Delta_{ij}$ .

**Remark 3.2.2.** *Let us make a few comments about this theorem.*

1. Our result establishes a Cauchy theory and trend to equilibrium around the macroscopic stationary state  $(\bar{\mathbf{c}}, \bar{\mathbf{u}})$ , which extends the previous works where either a closure assumption was made or the equilibrium considered was  $(\bar{\mathbf{c}}, \mathbf{0})$ . In particular, we give here a complete description of all possible studies (at order  $\varepsilon$ ) around a constant mass vector  $\bar{\mathbf{c}}$ .
2. The “mass compatibility” and the “moment compatibility” assumptions are not closure hypotheses, they actually exactly come from the system of equations (3.1.7)–(3.1.8) applied at time  $t = 0$ . We impose these conditions at the beginning, so that our initial datum is compatible with the Maxwell-Stefan system.

3. We emphasize again that we do not prove strong uniqueness for the solutions. Indeed, we can construct infinitely many solutions to the Maxwell-Stefan system, by considering different constant masses  $\bar{\mathbf{c}}$  and incompressible momenta  $\bar{\mathbf{u}}$ . However, these are all the possible solutions in a perturbative setting, and the uniqueness property has actually to be understood in this perturbative sense: as soon as a macroscopic equilibrium  $(\bar{\mathbf{c}}, \bar{\mathbf{u}})$  is fixed, we recover strong uniqueness around this specific state.
4. The solution we construct has actually more regularity with respect to  $t$ , provided that  $s > 4$  and  $\bar{\mathbf{u}} \in C^0(\mathbb{R}_+; H^s(\mathbb{T}^3))$ . Indeed, we point out that, in this case, the couple  $(\mathbf{c}, \mathbf{u})$  also belongs to  $C^0(\mathbb{R}_+; H^{s-1}(\mathbb{T}^3)) \times C^0(\mathbb{R}_+; H^{s-2}(\mathbb{T}^3))$ , allowing in particular to properly define the initial value problem. In the next section, we shall always choose  $(\mathbf{c}, \mathbf{u})$  to be continuous in time, as this property is necessary when proving the global existence of solutions to the Boltzmann equation.
5. The constants  $\delta_{MS}$ ,  $\lambda_{MS}$  and  $C_{MS}$  are not explicitly computed, but their values can be determined respectively from formulae (3.2.24), (3.2.26) and (3.2.27).

In order to investigate the existence and uniqueness of solutions to (3.1.7)–(3.1.8), it is common in the literature [96, 33, 138] to introduce the Maxwell-Stefan matrix

$$A(\mathbf{c}) = \left( \begin{array}{c} c_i c_j - \left( \sum_{k=1}^N c_i c_k \right) \delta_{ij} \\ \Delta_{ij} \end{array} \right)_{1 \leq i, j \leq N}, \quad (3.2.2)$$

which depends on  $(c_i)_{1 \leq i \leq N}$ . In this way, the Maxwell-Stefan system (3.1.7)–(3.1.9) can be rewritten (also using our notation for the scalar product between  $N$ -vectors) in a more convenient vectorial form as

$$\partial_t \mathbf{c} + \nabla_x \cdot (\mathbf{c} \mathbf{u}) = 0, \quad (3.2.3)$$

$$\nabla_x \mathbf{c} = A(\mathbf{c}) \mathbf{u}, \quad (3.2.4)$$

$$\partial_t \langle \mathbf{c}, \mathbf{1} \rangle = 0, \quad \nabla_x \cdot \langle \mathbf{c}, \mathbf{u} \rangle = 0. \quad (3.2.5)$$

In particular, a natural idea would be to invert the gradient relation (3.2.4) so that we can express  $\mathbf{u}$  in terms of  $\mathbf{c}$ , and recover an evolution equation for the sole unknown  $\mathbf{c}$ , by replacing  $\mathbf{u} = A(\mathbf{c})^{-1} \nabla_x \mathbf{c}$  into equation (3.2.3). Unfortunately, it is possible to prove [33, 138] that the matrix  $A$  is only positive semi-definite, with  $\ker A = \text{Span}(\mathbf{1})$ . Therefore, any existing [96, 33, 38, 138] Cauchy theory for the Maxwell-Stefan equations is based on the possibility of explicitly computing the pseudoinverse (or Penrose-Moore inverse [157, 170]) of  $A$ , which is defined on the space  $(\text{Span}(\mathbf{1}))^\perp$ . This can be achieved for example [33, 138] using the Perron-Frobenius theory for quasi-positive matrices. However, a major drawback of this strategy is that the computations giving the explicit form of  $A^{-1}$  are extremely intricate and do not offer a neat understanding of the action of  $A$  on the velocities  $\mathbf{u}$ . Moreover, as already pointed out in the introduction, since one cannot see the entire part of  $\mathbf{u}$  that evolves in  $\ker A$ , a closure assumption of type (3.1.14) is needed in order to compensate this lack of information.

In this work we propose another approach which takes inspiration from the micro-macro decomposition techniques commonly used in the kinetic theory of gases. More precisely, by introducing the orthogonal projection  $\pi_A$  onto  $\text{Span}(\mathbf{1})$ , associated to the non-injective operator  $A$ , we split  $\mathbf{u} = \pi_A(\mathbf{u}) + \mathbf{U}$  into a part projected onto  $\text{Span}(\mathbf{1})$  and an orthogonal part  $\mathbf{U}$  which is projected onto  $(\ker A)^\perp$ . Thanks to the incompressibility condition (3.2.5)



we are in particular able to get rid of the closure assumption (3.1.14) and to construct a new system of equations, equivalent to (3.2.3)–(3.2.5) for full velocities  $\mathbf{u}$ , in which the Maxwell-Stefan matrix only acts on  $\mathbf{U}$ . In such a way, we are able to deal with the pseudoinverse of  $A$  (which is always well-defined on  $(\ker A)^\perp$ ), without the need of computing its explicit structure. Moreover, our alternative strategy provides an original point of view in which we exhibit a clear separation between  $\pi_A(\mathbf{u})$  and  $\mathbf{U}$ , allowing to show explicitly the actual action of  $A$  on the sole vector  $\mathbf{U}$ . Eventually, starting from this new equivalent orthogonal system we derive all the required *a priori* energy estimates for the unknowns, which enables to recover global existence and uniqueness of the perturbative solution  $(\mathbf{c}, \mathbf{u})$ .

With this idea in mind, the section is divided into two parts. In the first one, we show how to derive the new orthogonal system equivalent to (3.2.3)–(3.2.5), and state the counterpart of Theorem 3.2.1 in terms of this new reformulation for the unknowns  $\mathbf{c}$  and  $\mathbf{U}$ . In the second part we then prove all the required properties (existence and uniqueness, positivity and exponential decay to equilibrium) for the couple  $(\mathbf{c}, \mathbf{U})$ , properties that will be also satisfied by the original unknowns  $(\mathbf{c}, \mathbf{u})$ .

### 3.2.2 An orthogonal incompressible Maxwell-Stefan system

Here we present the equivalent orthogonal reformulation of the Maxwell-Stefan system (3.2.3)–(3.2.5), which allows to transfer the study of existence and uniqueness for solutions  $(\mathbf{c}, \mathbf{u})$  to the development of a Cauchy theory for the new unknowns  $(\mathbf{c}, \mathbf{U})$ , where we denote with  $\mathbf{U} = \mathbf{u} - \pi_A(\mathbf{u})$  the part of  $\mathbf{u}$  that is projected onto  $(\ker A)^\perp$ .

Before stating our result, we introduce a useful notation that allows to preserve the vectorial structure of the Maxwell-Stefan system. We suppose that, for some  $V \in \mathbb{R}^3$  and some  $N$ -vector  $\mathbf{w} \in (\mathbb{R}^3)^N$  whose components lie in  $\mathbb{R}^3$ , the standard notation of the scalar product in  $\mathbb{R}^3$  is extended to any multiplication of type  $V \cdot \mathbf{w}$  in the following sense

$$V \cdot \mathbf{w} = (V \cdot w_i)_{1 \leq i \leq N}.$$

**Proposition 3.2.3.** *Let  $s \in \mathbb{N}^*$ ,  $C_0 > 0$ , and consider two functions  $\mathbf{c}^{\text{in}} \in H^s(\mathbb{T}^3)$  and  $\mathbf{u}^{\text{in}} \in H^{s-1}(\mathbb{T}^3)$  verifying, for almost every  $x \in \mathbb{T}^3$ ,*

$$\mathbf{c}^{\text{in}}(x) > 0 \quad \text{and} \quad \sum_{i=1}^N c_i^{\text{in}}(x) = C_0.$$

*Then,  $(\mathbf{c}, \mathbf{u}) \in L^\infty(\mathbb{R}_+; H^s(\mathbb{T}^3)) \times L^\infty(\mathbb{R}_+; H^{s-1}(\mathbb{T}^3))$  is a solution to the incompressible Maxwell-Stefan system (3.2.3)–(3.2.5), associated to the initial datum  $(\mathbf{c}^{\text{in}}, \mathbf{u}^{\text{in}})$ , if and only if there exist two functions  $\mathbf{U} : \mathbb{R}_+ \times \mathbb{T}^3 \rightarrow \mathbb{R}^{3N}$  and  $\bar{u} : \mathbb{R}_+ \times \mathbb{T}^3 \rightarrow \mathbb{R}^3$  in  $L^\infty(\mathbb{R}_+; H^{s-1}(\mathbb{T}^3))$  such that, for almost every  $(t, x) \in \mathbb{R}_+ \times \mathbb{T}^3$ ,*

$$\mathbf{U}(t, x) \in (\ker A)^\perp \quad \text{and} \quad \nabla_x \cdot \bar{u}(t, x) = 0, \quad (3.2.6)$$

$$\mathbf{U}(t, x) + \bar{u}(t, x) - \frac{1}{C_0} \langle \mathbf{c}, \mathbf{U} \rangle \mathbf{1} = \mathbf{u}(t, x), \quad (3.2.7)$$

$$\begin{cases} \partial_t \mathbf{c} + \nabla_x \cdot \left( \mathbf{c} \left( \mathbf{U} - \frac{\langle \mathbf{c}, \mathbf{U} \rangle}{\langle \mathbf{c}, \mathbf{1} \rangle} \mathbf{1} \right) \right) + \bar{u} \cdot \nabla_x \mathbf{c} = 0, \\ \nabla_x \mathbf{c} = A(\mathbf{c}) \mathbf{U}. \end{cases} \quad (3.2.8)$$

**Remark 3.2.4.** *This result is not difficult to prove but we underline again that it is of great importance, since it turns the incompressible Maxwell-Stefan system (3.2.3)–(3.2.5) with full velocity vectors  $\mathbf{u}$  into a system only depending on their orthogonal component  $\mathbf{U} \in (\ker A)^\perp$ , while the projection onto  $\ker A$  raises a simple transport term in the continuity equation (3.2.3). Notice in particular that we differentiate between  $C_0 = \langle \mathbf{c}^{\text{in}}, \mathbf{1} \rangle$  in (3.2.7) and  $\langle \mathbf{c}, \mathbf{1} \rangle$  in (3.2.8). As we shall see, in both equations it will turn out that these two quantities are equal, but keeping the notation  $\langle \mathbf{c}, \mathbf{1} \rangle$  offers a fully closed system.*

*Proof of Proposition 3.2.3.* Let  $\pi_A$  be the orthogonal projection operator onto  $\ker A$  and consider a solution  $(\mathbf{c}, \mathbf{u})$  of the Maxwell-Stefan system (3.2.3)–(3.2.5). The first implication directly follows from the decomposition

$$\mathbf{u} = \pi_A(\mathbf{u}) + (\mathbf{u} - \pi_A(\mathbf{u})) = \frac{\langle \mathbf{u}, \mathbf{1} \rangle}{\|\mathbf{1}\|} \mathbf{1} + \pi_A^\perp(\mathbf{u}),$$

where we recall that  $\|\cdot\|$  defines the Euclidean norm induced by the scalar product  $\langle \cdot, \cdot \rangle$  in  $\mathbb{R}^N$ , weighted by the vector  $\mathbf{1}$ .

First of all, observe that summing over the gradient equations (3.2.4) we get

$$\nabla_x \left( \sum_{i=1}^N c_i \right) = \sum_{1 \leq i, j \leq N} \frac{c_i c_j}{\Delta_{ij}} (u_j - u_i) = 0.$$

Therefore, the quantity  $\langle \mathbf{c}, \mathbf{1} \rangle$  is independent of  $x$ , but it is also independent of  $t$  thanks to the incompressibility condition (3.2.5). This allows to initially deduce that

$$\sum_{i=1}^N c_i(t, x) = \sum_{i=1}^N c_i^{\text{in}}(x) = C_0 \quad \text{a.e. on } \mathbb{R}_+ \times \mathbb{T}^3. \quad (3.2.9)$$

If we now define  $\mathbf{U} = \pi_A^\perp(\mathbf{u})$  and  $W = \frac{\langle \mathbf{u}, \mathbf{1} \rangle}{\|\mathbf{1}\|}$ , the transport equation (3.2.4) can be rewritten in terms of  $\mathbf{U}$  and  $W$  as

$$\partial_t \mathbf{c} + \nabla_x \cdot (\mathbf{c} \mathbf{U}) + \mathbf{c} \nabla_x \cdot W + W \cdot \nabla_x \mathbf{c} = 0. \quad (3.2.10)$$

In a similar way, the incompressibility condition (3.2.5) in these new unknowns reads

$$\begin{aligned} 0 &= \sum_{i=1}^N \nabla_x \cdot (c_i (U_i + W)) \\ &= \sum_{i=1}^N \nabla_x \cdot (c_i U_i) + \nabla_x \cdot \left( \sum_{i=1}^N c_i \right) \cdot W + (\nabla_x \cdot W) \sum_{i=1}^N c_i \\ &= \nabla_x \cdot \langle \mathbf{c}, \mathbf{U} \rangle + C_0 \nabla_x \cdot W, \end{aligned}$$

where we have used (3.2.9). We consequently infer the existence of a divergence-free function  $\bar{u} : \mathbb{R}_+ \times \mathbb{T}^3 \rightarrow \mathbb{R}^3$  such that, for almost every  $(t, x) \in \mathbb{T}^3 \times \mathbb{R}^3$ ,

$$\begin{cases} \nabla_x \cdot \bar{u}(t, x) = 0, \\ W(t, x) = -\frac{1}{C_0} \langle \mathbf{c}, \mathbf{U} \rangle(t, x) + \bar{u}(t, x), \end{cases}$$

and thus (3.2.6)–(3.2.7) easily follow.

Plugging the above relation into (3.2.10) and replacing  $C_0$  by its value  $\langle \mathbf{c}, \mathbf{1} \rangle$ , we then recover the first equation of (3.2.8). Finally, the decomposition (3.2.2) also yields the second relation of (3.2.8), since  $\pi_A(\mathbf{u}) \in \ker A$  and thus

$$A(\mathbf{c})\mathbf{u} = A(\mathbf{c})\mathbf{U},$$

proving that  $(\mathbf{c}, \mathbf{U}, \bar{u})$  is a solution of the orthogonal reformulation (3.2.6)–(3.2.8).

Consider now a triple  $(\mathbf{c}, \mathbf{U}, \bar{u})$  satisfying conditions (3.2.6)–(3.2.8). The reverse implication then follows by defining

$$\mathbf{u} = \mathbf{U} + \left( -\frac{1}{C_0} \langle \mathbf{c}, \mathbf{U} \rangle + \bar{u} \right) \mathbf{1}. \quad (3.2.11)$$

Indeed, summing over  $1 \leq i \leq N$  the gradient equations of (3.2.8), we get

$$\nabla_x \left( \sum_{i=1}^N c_i \right) = 0,$$

which is used when one also sums over  $1 \leq i \leq N$  the transport equations of (3.2.8), to deduce

$$\begin{aligned} 0 &= \partial_t \left( \sum_{i=1}^N c_i \right) + \nabla_x \left( \sum_{i=1}^N c_i U_i \right) - \nabla_x \cdot \left( \langle \mathbf{c}, \mathbf{U} \rangle \frac{\left( \sum_{i=1}^N c_i \right)}{\langle \mathbf{c}, \mathbf{1} \rangle} \right) \\ &= \partial_t \left( \sum_{i=1}^N c_i \right), \end{aligned}$$

since  $\langle \mathbf{c}, \mathbf{1} \rangle = \sum_{i=1}^N c_i$  by definition. Thus, the quantity  $\langle \mathbf{c}, \mathbf{1} \rangle$  is independent of  $(t, x)$ , allowing to infer that

$$\sum_{i=1}^N c_i(t, x) = \langle \mathbf{c}^{\text{in}}, \mathbf{1} \rangle = C_0 \quad \text{a.e. on } \mathbb{R}_+ \times \mathbb{T}^3.$$

This recovery of (3.2.9) not only implies the incompressibility condition (3.2.5) but also, with the divergence free property of  $\bar{u}$ , that

$$\begin{aligned} \nabla_x \cdot (\mathbf{c}\mathbf{u}) &= \nabla_x \cdot \left( \mathbf{c} \left( \mathbf{U} - \frac{\langle \mathbf{c}, \mathbf{U} \rangle}{C_0} \mathbf{1} \right) \right) + \bar{u} \cdot \nabla_x \mathbf{c} \\ &= \nabla_x \cdot \left( \mathbf{c} \left( \mathbf{U} - \frac{\langle \mathbf{c}, \mathbf{U} \rangle}{\langle \mathbf{c}, \mathbf{1} \rangle} \mathbf{1} \right) \right) + \bar{u} \cdot \nabla_x \mathbf{c}. \end{aligned}$$

Therefore, the first equation of (3.2.8) rewrites

$$\partial_t \mathbf{c} + \nabla_x \cdot (\mathbf{c}\mathbf{u}) = 0,$$

and, thanks again to the fact that  $\ker A = \text{Span}(\mathbf{1})$ , one finally sees that

$$\nabla_x \mathbf{c} = A(\mathbf{c})\mathbf{U} = A(\mathbf{c})\mathbf{u}.$$

This ensures that  $(\mathbf{c}, \mathbf{u})$ , with  $\mathbf{u}$  defined by (3.2.11), solves the Maxwell-Stefan system (3.2.3)–(3.2.4) with incompressibility condition (3.2.5). This concludes the proof.  $\square$

By means of this reformulation, we can now prove our main result.

### 3.2.3 Proof of Theorem 3.2.1

This last part is devoted to showing the validity of Theorem 3.2.1. We shall divide the proof into several steps which help in enlightening the basic ideas behind our strategy. We first restate our result about solutions  $(\mathbf{c}, \mathbf{u})$  in terms of the orthogonal reformulation (3.2.6)–(3.2.8), about solutions  $(\mathbf{c}, \mathbf{U}, \bar{u})$ . Thanks to some useful preliminary lemmata describing the main properties of the matrix  $A$  and of its pseudoinverse (whose technical proofs can be found in Appendix A), we then derive uniform (in  $\varepsilon$ ) *a priori* energy estimates for the solution  $(\mathbf{c}, \mathbf{U})$ , which provide the exponential relaxation towards the global equilibrium  $(\bar{\mathbf{c}}, \bar{\mathbf{u}})$ . Starting from this we are thus able to recover the positivity of  $\mathbf{c}$ , and to prove global existence and uniqueness for solutions to (3.2.8) having the specific perturbative forms  $\mathbf{c} = \bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}$  and  $\mathbf{U} = \varepsilon \tilde{\mathbf{U}}$ . The combination of these results will eventually allow to deduce global existence, uniqueness and exponential decay for the couple  $(\mathbf{c}, \mathbf{u})$ , using the reconstruction condition (3.2.7).

**Step 1 – Reformulation in terms of orthogonal velocities.** Let us begin with a simple lemma needed in order to understand the shape of the moments  $\mathbf{U}$  and  $\bar{u}$ , when they are associated to a constant state  $\bar{\mathbf{c}}$ .

**Lemma 3.2.5.** *Let  $s \in \mathbb{N}^*$  and let  $\bar{\mathbf{c}}$  be a positive constant  $N$ -vector. For any functions  $\mathbf{U}, \bar{u}$  in  $L^\infty(\mathbb{R}_+; H^{s-1}(\mathbb{T}^3))$  such that  $\mathbf{U} \in (\text{Span}(\mathbf{1}))^\perp$  and  $\nabla_x \cdot \bar{u} = 0$ , a triple  $(\bar{\mathbf{c}}, \mathbf{U}, \bar{u})$  is solution to the system of equations (3.2.6)–(3.2.8) if and only if*

$$\mathbf{U}(t, x) = 0 \quad \text{a.e. on } \mathbb{R}_+ \times \mathbb{T}^3.$$

*Proof.* The proof is very simple. Because  $\bar{\mathbf{c}}$  is constant, the gradient equation of (3.2.8) reads  $A(\bar{\mathbf{c}})\mathbf{U} = 0$ . But  $\mathbf{U}$  belongs to  $(\ker A)^\perp$ , which means that the pseudoinverse  $A^{-1}$  remains well-defined. Consequently, for almost every  $(t, x) \in \mathbb{R}_+ \times \mathbb{T}^3$ ,  $\mathbf{U}(t, x) = 0$ .

The reverse implication is direct. □

We are now interested in building a Cauchy theory for the orthogonal form of the Maxwell-Stefan system, around the stationary solutions given by Proposition 3.2.5. More precisely, we want to prove existence and uniqueness for perturbative solutions to (3.2.6)–(3.2.8) of the form

$$\begin{cases} \mathbf{c}(t, x) = \bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}, \\ \mathbf{U} = \varepsilon \tilde{\mathbf{U}}. \end{cases}$$

In terms of these particular solutions, the system (3.2.6)–(3.2.8) translates into

$$\partial_t \tilde{\mathbf{c}} + \bar{\mathbf{c}} \nabla_x \cdot \mathbf{V}_{\tilde{\mathbf{U}}} + \bar{u} \cdot \nabla_x \tilde{\mathbf{c}} + \varepsilon \nabla_x \cdot (\tilde{\mathbf{c}} \mathbf{V}_{\tilde{\mathbf{U}}}) = 0 \quad (3.2.12)$$

$$\nabla_x \tilde{\mathbf{c}} = A(\bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}) \tilde{\mathbf{U}} \quad (3.2.13)$$

with the notation  $\mathbf{V}_{\tilde{\mathbf{U}}} = \tilde{\mathbf{U}} - \frac{\langle \mathbf{c}, \tilde{\mathbf{U}} \rangle}{\langle \mathbf{c}, \mathbf{1} \rangle} \mathbf{1}$ .

The orthogonal reformulation of Theorem 3.2.1 then writes in the following way.

**Theorem 3.2.6.** *Let  $s > 3$  be and integer,  $\bar{u} : \mathbb{R}_+ \times \mathbb{T}^3 \rightarrow \mathbb{R}^3$  be in  $L^\infty(\mathbb{R}_+; H^s(\mathbb{T}^3))$  with  $\nabla_x \cdot \bar{u} = 0$ , and consider a constant  $N$ -vector  $\bar{\mathbf{c}} > 0$ . There exist  $\delta_s, C_s, \lambda_s > 0$  such that for all  $\varepsilon \in (0, 1]$  and for any  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{U}}^{\text{in}}) \in H^s(\mathbb{T}^3) \times H^{s-1}(\mathbb{T}^3)$  satisfying, for almost every  $x \in \mathbb{T}^3$  and for any  $1 \leq i \leq N$ ,*

$$(i) \text{ Mass compatibility: } \sum_{i=1}^N \tilde{c}_i^{\text{in}}(x) = 0 \quad \text{and} \quad \int_{\mathbb{T}^3} \tilde{c}_i^{\text{in}}(x) dx = 0,$$

$$(ii) \text{ Mass positivity: } \bar{c}_i + \varepsilon \tilde{c}_i^{\text{in}}(x) > 0,$$

$$(iii) \text{ Moment compatibility: } \tilde{\mathbf{U}}^{\text{in}}(x) = A(\bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}^{\text{in}}(x))^{-1} \nabla_x \tilde{\mathbf{c}}^{\text{in}}(x),$$

$$(iv) \text{ Smallness assumptions: } \|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s} \leq \delta_s \quad \text{and} \quad \|\tilde{\mathbf{u}}\|_{L_t^\infty H_x^s} \leq \delta_s,$$

there exists a unique weak solution  $(\tilde{\mathbf{c}}, \tilde{\mathbf{U}}) \in L^\infty(\mathbb{R}_+; H^s(\mathbb{T}^3)) \times L^\infty(\mathbb{R}_+; H^{s-1}(\mathbb{T}^3))$  to the system of equations (3.2.12)–(3.2.13), having  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{U}}^{\text{in}})$  as initial datum. In particular, for almost every  $(t, x) \in \mathbb{R}_+ \times \mathbb{T}^3$ , the vector  $\mathbf{c}(t, x) = \bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}(t, x)$  is positive and  $\tilde{\mathbf{U}}(t, x)$  belongs to  $(\ker A)^\perp$ .

Moreover, for almost every  $t \geq 0$

$$\|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})} \leq e^{-\lambda_s t} \|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})},$$

$$\|\tilde{\mathbf{U}}\|_{H_x^{s-1}} \leq C_s e^{-\lambda_s t} \|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}.$$

The constants  $\delta_s$ ,  $\lambda_s$  and  $C_s$  are constructive and are given respectively by (3.2.24), (3.2.26) and (3.2.27).

**Remark 3.2.7.** We underline that the reconstruction condition (3.2.7) does not involve the vector  $\mathbf{c}$ , but only the velocity vector. This means in particular that the solution  $\mathbf{c}$  provided by the above theorem coincides exactly with the one given by Theorem 3.2.1. However, there is a real difference when one reformulates Theorem 3.2.1 in terms of the orthogonal velocities. Indeed, it is important to notice that the velocity vectors  $\tilde{\mathbf{u}}$  and  $\tilde{\mathbf{U}}$  are not the same, since (3.2.7) tells us that actually  $\tilde{\mathbf{u}} = \mathbf{V}_{\tilde{\mathbf{c}}}$ , from which we only deduce the relation  $\langle \mathbf{c}, \tilde{\mathbf{u}} \rangle = 0$ , and no more the orthogonality  $\langle \tilde{\mathbf{u}}, \mathbf{1} \rangle = 0$ .

**Step 2 – Properties of the Maxwell-Stefan matrix.** For the reader's convenience, we present here three preliminary lemmata that exhibit some useful properties satisfied by the matrix  $A$  and by its pseudoinverse. Their technical proofs can be found in Appendix A.

We first recall the non-positivity property of the Maxwell-Stefan matrix [96, 33, 138, 35].

**Lemma 3.2.8.** For any  $\mathbf{c} \geq 0$  the matrix  $A(\mathbf{c})$  is nonpositive, in the sense that there exist two positive constants  $\lambda_A$  and  $\mu_A$  such that, for any  $\mathbf{X} \in \mathbb{R}^N$ ,

$$\|A(\mathbf{c})\mathbf{X}\| \leq \mu_A \langle \mathbf{c}, \mathbf{1} \rangle^2 \|\mathbf{X}\|,$$

$$\langle \mathbf{X}, A(\mathbf{c})\mathbf{X} \rangle \leq -\lambda_A \left( \min_{1 \leq i \leq N} c_i \right)^2 \left[ \|\mathbf{X}\|^2 - \langle \mathbf{X}, \mathbf{1} \rangle^2 \right] \leq 0.$$

Next, we provide some useful estimates on the  $x$ -derivatives of  $A$ , which will be crucial in order to correctly bound the quantities coming into play inside the proofs of existence, uniqueness and exponential decay of the solution  $(\mathbf{c}, \tilde{\mathbf{U}})$ .

**Lemma 3.2.9.** Consider a multi-index  $\alpha \in \mathbb{N}^3$  and let  $\mathbf{c}, \tilde{\mathbf{U}} \in H^{|\alpha|}(\mathbb{T}^3)$ , with  $\mathbf{c} \geq 0$ . Then, for any  $\mathbf{X} \in \mathbb{R}^N$ ,

$$\begin{aligned} \langle \partial_x^\alpha [A(\mathbf{c})\mathbf{U}], \mathbf{X} \rangle &\leq \langle A(\mathbf{c}) (\partial_x^\alpha \mathbf{U}), \mathbf{X} \rangle \\ &+ 2N^2 \mu_A \langle \mathbf{c}, \mathbf{1} \rangle \|\mathbf{X}\| \sum_{\substack{\alpha_1 + \alpha_3 = \alpha \\ |\alpha_1| \geq 1}} \|\partial_x^{\alpha_1} \mathbf{c}\| \|\partial_x^{\alpha_3} \mathbf{U}\| \\ &+ N^2 \mu_A \|\mathbf{X}\| \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1}} \|\partial_x^{\alpha_1} \mathbf{c}\| \|\partial_x^{\alpha_2} \mathbf{c}\| \|\partial_x^{\alpha_3} \mathbf{U}\|, \end{aligned}$$

where  $\mu_A$  is defined in Lemma 3.2.8.

We conclude with a control over the pseudoinverse of  $A(\mathbf{c})$ , that is defined on  $(\text{Span}(\mathbf{1}))^\perp$ . Note that this result is particularly important, since it provides an explicit negative return for  $A^{-1}$ , as long as the vector  $\mathbf{c}$  remains positive.

**Lemma 3.2.10.** For any  $\mathbf{c} \in (\mathbb{R}_+^*)^N$  and any  $\mathbf{U} \in (\text{Span}(\mathbf{1}))^\perp$ , the following estimates hold:

$$\begin{aligned} \|A(\mathbf{c})^{-1} \mathbf{U}\| &\leq \frac{1}{\lambda_A \left( \min_{1 \leq i \leq N} c_i \right)^2} \|\mathbf{U}\|, \\ \langle A(\mathbf{c})^{-1} \mathbf{U}, \mathbf{U} \rangle &\leq - \frac{\lambda_A \left( \min_{1 \leq i \leq N} c_i \right)^2}{\mu_A^2 \langle \mathbf{c}, \mathbf{1} \rangle^4} \|\mathbf{U}\|^2, \end{aligned}$$

where  $\lambda_A$  and  $\mu_A$  are defined in Lemma 3.2.8.

**Step 3 – A priori energy estimates and positivity.** The two *a priori* results (exponential decay and positivity of  $\mathbf{c}$ ) that we now derive are of crucial importance, as they will allow us to exhibit existence and uniqueness for the couple  $(\tilde{\mathbf{c}}, \tilde{\mathbf{U}})$  in the next section.

Before we start, we present a simple result which establishes two relevant properties satisfied by the solution of (3.2.12)–(3.2.13). We show in particular that  $\tilde{\mathbf{c}}$  has zero mean on the torus, a feature that will be exploited in the proof of the *a priori* estimates, in order to exploit Poincaré inequality on  $\tilde{\mathbf{c}}$ .

**Lemma 3.2.11.** Let  $\bar{c}, C_0 > 0$  such that  $\langle \bar{\mathbf{c}}, \mathbf{1} \rangle = C_0$ , and consider a triple  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{U}}^{\text{in}}, \bar{u})$  satisfying the hypotheses of Theorem 3.2.6. If  $(\tilde{\mathbf{c}}, \tilde{\mathbf{U}})$  is a weak solution of (3.2.12)–(3.2.13) with initial datum  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{U}}^{\text{in}})$ , then, for any  $1 \leq i \leq N$  and almost every  $(t, x) \in \mathbb{R}_+ \times \mathbb{T}^3$ ,

$$\sum_{i=1}^N \tilde{c}_i(t, x) = 0 \quad \text{and} \quad \int_{\mathbb{T}^3} \tilde{c}_i(t, x) dx = 0. \quad (3.2.14)$$

In particular, the conservation of the total mass  $\langle \mathbf{c}, \mathbf{1} \rangle = C_0$  holds almost everywhere on  $\mathbb{R}_+ \times \mathbb{T}^3$ .

*Proof.* We have already showed how to recover the preservation of the total mass inside the proof of Proposition 3.2.3.

The second property follows directly from the fact that  $\bar{\mathbf{c}}$  is a constant  $N$ -vector and  $\bar{u}$  is divergence-free. Indeed, using these two assumptions the mass equation (3.2.12) can be written under a divergent form as

$$\partial_t \tilde{\mathbf{c}} + \nabla_x \cdot (\mathbf{c} \mathbf{V}_{\tilde{U}} + \tilde{\mathbf{c}} \bar{\mathbf{u}}) = 0.$$

Integrating over the torus we thus obtain

$$\frac{d}{dt} \int_{\mathbb{T}^3} \tilde{\mathbf{c}}(t, x) dx = 0 \quad \text{for a.e. } t \geq 0,$$

which gives the expected result since  $\tilde{\mathbf{c}}^{\text{in}}$  has zero mean on the torus.  $\square$

The result providing the *a priori* energy estimates is then the following.

**Proposition 3.2.12.** *Let  $s > 3$  be an integer. There exists  $\delta_s, \lambda_s, C_s > 0$  such that, under the assumptions of Theorem 3.2.6, if  $(\tilde{\mathbf{c}}, \tilde{\mathbf{U}}, \bar{u})$  is a solution of the perturbed orthogonal system (3.2.12)–(3.2.13) satisfying the controls*

$$\|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s} \leq \delta_s \quad \text{and} \quad \|\bar{u}\|_{L_t^\infty H_x^s} \leq \delta_s,$$

then, for almost every  $t \geq 0$ ,

$$\|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})} \leq e^{-\lambda_s t} \|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})},$$

$$\|\tilde{\mathbf{U}}\|_{H_x^{s-1}} \leq C_s e^{-\lambda_s t} \|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}.$$

In particular,  $\lambda_s$  and  $C_s$  are explicit and only depend on  $s$ , the number of species  $N$ , the constant state  $\bar{\mathbf{c}}$  and the diffusion coefficients  $\Delta_{ij}$ .

*Proof.* We fix a multi-index  $\alpha \in \mathbb{N}^3$  such that  $|\alpha| \leq s$ . Recall that we have defined

$$\mathbf{V}_{\tilde{U}} = \tilde{\mathbf{U}} - \frac{\langle \mathbf{c}, \tilde{\mathbf{U}} \rangle}{\langle \mathbf{c}, \mathbf{1} \rangle} \mathbf{1}.$$

We successively apply the  $\alpha$ -derivative to the transport equation (3.2.12), take the scalar product with the vector  $\left(\frac{1}{\bar{c}_i} \partial_x^\alpha \tilde{c}_i\right)_{1 \leq i \leq N}$  and integrate over  $\mathbb{T}^3$ . This yields, after integrating by parts,

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\partial_x^\alpha \tilde{\mathbf{c}}\|_{L_x^2(\bar{\mathbf{c}}^{-\frac{1}{2}})}^2 &= \int_{\mathbb{T}^3} \langle \nabla_x \partial_x^\alpha \tilde{\mathbf{c}}, \partial_x^\alpha \mathbf{V}_{\tilde{U}} \rangle dx \\ &+ \int_{\mathbb{T}^3} \langle \nabla_x \partial_x^\alpha \tilde{\mathbf{c}}, \partial_x^\alpha (\tilde{\mathbf{c}} \bar{\mathbf{u}}) \rangle_{\bar{\mathbf{c}}^{-1}} dx \\ &+ \varepsilon \int_{\mathbb{T}^3} \langle \nabla_x \partial_x^\alpha \tilde{\mathbf{c}}, \partial_x^\alpha (\tilde{\mathbf{c}} \mathbf{V}_{\tilde{U}}) \rangle_{\bar{\mathbf{c}}^{-1}} dx. \end{aligned} \quad (3.2.15)$$

We estimate these three terms separately. We first notice that summing over  $1 \leq i \leq N$  the gradient equations (3.2.13) we obtain

$$\sum_{i=1}^N \nabla_x \tilde{c}_i(t, x) = 0 \quad \text{a.e. on } \mathbb{R}_+ \times \mathbb{T}^3,$$

which means that  $\nabla_x \tilde{\mathbf{c}}$  belongs to  $(\text{Span}(\mathbf{1}))^\perp$ . Applying the  $\alpha$ -derivative to both sides of this relation then gives

$$\sum_{i=1}^N \nabla_x \partial_x^\alpha \tilde{c}_i(t, x) = 0 \quad \text{a.e. on } \mathbb{R}_+ \times \mathbb{T}^3,$$

from which we deduce that also

$$\nabla_x \partial_x^\alpha \tilde{\mathbf{c}} \in (\text{Span}(\mathbf{1}))^\perp \quad \text{a.e. on } \mathbb{R}_+ \times \mathbb{T}^3. \quad (3.2.16)$$

Thanks to the orthogonality (3.2.16) of the higher derivatives and using the gradient relation (3.2.13), the first term on the right-hand side of (3.2.15) becomes

$$\begin{aligned} \int_{\mathbb{T}^3} \langle \nabla_x \partial_x^\alpha \tilde{\mathbf{c}}, \partial_x^\alpha \mathbf{V}_{\tilde{U}} \rangle dx &= \int_{\mathbb{T}^3} \langle \partial_x^\alpha \nabla_x \tilde{\mathbf{c}}, \partial_x^\alpha \tilde{\mathbf{U}} \rangle dx - \frac{1}{C_0} \partial_x^\alpha \langle \mathbf{c}, \tilde{\mathbf{U}} \rangle \int_{\mathbb{T}^3} \langle \nabla_x \partial_x^\alpha \tilde{\mathbf{c}}, \mathbf{1} \rangle dx \\ &= \int_{\mathbb{T}^3} \langle \partial_x^\alpha [A(\mathbf{c})\tilde{\mathbf{U}}], \partial_x^\alpha \tilde{\mathbf{U}} \rangle dx. \end{aligned}$$

We can now apply Proposition 3.2.9 with  $\mathbf{X} = \partial_x^\alpha \tilde{\mathbf{U}}$  and use the mass conservation given in Lemma 3.2.11, in combination with the spectral gap of  $A(\mathbf{c})$  from Proposition 3.2.8, to recover the initial bound

$$\begin{aligned} \int_{\mathbb{T}^3} \langle \nabla_x \partial_x^\alpha \tilde{\mathbf{c}}, \partial_x^\alpha \mathbf{V}_{\tilde{U}} \rangle dx &\leq \int_{\mathbb{T}^3} \langle A(\mathbf{c}) \partial_x^\alpha \tilde{\mathbf{U}}, \partial_x^\alpha \tilde{\mathbf{U}} \rangle dx \\ &\quad + 2N^2 \mu_A C_0 \int_{\mathbb{T}^3} \left\| \partial_x^\alpha \tilde{\mathbf{U}} \right\| \sum_{\substack{\alpha_1 + \alpha_3 = \alpha \\ |\alpha_1| \geq 1}} \left\| \partial_x^{\alpha_1} \mathbf{c} \right\| \left\| \partial_x^{\alpha_3} \tilde{\mathbf{U}} \right\| dx \\ &\quad + N^2 \mu_A \int_{\mathbb{T}^3} \left\| \partial_x^\alpha \tilde{\mathbf{U}} \right\| \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ \alpha_1, \alpha_2 \geq 1}} \left\| \partial_x^{\alpha_1} \mathbf{c} \right\| \left\| \partial_x^{\alpha_2} \mathbf{c} \right\| \left\| \partial_x^{\alpha_3} \tilde{\mathbf{U}} \right\| dx \\ &\leq -\lambda_A \left( \min_{1 \leq i \leq N} c_i \right) \left\| \partial_x^\alpha \tilde{\mathbf{U}} \right\|_{L_x^2}^2 \\ &\quad + 2\varepsilon N^2 \mu_A C_0 \left\| \tilde{\mathbf{U}} \right\|_{H_x^s} \left[ \int_{\mathbb{T}^3} \left( \sum_{\substack{\alpha_1 + \alpha_3 = \alpha \\ |\alpha_1| \geq 1}} \left\| \partial_x^{\alpha_1} \tilde{\mathbf{c}} \right\| \left\| \partial_x^{\alpha_3} \tilde{\mathbf{U}} \right\| \right)^2 dx \right]^{\frac{1}{2}} \\ &\quad + \varepsilon^2 N^2 \mu_A \left\| \tilde{\mathbf{U}} \right\|_{H_x^s} \left[ \int_{\mathbb{T}^3} \left( \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1}} \left\| \partial_x^{\alpha_1} \tilde{\mathbf{c}} \right\| \left\| \partial_x^{\alpha_2} \tilde{\mathbf{c}} \right\| \left\| \partial_x^{\alpha_3} \tilde{\mathbf{U}} \right\| \right)^2 dx \right]^{\frac{1}{2}}, \end{aligned}$$

where we have also used the Cauchy-Schwarz inequality and the fact that the  $L_x^2$  norm of  $\partial_x^\alpha \tilde{\mathbf{U}}$  is controlled by the  $H_x^s$  norm of  $\tilde{\mathbf{U}}$ .

Recalling our choice  $s > 3$ , in order to control the bi and tri-norm terms inside the integrals we use the continuous embedding of  $H_x^{s/2}$  in  $L_x^\infty$ , which holds as soon as  $s/2 > 3/2$ .



We detail our procedure for the tri-norm term, the bi-norm term being treated in the same way.

Since  $\alpha_1 + \alpha_2 + \alpha_3 = \alpha$ , at most one of the  $|\alpha_i|$  can be strictly larger than  $|\alpha|/2$ . Hence, at least two  $|\alpha_i|$  are lower or equal to  $|\alpha|/2 \leq s/2$ . Therefore, we split the tri-norm term into three sums as

$$\begin{aligned} & \int_{\mathbb{T}^3} \left( \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1}} \|\partial_x^{\alpha_1} \tilde{\mathbf{c}}\| \|\partial_x^{\alpha_2} \tilde{\mathbf{c}}\| \|\partial_x^{\alpha_3} \tilde{\mathbf{U}}\| \right)^2 dx \\ & \leq \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1 \\ |\alpha_1|, |\alpha_2| \leq \frac{s}{2}}} \int_{\mathbb{T}^3} \|\partial_x^{\alpha_1} \tilde{\mathbf{c}}\|^2 \|\partial_x^{\alpha_2} \tilde{\mathbf{c}}\|^2 \|\partial_x^{\alpha_3} \tilde{\mathbf{U}}\|^2 dx \\ & \quad + \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1 \\ |\alpha_1|, |\alpha_3| \leq \frac{s}{2}}} \int_{\mathbb{T}^3} \|\partial_x^{\alpha_1} \tilde{\mathbf{c}}\|^2 \|\partial_x^{\alpha_2} \tilde{\mathbf{c}}\|^2 \|\partial_x^{\alpha_3} \tilde{\mathbf{U}}\|^2 dx \\ & \quad + \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1 \\ |\alpha_2|, |\alpha_3| \leq \frac{s}{2}}} \int_{\mathbb{T}^3} \|\partial_x^{\alpha_1} \tilde{\mathbf{c}}\|^2 \|\partial_x^{\alpha_2} \tilde{\mathbf{c}}\|^2 \|\partial_x^{\alpha_3} \tilde{\mathbf{U}}\|^2 dx \end{aligned}$$

For any  $\alpha_k$ -derivative such that  $|\alpha_k| \leq s/2$ , we bound the corresponding factor by its  $L_x^\infty$  norm and we then exploit the mentioned embedding of  $H_x^{s/2}$  in  $L_x^\infty$  in order to recover the correct Sobolev norm. The first sum produces

$$\begin{aligned} & \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1 \\ |\alpha_1|, |\alpha_2| \leq \frac{s}{2}}} \int_{\mathbb{T}^3} \|\partial_x^{\alpha_1} \tilde{\mathbf{c}}\|^2 \|\partial_x^{\alpha_2} \tilde{\mathbf{c}}\|^2 \|\partial_x^{\alpha_3} \tilde{\mathbf{U}}\|^2 dx \\ & \leq \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1 \\ |\alpha_1|, |\alpha_2| \leq \frac{s}{2}}} \|\partial_x^{\alpha_1} \tilde{\mathbf{c}}\|_{L_x^\infty}^2 \|\partial_x^{\alpha_2} \tilde{\mathbf{c}}\|_{L_x^\infty}^2 \|\partial_x^{\alpha_3} \tilde{\mathbf{U}}\|_{L_x^2}^2 \\ & \leq \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1 \\ |\alpha_1|, |\alpha_2| \leq \frac{s}{2}}} \|\partial_x^{\alpha_1} \tilde{\mathbf{c}}\|_{H_x^{s/2}}^2 \|\partial_x^{\alpha_2} \tilde{\mathbf{c}}\|_{H_x^{s/2}}^2 \|\partial_x^{\alpha_3} \tilde{\mathbf{U}}\|_{L_x^2}^2 \\ & \leq s^2 \|\tilde{\mathbf{c}}\|_{H_x^s}^4 \|\tilde{\mathbf{U}}\|_{H_x^s}^2, \end{aligned}$$

and the two others are dealt with in the same way. Therefore, the tri-norm term can be finally estimated as

$$\int_{\mathbb{T}^3} \left( \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1}} \|\partial_x^{\alpha_1} \tilde{\mathbf{c}}\| \|\partial_x^{\alpha_2} \tilde{\mathbf{c}}\| \|\partial_x^{\alpha_3} \tilde{\mathbf{U}}\| \right)^2 dx \leq 3s^2 \|\tilde{\mathbf{c}}\|_{H_x^s}^4 \|\tilde{\mathbf{U}}\|_{H_x^s}^2. \quad (3.2.17)$$

Moreover, the previous Sobolev embedding also yields, for any  $1 \leq i \leq N$ ,

$$c_i(t, x) \geq \bar{c}_i - \varepsilon \|\tilde{\mathbf{c}}\|_{L_x^\infty} \geq \min_{1 \leq i \leq N} \bar{c}_i - \varepsilon \|\tilde{\mathbf{c}}\|_{H_x^s} \quad \text{a.e. on } \mathbb{R}_+ \times \mathbb{T}^3. \quad (3.2.18)$$

We thus infer the first upper bound

$$\begin{aligned} \int_{\mathbb{T}^3} \langle \nabla_x \partial_x^\alpha \tilde{\mathbf{c}}, \partial_x^\alpha \mathbf{V}_{\tilde{U}} \rangle dx &\leq -\lambda_A \left( \min_{1 \leq i \leq N} \bar{c}_i - \varepsilon \|\tilde{\mathbf{c}}\|_{H_x^s} \right) \left\| \partial_x^\alpha \tilde{\mathbf{U}} \right\|_{L_x^2}^2 \\ &\quad + \varepsilon N^2 \mu_A \left( 4C_0 + 6s\varepsilon \|\tilde{\mathbf{c}}\|_{H_x^s} \right) \|\tilde{\mathbf{c}}\|_{H_x^s} \left\| \tilde{\mathbf{U}} \right\|_{H_x^s}^2. \end{aligned} \quad (3.2.19)$$

The second and third term on the right-hand side of (3.2.15) are handled more easily. As we did for deriving (3.2.17), we apply the Leibniz derivation rule and the Cauchy-Schwarz inequality, together with the Sobolev embedding that allows to distribute the  $H_x^s$  norm to each factor of the products. In this way we obtain the estimates

$$\begin{aligned} \int_{\mathbb{T}^3} \langle \nabla_x \partial_x^\alpha \tilde{\mathbf{c}}, \partial_x^\alpha (\tilde{\mathbf{c}}\bar{\mathbf{u}}) \rangle_{\bar{\mathbf{c}}^{-1}} dx &\leq \frac{1}{\min_{1 \leq i \leq N} \bar{c}_i} \|\nabla_x \partial_x^\alpha \tilde{\mathbf{c}}\|_{L_x^2} \|\tilde{\mathbf{c}}\|_{H_x^s} \|\bar{\mathbf{u}}\|_{H_x^s}, \\ \int_{\mathbb{T}^3} \langle \nabla_x \partial_x^\alpha \tilde{\mathbf{c}}, \partial_x^\alpha (\tilde{\mathbf{c}}\mathbf{V}_{\tilde{U}}) \rangle_{\bar{\mathbf{c}}^{-1}} dx &\leq \frac{1}{\min_{1 \leq i \leq N} \bar{c}_i} \|\nabla_x \partial_x^\alpha \tilde{\mathbf{c}}\|_{L_x^2} \|\tilde{\mathbf{c}}\|_{H_x^s} \left( 1 + \frac{1}{C_0} \|\mathbf{c}\|_{H_x^s} \right) \|\tilde{\mathbf{U}}\|_{H_x^s}, \end{aligned}$$

where we have used that  $\frac{1}{\bar{c}_i} \leq \frac{1}{\min_i \bar{c}_i}$  for any  $1 \leq i \leq N$ . In order to control the  $L_x^2$  norm of  $\nabla_x \partial_x^\alpha \tilde{\mathbf{c}}$ , we exploit the gradient relation (3.2.13). By similar computations to the ones providing the estimate of Lemma 3.2.9, and thanks to the continuous Sobolev embedding  $H_x^{s/2} \hookrightarrow L_x^\infty$ , one infers

$$\begin{aligned} \|\nabla_x \partial_x^\alpha \tilde{\mathbf{c}}\|_{L_x^2} &\leq \|\nabla_x \tilde{\mathbf{c}}\|_{H_x^s} = \left\| A(\mathbf{c}) \tilde{\mathbf{U}} \right\|_{H_x^s} \\ &\leq (s^2 + C_0 s) \|\mathbf{c}\|_{H_x^s}^2 \left\| \tilde{\mathbf{U}} \right\|_{H_x^s} \\ &\leq 2(s^2 + C_0 s) \left( C_0^2 |\mathbb{T}^3| + \varepsilon^2 \|\tilde{\mathbf{c}}\|_{H_x^s}^2 \right) \left\| \tilde{\mathbf{U}} \right\|_{H_x^s} \\ &\leq C_s \left( 1 + \varepsilon^2 \|\tilde{\mathbf{c}}\|_{H_x^s}^2 \right) \left\| \tilde{\mathbf{U}} \right\|_{H_x^s}, \end{aligned} \quad (3.2.20)$$

where we have also used that

$$\begin{aligned} \int_{\mathbb{T}^3} (\bar{c}_i + \varepsilon \tilde{c}_i)^2 dx &\leq 2 \left( \int_{\mathbb{T}^3} \bar{c}_i^2 dx + \varepsilon^2 \int_{\mathbb{T}^3} \tilde{c}_i^2 dx \right), \\ 0 \leq \bar{c}_i &\leq \sum_{j=1}^N \bar{c}_j = C_0. \end{aligned}$$

Thanks to the same arguments one also controls the term  $1 + \frac{1}{C_0} \|\mathbf{c}\|_{H_x^s}$ , so that, since  $\varepsilon \leq 1$ , we finally deduce the upper bounds

$$\int_{\mathbb{T}^3} \langle \nabla_x \partial_x^\alpha \tilde{\mathbf{c}}, \partial_x^\alpha (\tilde{\mathbf{c}}\bar{\mathbf{u}}) \rangle_{\bar{\mathbf{c}}^{-1}} dx \leq \frac{C_s}{\min_{1 \leq i \leq N} \bar{c}_i} \|\tilde{\mathbf{c}}\|_{H_x^s} \left( 1 + \|\tilde{\mathbf{c}}\|_{H_x^s}^2 \right) \|\bar{\mathbf{u}}\|_{H_x^s} \|\tilde{\mathbf{U}}\|_{H_x^s}, \quad (3.2.21)$$

$$\int_{\mathbb{T}^3} \langle \nabla_x \partial_x^\alpha \tilde{\mathbf{c}}, \partial_x^\alpha (\tilde{\mathbf{c}}\mathbf{V}_{\tilde{U}}) \rangle_{\bar{\mathbf{c}}^{-1}} dx \leq \frac{C_s}{\min_{1 \leq i \leq N} \bar{c}_i} \|\tilde{\mathbf{c}}\|_{H_x^s} \left( 1 + \|\tilde{\mathbf{c}}\|_{H_x^s} \right)^3 \|\tilde{\mathbf{U}}\|_{H_x^s}^2, \quad (3.2.22)$$

by increasing the constant  $C_s$  if necessary.

To conclude, we gather (3.2.15) with the estimates (3.2.19), (3.2.21) and (3.2.22), and we sum over all  $|\alpha| \leq s$ . In this way, we obtain

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}^2 &\leq \frac{s^3 C_s}{\min_{1 \leq i \leq N} \bar{c}_i} \|\tilde{\mathbf{c}}\|_{H_x^s} \left(1 + \|\tilde{\mathbf{c}}\|_{H_x^s}^2\right) \|\bar{\mathbf{u}}\|_{H_x^s} \|\tilde{\mathbf{U}}\|_{H_x^s} \\ &\quad - \|\tilde{\mathbf{U}}\|_{H_x^s}^2 \left[ \lambda_A \min_{1 \leq i \leq N} \bar{c}_i - \varepsilon \|\tilde{\mathbf{c}}\|_{H_x^s} \left( \lambda_A + 4N^2 \mu_A C_0 s^3 \right. \right. \\ &\quad \left. \left. + 6N^2 \mu_A s^4 \|\tilde{\mathbf{c}}\|_{H_x^s} + \frac{s^3 C_s}{\min_{1 \leq i \leq N} \bar{c}_i} \left(1 + \|\tilde{\mathbf{c}}\|_{H_x^s}\right)^3 \right) \right]. \end{aligned}$$

In order to close the estimate above, since  $\bar{\mathbf{c}}$  is constant we first easily check that

$$\|\tilde{\mathbf{c}}\|_{H_x^s} \leq \max_{1 \leq i \leq N} \bar{c}_i \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})} \leq C_0 \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}.$$

Moreover, recalling Lemma 3.2.11, we can apply the Poincaré inequality to  $\tilde{\mathbf{c}}$ , which has zero mean on the torus. Denoting  $C_{\mathbb{T}^3} > 0$  the Poincaré constant, we can thus compute

$$\|\tilde{\mathbf{c}}\|_{H_x^s} \leq C_{\mathbb{T}^3} \|\nabla_x \tilde{\mathbf{c}}\|_{H_x^s} \leq C_{\mathbb{T}^3} C_s \left(1 + \varepsilon^2 \|\tilde{\mathbf{c}}\|_{H_x^s}^2\right) \|\tilde{\mathbf{U}}\|_{H_x^s}, \quad (3.2.23)$$

where we have also used (3.2.20).

Thanks to the above estimates, we can consequently infer the validity of the bound

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}^2 &\leq - \left[ \lambda_A \min_{1 \leq i \leq N} \bar{c}_i - \frac{s^3 C_{\mathbb{T}^3} C_s^2}{\min_{1 \leq i \leq N} \bar{c}_i} \left(1 + C_0 \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}\right)^4 \|\bar{\mathbf{u}}\|_{H_x^s} \right. \\ &\quad \left. - C_0 \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})} \left( \lambda_A + 6N^2 \mu_A C_0 s^4 \left(1 + \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}\right) \right) \right. \\ &\quad \left. - \frac{s^3 C_0 C_s}{\min_{1 \leq i \leq N} \bar{c}_i} \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})} \left(1 + C_0 \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}\right)^3 \right] \|\tilde{\mathbf{U}}\|_{H_x^s}^2 \\ &\leq - \left[ \lambda_A \min_{1 \leq i \leq N} \bar{c}_i - C_s \|\bar{\mathbf{u}}\|_{H_x^s} \left(1 + \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}\right)^4 \right. \\ &\quad \left. - C_s \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})} \left(1 + \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}\right)^3 \right] \|\tilde{\mathbf{U}}\|_{H_x^s}^2, \end{aligned}$$

where  $C_s > 0$  is fixed big enough in order to bound all the previous constants, and only depends on  $s$ ,  $N$ ,  $\lambda_A$ ,  $\mu_A$  and  $\bar{\mathbf{c}}$ . Therefore, if  $\|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s} \leq \delta_s$  and  $\|\bar{\mathbf{u}}\|_{H_x^s} \leq \delta_s$  for almost every  $t \geq 0$ , where  $\delta_s > 0$  is chosen such that

$$C_s \delta_s \left( (1 + \delta_s)^4 + (1 + \delta_s)^3 \right) \leq \frac{\lambda_A \min_{1 \leq i \leq N} \bar{c}_i}{2}, \quad (3.2.24)$$

we ensure that the  $H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})$  norm of  $\tilde{\mathbf{c}}$  keeps diminishing and satisfies

$$\frac{d}{dt} \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}^2 \leq - \frac{\lambda_A \min_{1 \leq i \leq N} \bar{c}_i}{2} \|\tilde{\mathbf{U}}\|_{H_x^s}^2 \quad \text{for a.e. } t \geq 0. \quad (3.2.25)$$

Moreover, since the Poincaré inequality (3.2.23) tells us that the norm of  $\tilde{\mathbf{U}}$  controls the one of  $\tilde{\mathbf{c}}$ , we recover the estimate

$$\frac{d}{dt} \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}^2 \leq -\frac{\lambda_A \min_{1 \leq i \leq N} \bar{c}_i}{2C_{\mathbb{T}^3}^2 C_s^2 (1 + \delta_s^2)^2} \|\tilde{\mathbf{c}}\|_{H_x^s}^2 \leq -\frac{\lambda_A \left( \min_{1 \leq i \leq N} \bar{c}_i \right)^2}{2C_{\mathbb{T}^3}^2 C_s^2 (1 + \delta_s^2)^2} \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}^2.$$

Setting

$$\lambda_s = \frac{\lambda_A \left( \min_{1 \leq i \leq N} \bar{c}_i \right)^2}{4C_{\mathbb{T}^3}^2 C_s^2 (1 + \delta_s^2)^2}, \quad (3.2.26)$$

Grönwall's lemma finally tells us that for almost every  $t \geq 0$

$$\|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})} \leq e^{-\lambda_s t} \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})},$$

and we also recover

$$\left\| \tilde{\mathbf{U}} \right\|_{H_x^{s-1}} = \|A(\mathbf{c})^{-1} \nabla_x \tilde{\mathbf{c}}\|_{H_x^{s-1}} \leq \tilde{C}_s \|\nabla_x \tilde{\mathbf{c}}\|_{H_x^{s-1}} \leq \tilde{C}_s \|\tilde{\mathbf{c}}\|_{H_x^s} \leq C_s \|\tilde{\mathbf{c}}\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})}, \quad (3.2.27)$$

by simply adjusting the value of  $C_s$ . The constant  $C_s = C_s(C_0, \lambda_A, \mu_A, s, \delta_s, \bar{\mathbf{c}}) > 0$  is obtained by inverting  $A(\mathbf{c})$  and repeating the previous computations, *via* the continuous Sobolev embedding previously mentioned. In particular, note that, for our choice of  $\delta_s$ , one sees from (3.2.18) that  $\mathbf{c}$  does not vanish anywhere and there is therefore no singularity in  $A(\mathbf{c})^{-1}$ .

This concludes the proof. □

Before going into details in the proofs of existence and uniqueness, we present here another result which establishes that the positivity of  $\mathbf{c}$  is obtained *a priori*. This will help the reader in clarifying the last statement we gave in the previous proof, about the invertibility of  $A(\mathbf{c})$ . Moreover, note that ensuring the positivity of  $\mathbf{c}$  *a priori* is crucial, since it will leave us free on the choice of the iterative scheme to be used in the next section in order to construct the solution of the system (3.2.12)–(3.2.13).

**Lemma 3.2.13.** *Consider an initial datum  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{U}}^{\text{in}})$  satisfying the assumptions of Theorem 3.2.6. If  $(\tilde{\mathbf{c}}, \tilde{\mathbf{U}})$  is a solution of (3.2.12)–(3.2.13) with initial datum  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{U}}^{\text{in}})$ , then, for almost every  $(t, x) \in \mathbb{R}_+ \times \mathbb{T}^3$  the vector  $\bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}(t, x)$  is positive.*

*Proof.* The proof is rather simple. Since we start from a positive initial datum  $\bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}^{\text{in}}$ , by inverting the gradient relation (3.2.13) as

$$\tilde{\mathbf{U}} = \frac{1}{\varepsilon} A(\mathbf{c})^{-1} \nabla_x \mathbf{c},$$

and plugging this identity into (3.2.12), we recover an elliptic equation for  $\mathbf{c} = \bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}$ . Standard elliptic weak minimum principles then apply to  $\mathbf{c}$ , ensuring its nonnegativity at least until a maximal finite time which we call  $T_0$ . But the previous *a priori* estimate obtained on  $\tilde{\mathbf{c}}$  tells us that in fact the positivity of  $\mathbf{c}$  is satisfied as long as  $\delta_s$  is also chosen in (3.2.18) to be strictly smaller than  $\min_{1 \leq i \leq N} \bar{c}_i$ . This guarantees that  $T_0 = +\infty$  and thus  $\mathbf{c}(t, x)$  is positive almost everywhere on  $\mathbb{R}_+ \times \mathbb{T}^3$ . □

**Step 4 – Existence and uniqueness of the couple  $(\tilde{\mathbf{c}}, \tilde{\mathbf{U}})$ .** We now have all the tools needed in order to construct our Cauchy theory for the couple  $(\tilde{\mathbf{c}}, \tilde{\mathbf{U}})$ . We shall first present the existence result and then prove the uniqueness of the constructed solution.

**Proposition 3.2.14.** *Let  $s > 3$  be an integer and consider a triple  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{U}}^{\text{in}}, \bar{u})$  which satisfies the assumptions of Theorem 3.2.6. There exists  $\delta_s > 0$  such that, for all  $\varepsilon \in (0, 1]$ , there exists a global weak solution  $(\tilde{\mathbf{c}}, \tilde{\mathbf{U}}) \in L^\infty(\mathbb{R}_+; H^s(\mathbb{T}^3)) \times L^\infty(\mathbb{R}_+; H^{s-1}(\mathbb{T}^3))$  of the system (3.2.12)–(3.2.13), with initial datum  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{U}}^{\text{in}})$ .*

*Proof.* The proof is standard and is based on an iterative scheme, where we first construct a solution on a well-chosen time interval  $[0, T_0]$ , and we then show that this interval can be extended to  $[0, +\infty)$ . Note however that one has to be careful with the estimates, since the conservation of the exact exponential decay rate is crucial. The underlying mechanism lies on the fact that our problem is actually quasilinear parabolic for small initial data. Indeed, noticing that

$$\tilde{\mathbf{U}} = A(\mathbf{c})^{-1} \nabla_x \tilde{\mathbf{c}},$$

we solely have to solve

$$\begin{aligned} \partial_t \tilde{\mathbf{c}} + \bar{\mathbf{c}} \nabla_x \cdot \left( A(\mathbf{c})^{-1} \nabla_x \tilde{\mathbf{c}} - \frac{\langle \mathbf{c}, A(\mathbf{c})^{-1} \nabla_x \tilde{\mathbf{c}} \rangle}{\langle \mathbf{c}, \mathbf{1} \rangle} \mathbf{1} \right) + \bar{u} \cdot \nabla_x \tilde{\mathbf{c}} \\ + \varepsilon \nabla_x \cdot \left( \tilde{\mathbf{c}} \left( A(\mathbf{c})^{-1} \nabla_x \tilde{\mathbf{c}} - \frac{\langle \mathbf{c}, A(\mathbf{c})^{-1} \nabla_x \tilde{\mathbf{c}} \rangle}{\langle \mathbf{c}, \mathbf{1} \rangle} \mathbf{1} \right) \right) = 0. \end{aligned}$$

From Lemma 3.2.10 we see that the higher order term is of order 2, symmetric and negative for  $\mathbf{c} > 0$ , which makes this equation quasilinear parabolic.

We initially set

$$\tilde{\mathbf{c}}^{(0)} = \tilde{\mathbf{c}}^{\text{in}}, \quad T_0 = 3 \frac{C_{\mathbb{T}^3} \min_{1 \leq i \leq N} \bar{c}_i}{4C_0 C_s (1 + 4\delta_s^2) \delta_s}, \quad (3.2.28)$$

where  $\delta_s$  and  $C_s$  respectively come from (3.2.24) and (3.2.27).

Suppose that an  $N$ -vector function  $\tilde{\mathbf{c}}^{(n)} \in L^\infty(0, T_0; H^s(\mathbb{T}^3))$  is given, satisfying

$$\left\| \tilde{\mathbf{c}}^{(n)} \right\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})} \leq 2\delta_s e^{-\lambda_s t}, \quad \sum_{i=1}^N \tilde{c}_i^{(n)}(t, x) = 0, \quad \text{a.e. on } (0, T_0) \times \mathbb{T}^3. \quad (3.2.29)$$

For  $s > 3$ , the Sobolev embedding  $H_x^s \hookrightarrow L_x^\infty$  makes applicable standard parabolic methods on the torus (see for instance [87, Section 7.1]) which raise the existence of a solution  $\tilde{\mathbf{c}}^{(n+1)} \in L^2(0, T_0; H^1(\mathbb{T}^3))$  to the following linear equation

$$\begin{aligned} \partial_t \tilde{\mathbf{c}}^{(n+1)} + \bar{u} \cdot \nabla_x \tilde{\mathbf{c}}^{(n)} \\ + \nabla_x \cdot \left( \mathbf{c}^{(n)} \left( A(\mathbf{c}^{(n)})^{-1} \nabla_x \tilde{\mathbf{c}}^{(n+1)} - \frac{\langle \mathbf{c}^{(n)}, A(\mathbf{c}^{(n)})^{-1} \nabla_x \tilde{\mathbf{c}}^{(n+1)} \rangle}{\langle \mathbf{c}^{(n)}, \mathbf{1} \rangle} \mathbf{1} \right) \right) = 0, \quad (3.2.30) \end{aligned}$$

with initial datum  $\tilde{\mathbf{c}}^{\text{in}}$ . Note that summing (3.2.30) over  $1 \leq i \leq N$  yields

$$\sum_{i=1}^N \tilde{c}_i^{(n+1)}(t, x) = \sum_{i=1}^N \tilde{c}_i^{(n+1)}(0, x) = 0 \quad \text{a.e. on } (0, T_0) \times \mathbb{T}^3$$

which shows, thanks to Lemma 3.2.10, that  $(\text{Span}(\mathbf{1}))^\perp$  is stable for (3.2.30), implying that  $A(\mathbf{c}^{(n)})^{-1} \nabla_x \tilde{\mathbf{c}}^{(n+1)}$  is well-defined at almost every time.

The same computations carried out to derive the *a priori* estimates in Proposition 3.2.12 give (see in particular (3.2.21) for the term containing  $\bar{u}$ )

$$\begin{aligned} & \frac{d}{dt} \left\| \tilde{\mathbf{c}}^{(n+1)} \right\|_{H_x^s(\bar{c}^{-\frac{1}{2}})}^2 \\ & \leq - \left( C_{\mathbb{T}^3} \min_{1 \leq i \leq N} \bar{c}_i \right) \left( \frac{2\lambda_A}{C_{\mathbb{T}^3}^2 C_s^2 (1 + \delta_s^2)^2} + C_s (1 + 4\varepsilon^2 \delta_s^2) \|\bar{u}\|_{H_x^s} \right) \left\| \nabla_x \tilde{\mathbf{c}}^{(n+1)} \right\|_{H_x^s}^2 \\ & \quad + C_s (1 + 4\varepsilon^2 \delta_s^2) \left\| \nabla_x \tilde{\mathbf{c}}^{(n+1)} \right\|_{H_x^s} \|\bar{u}\|_{H_x^s} \left\| \tilde{\mathbf{c}}^{(n)} \right\|_{H_x^s(\bar{c}^{-\frac{1}{2}})}, \end{aligned}$$

where we used that  $\|\tilde{\mathbf{c}}^{(n)}\|_{H_x^s} \leq 2\delta_s$ . Note that  $C_s(1 + \varepsilon^2 \delta_s^2) \|\bar{u}\|_{H_x^s}$  inside the negative term directly comes from the absence of  $\nabla_x \cdot (\tilde{\mathbf{c}}^{(n+1)} \bar{\mathbf{u}})$  in (3.2.30), whereas the multiplicative constant in front of it originates from the definition of  $\lambda_s$ . We now use Young's inequality to get

$$\begin{aligned} & \frac{d}{dt} \left\| \tilde{\mathbf{c}}^{(n+1)} \right\|_{H_x^s(\bar{c}^{-\frac{1}{2}})}^2 \\ & \leq - \left( C_{\mathbb{T}^3} \min_{1 \leq i \leq N} \bar{c}_i \right) \left( \frac{2\lambda_s}{\left( \min_{1 \leq i \leq N} \bar{c}_i \right)^2} + C_s (1 + 4\varepsilon^2 \delta_s^2) \|\bar{u}\|_{H_x^s} - \frac{\eta}{C_{\mathbb{T}^3} \min_{1 \leq i \leq N} \bar{c}_i} \right) \left\| \nabla_x \tilde{\mathbf{c}}^{(n+1)} \right\|_{H_x^s}^2 \\ & \quad + \frac{C_s^2 (1 + 4\varepsilon^2 \delta_s^2)^2 \|\bar{u}\|_{H_x^s}^2}{\eta} \left\| \tilde{\mathbf{c}}^{(n)} \right\|_{H_x^s}^2, \end{aligned}$$

for any  $\eta > 0$ . Therefore, if we choose

$$\eta = C_s (1 + 4\varepsilon^2 \delta_s^2) \|\bar{u}\|_{H_x^s} C_{\mathbb{T}^3} \min_{1 \leq i \leq N} \bar{c}_i,$$

thanks to Poincaré inequality (3.2.23) and to the assumption  $\|\bar{u}\|_{H_x^s} \leq \delta_s$ , we obtain

$$\frac{d}{dt} \left\| \tilde{\mathbf{c}}^{(n+1)} \right\|_{H_x^s(\bar{c}^{-\frac{1}{2}})}^2 \leq -2\lambda_s \left\| \tilde{\mathbf{c}}^{(n+1)} \right\|_{H_x^s(\bar{c}^{-\frac{1}{2}})}^2 + \frac{C_0 C_s (1 + 4\delta_s^2) \delta_s}{C_{\mathbb{T}^3} \min_{1 \leq i \leq N} \bar{c}_i} \left\| \tilde{\mathbf{c}}^{(n)} \right\|_{H_x^s(\bar{c}^{-\frac{1}{2}})}^2.$$

Eventually, we apply Grönwall's lemma using the exponential decay of  $\left\| \tilde{\mathbf{c}}^{(n)} \right\|_{H_x^s(\bar{c}^{-\frac{1}{2}})}^2$  given by the iterative assumption (3.2.29), and we successively get, for almost every  $t \in (0, T_0)$ ,

$$\begin{aligned} \left\| \tilde{\mathbf{c}}^{(n+1)} \right\|_{H_x^s(\bar{c}^{-\frac{1}{2}})}^2 & \leq \left( \left\| \tilde{\mathbf{c}}^{\text{in}} \right\|_{H_x^s(\bar{c}^{-\frac{1}{2}})}^2 + 4\delta_s^2 \frac{C_0 C_s (1 + 4\delta_s^2) \delta_s}{C_{\mathbb{T}^3} \min_{1 \leq i \leq N} \bar{c}_i} t \right) e^{-2\lambda_s t} \\ & \leq \delta_s^2 \left( 1 + 4 \frac{C_0 C_s (1 + 4\delta_s^2) \delta_s}{C_{\mathbb{T}^3} \min_{1 \leq i \leq N} \bar{c}_i} T_0 \right) e^{-2\lambda_s t} \\ & \leq 4\delta_s^2 e^{-2\lambda_s t}, \end{aligned}$$

thanks to the definition of  $T_0$  given in (3.2.28). This proves that  $\tilde{\mathbf{c}}^{(n+1)} \in L^\infty(0, T_0; H^s(\mathbb{T}^3))$  and satisfies the iterative assumptions (3.2.29).

By induction, we therefore construct a sequence  $(\tilde{\mathbf{c}}^{(n)})_{n \in \mathbb{N}}$  defined a.e. on  $(0, T_0) \times \mathbb{T}^3$ , belonging to  $(\text{Span}(\mathbf{1}))^\perp$  and bounded by  $2\delta_s$  in  $L^\infty(0, T_0; H^s(\mathbb{T}^3))$ . Moreover, the iterative equation (3.2.30) gives an explicit formula for  $\partial_t \tilde{\mathbf{c}}^{(n+1)}$  in terms of  $\tilde{\mathbf{c}}^{(n)}$ ,  $\tilde{\mathbf{c}}^{(n+1)}$  and  $\bar{u}$ . Again, the continuous Sobolev embedding  $H_x^{s/2} \hookrightarrow L_x^\infty$  for  $s > 3$  and Lemma 3.2.10 raise the existence of a polynomial  $P$  in two variables, with coefficients only depending on the constants  $s$ ,  $\bar{\mathbf{c}}$ ,  $\|\bar{u}\|_{H_x^s}$ ,  $\lambda_A$  and  $\mu_A$ , such that

$$\left\| \partial_t \tilde{\mathbf{c}}^{(n+1)} \right\|_{L_x^2} \leq P \left( \|\tilde{\mathbf{c}}^{(n)}\|_{H_x^s}, \|\tilde{\mathbf{c}}^{(n+1)}\|_{H_x^s} \right) \leq P(2\delta_s, 2\delta_s) \quad \text{for a.e. } t \in (0, T_0).$$

This shows that  $(\partial_t \tilde{\mathbf{c}}^{(n)})_{n \in \mathbb{N}}$  is bounded in  $L^\infty(0, T_0; L^2(\mathbb{T}^3))$ , uniformly with respect to  $n \in \mathbb{N}$ .

Therefore, choosing  $0 < s' < s - 2$ , by Sobolev embeddings there exists an  $N$ -vector function  $\tilde{\mathbf{c}}^\infty \in L^\infty(0, T_0; H^s(\mathbb{T}^3))$  such that, up to a subsequence,

1.  $(\tilde{\mathbf{c}}^{(n)})_{n \in \mathbb{N}}$  converges weakly-\* in  $L^\infty(0, T_0)$  and weakly in  $H_x^s$  to  $\tilde{\mathbf{c}}^\infty$ ,
2.  $(\tilde{\mathbf{c}}^{(n)})_{n \in \mathbb{N}}$ ,  $(\nabla_x \tilde{\mathbf{c}}^{(n)})_{n \in \mathbb{N}}$  and  $(\nabla_x \nabla_x \tilde{\mathbf{c}}^{(n)})_{n \in \mathbb{N}}$  converge weakly-\* in  $L^\infty(0, T_0)$  and strongly in  $H_x^{s'}$ ,
3.  $(\partial_t \tilde{\mathbf{c}}^{(n)})_{n \in \mathbb{N}}$  converges weakly-\* in  $L^\infty(0, T_0)$  and weakly in  $L_x^2$ .

Integrating our scheme (3.2.30) against test functions, we can then pass to the limit as  $n$  goes to  $+\infty$  (the nonlinear terms being bounded and dealt with thanks to the strong convergences in  $H_x^{s'}$ ) and we see that  $\tilde{\mathbf{c}}^\infty$  is a weak solution to

$$\begin{aligned} \partial_t \tilde{\mathbf{c}}^\infty + \bar{\mathbf{c}} \nabla_x \cdot \left( A(\mathbf{c}^\infty)^{-1} \nabla_x \tilde{\mathbf{c}}^\infty - \frac{\langle \mathbf{c}^\infty, A(\mathbf{c}^\infty)^{-1} \nabla_x \tilde{\mathbf{c}}^\infty \rangle}{\langle \mathbf{c}^\infty, \mathbf{1} \rangle} \mathbf{1} \right) + \bar{u} \cdot \nabla_x \tilde{\mathbf{c}}^\infty \\ + \varepsilon \nabla_x \cdot \left( \tilde{\mathbf{c}}^\infty \left( A(\mathbf{c}^\infty)^{-1} \nabla_x \tilde{\mathbf{c}}^\infty - \frac{\langle \mathbf{c}^\infty, A(\mathbf{c}^\infty)^{-1} \nabla_x \tilde{\mathbf{c}}^\infty \rangle}{\langle \mathbf{c}^\infty, \mathbf{1} \rangle} \mathbf{1} \right) \right) = 0. \end{aligned}$$

Denoting  $\tilde{\mathbf{U}}^\infty = A(\mathbf{c}^\infty)^{-1} \nabla_x \tilde{\mathbf{c}}^\infty$ , this proves that  $(\tilde{\mathbf{c}}^\infty, \tilde{\mathbf{U}}^\infty)$  is a weak solution to the system (3.2.12)–(3.2.13), which belongs to  $L^\infty(0, T_0; H^s(\mathbb{T}^3)) \times L^\infty(0, T_0; H^{s-1}(\mathbb{T}^3))$ . In particular, looking at equations (3.2.12)–(3.2.13), by means of the continuous embedding of  $H_x^{s/2}$  in  $L_x^\infty$  one easily checks that  $(\partial_t \tilde{\mathbf{c}}^\infty, \partial_t \tilde{\mathbf{U}}^\infty) \in L^\infty(0, T_0; L^2(\mathbb{T}^3)) \times L^\infty(0, T_0; L^2(\mathbb{T}^3))$  as soon as  $s > 4$ . Applying the Aubin-Lions-Simon theorem (see for example [42, Theorem II.5.16]), we thus also ensure that  $(\tilde{\mathbf{c}}^\infty, \tilde{\mathbf{U}}^\infty) \in C^0([0, T_0]; H^{s-1}(\mathbb{T}^3)) \times C^0([0, T_0]; H^{s-2}(\mathbb{T}^3))$  for any  $s > 4$ .

Therefore, using the continuity of  $\tilde{\mathbf{c}}^\infty$ , we can finally conclude thanks to the *a priori* estimates established in Proposition 3.2.12, which state that  $\|\tilde{\mathbf{c}}^\infty(T_0)\|_{H_x^s(\bar{\mathbf{c}}^{-\frac{1}{2}})} \leq \delta_s$ . Indeed, we can restart our scheme at  $T_0$  from this initial condition and we can obtain a solution on the time interval  $[T_0, 2T_0]$ . Again, using the continuity of  $\tilde{\mathbf{c}}^\infty$  with respect to  $t \in [T_0, 2T_0]$  and Proposition 3.2.12, the corresponding sequence will be bounded by  $\delta_s$  at  $2T_0$ , and by induction we can construct a weak solution of (3.2.12)–(3.2.13) on  $[0, +\infty)$ .  $\square$

In the next result we finally recover the uniqueness of the solution to the orthogonal system (3.2.12)–(3.2.13). We remind the reader that this property has to be understood in a perturbative sense, since we are only able to prove the uniqueness of the fluctuations  $(\tilde{\mathbf{c}}, \tilde{\mathbf{U}})$  around the macroscopic equilibrium state  $(\bar{\mathbf{c}}, \mathbf{0})$ .

**Proposition 3.2.15.** *Let  $s > 3$  be an integer, and consider a couple  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{U}}^{\text{in}})$  satisfying the assumptions of Theorem 3.2.6. There exists  $\delta_s > 0$  such that, if  $(\tilde{\mathbf{c}}, \tilde{\mathbf{U}})$  and  $(\tilde{\mathbf{d}}, \tilde{\mathbf{W}})$  are two solutions of (3.2.12)–(3.2.13) having the same initial datum  $(\tilde{\mathbf{c}}^{\text{in}}, \tilde{\mathbf{U}}^{\text{in}})$ , then  $\tilde{\mathbf{c}} = \tilde{\mathbf{d}}$  and  $\tilde{\mathbf{U}} = \tilde{\mathbf{W}}$ .*

*Proof.* Subtracting the two sets of equations satisfied by  $(\tilde{\mathbf{c}}, \tilde{\mathbf{U}})$  and  $(\tilde{\mathbf{d}}, \tilde{\mathbf{W}})$ , and denoting  $\tilde{\mathbf{h}} = \tilde{\mathbf{c}} - \tilde{\mathbf{d}}$  and  $\tilde{\mathbf{R}} = \tilde{\mathbf{U}} - \tilde{\mathbf{W}}$ , we initially establish the relations

$$\partial_t \tilde{\mathbf{h}} + \bar{\mathbf{c}} \nabla_x \cdot \mathbf{V}_{\tilde{\mathbf{R}}} + \bar{u} \cdot \nabla_x \tilde{\mathbf{h}} + \varepsilon \nabla_x \cdot (\tilde{\mathbf{h}} \mathbf{V}_{\tilde{\mathbf{U}}}) + \varepsilon \nabla_x \cdot (\tilde{\mathbf{d}} \mathbf{V}_{\tilde{\mathbf{R}}}) = 0, \quad (3.2.31)$$

$$\nabla_x \tilde{\mathbf{h}} = A(\mathbf{c}) \tilde{\mathbf{R}} + [A(\mathbf{c}) - A(\mathbf{d})] \tilde{\mathbf{W}}, \quad (3.2.32)$$

with an obvious meaning for the shorthand  $\mathbf{V}_{\tilde{\mathbf{R}}}$ .

We shall give similar computations to the ones derived for the *a priori* estimates, except that we here restrict our investigation to the sole  $L_x^2$  setting, since it will prove itself to be sufficient in order to deduce uniqueness. However, we still need the solutions to be in  $H_x^s$  for some  $s > 3$ , in order to again take advantage of the Sobolev embedding  $H_x^{s/2} \hookrightarrow L_x^\infty$ . We compute the scalar product between  $\bar{\mathbf{c}}^{-1} \tilde{\mathbf{h}}$  and the equation (3.2.31), and we integrate over the torus. As in the proof of Proposition 3.2.12, we use the gradient equation (3.2.32) and its orthogonal properties to recover

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\tilde{\mathbf{h}}\|_{L_x^2(\bar{\mathbf{c}}^{-\frac{1}{2}})}^2 &\leq \int_{\mathbb{T}^3} \langle A(\mathbf{c}) \tilde{\mathbf{R}}, \tilde{\mathbf{R}} \rangle dx + \int_{\mathbb{T}^3} \langle [A(\mathbf{c}) - A(\mathbf{d})] \tilde{\mathbf{W}}, \tilde{\mathbf{R}} \rangle_{\bar{\mathbf{c}}^{-1}} dx \\ &\quad + \int_{\mathbb{T}^3} \langle \nabla_x \tilde{\mathbf{h}}, \tilde{\mathbf{h}} (\bar{\mathbf{u}} + \varepsilon \mathbf{V}_{\tilde{\mathbf{R}}}) \rangle_{\bar{\mathbf{c}}^{-1}} dx + \varepsilon \int_{\mathbb{T}^3} \langle \nabla_x \tilde{\mathbf{h}}, \tilde{\mathbf{d}} \mathbf{V}_{\tilde{\mathbf{R}}} \rangle_{\bar{\mathbf{c}}^{-1}} dx. \end{aligned}$$

We use the spectral gap of  $A(\mathbf{c})$  for the first term on the right-hand side, while the remaining terms are dealt with thanks to the *a priori* estimates derived in Proposition 3.2.12 and the usual Sobolev embedding, in the following way:

$$|\tilde{\mathbf{c}}(t, x)| \leq \|\mathbf{c}\|_{H_x^s} \leq \delta_s, \quad |\bar{u}(t, x)| \leq \delta_s, \quad |\tilde{\mathbf{d}}(t, x)| \leq \delta_s, \quad \text{a.e. on } \mathbb{R}_+ \times \mathbb{T}^3.$$

This initially gives

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\tilde{\mathbf{h}}\|_{L_x^2(\bar{\mathbf{c}}^{-\frac{1}{2}})}^2 &\leq -\frac{\lambda_A}{2} \|\tilde{\mathbf{R}}\|_{L_x^2}^2 + \frac{\sum_{1 \leq i, j \leq N} \int_{\mathbb{T}^3} |\tilde{R}_i| |c_i c_j - d_i d_j| |\tilde{W}_j - \tilde{W}_i| dx}{\min_{1 \leq i \leq N} \bar{c}_i \min_{1 \leq i, j \leq N} \Delta_{ij}} \\ &\quad \left[ \delta_s + \varepsilon \delta_s \left( 1 + \frac{N \delta_s^2}{C_0} \right) \right] \|\tilde{\mathbf{h}}\|_{L_x^2} \|\nabla_x \tilde{\mathbf{h}}\|_{L_x^2} + \varepsilon \delta_s \|\nabla_x \tilde{\mathbf{h}}\|_{L_x^2} \|\tilde{\mathbf{R}}\|_{L_x^2}. \end{aligned} \quad (3.2.33)$$

Then, the algebraic manipulation

$$|c_i c_j - d_i d_j| = \left| \frac{1}{2} (c_i - d_i) (c_j + d_j) + \frac{1}{2} (c_i + d_i) (c_j - d_j) \right| \leq \varepsilon \frac{\delta_s}{2} (|h_i| + |h_j|),$$

and Cauchy-Schwarz inequality yield the control

$$\sum_{1 \leq i, j \leq N} \int_{\mathbb{T}^3} |\tilde{R}_i| |c_i c_j - d_i d_j| |\tilde{W}_j - \tilde{W}_i| dx \leq 2\varepsilon \delta_s^2 \|\tilde{\mathbf{R}}\|_{L_x^2} \|\tilde{\mathbf{h}}\|_{L_x^2}. \quad (3.2.34)$$



From the gradient relation (3.2.32) and from Poincaré inequality (3.2.23), we also deduce the existence of a constant  $C_s > 0$  such that

$$\left\| \tilde{\mathbf{R}} \right\|_{L_x^2} \geq C_s \left\| \nabla_x \tilde{\mathbf{h}} \right\| - \varepsilon \delta_s^2 \left\| \tilde{\mathbf{h}} \right\|_{L_x^2} \geq (C_s - \varepsilon \delta_s^2) \left\| \tilde{\mathbf{h}} \right\|_{L_x^2}. \quad (3.2.35)$$

We now use (3.2.34), (3.2.35) and the fact that  $0 < \varepsilon \leq 1$  inside (3.2.33) to finally infer the upper bound

$$\frac{1}{2} \frac{d}{dt} \left\| \tilde{\mathbf{h}} \right\|_{L_x^2(\bar{c}^{-\frac{1}{2}})}^2 \leq \left( -\frac{\lambda_A}{2} + \delta_s K(\delta_s) \right) \left\| \tilde{\mathbf{R}} \right\|_{L_x^2}^2$$

where  $K(\delta_s) > 0$  is a polynomial in  $\delta_s$  whose coefficients only depend on  $\bar{c}$  and the number of species  $N$ . By choosing  $\delta_s$  small enough so that both Proposition 3.2.12 holds and the inequality  $-\frac{\lambda_A}{2} + \delta_s K(\delta_s) \leq 0$  is satisfied, we conclude that  $\left\| \tilde{\mathbf{h}} \right\|_{L_x^2(\bar{c}^{-\frac{1}{2}})}$  decreases with time. Therefore, since initially  $\tilde{\mathbf{h}}^{\text{in}} = 0$ , we deduce that  $\tilde{\mathbf{h}} = 0$  at any time  $t \geq 0$ .

This implies that  $\tilde{\mathbf{c}} = \tilde{\mathbf{d}}$ , from which we also deduce that the gradient relation (3.2.32) becomes

$$A(\mathbf{c})\tilde{\mathbf{R}} = 0.$$

We thus infer that  $\tilde{\mathbf{R}} = 0$ , since  $\tilde{\mathbf{R}} \in (\ker A)^\perp$ . Consequently,  $\tilde{\mathbf{U}} = \tilde{\mathbf{V}}$ , and the uniqueness is established.  $\square$

**Step 5 – Conclusion.** We are finally able to conclude our study of the incompressible Maxwell-Stefan system (3.2.3)–(3.2.5).

Theorem 3.2.6 is a direct gathering of Proposition 3.2.12, Lemmata 3.2.11 and 3.2.13, and Propositions 3.2.14–3.2.15.

Our main Theorem 3.2.1 then directly follows from Theorem 3.2.6 with the unique orthogonal writing (3.2.7) established in Proposition 3.2.3. In fact, as soon as the unique solution  $(\bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}, \bar{\mathbf{u}} + \varepsilon \tilde{\mathbf{U}})$  of the orthogonal system (3.2.12)–(3.2.13) is established, the corresponding unique perturbative solution of the Maxwell-Stefan system (3.2.3)–(3.2.4) with incompressibility condition (3.2.5) is given by  $(\bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}, \bar{\mathbf{u}} + \varepsilon \tilde{\mathbf{u}})$ , where

$$\tilde{\mathbf{u}} = \tilde{\mathbf{U}} - \frac{1}{C_0} \langle \mathbf{c}, \tilde{\mathbf{U}} \rangle \mathbf{1}$$

satisfies  $\langle \mathbf{c}, \tilde{\mathbf{u}} \rangle = 0$ . In particular, the exponential decay of  $\tilde{\mathbf{u}}$  follows directly from the exponential decays of  $\tilde{\mathbf{c}}$  and  $\tilde{\mathbf{U}}$ .

### 3.3 Perturbative Cauchy theory for the Boltzmann multi-species equation

In this section we establish a Cauchy theory for the Boltzmann multi-species equation (3.1.11), perturbed around the local Maxwellian state (3.1.10). In view of the crucial importance of the choice of  $\mathbf{M}^\varepsilon$ , before starting our analysis let us fix in a more precise way its specific form.

Recall that we can select as unique global equilibrium of the mixture the global Maxwellian state  $\boldsymbol{\mu}$  defined by (3.1.5), where  $u_\infty = 0$  and  $\theta_\infty = 1$  are chosen in order to enlighten the computations. Thanks to the Cauchy theory built up in the previous section for the Maxwell-Stefan system, we can choose the macroscopic equilibrium state  $(\bar{c}_i, \bar{u})_{1 \leq i \leq N}$  to be compatible with the global (kinetic) equilibrium of the mixture  $\boldsymbol{\mu}$ , by taking  $\bar{c}_i = c_{i,\infty}$  for any  $1 \leq i \leq N$ . Therefore, supposing the uniform (in space) and constant (in time)

temperature  $\theta$  to be equal to 1 for simplicity, we introduce the local Maxwellian vector  $\mathbf{M}^\varepsilon = \mathbf{M}_{(\mathbf{c}, \varepsilon \mathbf{u}, \mathbf{1})} = (M_1^\varepsilon, \dots, M_N^\varepsilon)$ , given for any  $1 \leq i \leq N$  by

$$M_i^\varepsilon(t, x, v) = c_i(t, x) \left( \frac{m_i}{2\pi} \right)^{3/2} \exp \left\{ -m_i \frac{|v - \varepsilon u_i(t, x)|^2}{2} \right\}, \quad t \geq 0, x \in \mathbb{T}^3, v \in \mathbb{R}^3, \quad (3.3.1)$$

where  $(\mathbf{c}, \mathbf{u})$  is the unique weak solution of the Maxwell-Stefan system (3.1.7)–(3.1.9), perturbed around the macroscopic equilibrium state  $(\mathbf{c}_\infty, \bar{\mathbf{u}})$ . More precisely, the fluid quantities of  $\mathbf{M}^\varepsilon$  take the form

$$\begin{cases} c_i(t, x) = c_{i,\infty} + \varepsilon \tilde{c}_i(t, x), \\ u_i(t, x) = \bar{u}_i(t, x) + \varepsilon \tilde{u}_i(t, x), \quad \nabla_x \cdot \bar{\mathbf{u}}(t, x) = 0, \end{cases} \quad t \geq 0, x \in \mathbb{T}^3, \quad (3.3.2)$$

for any  $1 \leq i \leq N$ . In particular, we notice that under the assumptions of Theorem 3.2.1 the following fundamental properties are verified by the couple  $(\mathbf{c}_\infty + \varepsilon \tilde{\mathbf{c}}, \bar{\mathbf{u}} + \varepsilon \tilde{\mathbf{u}})$ :

$$(1) \quad \min_{1 \leq i \leq N} (c_{i,\infty} + \varepsilon \tilde{c}_i(t, x)) > 0 \quad \text{a.e. on } \mathbb{R}_+ \times \mathbb{T}^3,$$

$$(2) \quad \langle \mathbf{c}_\infty + \varepsilon \tilde{\mathbf{c}}(t, x), \mathbf{1} \rangle = C_0 > 0 \quad \text{a.e. on } \mathbb{R}_+ \times \mathbb{T}^3,$$

$$(3) \quad \|\tilde{\mathbf{c}}\|_{L_t^\infty H_x^s(\mathbf{c}_\infty^{-\frac{1}{2}})} \leq \delta_{\text{MS}},$$

$$(4) \quad \|\bar{\mathbf{u}}\|_{L_t^\infty H_x^s} \leq \delta_{\text{MS}} \quad \text{and} \quad \|\tilde{\mathbf{u}}\|_{L_t^\infty H_x^s} \leq \delta_{\text{MS}} C_{\text{MS}}.$$

Starting from this choice of the local Maxwellian, we consider solutions to the Boltzmann multi-species equation (3.1.6) of the form  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}$ , where the fluctuations  $\mathbf{f}$  satisfy the perturbed system (3.1.11). In this section we prove global existence, uniqueness and uniform (with respect to  $\varepsilon$ ) *a priori* estimates for the perturbations  $\mathbf{f}$ , providing a rigorous derivation of the Maxwell-Stefan system (3.1.7)–(3.1.9) in the limit  $\varepsilon \rightarrow 0$  of the perturbed Boltzmann equation (3.1.11).

### 3.3.1 Statement of the result

Our strategy is inspired by the works [161, 43] and aims at building a suitable Sobolev-equivalent norm which satisfies a Grönwall-type inequality among solutions of (3.1.11). The idea of the method originates from the hypocoercive behaviour shown by some classical kinetic equations in the mono-species framework, where the interaction of a degenerate coercive operator with a conservative operator may induce global dissipation in all variables, and consequently relaxation towards equilibrium. A typical example is precisely the inhomogeneous Boltzmann mono-species equation. In fact, the mono-species Boltzmann operator  $L$  linearized around a global equilibrium of the gaz exhibits a spectral gap which translates into a negative return in some Hilbert space depending on the sole velocity variable  $v$ . In particular,  $L$  is degenerate in the sense that its kernel is much larger than the set of global equilibria. Here, precisely comes into play the effect of the conservative transport operator  $v \cdot \nabla_x$ , that introduces a dependence on the space variable  $x$  which at first sight cannot be handled using the dissipation of  $L$  in  $v$ . Nevertheless, it is possible to prove [193, 161] that the association of these operators can actually produce a global negative return in both  $x$  and  $v$ , if one considers a well-designed Lyapunov functional that

is able to transfer the dissipation of  $L$  into a (hypo) dissipation of  $T = L - v \cdot \nabla_x$ . One possibility is for example to introduce [161] a modified Sobolev norm where we add to the usual  $H_{x,v}^s$  norm, new suitable terms based on commutators of higher derivatives, such as the well-known  $[v \cdot \nabla_x, \nabla_v] = -\nabla_x$ . In this way, the linear part is dealt with, and the full nonlinear Boltzmann equation (close to equilibrium) can be tackled [161] and its solution can be proved to relax towards a global equilibrium, with an exponential decay rate of convergence.

As already mentioned in the introduction, a similar strategy has been developed in [43] for the study of the hydrodynamic limit of the Boltzmann mono-species equation set under a standard diffusive scaling, leading to the same conclusions as [161]. Note however that such an extension was far from being obvious, since in this case the presence of the scaling parameter  $\varepsilon$  influences the choice for the correct Lyapunov functional. In particular, Briant has shown in [43] that a global dissipation can be obtained if one introduces a new Sobolev norm which is adapted from the one used in [161], by adding a dependence on  $\varepsilon$  in its terms. In such a way, the operator  $T^\varepsilon = \varepsilon^{-2}L - \varepsilon^{-1}v \cdot \nabla_x$  exhibits the required hypocoercive behaviour, which provides a control on the nonlinear stiff term  $\varepsilon^{-1}Q$  and allows to ensure a global negative return in both  $x$  and  $v$ , and the expected convergence to equilibrium for the solution.

Based on these initial considerations, our idea is simple. In the multi-species setting we consider here, even if the linearization around the non-equilibrium Maxwellian  $\mathbf{M}^\varepsilon$  gives rise to a linearized Boltzmann equation (3.1.11) involving the new operators  $\mathbf{L}^\varepsilon$  and  $\mathbf{S}^\varepsilon$ , we wish to prove that the underlying hypocoercive structure of our model is in fact almost formally identical to the one featured by the mono-species equation studied in [43]. Therefore, our point of view has a clear major advantage: once this analogy has been established, all the results obtained in [43] (in particular, existence and uniqueness of the solution) could be identically extended to our model.

The approach that will guide our presentation from now on will consist in adapting the tools and computations developed in [43], in order to study equation (3.1.11). However, we stress the fact that this is not a straightforward extension. Indeed, we have seen in Chapter 2 that already a full spectral gap property for  $\mathbf{L}^\varepsilon$  is missing when we settle our analysis in an Hilbert space weighted by the global equilibrium  $\boldsymbol{\mu}$ , which is incompatible with the operator  $\mathbf{L}^\varepsilon$ , linearized around the local Maxwellian  $\mathbf{M}^\varepsilon$ . In particular, we recall that we see the appearance of an extra positive term of order  $\varepsilon$ , which contains the projected part  $\pi_{\mathbf{L}}(\mathbf{f})$  and precisely takes into account this incompatibility. It is therefore fundamental to ensure that this loss in the spectral gap (as soon as it remains at a lower order in  $\varepsilon$ ) does not affect too much the computations derived in [43] and that  $\mathbf{L}^\varepsilon$  can still provide a complete negative return in combination with the transport operator  $v \cdot \nabla_x$ . This feature is indeed characteristic of our model and will appear any time the linearized operator  $\mathbf{L}^\varepsilon$  (and more specifically its higher derivatives in  $x$ ) is involved. It is at this point that the specific form of the fluid quantities (3.3.2) prominently comes into play in order to gain a lower order factor in  $\varepsilon$  or in  $\delta_{\text{MS}}$ . In particular, we underline the importance of having  $\delta_{\text{MS}}$  as a free parameter of the problem, since its choice shall be crucial in order to obtain a careful control on some of the extra terms produced by  $\mathbf{L}^\varepsilon$ , where the presence of the factor  $\varepsilon$  will not be enough to close the estimates as in [43]. Finally, we remind the reader the additional difficulties caused by the source term  $\mathbf{S}^\varepsilon$ , which displays an intricate dependence on the local Maxwellian  $\mathbf{M}^\varepsilon$ , and is at first glance of order  $\mathcal{O}(\varepsilon^{-3})$ . Again, the particular form of the solution  $(\mathbf{c}, \mathbf{u})$  is at the core of our derivation of the correct estimates to control  $\mathbf{S}^\varepsilon$ , and the perturbative setting we consider for the Maxwell-Stefan system will prove itself sufficient in order to handle the negative powers of  $\varepsilon$ .

Following [43], we begin by choosing the three basic tools needed in the analysis: the functional spaces, the hypocoercive operator and the modified Sobolev norm.

**Choice of the functional spaces.** We have already remarked in Chapter 2 that  $\mathbf{L}^\varepsilon$  exhibits no clear self-adjointness in the usual space of linearization  $L^2((\mathbf{M}^\varepsilon)^{-\frac{1}{2}}, \mathbb{R}^3)$ , and we saw that the only way to recover a partial spectral gap property is to link  $\mathbf{L}^\varepsilon$  to the Boltzmann operator  $\mathbf{L}$ , linearized around the global equilibrium  $\boldsymbol{\mu}$ . This connection is obtained by choosing  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  as the space of interest. Therefore, in order to exploit the result of Chapter 2, from now on we set our study in the corresponding weighted Sobolev spaces  $H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , defined for any  $s \in \mathbb{N}$ .

**Choice of the hypocoercive operator.** Next, we must identify the dissipative and the conservative operators that play a central role in the theory of hypocoercivity. Since it is crucial to determine the explicit expression of the equilibria of the mixture,  $\mathbf{L}^\varepsilon$  is not a valuable choice as we possess no information about the shape of its kernel. Therefore, as in the mono-species case [161, 43], we select the hypocoercive operator of interest to be defined for any  $\varepsilon \in (0, 1]$  by  $\mathbf{T}^\varepsilon = \varepsilon^{-2}\mathbf{L} - \varepsilon^{-1}v \cdot \nabla_x$ , acting on  $H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ . In particular, recall that the dissipative operator  $\mathbf{L} = (L_1, \dots, L_N)$  is defined for any  $1 \leq i \leq N$  by

$$L_i(\mathbf{f}) = \sum_{j=1}^N \left( Q_{ij}(\mu_i, f_j) + Q_{ij}(f_i, \mu_j) \right),$$

and is a closed self-adjoint operator in the space  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ . Moreover, its kernel is described by an orthonormal basis  $(\boldsymbol{\phi}^{(k)})_{1 \leq k \leq N+4}$  in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , that is

$$\ker \mathbf{L} = \text{Span}(\boldsymbol{\phi}^{(1)}, \dots, \boldsymbol{\phi}^{(N+4)}),$$

where

$$\left\{ \begin{array}{l} \boldsymbol{\phi}^{(i)} = \frac{1}{\sqrt{c_{i,\infty}}} \mu_i (\delta_{ij})_{1 \leq j \leq N} = \frac{1}{\sqrt{c_{i,\infty}}} \mu_i \mathbf{e}^{(i)}, \quad 1 \leq i \leq N, \\ \boldsymbol{\phi}^{(N+\ell)} = \frac{v_\ell}{\left( \sum_{j=1}^N m_j c_{j,\infty} \right)^{1/2}} (m_i \mu_i)_{1 \leq i \leq N}, \quad 1 \leq \ell \leq 3, \\ \boldsymbol{\phi}^{(N+4)} = \frac{1}{\left( \sum_{j=1}^N c_{j,\infty} \right)^{1/2}} \left( \frac{m_i |v|^2 - 3}{\sqrt{6}} \mu_i \right)_{1 \leq i \leq N}. \end{array} \right.$$

In this way, we can write the orthogonal projection onto  $\ker \mathbf{L}$  in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  as

$$\pi_{\mathbf{L}}(\mathbf{f})(v) = \sum_{k=1}^{N+4} \langle \mathbf{f}, \boldsymbol{\phi}^{(k)} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \boldsymbol{\phi}^{(k)}(v), \quad \forall \mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}). \quad (3.3.3)$$

In particular, its explicit expression is given by

$$\begin{aligned} \pi_{\mathbf{L}}(\mathbf{f}) &= \sum_{i=1}^N \left[ \frac{1}{c_{i,\infty}} \int_{\mathbb{R}^3} f_i dv \right] \mu_i \mathbf{e}^{(i)} \\ &+ \sum_{k=1}^3 \frac{v_k}{\sum_{i=1}^N m_i c_{i,\infty}} \left[ \sum_{i=1}^N \int_{\mathbb{R}^3} m_i v_k f_i dv \right] (m_i \mu_i)_{1 \leq i \leq N} \\ &+ \frac{1}{\sum_{i=1}^N c_{i,\infty}} \left[ \sum_{i=1}^N \int_{\mathbb{R}^3} \frac{m_i |v|^2 - 3}{\sqrt{6}} f_i dv \right] \left( \frac{m_i |v|^2 - 3}{\sqrt{6}} \mu_i \right)_{1 \leq i \leq N}. \end{aligned} \quad (3.3.4)$$

**Choice of the norm.** With the aim of deriving similar *a priori* estimates to [43], we choose the same Sobolev-equivalent norm. For any  $s \in \mathbb{N}^*$  and any  $\varepsilon \in (0, 1]$ , we introduce the following functional, defined on the space  $H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  by

$$\|\cdot\|_{\mathcal{H}_\varepsilon^s} = \left[ \sum_{|\alpha| \leq s} a_\alpha^{(s)} \|\partial_x^\alpha \cdot\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \varepsilon \sum_{\substack{|\alpha| \leq s \\ k, \alpha_k > 0}} b_{\alpha,k}^{(s)} \langle \partial_x^\alpha \cdot, \partial_v^{e_k} \partial_x^{\alpha - e_k} \cdot \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} + \varepsilon^2 \sum_{\substack{|\alpha| + |\beta| \leq s \\ |\beta| \geq 1}} d_{\alpha,\beta}^{(s)} \|\partial_v^\beta \partial_x^\alpha \cdot\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right]^{1/2}, \quad (3.3.5)$$

for some positive constants  $(a_\alpha^{(s)})_\alpha^s$ ,  $(b_{\alpha,k}^{(s)})_{\alpha,k}^s$  and  $(d_{\alpha,\beta}^{(s)})_{\alpha,\beta}^s$  to be appropriately fixed later.

Thanks to these choices, we can now establish our main result.

**Theorem 3.3.1.** *Let the collision kernels  $B_{ij}$  satisfy assumptions (H1)–(H4), and consider the local Maxwellian  $\mathbf{M}^\varepsilon$  defined by (3.3.1)–(3.3.2). There exist  $s_0 \in \mathbb{N}^*$ ,  $\bar{\delta}_{MS} > 0$  and  $\varepsilon_0 \in (0, 1]$  such that the following statements hold for any integer  $s \geq s_0$ .*

- (1) *There exist three sets of positive constants  $(a_\alpha^{(s)})_\alpha^s$ ,  $(b_{\alpha,k}^{(s)})_{\alpha,k}^s$  and  $(d_{\alpha,\beta}^{(s)})_{\alpha,\beta}^s$  such that, for all  $\varepsilon \in (0, \varepsilon_0]$ , both following norms are equivalent*

$$\|\cdot\|_{\mathcal{H}_\varepsilon^s} \sim \left( \|\cdot\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \sum_{|\alpha| \leq s} \|\partial_x^\alpha \cdot\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \varepsilon^2 \sum_{\substack{|\alpha| + |\beta| \leq s \\ |\beta| \geq 1}} \|\partial_v^\beta \partial_x^\alpha \cdot\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right)^{1/2}.$$

- (2) *There exists  $\delta_B > 0$  such that, for all  $\varepsilon \in (0, \varepsilon_0]$ , for all  $\delta_{MS} \in [0, \bar{\delta}_{MS}]$  and for any initial datum  $\mathbf{f}^{\text{in}}$  in  $H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  with*

$$\|\mathbf{f}^{\text{in}}\|_{\mathcal{H}_\varepsilon^s} \leq \delta_B, \quad \|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq C \delta_{MS},$$

for some positive constant  $C > 0$  independent of the parameters  $\varepsilon$  and  $\delta_{MS}$ , there exists a unique  $\mathbf{f} \in C^0(\mathbb{R}_+; H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}))$  such that  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}$  is the unique weak solution of the Boltzmann multi-species equation (3.1.11). Moreover,

if  $\mathbf{F}^{\varepsilon, \text{in}} = \mathbf{M}^{\varepsilon, \text{in}} + \varepsilon \mathbf{f}^{\text{in}} \geq 0$ , then  $\mathbf{F}^\varepsilon(t, x, v) \geq 0$  for a.e.  $(t, x, v) \in \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ . Finally, for any time  $t \geq 0$ ,  $\mathbf{F}^\varepsilon$  satisfies the stability property

$$\|\mathbf{F}^\varepsilon - \mathbf{M}^\varepsilon\|_{\mathcal{H}_\varepsilon^s} \leq \varepsilon \delta_B, \quad \forall \varepsilon \in (0, \varepsilon_0].$$

The constant  $\delta_B$  is explicit and only depend on the number of species  $N$ , on the atomic masses  $(m_i)_{1 \leq i \leq N}$ , and on the cross sections  $(B_{ij})_{1 \leq i, j \leq N}$ . In particular, it is independent of the parameters  $\varepsilon$  and  $\delta_{MS}$ .

The rest of this section is devoted to proving our result. In the first part we present the hypocoercive properties satisfied by the Boltzmann operators  $\mathbf{L}^\varepsilon$  and  $\mathbf{Q}$ , which allow to connect our analysis to the formalism used in [161, 43]. In the second part we sketch the actual proof of Theorem 3.3.1. Dividing our procedure into several steps for a sake of clarity, we initially show how to derive suitable uniform (in  $\varepsilon$ ) bounds for the problematic source term  $\mathbf{S}^\varepsilon$ . We then list the *a priori* energy estimates that we are able to recover for any solution  $\mathbf{f}$  of (3.1.11). To conclude, we shall notice that our estimates actually coincide (up to lower orders in  $\varepsilon$  or in  $\delta_{MS}$ ) to the ones obtained in [43], and we can thus apply the same computations as in [43] to state existence and uniqueness of the fluctuations  $\mathbf{f}$ .

### 3.3.2 Hypocoercive formalism

In this first part, we want to investigate the hypocoercivity aspects of the perturbed multi-species Boltzmann equation, in terms of mathematical properties for  $\mathbf{L}^\varepsilon$  and  $\mathbf{Q}$ . The idea is to adapt the method developed by Mouhot and Neumann in [161]. More specifically, we want to generalize to the multi-species setting the results obtained in [43]. The initial step consists in verifying some structural properties on  $\mathbf{L}^\varepsilon$  and  $\mathbf{Q}$ , necessary to recover the basic *a priori* energy estimates that will be presented in the following part. We shall see that the extension of the method is absolutely nontrivial and many new issues come up in the analysis. For this reason, we choose to keep the same order of presentation of the technical assumptions adopted in [43]. This will allow us to enlighten the similarities and especially the main differences between our strategies.

Before stating our lemmata, we here provide a brief description of the main features of the linearized Boltzmann operator  $\mathbf{L}^\varepsilon$ . We recall that  $\mathbf{L}^\varepsilon$  can be written under the form

$$\mathbf{L}^\varepsilon = \mathbf{K}^\varepsilon - \boldsymbol{\nu}^\varepsilon,$$

where  $\mathbf{K}^\varepsilon = (K_1^\varepsilon, \dots, K_N^\varepsilon)$  is defined, for any  $1 \leq i \leq N$ , by

$$K_i^\varepsilon(\mathbf{f})(v) = \sum_{j=1}^N \int_{\mathbb{R}^3 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) (M_i^{\varepsilon'} f_j'^* + M_j^{\varepsilon' *} f_i' - M_i^\varepsilon f_j^*) dv_* d\sigma, \quad (3.3.6)$$

and  $\boldsymbol{\nu}^\varepsilon = (\nu_1^\varepsilon, \dots, \nu_N^\varepsilon)$  acts like a multiplicative operator, namely, for any  $1 \leq i \leq N$ ,

$$\nu_i^\varepsilon(\mathbf{f})(v) = \sum_{j=1}^N \nu_{ij}^\varepsilon(v) f_j(v),$$

$$\nu_{ij}^\varepsilon(v) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) M_j^\varepsilon(v_*) dv_* d\sigma, \quad \forall v \in \mathbb{R}^3. \quad (3.3.7)$$

**Remark 3.3.2.** Note that throughout this initial presentation we shall suppose that the solution  $(\mathbf{c}, \mathbf{u})$  of the Maxwell-Stefan system we consider is always smooth enough to perform all the estimates, as stated in Theorem 3.2.1. The required regularity will be fixed afterwards and will allow to apply all the results obtained in this section. As such, the quantities  $\min_i c_i > 0$ ,  $C_0 = \langle \mathbf{c}, \mathbf{1} \rangle$ ,  $\|\mathbf{c}\|_{L_t^\infty H_x^s(\mathbf{c}_\infty^{-\frac{1}{2}})}$  and  $\|\mathbf{u}\|_{L_t^\infty H_x^s}$  are considered as constants and we only keep their track when the explicit order of magnitude  $\mathcal{O}(\delta_{MS})$  is needed in order to close the energy estimates at the kinetic level. Also, each time a constant is written, it is independent of  $\varepsilon$ . This is only done for a sake of simplicity and clarity, but nevertheless each of these constants will be computed explicitly inside the proofs.

We begin with a lemma which establishes some general controls on  $\boldsymbol{\nu}^\varepsilon$  and  $\mathbf{L}^\varepsilon$  (stating in particular the coercivity of  $\boldsymbol{\nu}^\varepsilon$ ). The proof mimics the one obtained in the mono-species case and is thus straightforward.

**Lemma 3.3.3** (Estimates on  $\boldsymbol{\nu}^\varepsilon$  and  $\mathbf{L}^\varepsilon$ ). *For any  $\varepsilon \in (0, 1]$ , the linearized operator  $\mathbf{L}^\varepsilon$  and its multiplicative part  $\boldsymbol{\nu}^\varepsilon$  satisfy the following explicit bounds. There exist some explicit positive constants  $C_1^\nu$ ,  $C_2^\nu$  and  $C_1^L$  such that, for any  $\mathbf{f}, \mathbf{g} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , we have*

$$C_1^\nu \|\mathbf{f}\|_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq C_1^\nu \|\mathbf{f}\|_{L_v^2(\langle v \rangle^{\frac{1}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq \langle \boldsymbol{\nu}^\varepsilon(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq C_2^\nu \|\mathbf{f}\|_{L_v^2(\langle v \rangle^{\frac{1}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2, \quad (3.3.8)$$

$$\left| \langle \mathbf{L}^\varepsilon(\mathbf{f}), \mathbf{g} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \right| \leq C_1^L \|\mathbf{f}\|_{L_v^2(\langle v \rangle^{\frac{1}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \|\mathbf{g}\|_{L_v^2(\langle v \rangle^{\frac{1}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}. \quad (3.3.9)$$

The constant  $C_1^\nu$  in (3.3.8) translates into a coercivity property for  $\boldsymbol{\nu}^\varepsilon$ . Our next result shows that  $\boldsymbol{\nu}^\varepsilon$  also exhibits a defect of coercivity along its  $v$ -derivatives.

**Lemma 3.3.4** (Defect of coercivity for  $\partial_v^\beta \partial_x^\alpha \boldsymbol{\nu}^\varepsilon$ ). *For any  $s \in \mathbb{N}^*$ , and for all multi-indices  $\alpha, \beta$  such that  $|\alpha| + |\beta| = s$  and  $|\beta| \geq 1$ , there exist some positive constants  $C_k^\nu$ , with  $k \in \{3, \dots, 7\}$ , such that, for any  $\mathbf{f} \in H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ ,*

$$\begin{aligned} & \left\langle \partial_v^\beta \partial_x^\alpha \boldsymbol{\nu}^\varepsilon(\mathbf{f}), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \geq \\ & (C_3^\nu - \varepsilon \mathbf{1}_{\{|\alpha| \geq 1\}} C_4^\nu) \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{1}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ & - (C_5^\nu + \varepsilon \mathbf{1}_{\{|\alpha| \geq 1\}} C_6^\nu) \|\mathbf{f}\|_{H_{x,v}^{s-1}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ & - \varepsilon \mathbf{1}_{\{|\alpha| \geq 1\}} C_7^\nu \sum_{0 < |\alpha'| + |\beta'| \leq s-1} \left\| \partial_v^{\beta'} \partial_x^{\alpha'} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{1}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \end{aligned} \quad (3.3.10)$$

We here notice for the first time the main difference with the mono-species case treated in [43], where the Boltzmann equation is perturbed around a global equilibrium. Since the Maxwellian  $\mathbf{M}^\varepsilon$  we consider depends on the space variable, we see the appearance of several new terms in the estimates, coming precisely from the  $x$ -derivatives of  $\mathbf{M}^\varepsilon$ . Nevertheless, each of these correction terms is at a lower order in  $\varepsilon$  and they are thus likely to be controlled by the main terms, which correspond to the ones derived in [43].

Let us now turn to the analysis of  $\mathbf{K}^\varepsilon$ . Following again the strategy of Mouhot and Neumann [161], we want to prove that this operator exhibits a regularizing behaviour whenever we consider some  $v$ -derivatives. More precisely, we shall see that  $\partial_v^\beta \partial_x^\alpha \mathbf{K}^\varepsilon$  is controlled by a main term only depending on lower derivatives of  $\mathbf{f}$  plus a correction term (which can be made arbitrary small) involving the same order of derivatives  $\partial_v^\beta \partial_x^\alpha \mathbf{f}$ . We can think of this property as the counterpart of the defect of coercivity shown previously on  $\partial_v^\beta \partial_x^\alpha \boldsymbol{\nu}^\varepsilon$ , in the sense that the correction term appearing in the bound of  $\partial_v^\beta \partial_x^\alpha \mathbf{K}^\varepsilon$  will be controlled by the negative contribution coming from  $\partial_v^\beta \partial_x^\alpha \boldsymbol{\nu}^\varepsilon$ . The dependence of  $\mathbf{M}^\varepsilon$  on the space variable will again produce the appearance of some new extra terms associated to the  $x$ -derivatives of the local Maxwellian. As before, it is only a partial issue since these terms will come at a lower order in  $\varepsilon$ .

The study of  $\mathbf{K}^\varepsilon$  is much more complicated than the one needed for  $\boldsymbol{\nu}^\varepsilon$ . Indeed, in order to obtain a bound for its  $v$ -derivatives, we shall dive deeper into the structure of the operator, encountering two major issues. As an initial step in our investigation, we shall use the fact that  $\mathbf{K}^\varepsilon$  can be written under a kernel form. The first issue is that we also want to avoid any kind of estimate at this level and we thus need to recover a full explicit expression of the kernel, which is not just a simple extension of the mono-species case. This is done in Appendix B by deriving a precise Carleman representation of  $\mathbf{K}^\varepsilon$ , following the work of [45], with integration domains independent of the variable  $v$ . The second issue arises because the kernel operator strongly depends on  $|v - v_*|$  and we need to properly treat the  $v$ -derivatives in the small region where the relative velocity is close to zero. We solve the problem by simply changing the point of view. By means of a standard technique [105, 106], we introduce a new variable  $\eta = v - v_*$  and we observe that in this configuration  $(v, v_*) \mapsto (v, \eta)$  the kernel operator is actually smooth in the variable  $v$ , allowing to easily compute the derivative and close the estimates. This last step will in particular involve dealing with the different decay rates of the global equilibria  $\mu_i$ , but the analysis will follow exactly the same strategy used in Chapter 2.

**Lemma 3.3.5** (Mixing properties in velocity for  $\partial_v^\beta \partial_x^\alpha \mathbf{K}^\varepsilon$ ). *Let  $s \in \mathbb{N}^*$  and consider two multi-indices  $\alpha, \beta$  such that  $|\alpha| + |\beta| = s$  and  $|\beta| \geq 1$ . Then, for any  $\xi \in (0, 1)$ , there exist two constants  $C_1^\mathbf{K}(\xi), C_2^\mathbf{K} > 0$  such that, for all  $\mathbf{f} \in H_{x,v}^s(\boldsymbol{\mu}^{-\frac{1}{2}})$ ,*

$$\left\langle \partial_v^\beta \partial_x^\alpha \mathbf{K}^\varepsilon(\mathbf{f}), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq C_1^\mathbf{K}(\xi) \|\mathbf{f}\|_{H_{x,v}^{s-1}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \xi C_2^\mathbf{K} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (3.3.11)$$

The constants  $C_1^\mathbf{K}(\xi)$  and  $C_2^\mathbf{K}$  are explicit, and in particular  $C_2^\mathbf{K}$  does not depend on the parameter  $\xi$ .

The next crucial step in establishing a solid hypocoercivity framework is to determine whether  $\mathbf{L}^\varepsilon$  possesses a spectral gap in the space of interest  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ . This question is far from being obvious in the context of the multi-species Boltzmann equation, the main difficulties coming from the linearization of the Boltzmann operator around a non-equilibrium Maxwellian state  $\mathbf{M}^\varepsilon$ . The main issue is linked to the fact that  $\mathbf{L}^\varepsilon$  is not self-adjoint in this setting and thus all the tools from classical spectral theory, as well as methods from [65, 45], cannot be applied directly. Nevertheless, a partial answer to this problem has been already provided in Chapter 2, where we were able to recover a quantitative upper bound for the Dirichlet form of the linearized operator  $\mathbf{L}^\varepsilon$  in the space  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ . We recall that the idea is to look for a penalization of type  $\mathbf{L}^\varepsilon = \mathbf{L} + (\mathbf{L}^\varepsilon - \mathbf{L})$ , where  $\mathbf{L}$  is the Boltzmann operator linearized around the global equilibrium  $\boldsymbol{\mu}$ . Since  $\mathbf{L}$  is known to possess a spectral gap in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , it is then sufficient to prove that the penalization term can be controlled, too. In this way, the Dirichlet form of  $\mathbf{L}^\varepsilon$  can be upper bounded



by the usual spectral gap plus two correction terms of order  $\varepsilon$ . The first term gives the distance between the non-equilibrium Maxwellian  $\mathbf{M}^\varepsilon$  (of the linearization) and the global equilibrium  $\boldsymbol{\mu}$ , while the second one translates the fact that the spectral projection is taken with respect to the space of equilibria of  $\mathbf{L}$ , which does not correspond to the space of equilibria of  $\mathbf{L}^\varepsilon$ . We present a slightly different version of the estimate obtained in Chapter 2, since our study requires more control on the term accounting for the projection onto  $\ker \mathbf{L}$  (say a control of order  $\varepsilon^2$ ). The reason is that we need to handle the factor  $1/\varepsilon^2$  in front of  $\mathbf{L}^\varepsilon$ . In particular, we want to emphasize that the following statement is in fact an extension of Theorem 2.3.2 of Chapter 2, as we shall consider here the number of particles  $c_i(t, x) = c_{i,\infty} + \varepsilon \tilde{c}_i(t, x)$  of each species of the mixture to be dependent on time and space. The issue is that the spectral gap for  $\mathbf{L}$  recovered in [45] holds on the space  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , for constant numbers of particles  $c_{i,\infty}$ ,  $1 \leq i \leq N$ . To overcome this problem, we shall then split the operator  $\mathbf{L}^\varepsilon$  into a close-to-equilibrium part corresponding to  $c_{i,\infty}$  (satisfying Theorem 2.3.2) and a lower order term corresponding to  $\varepsilon \tilde{c}_i$ , which will be easily estimated. At last, we stress the fact that it is also crucial at this point to keep track of the quantity  $\delta_{\text{MS}}$  that uniformly bounds the  $L_x^\infty$  norms of  $\tilde{\mathbf{c}}$  and  $\mathbf{u}$ . Indeed, in what follows we shall eventually need the freedom in the choice of  $\delta_{\text{MS}}$ , in order to take it small enough to close the *a priori* estimates and recover the correct negative return in the Sobolev norm  $\|\cdot\|_{\mathcal{H}_\varepsilon^s}$ .

**Lemma 3.3.6** (Local coercivity of  $\mathbf{L}^\varepsilon$ ). *Let the collision kernels  $B_{ij}$  satisfy assumptions (H1)–(H4), and let  $\lambda_{\mathbf{L}} > 0$  be the spectral gap in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  of the operator  $\mathbf{L}$ . There exists an explicit constant  $C_2^{\mathbf{L}} > 0$  such that, for all  $\varepsilon \in (0, 1]$  and for any  $\eta_1 > 0$ , the operator  $\mathbf{L}^\varepsilon$  satisfies the following estimate. For any  $\mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$*

$$\begin{aligned} \langle \mathbf{L}^\varepsilon(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} &\leq -\left(\lambda_{\mathbf{L}} - (\varepsilon + \eta_1)C_2^{\mathbf{L}}\right) \|\mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \varepsilon^2 \delta_{\text{MS}} \frac{C_2^{\mathbf{L}}}{\eta_1} \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2, \end{aligned} \quad (3.3.12)$$

where  $\pi_{\mathbf{L}}$  is the orthogonal projection onto  $\ker \mathbf{L}$  in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , and we recall that  $\delta_{\text{MS}} > 0$  can be chosen as small as desired from Theorem 3.2.1.

We now turn to the study of the full nonlinear Boltzmann operator  $\mathbf{Q}$ . Basically, we recover for  $\mathbf{Q}$  the equivalent property that was needed in [43] to handle the mono-species Boltzmann operator. We also include in this result a well-known and fundamental feature of both  $\mathbf{L}^\varepsilon$  and  $\mathbf{Q}$ : the orthogonality to  $\ker \mathbf{L}$ , the space of local equilibria of the mixture.

**Lemma 3.3.7** (Orthogonality to  $\ker \mathbf{L}$  and general controls on  $\mathbf{Q}$ ). *The linear operator  $\mathbf{L}^\varepsilon$  and the bilinear operator  $\mathbf{Q}$  are orthogonal to the kernel of  $\mathbf{L}$ , namely*

$$\pi_{\mathbf{L}}(\mathbf{L}^\varepsilon(\mathbf{f})) = \pi_{\mathbf{L}}(\mathbf{Q}(\mathbf{g}, \mathbf{h})) = 0, \quad \forall \mathbf{f}, \mathbf{g}, \mathbf{h} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}). \quad (3.3.13)$$

Moreover,  $\mathbf{Q}$  satisfies the following estimate. For any  $s \in \mathbb{N}$  and for all multi-indices  $\alpha, \beta$  such that  $|\alpha| + |\beta| = s$ , there exist two nonnegative functionals  $\mathcal{G}_x^s$  and  $\mathcal{G}_{x,v}^s$  satisfying  $\mathcal{G}_x^{s+1} \leq \mathcal{G}_x^s$ ,  $\mathcal{G}_{x,v}^{s+1} \leq \mathcal{G}_{x,v}^s$ , and such that

$$\left| \langle \partial_v^\beta \partial_x^\alpha \mathbf{Q}(\mathbf{g}, \mathbf{h}), \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \right| \leq \begin{cases} \mathcal{G}_x^s(\mathbf{g}, \mathbf{h}) \|\mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} & \text{if } |\beta| = 0, \\ \mathcal{G}_{x,v}^s(\mathbf{g}, \mathbf{h}) \|\mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} & \text{if } |\beta| \geq 1. \end{cases} \quad (3.3.14)$$

In particular, there exists  $s_0 \in \mathbb{N}^*$  such that, for any integer  $s \geq s_0$ , there exists an explicit constant  $C_s^{\mathbf{Q}} > 0$  verifying

$$\begin{aligned} \mathcal{G}_x^s(\mathbf{g}, \mathbf{h}) &\leq C_s^{\mathbf{Q}} \left( \|\mathbf{g}\|_{H_x^s L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \|\mathbf{h}\|_{H_x^s L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} + \|\mathbf{h}\|_{H_x^s L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \|\mathbf{g}\|_{H_x^s L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \right), \\ \mathcal{G}_{x,v}^s(\mathbf{g}, \mathbf{h}) &\leq C_s^{\mathbf{Q}} \left( \|\mathbf{g}\|_{H_{x,v}^s(\boldsymbol{\mu}^{-\frac{1}{2}})} \|\mathbf{h}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} + \|\mathbf{h}\|_{H_{x,v}^s(\boldsymbol{\mu}^{-\frac{1}{2}})} \|\mathbf{g}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \right). \end{aligned} \quad (3.3.15)$$

This last lemma completes the investigation of the hypocoercivity properties satisfied by our kinetic model. We can finally step forward to the actual proof of Theorem 3.3.1.

### 3.3.3 Proof of Theorem 3.3.1

The last part of this section contains the proof of Theorem 3.3.1. For the sake of clarity, we divide our presentation into several steps. We begin by studying the source term  $\mathbf{S}^\varepsilon$ , which constitutes the main novelty of this work. Its correct estimate can in fact be seen as the last feature in providing a satisfactory hypocoercive framework. We then present some basic properties of the macroscopic projector  $\pi_{\mathbf{L}}$  which is used in the next step in order to derive the *a priori* energy estimates satisfied by the perturbations  $\mathbf{f}$ . In the last step, we adapt the computations carried out in [43] to recover the conclusions of Theorem 3.3.1.

**Step 1 – Estimates on the source term  $\mathbf{S}^\varepsilon$ .** We here provide the study of the source term

$$\mathbf{S}^\varepsilon = \frac{1}{\varepsilon^3} \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon) - \frac{1}{\varepsilon} \partial_t \mathbf{M}^\varepsilon - \frac{1}{\varepsilon^2} v \cdot \nabla_x \mathbf{M}^\varepsilon.$$

This term gives the distance between the Maxwell-Stefan system and the fluid part of the Boltzmann equation, and it represents one of the main differences from the model considered in [43], and also one of the main drawbacks. In fact, since  $\mathbf{S}^\varepsilon$  strongly depends on inverse powers of  $\varepsilon$  and on  $\mathbf{M}^\varepsilon$  and its derivatives, it is crucial to determine its leading order of magnitude with respect to  $\varepsilon$  and to understand the role played by the macroscopic quantities  $\mathbf{c}$  and  $\mathbf{u}$ .

The idea at the basis of our analysis is simple. The Lyapunov functional (3.3.5) we chose is essentially made up of three terms: the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm which accounts for pure spatial derivatives and for mixed derivatives, and the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  scalar product which corresponds to a higher order commutator. In particular, as soon as one derivative in velocity is considered, the weights  $\varepsilon$  and  $\varepsilon^2$  are used in order to balance out the energy estimates by cancelling the stiffest terms. Therefore, when dealing with  $\mathbf{S}^\varepsilon$ , we just need to ensure that it can be uniformly bounded in the norm  $\|\cdot\|_{\mathcal{H}_\varepsilon^s}$ , or, in other words, that its highest order of magnitude does not exceed the control provided by the weights that appear in the modified Sobolev norm (3.3.5), *i.e.*  $(a_\alpha^{(s)})_\alpha^s$ ,  $(\varepsilon b_{\alpha,k}^{(s)})_{\alpha,k}^s$  and  $(\varepsilon^2 a_{\alpha,\beta}^{(s)})_{\alpha,\beta}^s$ .

With this idea in mind, we consider three cases, each referring to one of the three sums appearing in the Sobolev norm (3.3.5). Their investigation is similar and essentially based on the separated study of the linear part and of the nonlinear term  $\mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon)$ . On the one side, the linear part accounts for an order  $\varepsilon^{-1}$  since we can check that  $\nabla_x \mathbf{M}^\varepsilon = \mathcal{O}(\varepsilon)$ . On the other hand, we handle the nonlinear term by exploiting the form of  $\mathbf{u} = \bar{\mathbf{u}} + \varepsilon \tilde{\mathbf{u}}$ . More precisely, using the penalization method of Chapter 2, we show that  $\mathbf{M}^\varepsilon$  is close to a local equilibrium of the mixture (with common macroscopic velocity  $\varepsilon \bar{\mathbf{u}}$ ) up to an order  $\varepsilon^2$ ,

allowing to prove that  $\partial_v^\beta \partial_x^\alpha \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon) = \mathcal{O}(\varepsilon^2)$  for any multi-indices  $\alpha, \beta \geq 0$ . In such a way, we are able to deduce that the general leading order of the source term (and of its derivatives) is actually  $\mathcal{O}(\varepsilon^{-1})$ , which can be easily handled in the  $\mathcal{H}_\varepsilon^s$  norm by the factors  $\varepsilon$  and  $\varepsilon^2$ , as soon as one derivative in  $v$  is considered. Unfortunately, since  $x$ -derivatives are instead controlled by a mere factor of order 1, the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm of  $\partial_x^\alpha \mathbf{S}^\varepsilon$  could blow up at a rate of  $\mathcal{O}(\varepsilon^{-1})$ .

That is why we derive a more precise estimate for the source term, in the case where only  $x$ -derivatives are taken into account. In particular, the strategy consists in decomposing  $\partial_x^\alpha \mathbf{S}^\varepsilon$  into a fluid and a microscopic part as  $\partial_x^\alpha \mathbf{S}^\varepsilon = \pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{S}^\varepsilon) + \partial_x^\alpha \mathbf{S}^{\varepsilon\perp}$ , in order to show that the stiff terms are actually concentrated in the sole orthogonal component  $\partial_x^\alpha \mathbf{S}^{\varepsilon\perp}$ . Indeed, the fluid part can be handled thanks to the orthogonality of the Boltzmann operator to  $\ker \mathbf{L}$ , which allows one to get rid of the nonlinear term  $\varepsilon^{-3} \partial_x^\alpha \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon)$ . This, together with the fact that  $\mathbf{c}$  and  $\mathbf{u}$  satisfy the Maxwell-Stefan system (3.1.7)–(3.1.9), will be sufficient to prove that actually  $\pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{S}^\varepsilon) = \mathcal{O}(1)$ . Thanks to the previous considerations, we shall eventually recover the leading order  $\partial_x^\alpha \mathbf{S}^{\varepsilon\perp} = \mathcal{O}(\varepsilon^{-1})$ , but in this case it will no more constitute an issue since the spectral gap of  $\partial_x^\alpha \mathbf{L}^\varepsilon$  will provide the needed negative return.

For the sake of exhaustiveness, in the following result we separately state the three mentioned cases, even if the bounds which we obtain are quite similar in their structure. The deeper reason for their particular form will be clearer later on, during the derivation of the energy estimates.

**Lemma 3.3.8** (Estimates on  $\mathbf{S}^\varepsilon$ ). *Let  $s \in \mathbb{N}$  and  $\mathbf{f} \in H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , and consider two multi-indices  $\alpha, \beta$  such that  $|\alpha| + |\beta| = s$ . If  $|\beta| \geq 1$ , there exists a positive constant  $C_{\alpha,\beta}^{\mathbf{S}}$ , such that, for any  $\varepsilon \in (0, 1]$  and any  $\eta_2 > 0$ ,*

$$\left| \left\langle \partial_v^\beta \partial_x^\alpha \mathbf{S}^\varepsilon, \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \right| \leq \frac{\delta_{MS}^2 C_{\alpha,\beta}^{\mathbf{S}}}{\eta_2} + \frac{\eta_2}{\varepsilon^2} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{7}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (3.3.16)$$

*In particular, if  $\alpha_k > 0$  for some  $k \in \{1, 2, 3\}$  and  $\beta = e_k$ , there exists  $C_{\alpha,k}^{\mathbf{S}} > 0$  such that, for any  $\varepsilon \in (0, 1]$  and any  $\eta_3 > 0$ ,*

$$\left| \left\langle \partial_x^\alpha \mathbf{S}^\varepsilon, \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \right| \leq \frac{\delta_{MS}^2 C_{\alpha,k}^{\mathbf{S}}}{\varepsilon \eta_3} + \frac{\eta_3}{\varepsilon} \left\| \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{7}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (3.3.17)$$

*Finally, if  $|\beta| = 0$ , we ask for a stronger control on the projection  $\pi_{\mathbf{L}}(\mathbf{S}^\varepsilon)$ . There exists a positive constant  $C_\alpha^{\mathbf{S}}$  such that, for any  $\varepsilon \in (0, 1]$  and any  $\eta_4, \eta_5 > 0$ ,*

$$\left| \left\langle \partial_x^\alpha \mathbf{S}^\varepsilon, \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \right| \leq \frac{\delta_{MS}^2 C_\alpha^{\mathbf{S}}}{\eta_4 \eta_5} + \eta_4 \left\| \pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{f}) \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{\eta_5}{\varepsilon^2} \left\| \partial_x^\alpha \mathbf{f}^\perp \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{7}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (3.3.18)$$

*The constants  $C_{\alpha,\beta}^{\mathbf{S}}$ ,  $C_{\alpha,k}^{\mathbf{S}}$  and  $C_\alpha^{\mathbf{S}}$  are explicit and only depend on the physical parameters of the problem, and on polynomials in the variables  $\|\mathbf{c}\|_{L_t^\infty H_x^{|\alpha|+4}(\mathbf{c}_\infty^{-\frac{1}{2}})}$  and  $\|\mathbf{u}\|_{L_t^\infty H_x^{|\alpha|+4}}$ .*

*In particular, they are independent of  $\varepsilon$ .*

The proof of this result is technical and is thus provided at the end of the next section, together with the proofs of the hypocoercivity lemmata.

**Step 2 – Properties of the fluid projection  $\pi_{\mathbf{L}}$ .** The derivation of the *a priori* energy estimates finally requires a deeper understanding of the properties of the projectors  $\pi_{\mathbf{T}^\varepsilon}$

and  $\pi_{\mathbf{L}}$ . We present in this step three lemmata which are preliminary to our following study, the main one being a result establishing a fundamental Poincaré-type inequality satisfied by  $\pi_{\mathbf{L}}$ .

We begin by describing the structure of the hypocoercive operator  $\mathbf{T}^\varepsilon$ .

**Lemma 3.3.9.** *For any  $\varepsilon > 0$ , the operator  $\mathbf{T}^\varepsilon = \frac{1}{\varepsilon^2} \mathbf{L} - \frac{1}{\varepsilon} v \cdot \nabla_x$ , acting on  $H^1(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , satisfies  $\ker \mathbf{T}^\varepsilon = \ker \mathbf{L} \cap \ker v \cdot \nabla_x$ . Moreover, the associated projection  $\pi_{\mathbf{T}^\varepsilon}$  explicitly writes*

$$\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}) = \int_{\mathbb{T}^3} \pi_{\mathbf{L}}(\mathbf{f}) dx, \quad (3.3.19)$$

for any  $\mathbf{f} \in H^1(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ .

The proof of this lemma is very simple and is therefore omitted. It can be found for example as an initial remark in [45, Section 4].

Next, we present a very useful property of the projection  $\pi_{\mathbf{L}}$ , which is intensively used in what follows: the equivalence of the  $L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  and  $L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})$  norms on the space  $\ker \mathbf{L}$ .

**Lemma 3.3.10.** *There exists a positive explicit constant  $C_\pi$  such that*

$$\|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq C_\pi \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2, \quad (3.3.20)$$

for any  $\mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ .

*Proof.* Recalling the explicit expression of  $\pi_{\mathbf{L}}(\mathbf{f})$  from (3.3.3) by means of the orthonormal basis  $(\boldsymbol{\phi}^{(k)})_{1 \leq k \leq N+4}$  in  $L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , we can successively write

$$\begin{aligned} \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 &= \sum_{i=1}^N \int_{\mathbb{R}^3} \left| \sum_{k=1}^{N+4} \langle \mathbf{f}, \boldsymbol{\phi}^{(k)} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \phi_i^{(k)}(v) \right|^2 \langle v \rangle^\gamma \mu_i^{-1} dv \\ &= \sum_{k,\ell=1}^{N+4} \langle \mathbf{f}, \boldsymbol{\phi}^{(k)} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \langle \mathbf{f}, \boldsymbol{\phi}^{(\ell)} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \sum_{i=1}^N \int_{\mathbb{R}^3} \phi_i^{(k)} \phi_i^{(\ell)} \langle v \rangle^\gamma \mu_i^{-1} dv \\ &= \sum_{k,\ell=1}^{N+4} \langle \mathbf{f}, \boldsymbol{\phi}^{(k)} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \langle \mathbf{f}, \boldsymbol{\phi}^{(\ell)} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \langle \boldsymbol{\phi}^{(k)}, \boldsymbol{\phi}^{(\ell)} \rangle_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \\ &\leq \frac{1}{2} \max_{1 \leq k, \ell \leq N+4} \left| \langle \boldsymbol{\phi}^{(k)}, \boldsymbol{\phi}^{(\ell)} \rangle_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \right| \\ &\quad \times \sum_{k,\ell=1}^{N+4} \left( \langle \mathbf{f}, \boldsymbol{\phi}^{(k)} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \langle \mathbf{f}, \boldsymbol{\phi}^{(\ell)} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right) \\ &= (N+4) \max_{1 \leq k, \ell \leq N+4} \left| \langle \boldsymbol{\phi}^{(k)}, \boldsymbol{\phi}^{(\ell)} \rangle_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \right| \sum_{k=1}^{N+4} \langle \mathbf{f}, \boldsymbol{\phi}^{(k)} \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &= (N+4) \max_{1 \leq k, \ell \leq N+4} \left| \langle \boldsymbol{\phi}^{(k)}, \boldsymbol{\phi}^{(\ell)} \rangle_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \right| \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2, \end{aligned}$$

thanks to Parseval's identity.

In particular, the specific form of the elements of the orthonormal basis allows to easily show that  $\boldsymbol{\phi}^{(k)} \in L_v^2(\mathbb{R}^3, \langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})$  for any  $1 \leq k \leq N+4$ . Therefore, the maximum of the scalar products is a bounded quantity, and we can finally choose

$$C_\pi = (N+4) \max_{1 \leq k, \ell \leq N+4} \left| \langle \boldsymbol{\phi}^{(k)}, \boldsymbol{\phi}^{(\ell)} \rangle_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \right|$$

to infer the validity of (3.3.20).  $\square$

To conclude this preliminary step, we establish a Poincaré-type inequality for  $\pi_{\mathbf{L}}$  which represents a tool of crucial importance in order to apply the hypocoercive strategy of [161, 43]. Note however that, as opposed to the works in the mono-species setting, where the solution of the Boltzmann equation is perturbed around a global equilibrium, the linearization around  $\mathbf{M}^\varepsilon$  we perform here does not give access to a perfect Poincaré inequality. Indeed, the projection part  $\pi_{\mathbf{L}}(\mathbf{f})$  does not have zero mean on the torus because of the presence of the source term  $\mathbf{S}^\varepsilon$  in (3.1.11). We evade this obstacle by showing that a Poincaré inequality can still be recovered at a lower order, allowing the appearance of a small correction of order  $\mathcal{O}(\delta_{MS}^2)$ .

**Lemma 3.3.11.** *Let us denote with  $C_{\mathbb{T}^3}$  the Poincaré constant on the torus and let  $\delta_{MS} > 0$ . Consider a solution  $\mathbf{f} \in H^1(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  of the perturbed Boltzmann equation (3.1.11), satisfying initially*

$$\|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq C\delta_{MS},$$

for some constant  $C > 0$  independent of the parameters  $\varepsilon$  and  $\delta_{MS}$ . There exists a positive constant  $C^{\mathbf{T}}$  such that

$$\|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq 2C_{\mathbb{T}^3} \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \delta_{MS}^2 C^{\mathbf{T}}. \quad (3.3.21)$$

In particular,  $C^{\mathbf{T}}$  is explicit and does not depend on the parameter  $\varepsilon$ .

*Proof.* Pick a solution  $\mathbf{f} \in H^1(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  of (3.1.11). Recalling the relation (3.3.19) between the projectors, we observe that we can express  $\pi_{\mathbf{L}}(\mathbf{f})$  in terms of  $\pi_{\mathbf{T}^\varepsilon}(\mathbf{f})$ . Applying Poincaré inequality, we first obtain

$$\begin{aligned} \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &\leq 2 \left\| \pi_{\mathbf{L}}(\mathbf{f}) - \frac{1}{|\mathbb{T}^3|} \pi_{\mathbf{T}^\varepsilon}(\mathbf{f}) \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2}{|\mathbb{T}^3|^2} \|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\leq 2C_{\mathbb{T}^3} \|\nabla_x \pi_{\mathbf{L}}(\mathbf{f})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2}{|\mathbb{T}^3|^2} \|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2. \end{aligned} \quad (3.3.22)$$

Note that for the models in [161, 43], the authors are able to prove that  $\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}) = 0$ , starting from an initial datum satisfying  $\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}}) = 0$ . This is a peculiarity of the Boltzmann equation, which naturally preserves the action of the projection  $\pi_{\mathbf{T}^\varepsilon}$  on it. Clearly, in our case we do not have the same property, and in fact our aim is to show that actually the second term accounts for an order  $\mathcal{O}(\delta_{MS}^2)$ . To do this, we need to recover an equation for  $\pi_{\mathbf{T}^\varepsilon}(\mathbf{f})$ .

As mentioned, the idea is to apply the projector  $\pi_{\mathbf{T}^\varepsilon}$  to both sides of the Boltzmann equation (3.1.11). Using Lemma 3.3.9, thanks to the linearity of  $\pi_{\mathbf{T}^\varepsilon}$  and to the orthogonality of  $\mathbf{L}^\varepsilon$  and  $\mathbf{Q}$  to  $\ker \mathbf{L}$  given by (3.3.13), one can see that the transport terms and

the Boltzmann operators cancel out, so that we are left with the identity, holding a.e. on  $\mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ ,

$$\partial_t \pi_{\mathbf{T}^\varepsilon}(\mathbf{f}) = -\frac{1}{\varepsilon} \partial_t \pi_{\mathbf{T}^\varepsilon}(\mathbf{M}^\varepsilon),$$

where we have also used the fact that the projection operator commutes with the time derivative. In particular, integrating over  $[0, t]$  the above identity, we obtain the desired equation for  $\pi_{\mathbf{T}^\varepsilon}(\mathbf{f})$ , which reads

$$\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}) = \pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}}) - \frac{1}{\varepsilon} \pi_{\mathbf{T}^\varepsilon}(\mathbf{M}^\varepsilon - \mathbf{M}^{\varepsilon, \text{in}}). \quad (3.3.23)$$

Consequently, since  $\mathbf{M}^\varepsilon$  and  $\mathbf{M}^{\varepsilon, \text{in}}$  only depend on the macroscopic quantities  $(\mathbf{c}, \mathbf{u})$  and  $(\mathbf{c}^{\text{in}}, \mathbf{u}^{\text{in}})$ , using the relation (3.3.19) together with the formula (3.3.4) of the projection  $\pi_{\mathbf{L}}$ , it is possible to explicitly compute the value of  $\pi_{\mathbf{T}^\varepsilon}(\mathbf{M}^\varepsilon - \mathbf{M}^{\varepsilon, \text{in}})$ . It is first easy to check that, for any  $1 \leq i \leq N$ ,

$$\int_{\mathbb{R}^3} M_i^\varepsilon(t, x, v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = \begin{pmatrix} c_i(t, x) \\ \varepsilon c_i(t, x) u_i(t, x) \\ \frac{3}{m_i} c_i(t, x) + \varepsilon^2 c_i(t, x) |u_i(t, x)|^2 \end{pmatrix},$$

and the equivalent holds for  $\mathbf{M}^{\varepsilon, \text{in}}$ . It thus follows that

$$\begin{aligned} \pi_{\mathbf{T}^\varepsilon}(\mathbf{M}^\varepsilon - \mathbf{M}^{\varepsilon, \text{in}}) &= \int_{\mathbb{T}^3} \pi_{\mathbf{L}}(\mathbf{M}^\varepsilon - \mathbf{M}^{\varepsilon, \text{in}}) dx \\ &= \sum_{i=1}^N \left[ \frac{\varepsilon}{c_{i, \infty}} \int_{\mathbb{T}^3} (\tilde{c}_i(t, x) - \tilde{c}_i^{\text{in}}(x)) dx \right] \mu_i \mathbf{e}^{(i)} \\ &\quad + \frac{\varepsilon v}{\sum_{i=1}^N m_i c_{i, \infty}} \cdot \left[ \sum_{i=1}^N \int_{\mathbb{T}^3} m_i (c_i u_i - c_i^{\text{in}} u_i^{\text{in}}) dx \right] (m_i \mu_i)_{1 \leq i \leq N} \\ &\quad + \frac{\varepsilon^2}{\sqrt{6} \sum_{i=1}^N c_{i, \infty}} \left[ \sum_{i=1}^N \int_{\mathbb{T}^3} m_i (c_i |u_i|^2 - c_i^{\text{in}} |u_i^{\text{in}}|^2) dx \right] \left( \frac{m_i |v|^2 - 3}{\sqrt{6}} \mu_i \right)_{1 \leq i \leq N}. \end{aligned}$$

In particular, the couple  $(\mathbf{c}, \mathbf{u})$  is solution of the Maxwell-Stefan system (3.1.7)–(3.1.9), so that, from Lemma 3.2.11, one gets that the zeroth-order terms disappear, because both  $\tilde{c}_i$  and  $\tilde{c}_i^{\text{in}}$  have zero mean on the torus. Therefore, replacing the above identity in (3.3.23), we finally recover the expression of  $\pi_{\mathbf{T}^\varepsilon}(\mathbf{f})$ , which writes explicitly

$$\begin{aligned} \pi_{\mathbf{T}^\varepsilon}(\mathbf{f}) &= \pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}}) - \frac{v}{\sum_{i=1}^N m_i c_{i, \infty}} \cdot \left[ \sum_{i=1}^N \int_{\mathbb{T}^3} m_i (c_i u_i - c_i^{\text{in}} u_i^{\text{in}}) dx \right] (m_i \mu_i)_{1 \leq i \leq N} \\ &\quad - \frac{\varepsilon}{\sqrt{6} \sum_{i=1}^N c_{i, \infty}} \left[ \sum_{i=1}^N \int_{\mathbb{T}^3} m_i (c_i |u_i|^2 - c_i^{\text{in}} |u_i^{\text{in}}|^2) dx \right] \left( \frac{m_i |v|^2 - 3}{\sqrt{6}} \mu_i \right)_{1 \leq i \leq N}. \end{aligned}$$

Then, we can repeat the same computations used to derive the *a priori* estimates for the Maxwell-Stefan system, in order to bound the first and second order terms. In particular,

recalling the uniform controls obtained for  $\mathbf{c}$  and  $\mathbf{u}$  through the application of the continuous Sobolev embedding of  $H_x^{s/2}$  in  $L_x^\infty$  for  $s > 3$ , one easily infers the existence of a positive constant  $C^{\mathbf{T}}$  such that

$$\begin{aligned}
& \left| \frac{v}{\sum_{i=1}^N m_i c_{i,\infty}} \cdot \sum_{i=1}^N \int_{\mathbb{T}^3} m_i (c_i u_i - c_i^{\text{in}} u_i^{\text{in}}) dx \right| \\
& \leq |v| \frac{N |\mathbb{T}^3|}{C_0} \left( \max_{1 \leq i \leq N} m_i c_{i,\infty} \right) \\
& \quad \times \left( \|\mathbf{c}\|_{H_x^s(\mathbf{c}_\infty^{-\frac{1}{2}})} \|\mathbf{u}\|_{H_x^{s-1}} + \|\mathbf{c}^{\text{in}}\|_{H_x^s(\mathbf{c}_\infty^{-\frac{1}{2}})} \|\mathbf{u}^{\text{in}}\|_{H_x^{s-1}} \right) \\
& \leq C^{\mathbf{T}} |v| \left( 2 \|\mathbf{c}_\infty\|_{L_x^2(\mathbf{c}_\infty^{-\frac{1}{2}})} + \varepsilon \|\tilde{\mathbf{c}}\|_{H_x^s(\mathbf{c}_\infty^{-\frac{1}{2}})} + \varepsilon \|\tilde{\mathbf{c}}^{\text{in}}\|_{H_x^s(\mathbf{c}_\infty^{-\frac{1}{2}})} \right) \\
& \quad \times \left( 2 \|\bar{\mathbf{u}}\|_{H_x^{s-1}} + \varepsilon \|\tilde{\mathbf{u}}\|_{H_x^{s-1}} + \varepsilon \|\tilde{\mathbf{u}}^{\text{in}}\|_{H_x^{s-1}} \right) \\
& \leq C^{\mathbf{T}} \delta_{\text{MS}} |v| (\sqrt{N |\mathbb{T}^3|} + \varepsilon \delta_{\text{MS}}) (1 + \varepsilon C_{\text{MS}}),
\end{aligned}$$

and a similar result can be recovered for the second order terms. As  $\varepsilon \leq 1$ , we can thus successively increase the value of  $C^{\mathbf{T}} > 0$  to derive the final control

$$\begin{aligned}
\|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 & \leq 2 \|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + C^{\mathbf{T}} \delta_{\text{MS}}^2 \|(1 + |v| + |v|^2) \boldsymbol{\mu}\|_{L_x^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \leq C^{\mathbf{T}} \delta_{\text{MS}}^2,
\end{aligned}$$

since the norm on the right-hand side is clearly finite, and we have also used the hypothesis on the initial datum  $\mathbf{f}^{\text{in}}$ .

Moreover, since  $\pi_{\mathbf{L}}$  commutes with  $x$ -derivatives, we can use the unique orthogonal writing  $\nabla_x \mathbf{f} = \pi_{\mathbf{L}}(\nabla_x \mathbf{f}) + \nabla_x \mathbf{f}^\perp$  to get

$$\|\nabla_x \pi_{\mathbf{L}}(\mathbf{f})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2.$$

Plugging both last inequalities into (3.3.22) and redefining accordingly  $C^{\mathbf{T}}$  allow to end the proof.  $\square$

**Step 3 – A priori energy estimates.** It is crucial at this point to show the strict similarities between the *a priori* estimates that we obtain here, with the one derived in [43, Section 3]. Indeed, it is enough to prove this analogy in order to deduce that the exact same computations of [43] apply in our case, leading to the expected results of existence and uniqueness. To do this, we write down all the estimates for the terms appearing in the modified Sobolev norm (3.3.5), whose structure has been fixed at the beginning of this section. The link with [43, Section 3] is established in this way. We list all the estimates, separating inside square brackets the extra terms that appear in our study. In particular, the extra terms involving the norms of  $\mathbf{f}$  and its derivatives are estimated either by a factor of order  $\varepsilon$  or by a factor of order  $\delta_{\text{MS}}$ , both of which can be taken as small as desired in order to close the estimates as in [43]. Note however that we cannot recover the exponential decay in time obtained in [161, 43], as the presence of the source term strongly influences

the shape of the energy estimates. Despite this inconvenience, we mention that our analysis is not the sharpest possible, and we guess that an exponential decay rate could probably be recovered in the particular case when  $\bar{u} = 0$ . We shall give a brief discussion on the topic later on, after the presentation of our result establishing the *a priori* energy estimates (see Corollary 3.3.13).

For the sake of simplicity, we shall use the notations  $C^{(k)}$  and  $\tilde{C}_k^{\mathbf{s}}$  for the technical constants appearing in the following *a priori* estimates. Their explicit values can be found in Appendix C, together with the detailed derivation of all the inequalities. In addition to this, in order to enlighten the computations, we suppose from now on that  $\delta_{\text{MS}} \leq 1$ , even if this requirement may not be optimal.

Let  $s \in \mathbb{N}^*$  and consider a function  $\mathbf{f}$  in  $H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  which solves the perturbed Boltzmann equation (3.1.11) and satisfies initially  $\|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \mathcal{O}(\delta_{\text{MS}})$ , as in the statement of Theorem 3.3.1. Moreover, let us introduce the standard notation  $\mathbf{f}^\perp = \mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f})$  for the part of  $\mathbf{f}$  that is projected onto  $(\ker \mathbf{L})^\perp$ .

The estimate for the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm of  $\mathbf{f}$  reads

$$\begin{aligned} \frac{d}{dt} \|\mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &\leq -\frac{\lambda_{\mathbf{L}}}{\varepsilon^2} \|\mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{8(C_2^{\mathbf{L}} + 1)}{\lambda_{\mathbf{L}}} \mathcal{G}_x^0(\mathbf{f}, \mathbf{f})^2 \\ &\quad + \left[ \delta_{\text{MS}} C^{(1)} \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \tilde{C}_0^{\mathbf{s}} \delta_{\text{MS}} \right]. \end{aligned} \quad (3.3.24)$$

The time evolution of the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm of  $\nabla_x \mathbf{f}$  is estimated as

$$\begin{aligned} \frac{d}{dt} \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &\leq -\frac{\lambda_{\mathbf{L}}}{\varepsilon^2} \|\nabla_x \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{8(2 + 2C_2^{\mathbf{L}} + C_1^{\mathbf{L}} K_x)}{\lambda_{\mathbf{L}}} \mathcal{G}_x^1(\mathbf{f}, \mathbf{f})^2 \\ &\quad + \left[ \delta_{\text{MS}} C^{(2)} \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{\varepsilon \delta_{\text{MS}} C^{(3)}}{\varepsilon^2} \|\mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \tilde{C}_x^{\mathbf{s}} \delta_{\text{MS}} \right]. \end{aligned} \quad (3.3.25)$$

The estimate for the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm of  $\nabla_v \mathbf{f}$  reads

$$\begin{aligned} \frac{d}{dt} \|\nabla_v \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &\leq \frac{K_1}{\varepsilon^2} \|\mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{K_{\text{dx}}}{\varepsilon^2} \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad - \frac{C_3^{\mathbf{v}}}{\varepsilon^2} \|\nabla_v \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{4(3 + C_2^{\mathbf{K}})}{C_3^{\mathbf{v}}} \mathcal{G}_{x,v}^1(\mathbf{f}, \mathbf{f})^2 + \left[ \frac{\tilde{C}_v^{\mathbf{s}} \delta_{\text{MS}}}{\varepsilon^2} \right]. \end{aligned} \quad (3.3.26)$$



The estimate for the commutator reads, for any  $e > 0$ ,

$$\begin{aligned}
& \frac{d}{dt} \langle \nabla_x \mathbf{f}, \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\
& \leq \frac{2C_1^{\mathbf{L}} e}{\varepsilon^3} \|\nabla_x \mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 - \frac{1}{\varepsilon} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{C^{(4)}}{e\varepsilon} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \quad + \frac{2e}{\varepsilon} \mathcal{G}_x^1(\mathbf{f}, \mathbf{f})^2 + \left[ \delta_{\text{MS}} e C^{(5)} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right. \\
& \quad \quad \left. + \frac{\varepsilon^2 e C^{(6)}}{\varepsilon^3} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{\delta_{\text{MS}}^2 e \tilde{C}_{x,v}^s}{\varepsilon} \right]. \quad (3.3.27)
\end{aligned}$$

We then consider two multi-indices  $\alpha, \beta \in \mathbb{N}^3$  such that  $|\alpha| + |\beta| = s$ . If  $|\beta| = 0$ , the estimate for higher  $x$ -derivatives reads

$$\begin{aligned}
& \frac{d}{dt} \|\partial_x^\alpha \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq -\frac{\lambda_{\mathbf{L}}}{\varepsilon^2} \|\partial_x^\alpha \mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + C^{(7)} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 \\
& \quad + \left[ \frac{\varepsilon \delta_{\text{MS}} K_\alpha}{\varepsilon^2} \sum_{|\alpha'| \leq s-1} \|\partial_x^{\alpha'} \mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right. \\
& \quad \quad \left. + \delta_{\text{MS}} C^{(8)} \|\partial_x^\alpha \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \tilde{C}_\alpha^s \delta_{\text{MS}} \right]. \quad (3.3.28)
\end{aligned}$$

In the case when we have at least one derivative in  $v$ , that is when  $|\beta| \geq 1$ , we obtain the estimate on mixed derivatives

$$\begin{aligned}
& \frac{d}{dt} \|\partial_v^\beta \partial_x^\alpha \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \leq -\frac{C_3^\nu}{\varepsilon^2} \|\partial_v^\beta \partial_x^\alpha \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{K_{s-1}}{\varepsilon^2} \|\mathbf{f}\|_{H_{x,v}^{s-1}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \quad + C^{(9)} \sum_{k, \beta_k > 0} \|\partial_v^{\beta - e_k} \partial_x^{\alpha + e_k} \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{4(5 + C_2^{\mathbf{K}} + C_4^\nu)}{C_3^\nu} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 \\
& \quad + \left[ \frac{\varepsilon C_7^\nu}{\varepsilon^2} \|\mathbf{f}\|_{H_{x,v}^{s-1}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \tilde{C}_{\alpha,\beta}^s \delta_{\text{MS}} \right]. \quad (3.3.29)
\end{aligned}$$

In the following, we also need to consider the particular case when we replace  $\alpha$  with  $\alpha - e_k$

and  $\beta$  with  $e_k$  in the previous estimate. Inequality (3.3.29) becomes

$$\begin{aligned}
& \frac{d}{dt} \left\| \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \leq -\frac{C_3^\nu}{\varepsilon^2} \left\| \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{K_{s-1}}{\varepsilon^2} \|\mathbf{f}\|_{H_{x,v}^{s-1}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \quad + C^{(9)} \|\partial_x^\alpha \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{4(5 + C_2^K + C_4)}{C_3^\nu} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 \\
& \quad + \left[ \frac{\varepsilon C_7^\nu}{\varepsilon^2} \|\mathbf{f}\|_{H_{x,v}^{s-1}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \tilde{C}_{\alpha,\beta}^s \delta_{\text{MS}} \right]. \quad (3.3.30)
\end{aligned}$$

Finally, we need to upper bound the commutator for higher derivatives

$$\begin{aligned}
& \frac{d}{dt} \langle \partial_x^\alpha \mathbf{f}, \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\
& \leq \frac{2C_1^L e}{\varepsilon^3} \left\| \partial_x^\alpha \mathbf{f}^\perp \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 - \frac{1}{\varepsilon} \|\partial_x^\alpha \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \quad + \frac{C^{(10)}}{\varepsilon e} \left\| \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2e}{\varepsilon C_1^L} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 \\
& \quad + \left[ \frac{\delta_{\text{MS}} e K_{\alpha,k}}{\varepsilon} \|\mathbf{f}\|_{H_{x,v}^{s-1}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \delta_{\text{MS}} e C^{(11)} \|\partial_x^\alpha \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right. \\
& \quad \left. + \frac{\delta_{\text{MS}}^2 e \tilde{C}_{\alpha,k}^s}{\varepsilon} - \frac{1}{\varepsilon} \langle \partial_x^{\alpha - e_k} (v \cdot \nabla_x \mathbf{f}), v_k \partial_x^\alpha \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \right], \quad (3.3.31)
\end{aligned}$$

where the estimate holds for any  $e > 0$ , and we remember that the last term satisfies the fundamental property

$$- \sum_{\substack{|\alpha|=s \\ k, \alpha_k > 0}} \langle \partial_x^{\alpha - e_k} (v \cdot \nabla_x \mathbf{f}), v_k \partial_x^\alpha \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = - \sum_{|\alpha'|=s-1} \left\| v \cdot \nabla_x \partial_x^{\alpha'} \mathbf{f} \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq 0. \quad (3.3.32)$$

Starting from these inequalities, we are now able to establish the link with [43]. For the sake of clarity, we divide the derivation of the *a priori* energy estimates into two successive results. In the first one, we recover a preliminary upper bound which provides a partial negative return.

**Proposition 3.3.12.** *There exist  $\bar{\delta}_{\text{MS}} > 0$  and  $\varepsilon_0 \in (0, 1]$  such that the following statements hold for any  $s \in \mathbb{N}^*$ .*

- (1) There exist three sets of positive constants  $(a_\alpha^{(s)})_\alpha$ ,  $(b_{\alpha,k}^{(s)})_{\alpha,k}$  and  $(d_{\alpha,\beta}^{(s)})_{\alpha,\beta}$  such that, for all  $\varepsilon \in (0, \varepsilon_0]$ ,

$$\|\cdot\|_{\mathcal{H}_\varepsilon^s} \sim \left( \|\cdot\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \sum_{|\alpha| \leq s} \|\partial_x^\alpha \cdot\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \varepsilon^2 \sum_{\substack{|\alpha|+|\beta| \leq s \\ |\beta| \geq 1}} \|\partial_v^\beta \partial_x^\alpha \cdot\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right)^{1/2}. \quad (3.3.33)$$

- (2) There exist four positive constants  $K_0^{(s)}$ ,  $K_1^{(s)}$ ,  $K_2^{(s)}$  and  $C^{(s)}$  such that, for any values of  $\varepsilon \in (0, \varepsilon_0]$  and  $\delta_{MS} \in [0, \bar{\delta}_{MS}]$ , if  $\mathbf{f} \in H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  solves the perturbed Boltzmann equation (3.1.11) with initial datum  $\mathbf{f}^{\text{in}} \in H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  satisfying  $\|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \mathcal{O}(\delta_{MS})$ , then, for every time  $t \geq 0$ ,

$$\begin{aligned} \frac{d}{dt} \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s}^2 &\leq -K_0^{(s)} \left( \|\mathbf{f}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{1}{\varepsilon^2} \sum_{|\alpha| \leq s} \|\partial_x^\alpha \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right) \\ &\quad + K_1^{(s)} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 + \varepsilon^2 K_2^{(s)} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 + C_s^s \delta_{MS}. \end{aligned} \quad (3.3.34)$$

*Proof.* Let  $\mathbf{f} \in H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  be any solution of (3.1.11) with initial condition satisfying the hypothesis of our statement, and consider a solution  $(\mathbf{c}, \mathbf{u}) \in H_x^{s+5} \times H_x^{s+4}$  of the Maxwell-Stefan system (3.1.7)-(3.1.9). Moreover, suppose  $\delta_{MS} \leq 1$  for simplicity. Under these hypotheses, estimates (3.3.24)–(3.3.31) hold and can be applied.

Following [43, Section 5], we proceed by induction on  $s \in \mathbb{N}^*$ . For  $s = 1$ , the modified Sobolev norm  $\mathcal{H}_\varepsilon^1$  reads, for any  $\mathbf{f} \in H^1(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ ,

$$\begin{aligned} \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^1}^2 &= A \|\mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + a \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + b\varepsilon \langle \nabla_x \mathbf{f}, \nabla_v \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} + d\varepsilon^2 \|\nabla_v \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2. \end{aligned}$$

Therefore, we consider the linear combination  $A(3.3.24) + a(3.3.25) + d\varepsilon^2(3.3.26) + b\varepsilon(3.3.27)$ . Recalling from Lemma 3.3.7 that we have the monotone behaviour  $\mathcal{G}_x^0 \leq \mathcal{G}_x^1$ , we can easily

find some positive constants  $K_1^{(1)}$ ,  $K_2^{(1)}$  and  $C_1^S$  such that, at first,

$$\begin{aligned}
\frac{d}{dt} \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^1}^2 &\leq \frac{1}{\varepsilon^2} \left[ \varepsilon (a\delta_{\text{MS}}C^{(3)} + \varepsilon K_1 d + b\varepsilon C^{(6)}) - \frac{A\lambda_{\mathbf{L}}}{2} \right] \|\mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
&\quad + \frac{1}{\varepsilon^2} \left[ 2C_1^L e b - \frac{a\lambda_{\mathbf{L}}}{2} \right] \|\nabla_x \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
&\quad + \left[ \delta_{\text{MS}}(AC^{(1)} + aC^{(2)}) + K_{\text{dx}}d - b(1 - \delta_{\text{MS}}eC^{(5)}) \right] \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
&\quad + \left[ \frac{C^{(4)}b}{e} - dC_3^v \right] \|\nabla_v \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
&\quad - \frac{A\lambda_{\mathbf{L}}}{2\varepsilon^2} \|\mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 - \frac{a\lambda_{\mathbf{L}}}{2\varepsilon^2} \|\nabla_x \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
&\quad + K_1^{(1)} \mathcal{G}_x^1(\mathbf{f}, \mathbf{f})^2 + \varepsilon^2 K_2^{(1)} \mathcal{G}_{x,v}^1(\mathbf{f}, \mathbf{f})^2 + C_1^S \delta_{\text{MS}}.
\end{aligned}$$

If we now choose

$$\bar{\delta}_{\text{MS}} \leq \min \left\{ 1, \frac{K_{\text{dx}}d}{AC^{(1)} + aC^{(2)}}, \frac{1}{2eC^{(5)}} \right\}, \quad \varepsilon_0 \leq \min \left\{ 1, \frac{K_1 d}{aC^{(3)} + K_1 d + bC^{(6)}} \right\},$$

we can repeat the same computations in [43] in order to fix the values of  $A$ ,  $a$ ,  $b$ ,  $d$  and  $e$ . In particular, the equivalence between the modified norm  $\mathcal{H}_\varepsilon^1$  and the standard Sobolev norm  $H_x^1 L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  immediately follows, and we also recover, because  $\varepsilon \in (0, 1]$ , the estimate

$$\begin{aligned}
\frac{d}{dt} \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^1}^2 &\leq - \left( \|\mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \|\nabla_x \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right. \\
&\quad \left. + \|\nabla_v \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right) \\
&\quad - \frac{A\lambda_{\mathbf{L}}}{2\varepsilon^2} \|\mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 - \frac{a\lambda_{\mathbf{L}}}{2\varepsilon^2} \|\nabla_x \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
&\quad + K_1^{(1)} \mathcal{G}_x^1(\mathbf{f}, \mathbf{f})^2 + \varepsilon^2 K_2^{(1)} \mathcal{G}_{x,v}^1(\mathbf{f}, \mathbf{f})^2 + C_1^S \delta_{\text{MS}}. \quad (3.3.35)
\end{aligned}$$

Note that we have kept the constants  $A$  and  $a$  in the extra negative contributions coming from  $\mathbf{f}^\perp$ , for the sake of clarity. In particular, we stress the fact that  $A$  and  $a$  have been fixed independently of  $\delta_{\text{MS}}$  and  $\varepsilon$ .

To conclude, we observe that thanks to the Poincaré inequality (3.3.21) and the equivalence between the  $L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})$  and  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norms on  $\ker \mathbf{L}$ , the following upper bounds hold

$$\begin{aligned}
\|\mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 &\leq C' \left( \|\mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{1}{2} \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \delta_{\text{MS}}^2 \right), \\
\|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 &\leq \tilde{C}' \left( \|\nabla_x \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{1}{2} \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right),
\end{aligned}$$

for some positive constants  $C'$  and  $\tilde{C}'$  computed from (3.3.20) and (3.3.21), which are independent of the parameters  $\delta_{\text{MS}}$  and  $\varepsilon$ . By plugging the above inequalities into (3.3.35) and by adding the small extra term  $\delta_{\text{MS}}^2$  to the same one multiplying  $C_1^{\text{S}}$ , we deduce the existence of a positive constant  $K_0^{(1)}$  (independent of  $\delta_{\text{MS}}$  and  $\varepsilon$ ) such that

$$\begin{aligned} \frac{d}{dt} \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^1}^2 &\leq -K_0^{(1)} \|\mathbf{f}\|_{H_{x,v}^1(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad - \frac{\lambda_{\mathbf{L}} \min\{A, a\}}{2\varepsilon^2} \left( \|\mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \|\nabla_x \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right) \\ &\quad + K_1^{(1)} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 + \varepsilon^2 K_2^{(1)} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 + C_1^{\text{S}} \delta_{\text{MS}}, \end{aligned}$$

Therefore, redefining  $K_0^{(1)}$  small enough to ensure that also  $K_0^{(1)} \leq \lambda_{\mathbf{L}} \min\{A, a\}/2$ , we finally recover estimate (3.3.34) in the case  $s = 1$ .

For the general case, we suppose that the result is true up to the integer  $s - 1$ , and we prove that it also holds for  $s$ . The first statement, about the equivalence between the  $\mathcal{H}_\varepsilon^s$  and  $H_x^s L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norms, is straightforward. For the second property, regarding the *a priori* estimate, in a similar way to what we have done for  $s = 1$ , we define this time

$$F_s(t) = \varepsilon^2 B \sum_{\substack{|\alpha|+|\beta|=s \\ |\alpha| \geq 2}} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + B' \sum_{\substack{|\alpha|=s \\ k, \alpha_k > 0}} Q_{\alpha,k}(t), \quad (3.3.36)$$

$$\begin{aligned} Q_{\alpha,k}(t) &= a \|\partial_x^\alpha \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + b\varepsilon \langle \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f}, \partial_x^\alpha \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &\quad + d\varepsilon^2 \|\partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2, \end{aligned} \quad (3.3.37)$$

and the positive constants have to be fixed as previously.

By taking the linear combination  $a(3.3.28) + b\varepsilon(3.3.31) + d\varepsilon^2(3.3.30)$ , we compute

$$\begin{aligned} \frac{d}{dt} Q_{\alpha,k}(t) &\leq \frac{1}{\varepsilon^2} \left[ 2C_1^{\text{L}} e b - \frac{a\lambda_{\mathbf{L}}}{2} \right] \|\partial_x^\alpha \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \left[ \frac{C^{(10)} b}{e} - C_3^{\text{V}} d \right] \|\partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \left[ \delta_{\text{MS}} C^{(8)} a + \varepsilon^2 C^{(9)} d - b \left( 1 - \delta_{\text{MS}} e C^{(11)} \right) \right] \|\partial_x^\alpha \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad - \frac{a\lambda_{\mathbf{L}}}{2\varepsilon^2} \|\partial_x^\alpha \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{a\varepsilon \delta_{\text{MS}} K_\alpha}{\varepsilon^2} \sum_{|\alpha'| \leq s-1} \|\partial_x^{\alpha'} \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + K_{s-1} d \|\mathbf{f}\|_{H_{x,v}^{s-1}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \left( \delta_{\text{MS}} e K_{\alpha,k} b + \varepsilon C_7^{\text{V}} d \right) \|\mathbf{f}\|_{H_{x,v}^{s-1}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \tilde{K}_1^{(s)} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 + \varepsilon^2 \tilde{K}_2^{(2)} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 + \tilde{C}_s^{\text{S}} \delta_{\text{MS}} \\ &\quad - b \langle \partial_x^{\alpha - e_k} (v \cdot \nabla_x \mathbf{f}), v_k \partial_x^\alpha \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}. \end{aligned}$$

In particular, similarly to the case  $s = 1$ , we can redefine  $\bar{\delta}_{\text{MS}}$  to satisfy also

$$\bar{\delta}_{\text{MS}} \leq \min \left\{ \frac{C^{(9)}d}{C^{(8)}a}, \frac{1}{2eC^{(11)}} \right\},$$

so that the first three contributions are the same as in [43, Section 5]. Therefore, we can set the values of  $a$ ,  $b$ ,  $d$  and  $e$  in such a way that

$$\begin{aligned} \frac{d}{dt} Q_{\alpha,k}(t) &\leq -K_0^{(s)} \left( \|\partial_x^\alpha \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \|\partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right) \\ &\quad - \frac{a\lambda_{\mathbf{L}}}{2\varepsilon^2} \|\partial_x^\alpha \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{a\varepsilon\delta_{\text{MS}}K_\alpha}{\varepsilon^2} \sum_{|\alpha'| \leq s-1} \|\partial_x^{\alpha'} \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \tilde{K}_{s-1} \|\mathbf{f}\|_{H_{x,v}^{s-1}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \tilde{K}_1^{(s)} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 + \varepsilon^2 \tilde{K}_2^{(2)} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 + \tilde{C}_s^s \delta_{\text{MS}} \\ &\quad - b \langle \partial_x^{\alpha-e_k} (v \cdot \nabla_x \mathbf{f}), v_k \partial_x^\alpha \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}, \end{aligned} \tag{3.3.38}$$

where we have used the equivalence between the  $L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})$  and the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norms on  $\ker \mathbf{L}$ , and we have also accordingly redefined all the main constants of interest to enlighten the computations. In particular, we stress again the fact that all these constants remain independent of the parameters  $\delta_{\text{MS}}$  and  $\varepsilon$ .

Now, note that if we sum (3.3.38) over  $|\alpha| = s$  and  $k = 1, 2, 3$ , such that  $\alpha_k > 0$ , the terms accounting for the scalar products disappear, thanks to the property (3.3.32). Therefore, going back to the definition (3.3.36) of  $F_s(t)$ , combining  $B'$ (3.3.38) with  $\varepsilon^2 B$ (3.3.29) we obtain

$$\begin{aligned} \frac{d}{dt} F_s(t) &\leq -C_3^v B \sum_{\substack{|\alpha|+|\beta|=s \\ |\beta| \geq 2}} \|\partial_v^\beta \partial_x^\alpha \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \sum_{\substack{|\alpha|+|\beta|=s \\ |\beta| \geq 2}} C^{(9)} B \varepsilon^2 \sum_{k, \beta_k > 0} \|\partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad - B' \tilde{K}_0^{(s)} \sum_{\substack{|\alpha|=s \\ k, \alpha_k > 0}} \left( \|\partial_x^\alpha \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \|\partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right) \\ &\quad - B' \sum_{\substack{|\alpha|=s \\ k, \alpha_k > 0}} \left( \frac{a\lambda_{\mathbf{L}}}{2\varepsilon^2} \|\partial_x^\alpha \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 - \frac{a\varepsilon\delta_{\text{MS}}K_\alpha}{\varepsilon^2} \sum_{|\alpha'| \leq s-1} \|\partial_x^{\alpha'} \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right) \\ &\quad + \left( B' \tilde{K}_{s-1} + B(K_{s-1} + \varepsilon C_7^v) \right) \|\mathbf{f}\|_{H_{x,v}^{s-1}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + K_1^{(s)} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 + \varepsilon^2 K_2^{(2)} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 + C_s^s \delta_{\text{MS}}^2. \end{aligned}$$

Redefining the constants if necessary, we can then copy the arguments used in [43, Section 5] to finally obtain the existence of  $\varepsilon_0 \in (0, 1]$  such that, for all  $\varepsilon \in (0, \varepsilon_0]$ ,

$$\begin{aligned} \frac{d}{dt} F_s(t) &\leq \tilde{K}_{s-1} \|\mathbf{f}\|_{H_{x,v}^{s-1}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 - \left( \sum_{|\alpha|+|\beta|=s} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right) \\ &\quad - B' \frac{a\lambda_{\mathbf{L}}}{2\varepsilon^2} \sum_{|\alpha|=s} \left\| \partial_x^\alpha \mathbf{f}^\perp \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \tilde{B}' \frac{a\varepsilon \delta_{\text{MS}} K_\alpha}{\varepsilon^2} \sum_{|\alpha'| \leq s-1} \left\| \partial_x^{\alpha'} \mathbf{f}^\perp \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + K_1^{(s)} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 + \varepsilon^2 K_2^{(2)} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 + C_s^s \delta_{\text{MS}}. \end{aligned}$$

To conclude, for some positive constants  $(K_p)_{p \leq s}$ , we only have to consider a linear combination  $\sum_{p=1}^s K_p F_p(t)$  and use the induction hypothesis, together with  $\varepsilon \leq 1$  and the last requirement

$$\bar{\delta}_{\text{MS}} \leq \frac{\min_p K_p}{2\tilde{B}' a K_\alpha}.$$

Recalling that the functionals  $\mathcal{G}_x^p$  and  $\mathcal{G}_{x,v}^p$  are monotonically increasing in  $p$ , we can finally recover the following estimate, valid for any  $\varepsilon \in (0, \varepsilon_0]$  and any  $\delta_{\text{MS}} \in [0, \bar{\delta}_{\text{MS}}]$ ,

$$\begin{aligned} \frac{d}{dt} \left( \sum_{p=1}^s K_p F_p(t) \right) &\leq -K_0^{(s)} \left( \sum_{|\alpha|+|\beta| \leq s} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{1}{\varepsilon^2} \sum_{|\alpha| \leq s} \left\| \partial_x^\alpha \mathbf{f}^\perp \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right) \\ &\quad + K_1^{(s)} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 + \varepsilon^2 K_2^{(2)} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 + C_s^s \delta_{\text{MS}}. \end{aligned}$$

which is the expected result.  $\square$

Starting from this general preliminary estimate, we can finally prove the result that establishes the uniform *a priori* control on  $\mathbf{f}$ , which in turn ensures the stability of the expansion around  $\mathbf{M}^\varepsilon$ .

**Corollary 3.3.13.** *There exist  $s_0 \in \mathbb{N}^*$ ,  $\bar{\delta}_{\text{MS}} > 0$  and  $\varepsilon_0 \in (0, 1]$  such that, for any integer  $s \geq s_0$ , there exists  $\delta_B > 0$  such that, for any  $\varepsilon \in (0, \varepsilon_0]$  and any  $\delta_{\text{MS}} \in [0, \bar{\delta}_{\text{MS}}]$ , if  $\mathbf{f} \in H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  solves the perturbed Boltzmann equation (3.1.11), and satisfies initially*

$$\|\mathbf{f}^{\text{in}}\|_{\mathcal{H}_\varepsilon^s} \leq \delta_B, \quad \|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \mathcal{O}(\delta_{\text{MS}}),$$

then  $\|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s} \leq \|\mathbf{f}^{\text{in}}\|_{\mathcal{H}_\varepsilon^s}$  for all  $t \geq 0$ .

*Proof.* Since we are under the same hypotheses of Proposition 3.3.12, we have seen how to fix the values of  $\bar{\delta}_{\text{MS}} > 0$  and  $\varepsilon_0 \in (0, 1]$ , so that, for any  $s \in \mathbb{N}^*$ , the *a priori* estimate (3.3.34) holds for any time  $t \geq 0$ . Note in particular that we can get rid of the negative terms involving the pure  $x$ -derivatives of  $\mathbf{f}$ , as their presence was needed in the previous

result only to ensure the control of the small positive extra terms of  $\mathcal{O}(\varepsilon)$ , in order to close the induction procedure. Therefore, for any  $s \in \mathbb{N}^*$  and any  $t \geq 0$ , the time evolution of the  $\mathcal{H}_\varepsilon^s$  norm of  $\mathbf{f}$  is uniformly controlled in  $\varepsilon \in (0, \varepsilon_0]$  and  $\delta_{\text{MS}} \in [0, \bar{\delta}_{\text{MS}}]$  as

$$\frac{d}{dt} \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s}^2 \leq -K_0^{(s)} \|\mathbf{f}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 + K_1^{(s)} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 + \varepsilon^2 K_2^{(s)} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 + C_s^{\text{S}} \delta_{\text{MS}}. \quad (3.3.39)$$

The idea is then to properly bound the functionals  $\mathcal{G}_x^s$  and  $\mathcal{G}_{x,v}^s$ . For this, recall from Lemma 3.3.7 that we can find an integer  $s_0 \in \mathbb{N}^*$  for which estimates (3.3.15) hold for any integer  $s \geq s_0$ . Moreover, thanks to the equivalence between the  $\mathcal{H}_\varepsilon^s$  norm and the standard Sobolev norm given by (3.3.33), we can infer the existence of two positive constants  $C_{\text{eq}}$  and  $C_{\text{EQ}}$  such that

$$\begin{aligned} C_{\text{eq}} \left( \|\cdot\|_{L_{x,v}^2(\mu^{-\frac{1}{2}})}^2 + \sum_{|\alpha| \leq s} \|\partial_x^\alpha \cdot\|_{L_{x,v}^2(\mu^{-\frac{1}{2}})}^2 + \varepsilon^2 \sum_{\substack{|\alpha|+|\beta| \leq s \\ |\beta| \geq 1}} \|\partial_v^\beta \partial_x^\alpha \cdot\|_{L_{x,v}^2(\mu^{-\frac{1}{2}})}^2 \right) \\ \leq \|\cdot\|_{\mathcal{H}_\varepsilon^s}^2 \leq C_{\text{EQ}} \|\cdot\|_{H_{x,v}^s(\mu^{-\frac{1}{2}})}^2. \end{aligned} \quad (3.3.40)$$

Therefore,  $\mathcal{G}_x^s$  can be successively estimated as

$$\begin{aligned} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 &\leq 2(C_s^{\text{Q}})^2 \|\mathbf{f}\|_{H_x^s L_v^2(\mu^{-\frac{1}{2}})}^2 \|\mathbf{f}\|_{H_x^s L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 \\ &\leq \frac{2(C_s^{\text{Q}})^2}{C_{\text{eq}}} \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s}^2 \|\mathbf{f}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2, \end{aligned}$$

and similarly, for  $\mathcal{G}_{x,v}^s$ , we get

$$\mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 \leq \frac{2(C_s^{\text{Q}})^2}{\varepsilon^2 C_{\text{eq}}} \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s}^2 \|\mathbf{f}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2.$$

Plugging the above inequalities into (3.3.39), we thus obtain

$$\frac{d}{dt} \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s}^2 \leq \left( \frac{2(C_s^{\text{Q}})^2}{C_{\text{eq}}} (K_1^{(s)} + K_2^{(s)}) \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s}^2 - K_0^{(s)} \right) \|\mathbf{f}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 + C_s^{\text{S}} \delta_{\text{MS}}.$$

If we now choose  $\delta_{\text{B}} > 0$  satisfying

$$\frac{2(C_s^{\text{Q}})^2}{C_{\text{eq}}} (K_1^{(s)} + K_2^{(s)}) \delta_{\text{B}}^2 \leq \frac{K_0^{(s)}}{2},$$

thanks to (3.3.40), we can also infer

$$\begin{aligned} \frac{d}{dt} \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s}^2 &\leq -\frac{K_0^{(s)}}{2} \|\mathbf{f}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 + C_s^{\text{S}} \delta_{\text{MS}} \\ &\leq -\frac{K_0^{(s)}}{2C_{\text{EQ}}} \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s}^2 + C_s^{\text{S}} \delta_{\text{MS}}, \end{aligned}$$



as long as  $\|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s} \leq \delta_B$ . But now setting  $\lambda_B = K_0^{(s)}/2C_{\text{EQ}}$ , from Grönwall's lemma, we deduce that, for any  $s \geq s_0$ , for any  $\varepsilon \in (0, \varepsilon_0]$  and for all  $\delta_{\text{MS}} \in [0, \bar{\delta}_{\text{MS}}]$ ,

$$\|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s}^2 \leq \|\mathbf{f}^{\text{in}}\|_{\mathcal{H}_\varepsilon^s}^2 e^{-\lambda_B t} + \frac{C_s^{\text{S}} \delta_{\text{MS}}}{\lambda_B} (1 - e^{-\lambda_B t}), \quad (3.3.41)$$

or, more explicitly,

$$\|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s} \leq \max \left\{ \delta_B, \left( \frac{\delta_{\text{MS}} C_s^{\text{S}}}{\lambda_B} \right)^{1/2} \right\}.$$

Therefore, recalling that  $\delta_B$  has been chosen independently of the parameter  $\bar{\delta}_{\text{MS}} > 0$ , if we impose

$$\bar{\delta}_{\text{MS}} \leq \frac{\delta_B^2 \lambda_B}{4 C_s^{\text{S}}},$$

we finally ensure the validity of the estimate  $\|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s} \leq \delta_B$  for any time  $t \geq 0$ , hence concluding the proof.  $\square$

**Remark 3.3.14.** We emphasize that the above result only provides a stability condition for the expansion around  $\mathbf{M}^\varepsilon$ , in the sense that the  $\mathcal{H}_\varepsilon^s$  norm of  $\mathbf{f}$  can be bounded uniformly in time by the constant  $\delta_B > 0$ . Unfortunately, we cannot obtain a full exponential decay in time because of the presence of the extra term  $C_s^{\text{S}} \delta_{\text{MS}}^2$  which accounts for the macroscopic quantities that define  $\mathbf{M}^\varepsilon$ . It is particularly important to emphasize that the constant  $C^{(s)}$  contains factors depending on  $\|\mathbf{c}_\infty\|_{L_x^2}$  and  $\|\bar{\mathbf{u}}\|_{L_t^\infty H_x^{s+4}}$ , which are uniformly controlled by some positive constants, but cannot exhibit an exponential decay. To be more specific about this issue, we actually guess that the only problematic quantity is the incompressible velocity  $\bar{\mathbf{u}}$ , because it appears as a multiplicative factor in some of the terms composing  $C^{(s)}$ . In particular, if we get rid of  $\bar{\mathbf{u}}$  by looking at the stationary macroscopic state  $(\mathbf{c}_\infty, \mathbf{0})$ , we can probably recover a global exponential decay in time for  $\mathbf{f}$ , by means of the exponential decays obtained for  $\tilde{\mathbf{c}}$  and  $\tilde{\mathbf{u}}$ . Besides, this feature can be explained with the perturbative theory of convergence towards equilibrium which, in our case, prescribes the exponential-in-time relaxation towards the sole global equilibrium  $\boldsymbol{\mu}$ , having macroscopic velocity  $\mathbf{u}_\infty = \mathbf{0}$ . Therefore, the only physically meaningful incompressible velocity  $\bar{\mathbf{u}}$  should precisely be  $\mathbf{0}$ .

By now, however, we stick to the partial result that we have established, since it is enough to get global existence and uniqueness of the perturbation  $\mathbf{f}$ .

**Step 3 – Existence and uniqueness of the perturbation  $\mathbf{f}$ .** We are finally able to prove that the solution  $\mathbf{f}$  to the perturbed Boltzmann equation (3.1.11) exists uniquely in time, on  $\mathbb{R}_+$ . Even if the proofs are very standard, we sketch the ideas behind and the computations, for the sake of completeness.

**Proposition 3.3.15.** *Let the collision kernels  $B_{ij}$  satisfy assumptions (H1)–(H4), and consider the local Maxwellian  $\mathbf{M}^\varepsilon$  defined by (3.3.1)–(3.3.2). Let  $s \geq s_0$ , given by Lemma 3.3.7. There exist  $\varepsilon_0 \in (0, 1]$  and  $\bar{\delta}_{\text{MS}}, \delta_B > 0$  such that, for all  $\varepsilon \in (0, \varepsilon_0]$ , all  $\delta_{\text{MS}} \in [0, \bar{\delta}_{\text{MS}}]$ , and for any initial datum  $\mathbf{f}^{\text{in}}$  in  $H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  satisfying*

$$\|\mathbf{f}^{\text{in}}\|_{\mathcal{H}_\varepsilon^s} \leq \delta_B, \quad \|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \mathcal{O}(\delta_{\text{MS}}),$$

there exists  $\mathbf{f} \in C^0(\mathbb{R}_+; H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}))$  such that  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}$  is a weak solution of the Boltzmann multi-species equation (3.1.11). Moreover, if  $\mathbf{F}^{\varepsilon, \text{in}} = \mathbf{M}^{\varepsilon, \text{in}} + \varepsilon \mathbf{f}^{\text{in}} \geq 0$ , then also  $\mathbf{F}^\varepsilon(t, x, v) \geq 0$  for a.e.  $(t, x, v) \in \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ .

*Proof.* The proof of the existence is based on a standard iterative method, where we construct a solution on a finite time interval  $[0, T_0]$ , and we then show that  $T_0$  can be extended up to  $+\infty$ . Let  $s \geq s_0$ , given by Lemma 3.3.7 and consider a solution  $(\mathbf{c}, \mathbf{u})$  of the Maxwell-Stefan system (3.1.7)–(3.1.9) which is at least  $L^\infty(\mathbb{R}_+; H^{s+5}(\mathbb{T}^3)) \times L^\infty(\mathbb{R}_+; H^{s+4}(\mathbb{T}^3))$ . In particular, recall that  $(\mathbf{c}, \mathbf{u})$  also belongs to  $C^0(\mathbb{R}_+; H^{s+4}(\mathbb{T}^3)) \times C^0(\mathbb{R}_+; H^{s+3}(\mathbb{T}^3))$ , so that the local Maxwellian  $\mathbf{M}^\varepsilon$  is continuous with respect to  $t \geq 0$ .

With these choices, set initially

$$\mathbf{f}^{(0)} = \mathbf{f}^{\text{in}}, \quad T_0 = \frac{\delta_B \min \left\{ 1, \frac{K_0^{(s)}}{2} \right\}}{4C_s^s \delta_{\text{MS}}}, \quad (3.3.42)$$

and suppose that on  $[0, T_0]$  a sequence of functions  $(f^{(\bar{n})})_{0 < \bar{n} \leq n}$  is given up to an integer  $n \in \mathbb{N}^*$ , satisfying, for any  $0 < \bar{n} \leq n$  and for any  $t \in [0, T_0]$ ,

$$\mathbf{f}^{(\bar{n})} \in H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}), \quad \left\| \pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{(\bar{n})}) \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \mathcal{O}(\delta_{\text{MS}}).$$

By induction on  $n > 0$ , we define the function  $\mathbf{f}^{(n+1)}$  such that

$$\begin{cases} \partial_t \mathbf{f}^{(n+1)} + \frac{1}{\varepsilon} v \cdot \nabla_x \mathbf{f}^{(n+1)} = \frac{1}{\varepsilon^2} \mathbf{L}^\varepsilon(\mathbf{f}^{(n+1)}) + \frac{1}{\varepsilon} \mathbf{Q}(\mathbf{f}^{(n)}, \mathbf{f}^{(n+1)}) + \mathbf{S}^\varepsilon, \\ \mathbf{f}^{(n+1)}|_{t=0} = \mathbf{f}^{\text{in}}. \end{cases} \quad (3.3.43)$$

It is now a classical result the existence of a solution  $\mathbf{f}^{(n+1)} \in H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  for the above evolution equation. Indeed, recalling the definition of  $\mathbf{T}^\varepsilon = \frac{1}{\varepsilon^2} \mathbf{L} - \frac{1}{\varepsilon} v \cdot \nabla_x$ , we can rewrite

$$\partial_t \mathbf{f}^{(n+1)} = \mathbf{T}^\varepsilon(\mathbf{f}^{(n+1)}) + \frac{1}{\varepsilon^2} (\mathbf{L}^\varepsilon - \mathbf{L})(\mathbf{f}^{(n+1)}) + \frac{1}{\varepsilon} \mathbf{Q}(\mathbf{f}^{(n)}, \mathbf{f}^{(n+1)}) + \mathbf{S}^\varepsilon. \quad (3.3.44)$$

Since  $\mathbf{L}$  is self-adjoint in  $L^2(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  and possesses a spectral gap  $\lambda_{\mathbf{L}}$ , and  $v \cdot \nabla_x$  is anti-symmetric, it is easy to prove that  $\mathbf{T}^\varepsilon$  generates a strongly continuous semigroup in  $H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  (see [139] for the general theory, and [45, Section 4.2] for the specific case of the Boltzmann multi-species equation). In particular, as done in [43, Section 6], introducing the following functional defined on  $H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$

$$E_{[0, T_0]}(\mathbf{f}) = \sup_{t \in [0, T_0]} \left( \|\mathbf{f}(t)\|_{\mathcal{H}_\varepsilon^s}^2 + \int_0^t \|\mathbf{f}(\tau)\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 d\tau \right),$$

from estimates (3.3.14)–(3.3.15) of Lemma 3.3.7, it immediately follows that

$$\mathbf{Q}(\mathbf{f}^{(n)}, \cdot) : \left( H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}), E_{[0, T_0]}(\cdot) \right) \rightarrow \left( H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}), \|\cdot\|_{H_{x,v}^s(\boldsymbol{\mu}^{-\frac{1}{2}})} \right)$$

is a bounded linear operator, and the same holds for the penalization  $\mathbf{L}^\varepsilon - \mathbf{L}$ . To ease the computations, from now on let us drop the subscript  $[0, T_0]$  in  $E_{[0, T_0]}$ . By means of the functional  $E$ , one can then apply Duhamel's formula in combination with a suitable fixed point argument to show that, as long as  $\|\mathbf{f}^{\text{in}}\|_{\mathcal{H}_\varepsilon^s}$  is chosen small enough, there exists a solution  $\mathbf{f}^{(n+1)}$  to (3.3.44), which is in  $H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  for any time  $t \in [0, T_0]$ . Moreover,

applying  $\pi_{\mathbf{T}^\varepsilon}$  to (3.3.44) and performing an identical study to the one carried out in the proof of Lemma 3.3.11 to derive the Poincaré inequality (3.3.21), we also ensure that

$$\left\| \pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{(n+1)}) \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq C^{\mathbf{T}} \delta_{\text{MS}}, \quad \forall t \in [0, T_0],$$

so that, by induction, the sequence  $(\mathbf{f}^{(n)})_{n \in \mathbb{N}}$  remains well-defined.

Starting from these considerations, one then aims at proving that the constructed sequence  $(\mathbf{f}^{(n)})_{n \in \mathbb{N}}$  can be uniformly bounded in the  $E$  norm. For this, since obviously  $E(\mathbf{f}^{(0)}) = \|\mathbf{f}^{\text{in}}\|_{\mathcal{H}_\varepsilon^s} \leq \delta_{\text{B}}$  from our initial choice (3.3.42), we proceed by induction on  $n \in \mathbb{N}$ , supposing that we can uniformly bound  $E(\mathbf{f}^{(n)}) \leq \delta_{\text{B}}$  up to some integer  $n > 0$ , and proving that also  $E(\mathbf{f}^{(n+1)}) \leq \delta_{\text{B}}$ .

Now, each  $\mathbf{f}^{(n)}$  satisfies all the hypotheses needed in order to copy the computations used to derive the *a priori* estimates in the previous step. More precisely, from Proposition 3.3.12, we know that there exist  $\bar{\delta}_{\text{MS}} > 0$  and  $\varepsilon_0 \in (0, 1]$  such that, for any  $s \geq s_0$ , for any  $\delta_{\text{MS}} \in [0, \bar{\delta}_{\text{MS}}]$  and  $\varepsilon \in (0, \varepsilon_0]$ , one recovers the estimate

$$\begin{aligned} \frac{d}{dt} \left\| \mathbf{f}^{(n+1)} \right\|_{\mathcal{H}_\varepsilon^s}^2 &\leq -K_0^{(s)} \left\| \mathbf{f}^{(n+1)} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + K_1^{(s)} \mathcal{G}_x^s(\mathbf{f}^{(n)}, \mathbf{f}^{(n+1)})^2 + \varepsilon^2 K_2^{(s)} \mathcal{G}_{x,v}^s(\mathbf{f}^{(n)}, \mathbf{f}^{(n+1)})^2 + C_s^{\delta_{\text{MS}}}. \end{aligned}$$

Moreover, thanks to (3.3.40) and proceeding like in the proof of Corollary 3.3.13, we also establish the bounds

$$\begin{aligned} \mathcal{G}_x^s(\mathbf{f}^{(n)}, \mathbf{f}^{(n+1)})^2 &\leq \frac{4(C_s^{\mathbf{Q}})^2}{C_{\text{eq}}} \left( \left\| \mathbf{f}^{(n)} \right\|_{\mathcal{H}_\varepsilon^s}^2 \left\| \mathbf{f}^{(n+1)} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \left\| \mathbf{f}^{(n+1)} \right\|_{\mathcal{H}_\varepsilon^s}^2 \left\| \mathbf{f}^{(n)} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right), \end{aligned}$$

$$\begin{aligned} \mathcal{G}_{x,v}^s(\mathbf{f}^{(n)}, \mathbf{f}^{(n+1)})^2 &\leq \frac{4(C_s^{\mathbf{Q}})^2}{\varepsilon^2 C_{\text{eq}}} \left( \left\| \mathbf{f}^{(n)} \right\|_{\mathcal{H}_\varepsilon^s}^2 \left\| \mathbf{f}^{(n+1)} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \left\| \mathbf{f}^{(n+1)} \right\|_{\mathcal{H}_\varepsilon^s}^2 \left\| \mathbf{f}^{(n)} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \right). \end{aligned}$$

Consequently, naming  $K^{(s)} = \frac{4(C_s^{\mathbf{Q}})^2}{C_{\text{eq}}}(K_1^{(s)} + K_2^{(s)})$ , we deduce the following estimate

$$\begin{aligned} \frac{d}{dt} \left\| \mathbf{f}^{(n+1)} \right\|_{\mathcal{H}_\varepsilon^s}^2 &\leq -K_0^{(s)} \left\| \mathbf{f}^{(n+1)} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + K^{(s)} \left\| \mathbf{f}^{(n)} \right\|_{\mathcal{H}_\varepsilon^s}^2 \left\| \mathbf{f}^{(n+1)} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + K^{(s)} \left\| \mathbf{f}^{(n+1)} \right\|_{\mathcal{H}_\varepsilon^s}^2 \left\| \mathbf{f}^{(n)} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + C^{(s)} \delta_{\text{MS}} \\ &\leq \left( K^{(s)} E(\mathbf{f}^{(n)}) - K_0^{(s)} \right) \left\| \mathbf{f}^{(n+1)} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + K^{(s)} E(\mathbf{f}^{(n+1)}) \left\| \mathbf{f}^{(n)} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + C_s^{\delta_{\text{MS}}}, \end{aligned}$$

holding for any  $t \in [0, T_0]$ .

Choosing  $\delta_B > 0$  such that  $E(\mathbf{f}^{(n)}) \leq K_0^{(s)}/2K^{(s)}$ , we can thus integrate the previous inequality on  $[0, t]$ , with  $t \leq T_0$ , to obtain

$$\begin{aligned} \|\mathbf{f}^{(n+1)}\|_{\mathcal{H}_\varepsilon^s}^2 + \frac{K_0^{(s)}}{2} \int_0^t \|\mathbf{f}^{(n+1)}(\tau)\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 d\tau \\ \leq \|\mathbf{f}^{\text{in}}\|_{\mathcal{H}_\varepsilon^s}^2 + K^{(s)} E(\mathbf{f}^{(n+1)}) E(\mathbf{f}^{(n)}) + t C_s^{\mathbf{S}} \delta_{\text{MS}}. \end{aligned}$$

Therefore, if we also suppose that

$$\delta_B \leq \min \left\{ 1, \frac{K_0^{(s)}}{2} \right\} / 2K^{(s)} \quad \text{and} \quad \delta_B \leq \min \left\{ 1, \frac{K_0^{(s)}}{2} \right\} / 4,$$

thanks to the induction hypothesis on  $E(\mathbf{f}^{(n)})$ , we deduce that

$$E(\mathbf{f}^{(n+1)}) \leq \frac{2}{\min \left\{ 1, \frac{K_0^{(s)}}{2} \right\}} \|\mathbf{f}^{\text{in}}\|_{\mathcal{H}_\varepsilon^s}^2 + \frac{2C_s^{\mathbf{S}} \delta_{\text{MS}}}{\min \left\{ 1, \frac{K_0^{(s)}}{2} \right\}} T_0 \leq \delta_B,$$

thanks to our choice of  $T_0$ . Hence, the sequence  $(\mathbf{f}^{(n)})_{n \in \mathbb{N}}$  is uniformly bounded by  $\delta_B$  in the  $E$  norm, and thus also in  $L^\infty(0, T_0; H_{x,v}^s(\boldsymbol{\mu}^{-\frac{1}{2}})) \cap L^1(0, T_0; H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}}))$ . Therefore, thanks to the Rellich-Kondrachov theorem on compact embeddings into less regular Sobolev spaces, we can take the limit  $n \rightarrow +\infty$  in (3.3.43), since  $\mathbf{T}^\varepsilon$ ,  $\mathbf{L}^\varepsilon - \mathbf{L}$  and  $\mathbf{Q}$  are continuous. In particular, we can extract a subsequence that converges towards a function  $\mathbf{f}^\infty$  which belongs to  $C^0([0, T_0]; H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}))$  and solves the initial value problem

$$\begin{cases} \partial_t \mathbf{f}^\infty + \frac{1}{\varepsilon} v \cdot \nabla_x \mathbf{f}^\infty = \frac{1}{\varepsilon^2} \mathbf{L}^\varepsilon(\mathbf{f}^\infty) + \frac{1}{\varepsilon} \mathbf{Q}(\mathbf{f}^\infty, \mathbf{f}^\infty) + \mathbf{S}^\varepsilon, \\ \mathbf{f}^\infty|_{t=0} = \mathbf{f}^{\text{in}}. \end{cases}$$

This proves our result on the interval  $[0, T_0]$ . Moreover,  $\mathbf{f}^\infty$  satisfies

$$\|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^\infty)\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq C^{\mathbf{T}} \delta_{\text{MS}}, \quad \forall t \in [0, T_0],$$

and the estimate  $\|\mathbf{f}^\infty\|_{\mathcal{H}_\varepsilon^s} \leq \delta_B$ , thanks to Corollary 3.3.13. By simply restarting this procedure on a new time interval  $[T_0, 2T_0]$  using  $\mathbf{f}^\infty(T_0)$  as initial datum and considering the corresponding functional  $E_{[T_0, 2T_0]}$ , one can repeat the previous computations, so that we recover the existence of a solution  $\mathbf{f} \in C^0(\mathbb{R}_+; H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}))$ , as desired. In particular, thanks to the *a priori* estimates that we previously established, this solution satisfies the uniform control

$$\|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s}^2 \leq \delta_B, \quad \forall t \geq 0,$$

holding for any  $\varepsilon \in (0, \varepsilon_0]$ .

The positivity of the solution  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{f}$  is finally showed using a standard method, which can be found for example in [45, Section 6.3]. This ends the proof.  $\square$

Finally, the constructed solution is unique, providing the full Cauchy theory of our problem.

**Proposition 3.3.16.** *Let  $s \geq s_0$  and consider a function  $\mathbf{f}^{\text{in}}$  satisfying the assumptions of Proposition 3.3.15. There exist  $\bar{\delta}_{MS} > 0$  and  $\varepsilon_0 \in (0, 1]$  such that, if  $\mathbf{f}$  and  $\mathbf{g}$  are two solutions of (3.1.11) having the same initial datum  $\mathbf{f}^{\text{in}}$ , then  $\mathbf{f} = \mathbf{g}$ .*

*Proof.* As in the proof of the previous result, fix initially a time

$$T_0 = \frac{\delta_B \min \left\{ 1, \frac{K_0^{(s)}}{2} \right\}}{4C_s^s \delta_{MS}}.$$

Next, define  $\mathbf{h} = \mathbf{f} - \mathbf{g}$ . Subtracting the equations satisfied by  $\mathbf{f}$  and  $\mathbf{g}$ , we see that  $\mathbf{h}$  is solution on  $[0, T_0] \times \mathbb{T}^3 \times \mathbb{R}^3$  of

$$\begin{cases} \partial_t \mathbf{h} + \frac{1}{\varepsilon} v \cdot \nabla_x \mathbf{h} = \frac{1}{\varepsilon^2} \mathbf{L}^\varepsilon(\mathbf{h}) + \frac{1}{\varepsilon} \left( \mathbf{Q}(\mathbf{h}, \mathbf{f}) + \mathbf{Q}(\mathbf{g}, \mathbf{h}) \right), \\ \mathbf{h}|_{t=0} = 0. \end{cases}$$

The idea is to derive similar estimates to the ones obtained in the proof of the previous result. For this, note the linear part obeys the same upper bounds, and for the nonlinear terms we shall again use estimates (3.3.15) of Lemma 3.3.7.

More precisely, using the *a priori* estimate of Proposition 3.3.12, we get

$$\begin{aligned} \frac{d}{dt} \|\mathbf{h}\|_{\mathcal{H}_\varepsilon^s}^2 &\leq -K_0^{(s)} \|\mathbf{h}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 + K_1^{(s)} \left( \mathcal{G}_x^s(\mathbf{h}, \mathbf{f})^2 + \mathcal{G}_x^s(\mathbf{g}, \mathbf{h})^2 \right) \\ &\quad + \varepsilon^2 K_2^{(s)} \left( \mathcal{G}_{x,v}^s(\mathbf{h}, \mathbf{f})^2 + \mathcal{G}_{x,v}^s(\mathbf{g}, \mathbf{h})^2 \right). \end{aligned}$$

The terms inside the parentheses are then bounded in the same way as before, using (3.3.15) and the norm equivalences provided by (3.3.40). Skipping the computations and denoting  $E = E_{[0, T_0]}$ , we recover the existence of a positive constant  $\tilde{K}$  such that

$$\begin{aligned} \frac{d}{dt} \|\mathbf{h}\|_{\mathcal{H}_\varepsilon^s}^2 &\leq \left( \tilde{K} \left( \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s}^2 + \|\mathbf{g}\|_{\mathcal{H}_\varepsilon^s}^2 \right) - K_0^{(s)} \right) \|\mathbf{h}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 \\ &\quad + \tilde{K} \left( \|\mathbf{f}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 + \|\mathbf{g}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 \right) \|\mathbf{h}\|_{\mathcal{H}_\varepsilon^s}^2 \\ &\leq \left( \tilde{K} \left( E(\mathbf{f}) + E(\mathbf{g}) \right) - K_0^{(s)} \right) \|\mathbf{h}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 \\ &\quad + \tilde{K} \left( \|\mathbf{f}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 + \|\mathbf{g}\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 \right) E(\mathbf{h}). \end{aligned}$$

In particular, since  $\mathbf{f}$  is a solution of the Boltzmann multi-species equation (3.1.11), we have seen previously that it satisfies the estimate  $E(\mathbf{f}) \leq \delta_B$  on  $[0, T_0]$ , and the same holds for  $\mathbf{g}$ . Therefore, choosing initially  $\delta_B \leq K_0^{(s)}/4\tilde{K}$  and integrating on  $[0, t]$ , with  $t \leq T_0$ , since  $\mathbf{h}^{\text{in}} = 0$  we obtain this time

$$\|\mathbf{h}\|_{\mathcal{H}_\varepsilon^s}^2 + \frac{K_0^{(s)}}{2} \int_0^t \|\mathbf{h}(\tau)\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 d\tau \leq \tilde{K} E(\mathbf{h}) \left( E(\mathbf{f}) + E(\mathbf{g}) \right),$$

from which immediately follows that

$$E(\mathbf{h}) \leq \frac{2\tilde{K}\delta_B}{\min\left\{1, \frac{K_0^{(s)}}{2}\right\}} E(\mathbf{h}).$$

Taking  $\delta_B > 0$  sufficiently small allows to conclude that  $E(\mathbf{h}) = 0$ , and thus  $\mathbf{f} = \mathbf{g}$  for any time  $t \in [0, T_0]$ . We can then repeat the computations on the time interval  $[T_0, 2T_0]$  with  $E = E_{[T_0, 2T_0]}$ , recovering the same conclusions. An iteration of this procedure finally allows to deduce that  $\mathbf{f} = \mathbf{g}$  for all  $t \geq 0$ . This ends the proof.  $\square$

**Step 4 – Conclusion.** Theorem 3.3.1 is a direct gathering of Propositions 3.3.12, 3.3.15, 3.3.16 and Corollary 3.3.13. Moreover, thanks to Theorems 3.2.1 and 3.3.1, both the local Maxwellian  $\mathbf{M}^\varepsilon$  and the perturbation  $\mathbf{f}$  are well-defined, are unique and exist globally in time. Therefore, we can now reconstruct  $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon\mathbf{f}$ , which is the unique global weak solution of the Boltzmann multi-species equation (3.1.11), perturbed around the non-equilibrium state  $\mathbf{M}^\varepsilon$ . To conclude, since the perturbation  $\mathbf{f}$  is uniformly bounded in the  $\mathcal{H}_\varepsilon^s$  norm by the constant  $\delta_B$  (independent of  $\varepsilon$  and computed in the Corollary 3.3.13), we also deduce the stability property

$$\|\mathbf{F}^\varepsilon - \mathbf{M}^\varepsilon\|_{\mathcal{H}_\varepsilon^s} = \varepsilon \|\mathbf{f}\|_{\mathcal{H}_\varepsilon^s} \leq \varepsilon\delta_B, \quad \forall \varepsilon \in (0, \varepsilon_0],$$

which finally guarantees a rigorous derivation of the Maxwell-Stefan system (3.1.7)–(3.1.9), in the diffusive limit  $\varepsilon \rightarrow 0$  of the Boltzmann multi-species equation (3.1.6).

## 3.4 Technical proofs of the hypocoercivity properties

In this last section we collect all the proofs of the lemmata which lead to the hypocoercive structure of our model.

Since, in what follows, we often estimate the Euclidean distance between  $\mathbf{M}^\varepsilon$  and  $\boldsymbol{\mu}$ , in order to enlighten our computations we here introduce the local and global Maxwellians  $\mathcal{M}^\varepsilon = \mathbf{M}_{(1, \varepsilon \mathbf{u}, 1)}$  and  $\mathcal{M} = \mathbf{M}_{(1, 0, 1)}$  which will allow us to write  $\boldsymbol{\mu} = \mathbf{c}_\infty \mathcal{M}$  and, in this way, separate  $\mathbf{M}^\varepsilon$  into a close-to-equilibrium part and a lower order term as  $\mathbf{M}^\varepsilon = \mathbf{c}_\infty \mathcal{M}^\varepsilon + \varepsilon \tilde{\mathbf{c}} \mathcal{M}^\varepsilon$ .

### 3.4.1 Proof of Lemma 3.3.3

Fix  $\delta \in (0, 1)$ . In order to prove (3.3.8), we initially observe that, since  $M_i^\varepsilon = c_i \mathcal{M}_i^\varepsilon$ , we can apply to  $\mathcal{M}_i^\varepsilon$  similar estimates to the ones derived in Lemma 2.4.1 of Chapter 2 to obtain for any  $1 \leq i \leq N$  the upper bound

$$M_i^\varepsilon(t, x, v) \leq C_\delta^{\text{up}} \left( 1 + \exp \left\{ \frac{4m_i}{1-\delta} \varepsilon^2 |u_i(t, x)|^2 \right\} \right) c_i \mathcal{M}_i^\delta(v), \quad t \geq 0, x \in \mathbb{T}^3, v \in \mathbb{R}^3, \quad (3.4.1)$$

where

$$C_\delta^{\text{up}} = \max_{1 \leq i \leq N} \left( \frac{m_i}{2\pi} \right)^{\frac{3(1-\delta)}{2}} \left( \sup_{|v| \in \mathbb{R}_+} e^{-(1-\delta)\frac{m_i}{4}|v|^2} + 1 \right) > 0.$$

Similarly we can recover a lower bound for  $M_i^\varepsilon$  as follows. For any  $1 \leq i \leq N$ , we can write

$$\mathcal{M}_i^\varepsilon(t, x, v) = \mathcal{M}_i^{1/\delta}(v) \mathcal{M}_i^\varepsilon(t, x, v) \mathcal{M}_i^{-1/\delta}(v), \quad t \geq 0, x \in \mathbb{T}^3, v \in \mathbb{R}^3.$$

Then, the product  $\mathcal{M}^\varepsilon \mathcal{M}_i^{-1/\delta}$  can be lower estimated as

$$\mathcal{M}_i^\varepsilon(v) \mathcal{M}_i^{-1/\delta}(v) \geq \left(\frac{m_i}{2\pi}\right)^{\frac{3(\delta-1)}{2\delta}} \exp\left\{\frac{m_i(1-\delta)}{2\delta}|v|^2 - m_i\varepsilon|v||u_i| - \varepsilon^2 \frac{m_i}{2}|u_i|^2\right\},$$

where we have dropped the dependence on both variables  $(t, x)$  for the sake of simplicity. We then distinguish two cases.

1. For  $|v| \geq \frac{4\delta\varepsilon|u_i|}{1-\delta}$ , we have

$$\mathcal{M}_i^\varepsilon(v) \mathcal{M}_i^{-1/\delta}(v) \geq \left(\frac{m_i}{2\pi}\right)^{\frac{3(\delta-1)}{2\delta}} \exp\left\{-\frac{m_i}{2}\varepsilon^2|u_i|^2\right\}.$$

2. For  $|v| \leq \frac{4\delta\varepsilon|u_i|}{1-\delta}$ , we get

$$\mathcal{M}_i^\varepsilon(v) \mathcal{M}_i^{-1/\delta}(v) \geq \left(\frac{m_i}{2\pi}\right)^{\frac{3(\delta-1)}{2\delta}} \exp\left\{-4m_i \frac{\delta}{1-\delta} \varepsilon^2 |u_i|^2 - \frac{m_i}{2} \varepsilon^2 |u_i|^2\right\}.$$

These estimates allow to deduce that

$$M_i^\varepsilon(v) \geq C_\delta^{\text{low}} \exp\left\{-m_i \frac{7\delta+1}{2(1-\delta)} \varepsilon^2 |u_i|^2\right\} c_i \mathcal{M}_i^{1/\delta}, \quad \forall v \in \mathbb{R}^3, \quad (3.4.2)$$

where we simply set

$$C_\delta^{\text{low}} = \min_{1 \leq i \leq N} \left(\frac{m_i}{2\pi}\right)^{\frac{3(\delta-1)}{2\delta}} > 0.$$

Gathering now (3.4.1) and (3.4.2), it is easy to deduce that, for any  $1 \leq i, j \leq N$ , there exist two positive constants  $\bar{\nu}_{ij}^{(\delta)}, \tilde{\nu}_{ij}^{(\delta)}$  such that, for all  $v \in \mathbb{R}^3$ ,

$$0 < \bar{\nu}_{ij}^{(\delta)} e^{-m_j \frac{7\delta+1}{2(1-\delta)} \varepsilon^2 |u_j|^2} c_j \langle v \rangle^\gamma \leq \nu_{ij}^\varepsilon(v) \leq \tilde{\nu}_{ij}^{(\delta)} \left(1 + e^{\frac{4m_j}{1-\delta} \varepsilon^2 |u_j|^2}\right) c_j \langle v \rangle^\gamma.$$

This in turns implies that, for any  $1 \leq i \leq N$ , there also exist  $\bar{\nu}_i^{(\delta)}, \tilde{\nu}_i^{(\delta)} > 0$  such that, for all  $v \in \mathbb{R}^3$ ,

$$\begin{aligned} 0 < \bar{\nu}_i^{(\delta)} \exp\left\{-\max_{1 \leq i \leq N} m_i \frac{7\delta+1}{2(1-\delta)} \varepsilon^2 \|\mathbf{u}\|_{L_t^\infty L_x^\infty}^2\right\} & \left(\min_{1 \leq i \leq N} c_i\right) \langle v \rangle^\gamma \\ & \leq \nu_i^\varepsilon(v) \leq \tilde{\nu}_i^{(\delta)} \left(1 + \exp\left\{\max_{1 \leq i \leq N} m_i \frac{4\varepsilon^2}{1-\delta} \|\mathbf{u}\|_{L_t^\infty L_x^\infty}^2\right\}\right) \|\mathbf{c}\|_{L_t^\infty L_x^\infty} \langle v \rangle^\gamma, \end{aligned} \quad (3.4.3)$$

recalling that  $\min_i c_i > 0$  a.e. on  $\mathbb{R}_+ \times \mathbb{T}^3$ , thanks to Lemma 3.2.13.

Since  $\nu^\varepsilon$  is a multiplicative operator, from these bounds it is finally easy to compute explicitly the values of  $C_1^\nu$  and  $C_2^\nu$  such that

$$C_1^\nu \|\mathbf{f}\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 \leq \langle \nu^\varepsilon(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\mu^{-\frac{1}{2}})} \leq C_2^\nu \|\mathbf{f}\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2$$

is satisfied. Moreover, since  $\langle v \rangle^\gamma \geq 1$ , it is then straightforward that the  $L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})$  norm upper bounds the  $L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm. Thus (3.3.8) is proved for any  $\delta \in (0, 1)$ .

At last, estimate (3.3.9) can be proved in a very similar way using the fact that  $\mathbf{K}^\varepsilon$  can be written under a kernel form and applying (3.4.1) to obtain the same bounds as in Chapter 2. From this and from (3.3.8), using the Cauchy-Schwarz inequality, we infer (3.3.9) by choosing

$$C_1^\varepsilon = C(\delta) \|\mathbf{c}\|_{L_t^\infty L_x^\infty} \left( 1 + \exp \left\{ \max_{1 \leq i \leq N} m_i \frac{4\varepsilon^2}{1 - \delta} \|\mathbf{u}\|_{L_t^\infty L_x^\infty} \right\} \right) \max_{1 \leq i, j \leq N} \sqrt{\frac{\bar{c}_j}{\bar{c}_i}} > 0.$$

Here  $C(\delta)$  is a constant only depending on the masses  $(m_i)_{1 \leq i \leq N}$ , the number of species  $N$  and an arbitrary parameter  $\delta \in (\bar{\delta}, 1)$ , where  $\bar{\delta}$  is fixed as in Chapter 2 independently of  $\varepsilon$ . This concludes the proof.

### 3.4.2 Proof of Lemma 3.3.4

We prove the result in the simple case where  $|\alpha| = |\beta| = 1$  (the case  $|\alpha| = 0$  being included). The general case can then be obtained in a similar way, by iterating our computations.

We first notice that, thanks to our assumptions on the collision kernels  $B_{ij}$ , it is easy to check that  $\nabla_v \nu_i^\varepsilon \in L_v^\infty(\mathbb{R}^3)$  for any  $1 \leq i \leq N$ . In fact, choosing  $\delta \in (0, 1)$  independently of  $\varepsilon$  and using the upper bound (3.4.1) on  $M_j^\varepsilon$ , we obtain, for any  $v \in \mathbb{R}^3$ ,

$$\begin{aligned} |\nabla_v \nu_i^\varepsilon(v)| &= \left| \sum_{j=1}^N \int_{\mathbb{R}^3 \times \mathbb{S}^2} b_{ij}(\cos \vartheta) \gamma |v - v_*|^{\gamma-1} \frac{v - v_*}{|v - v_*|} M_j^\varepsilon(v_*) dv_* d\sigma \right| \\ &\leq C(\delta) \sum_{j=1}^N c_j \int_{\mathbb{R}^3} \gamma |v - v_*|^{\gamma-1} e^{-\delta m_j \frac{|v_*|^2}{2}} dv_* \leq C(\delta) \langle \mathbf{c}, \mathbf{1} \rangle < +\infty, \end{aligned}$$

since  $\gamma \in [0, 1]$  and thus the above integral is clearly finite.

Next, considering the  $(x_k, v_\ell)$  derivatives, we can write

$$\begin{aligned} \langle \partial_{v_\ell} \partial_{x_k} \boldsymbol{\nu}^\varepsilon(\mathbf{f}), \partial_{v_\ell} \partial_{x_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} &= \sum_{i=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} \partial_{v_\ell} (\nu_i^\varepsilon \partial_{x_k} f_i) \partial_{v_\ell} \partial_{x_k} f_i \mu_i^{-1} dx dv \\ &\quad + \sum_{i=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} \partial_{v_\ell} (\partial_{x_k} \nu_i^\varepsilon f_i) \partial_{v_\ell} \partial_{x_k} f_i \mu_i^{-1} dx dv. \end{aligned}$$

Denote by  $I_1$  and  $I_2$ , respectively, the first and second term on the right-hand side. Using Young's inequality, the first term can be estimated as

$$\begin{aligned} I_1 &= \sum_{i=1}^N \left( \int_{\mathbb{T}^3 \times \mathbb{R}^3} \partial_{v_\ell} \nu_i^\varepsilon \partial_{x_k} f_i \partial_{v_\ell} \partial_{x_k} f_i \mu_i^{-1} dx dv + \int_{\mathbb{T}^3 \times \mathbb{R}^3} \nu_i^\varepsilon |\partial_{v_\ell} \partial_{x_k} f_i|^2 \mu_i^{-1} dx dv \right) \\ &\geq \sum_{i=1}^N \left( -\frac{1}{2} \int_{\mathbb{T}^3 \times \mathbb{R}^3} \frac{(\partial_{v_\ell} \nu_i^\varepsilon)^2}{\nu_i^\varepsilon} (\partial_{x_k} f_i)^2 \mu_i^{-1} dx dv + \frac{1}{2} \int_{\mathbb{T}^3 \times \mathbb{R}^3} \nu_i^\varepsilon |\partial_{v_\ell} \partial_{x_k} f_i|^2 \mu_i^{-1} dx dv \right) \\ &\geq C_3^\nu \|\partial_{v_\ell} \partial_{x_k} \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 - C_5^\nu \|\mathbf{f}\|_{H_{x,v}^1(\boldsymbol{\mu}^{-\frac{1}{2}})}^2, \end{aligned}$$



where  $C_3^\nu$  is obtained from (3.4.3) as

$$C_3^\nu = \frac{1}{2} \left( \min_{1 \leq i \leq N} \bar{\nu}_i^{(\delta)} c_i \right) \exp \left\{ - \max_{1 \leq i \leq N} m_i \frac{7\delta + 1}{2(1 - \delta)} \varepsilon^2 \|\mathbf{u}\|_{L_t^\infty L_x^\infty} \right\} > 0,$$

and

$$C_5^\nu = \max_{1 \leq i \leq N} \sup_{v \in \mathbb{R}^3} \frac{(\partial_{v_\ell} \nu_i^\varepsilon)^2}{2\nu_i^\varepsilon}$$

is positive and finite thanks again to the lower bound (3.4.3) and the fact that  $\nabla_v \nu_i^\varepsilon$  belongs to  $L_v^\infty(\mathbb{R}^3)$  for any  $1 \leq i \leq N$ .

To estimate the second term, we first notice that from  $\mathbf{M}^\varepsilon = \mathbf{c}_\infty \mathcal{M}^\varepsilon + \varepsilon \tilde{\mathbf{c}} \mathcal{M}^\varepsilon$  we get, for any  $(t, x, v) \in \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ ,

$$\begin{aligned} & \partial_{x_k} \nu_i^\varepsilon(t, x, v) \\ &= \sum_{j=1}^N \int_{\mathbb{R}^3 \times \mathbb{S}^2} b_{ij}(\cos \vartheta) |v - v_*|^\gamma \partial_{x_k} M_j^\varepsilon(v_*) dv_* d\sigma \\ &= \varepsilon \sum_{j=1}^N \int_{\mathbb{R}^3 \times \mathbb{S}^2} b_{ij}(\cos \vartheta) |v - v_*|^\gamma \left( \partial_{x_k} \tilde{c}_j + m_j c_j(v_* - \varepsilon u_j) \cdot \partial_{x_k} u_j \right) \mathcal{M}_j^\varepsilon(v_*) dv_* d\sigma \\ &= \varepsilon \tilde{\nu}_i^\varepsilon(t, x, v), \end{aligned}$$

hence  $\tilde{\nu}_i^\varepsilon$  and  $\nu_i^\varepsilon$  have the same structure. In particular, as done for  $\nu_i^\varepsilon$ , it is easy to show that  $\nabla_v \tilde{\nu}_i^\varepsilon \in L_v^\infty(\mathbb{R}^3)$  and that the following upper bound, similar to (3.4.3), is satisfied for all  $v \in \mathbb{R}^3$ :

$$\begin{aligned} \tilde{\nu}_i^\varepsilon(v) &\leq C_i(\delta) \exp \left\{ \max_{1 \leq i \leq N} m_i \frac{7 + \delta}{2(1 - \delta)} \varepsilon^2 \|\mathbf{u}\|_{L_t^\infty L_x^\infty}^2 \right\} \\ &\quad \times \left( \|\partial_{x_k} \tilde{\mathbf{c}}\|_{L_t^\infty L_x^\infty} + \|\mathbf{c}\|_{L_t^\infty L_x^\infty} (1 + \|\mathbf{u}\|_{L_t^\infty L_x^\infty}) \|\partial_{x_k} \mathbf{u}\|_{L_t^\infty L_x^\infty} \right) \langle v \rangle^\gamma. \end{aligned} \quad (3.4.4)$$

Note that, in this case, we are no more able to prove a lower bound for  $\tilde{\nu}_i^\varepsilon$ , as it was done in (3.4.3) for  $\nu_i^\varepsilon$ . From this lack of positivity comes the last term in the estimate. In fact, using again Young's inequality, we easily see that  $I_2$  can be estimated as

$$\begin{aligned} I_2 &= \varepsilon \sum_{i=1}^N \left( \int_{\mathbb{T}^3 \times \mathbb{R}^3} \partial_{v_\ell} \tilde{\nu}_i^\varepsilon f_i \partial_{v_\ell} \partial_{x_k} f_i \mu_i^{-1} dx dv + \int_{\mathbb{T}^3 \times \mathbb{R}^3} \tilde{\nu}_i^\varepsilon \partial_{v_\ell} f_i \partial_{v_\ell} \partial_{x_k} f_i \mu_i^{-1} dx dv \right) \\ &\geq \varepsilon \sum_{i=1}^N \left( -\frac{1}{2} \int_{\mathbb{T}^3 \times \mathbb{R}^3} \frac{(\partial_{v_\ell} \tilde{\nu}_i^\varepsilon)^2}{\nu_i^\varepsilon} f_i^2 \mu_i^{-1} dx dv - \frac{1}{2} \int_{\mathbb{T}^3 \times \mathbb{R}^3} \tilde{\nu}_i^\varepsilon (\partial_{v_\ell} f_i)^2 \mu_i^{-1} dx dv \right. \\ &\quad \left. - \frac{1}{2} \int_{\mathbb{T}^3 \times \mathbb{R}^3} (\nu_i^\varepsilon + \tilde{\nu}_i^\varepsilon) |\partial_{v_\ell} \partial_{x_k} f_i|^2 \mu_i^{-1} dx dv \right) \\ &\geq -\varepsilon C_4^\nu \|\partial_{v_\ell} \partial_{x_k} \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{7}{2}} \mu^{-\frac{1}{2}})}^2 - \varepsilon C_6^\nu \|\mathbf{f}\|_{H_{x,v}^1(\mu^{-\frac{1}{2}})}^2 - \varepsilon C_7^\nu \|\partial_{v_\ell} \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{7}{2}} \mu^{-\frac{1}{2}})}, \end{aligned}$$

where  $C_4^\nu, C_7^\nu$  are easily recovered from (3.4.3) and (3.4.4), and

$$C_6^\nu = \max_{1 \leq i \leq N} \sup_{v \in \mathbb{R}^3} \frac{(\partial_{v_\ell} \tilde{\nu}_i^\varepsilon)^2}{2\nu_i^\varepsilon} > 0.$$

Gathering the estimates for  $I_1$  and  $I_2$  concludes the proof.

### 3.4.3 Proof of Lemma 3.3.5

We prove the result in the simplest case where  $|\alpha| = 0$  and  $|\beta| = 1$ . The extension to the general case is again straightforward. We emphasize that compared to the usual case when the Maxwellian only depends on  $v$ ,  $x$ -derivatives of  $\mathbf{M}^\varepsilon$  generate new terms involving products of the form  $\varepsilon \partial_x^{\alpha'} \mathbf{u} \partial_x^\alpha \tilde{\mathbf{c}}$ , displaying a lower order in  $\varepsilon$ .

We want to estimate the term

$$\langle \nabla_v \mathbf{K}^\varepsilon(\mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\mu^{-\frac{1}{2}})} = \sum_{i=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} \nabla_v K_i^\varepsilon(\mathbf{f}) \nabla_v f_i \mu_i^{-1} dx dv,$$

where, for any  $1 \leq i \leq N$ ,  $K_i^\varepsilon$  is written under its kernel form (explicitly recovered in Appendix B) as

$$K_i^\varepsilon(\mathbf{f})(v) = \sum_{j=1}^N \left\{ \int_{\mathbb{R}^3} \kappa_{ij}^{(1)}(v, v_*) f_j^* dv_* + \int_{\mathbb{R}^3} \kappa_{ij}^{(2)}(v, v_*) f_i^* dv_* - \int_{\mathbb{R}^3} \kappa_{ij}^{(3)}(v, v_*) f_j^* dv_* \right\}.$$

For any fixed  $i, j$ , we shall treat separately the three kernels.

**Step 1 - Estimates for  $\kappa_{ij}^{(1)}$ .** Starting from  $\kappa_{ij}^{(1)}$ , we recall that its full explicit expression is given in Appendix B by (B.1.1). We compute its  $v$ -derivatives and immediately note that the singularity of the operator coming from  $|v - v_*|$  imposes to introduce a proper splitting (depending on a small parameter) in order to deal with a smooth part that we can derive infinitely many times and a remainder part (taking into account the region where  $v - v_*$  is close to 0) which goes to zero with the small parameter. Let us relabel the relative velocity  $\eta = v - v_*$  and choose  $v$  and  $\eta$  as new variables of  $\kappa_{ij}^{(1)}$ , rewriting  $v_* = v - \eta$ . Thus, denoting  $\bar{R} = R(v, \eta)$  and  $\bar{O} = O(v, \eta)$  the quantities

$$\begin{aligned} \bar{R} &= \frac{m_j}{|m_i - m_j|} |\eta|, \\ \bar{O} &= \frac{m_i}{m_i - m_j} v - \frac{m_j}{m_i - m_j} (v - \eta), \end{aligned}$$

defined for  $i \neq j$ , the operator  $\kappa_{ij}^{(1)}$  reads

$$\begin{aligned} \kappa_{ij}^{(1)}(v, \eta) &= C_{ij} c_i |\eta|^\gamma \int_{\mathbb{S}^2} \frac{b_{ij} \left( \omega \cdot \frac{\eta}{|\eta|} \right)}{\left| \frac{m_i^2 + m_j^2}{(m_i - m_j)^2} + \frac{2m_i m_j}{(m_i - m_j)|m_i - m_j|} \left( \omega \cdot \frac{\eta}{|\eta|} \right) \right|^{1-\gamma}} \\ &\quad \times e^{-\frac{m_i}{2} |\bar{R}\omega + \bar{O}|^2 + \varepsilon m_i (\bar{R}\omega + \bar{O}) \cdot u_i - \varepsilon^2 \frac{m_i}{2} |u_i|^2} d\omega. \end{aligned}$$

In particular,

$$b_{ij} \left( \omega \cdot \frac{\eta}{|\eta|} \right) = b_{ij} \left( \frac{\frac{2m_i m_j}{(m_i - m_j)^2} + \frac{m_i^2 + m_j^2}{(m_i - m_j)|m_i - m_j|} \left( \omega \cdot \frac{\eta}{|\eta|} \right)}{\frac{m_i^2 + m_j^2}{(m_i - m_j)^2} + \frac{2m_i m_j}{(m_i - m_j)|m_i - m_j|} \left( \omega \cdot \frac{\eta}{|\eta|} \right)} \right),$$

and

$$\begin{aligned} |\bar{R}\omega + \bar{O}|^2 &= \frac{2m_j^2}{(m_i - m_j)^2} |\eta|^2 + \frac{2m_j |\eta|}{|m_i - m_j|} (v \cdot \omega) + \frac{2m_j^2 |\eta|}{(m_i - m_j) |m_i - m_j|} (\eta \cdot \omega) \\ &\quad + |v|^2 + \frac{2m_j}{m_i - m_j} (v \cdot \eta), \\ (\bar{R}\omega + \bar{O}) \cdot u_i &= \frac{m_j}{|m_i - m_j|} |\eta| (\omega \cdot u_i) + v \cdot u_i + \frac{m_j}{m_i - m_j} (\eta \cdot u_i). \end{aligned}$$

The operator  $\kappa_{ij}^{(1)}(v, \eta)$  is clearly regular with respect to the variable  $v$ , thus we only need to ensure that we can take derivatives also with respect to  $\eta$ . For some small parameter  $\xi > 0$ , let us introduce a mollified indicator function  $\mathbb{1}_{\{|\cdot| \geq \xi\}}$  and define the splitting

$$\kappa_{ij}^{(1)} = \kappa_{ij}^{(1),S} + \kappa_{ij}^{(1),R},$$

where we have called the smooth part

$$\kappa_{ij}^{(1),S}(v, \eta) = \mathbb{1}_{\{|\eta| \geq \xi\}} \kappa_{ij}^{(1)}(v, \eta),$$

and  $\kappa_{ij}^{(1),R}$  is the remainder. It is straightforward to check that  $\kappa_{ij}^{(1),S}(v, \eta)$  is smooth in both variables  $v$  and  $\eta$ , and that  $\kappa_{ij}^{(1),R}$  is integrable with respect to  $\eta$  near 0. More precisely, one can prove (see the proofs of Lemmata 2.4.4 and 2.4.6 of Chapter 2) that there exists  $\bar{\delta} \in (0, 1)$ , depending on  $\|\mathbf{u}\|$  and  $\|\mathbf{c}\|$  but not on  $\varepsilon$ , such that  $\kappa_{ij}^{(1),R}$  is uniformly bounded with respect to  $v$ , namely

$$\kappa_{ij}^{(1),R}(v, \eta) \sqrt{\frac{\mu_j(v - \eta)}{\mu_i(v)}} \leq C_{ij}(\delta) |\eta|^\gamma e^{-C(\delta)|\eta|^2}, \quad \forall v \in \mathbb{R}^3,$$

where  $C_{ij}(\delta), C(\delta) > 0$  are two explicitly computable constants depending on an arbitrary parameter  $\delta \in (\bar{\delta}, 1)$ . This last fact allows to easily deduce that

$$\left\| \kappa_{ij}^{(1),R}(v, \eta) \sqrt{\frac{\mu_j(v - \eta)}{\mu_i(v)}} \right\|_{L_\eta^1} \leq C_{ij}^{(1)}(\delta) \xi^{\gamma+3}, \quad \forall v \in \mathbb{R}^3. \quad (3.4.5)$$

Now, setting

$$W_{ij}^{(1)} \left( \omega \cdot \frac{\eta}{|\eta|} \right) = \left| \frac{m_i^2 + m_j^2}{(m_i - m_j)^2} + \frac{2m_i m_j}{(m_i - m_j) |m_i - m_j|} \left( \omega \cdot \frac{\eta}{|\eta|} \right) \right|^{\gamma-1}$$

to ease the computations, we can take the  $\eta$ -derivative of  $\kappa_{ij}^{(1),S}$  to obtain

$$\begin{aligned} \nabla_{\eta} \kappa_{ij}^{(1),S}(v, \eta) &= C_{ij} \nabla_{\eta} \mathbf{1}_{\{|\eta| \geq \xi\}} |\eta|^{\gamma} \int_{\mathbb{S}^2} b_{ij} W_{ij}^{(1)} M_i^{\varepsilon}(\bar{R}\omega + \bar{O}) d\omega \\ &\quad + C_{ij} \mathbf{1}_{\{|\eta| \geq \xi\}} \nabla_{\eta} |\eta|^{\gamma} \int_{\mathbb{S}^2} b_{ij} W_{ij}^{(1)} M_i^{\varepsilon}(\bar{R}\omega + \bar{O}) d\omega \\ &\quad + C_{ij} \mathbf{1}_{\{|\eta| \geq \xi\}} |\eta|^{\gamma} \int_{\mathbb{S}^2} \nabla_{\eta} b_{ij} W_{ij}^{(1)} M_i^{\varepsilon}(\bar{R}\omega + \bar{O}) d\omega \\ &\quad + C_{ij} \mathbf{1}_{\{|\eta| \geq \xi\}} |\eta|^{\gamma} \int_{\mathbb{S}^2} b_{ij} \nabla_{\eta} W_{ij}^{(1)} M_i^{\varepsilon}(\bar{R}\omega + \bar{O}) d\omega \\ &\quad + C_{ij} \mathbf{1}_{\{|\eta| \geq \xi\}} |\eta|^{\gamma} \int_{\mathbb{S}^2} b_{ij} W_{ij}^{(1)} \nabla_{\eta} M_i^{\varepsilon}(\bar{R}\omega + \bar{O}) d\omega \\ &:= I_{1,1}^S + I_{1,2}^S + I_{1,3}^S + I_{1,4}^S + I_{1,5}^S. \end{aligned}$$

Direct computations yield the four derivatives

$$(1) \quad \nabla_{\eta} |\eta|^{\gamma} = \gamma |\eta|^{\gamma-1} \frac{\eta}{|\eta|},$$

$$(2) \quad \nabla_{\eta} b_{ij} \left( \omega \cdot \frac{\eta}{|\eta|} \right) = b'_{ij} \left( \omega \cdot \frac{\eta}{|\eta|} \right) \frac{\frac{(m_i+m_j)^2}{(m_i-m_j)|m_i-m_j|} \left( \frac{\omega}{|\eta|} - \frac{\eta \cdot \omega}{|\eta|^2} \frac{\eta}{|\eta|} \right)}{\left( \frac{m_i^2+m_j^2}{(m_i-m_j)^2} + \frac{2m_i m_j}{(m_i-m_j)|m_i-m_j|} \left( \omega \cdot \frac{\eta}{|\eta|} \right) \right)^2},$$

$$(3) \quad \nabla_{\eta} W_{ij}^{(1)} \left( \omega \cdot \frac{\eta}{|\eta|} \right) = \frac{\frac{2(\gamma-1)m_i m_j}{(m_i-m_j)|m_i-m_j|} \left( \frac{\omega}{|\eta|} - \frac{\eta \cdot \omega}{|\eta|^2} \frac{\eta}{|\eta|} \right)}{\left| \frac{m_i^2+m_j^2}{(m_i-m_j)^2} + \frac{2m_i m_j}{(m_i-m_j)|m_i-m_j|} \left( \omega \cdot \frac{\eta}{|\eta|} \right) \right|^{2-\gamma}},$$

$$(4) \quad \nabla_{\eta} M_i^{\varepsilon}(\bar{R}\omega + \bar{O}) = -\frac{m_i}{2} M_i^{\varepsilon}(\bar{R}\omega + \bar{O}) \left( \nabla_{\eta} |\bar{R}\omega + \bar{O}|^2 - 2\varepsilon \nabla_{\eta} \left( (\bar{R}\omega + \bar{O}) \cdot u_i \right) \right),$$

where

$$\begin{aligned} \nabla_{\eta} |\bar{R}\omega + \bar{O}|^2 &= \frac{4m_j^2}{(m_i-m_j)^2} \eta + \frac{2m_j}{|m_i-m_j|} \frac{\eta}{|\eta|} (v \cdot \omega) + \frac{2m_j}{m_i-m_j} v \\ &\quad + \frac{2m_j^2}{(m_i-m_j)|m_i-m_j|} \left( \frac{\eta}{|\eta|} (\eta \cdot \omega) + |\eta| \omega \right), \end{aligned}$$

and

$$\nabla_{\eta} \left( (\bar{R}\omega + \bar{O}) \cdot u_i \right) = \frac{m_j}{|m_i-m_j|} \frac{\eta}{|\eta|} (\omega \cdot u_i) + \frac{m_j}{m_i-m_j} u_i.$$

Our aim is now to bound each term  $I_{1,k}^S$  uniformly with respect to  $v \in \mathbb{R}^3$ . The estimate for  $I_{1,1}^S$  is straightforward, since  $|b_{ij}| \leq C$  from Grad's cutoff assumption we have made on the collision kernels, and

$$\left| \frac{m_i^2 + m_j^2}{(m_i - m_j)^2} + \frac{2m_i m_j}{(m_i - m_j)|m_i - m_j|} \left( \omega \cdot \frac{\eta}{|\eta|} \right) \right|^{\gamma-1} \leq \left| \frac{m_i^2 + m_j^2 - 2m_i m_j}{(m_i - m_j)^2} \right|^{\gamma-1} = 1,$$

thanks to the hypothesis that  $\gamma \in [0, 1]$ . Thus,  $|W_{ij}^{(1)}| \leq 1$  and we can apply the upper bound (3.4.1) for the local Maxwellian  $M_i^\varepsilon$  to initially infer that

$$|I_{1,1}^S| \leq C(\delta_1)c_i|\eta|^\gamma \int_{\mathbb{S}^2} \mathcal{M}_i^{\delta_1}(\bar{R}\omega + \bar{O})d\omega,$$

for any  $\delta_1 \in (0, 1)$ . Then, using the same estimates as in [45, Lemma 5.1], we recover the bound

$$|I_{1,1}^S| \leq C(\delta_1)c_i|\eta|^\gamma e^{-\delta_1\lambda(m_i, m_j)|\eta|^2 - \delta_1\lambda(m_i, m_j)\frac{|\eta|^2 - 2(v \cdot \eta)|^2}{|\eta|^2}} \sqrt{\frac{\mathcal{M}_i^{\delta_1}(v)}{\mathcal{M}_j^{\delta_1}(v - \eta)}}.$$

For  $I_{1,2}^S$ ,  $I_{1,3}^S$  and  $I_{1,4}^S$ , we obtain a similar result, since

$$\nabla_\eta |\eta|^\gamma \leq \gamma |\eta|^{\gamma-1}, \quad \nabla_\eta b_{ij} \leq C_{ij} |\eta|^{-1} \quad \text{and also} \quad \nabla_\eta W_{ij}^{(1)} \leq C_{ij} |\eta|^{-1},$$

thanks to the assumption that  $|b'_{ij}(\cos \vartheta)| \leq C$ . Thus, for  $k \in \{2, 3, 4\}$ , we deduce that

$$|I_{1,k}^S| \leq C(\delta_k)c_i|\eta|^{\gamma-1} e^{-\delta_k\lambda(m_i, m_j)\left(|\eta|^2 - \frac{|\eta|^2 - 2(v \cdot \eta)|^2}{|\eta|^2}\right)} \sqrt{\frac{\mathcal{M}_i^{\delta_k}(v)}{\mathcal{M}_j^{\delta_k}(v - \eta)}},$$

for any  $\delta_k \in (0, 1)$ ,  $k = 2, 3, 4$ . A bit different is the last term  $I_{1,5}^S$ . We observe that

$$\nabla_\eta |\bar{R}\omega + \bar{O}|^2 \leq C_{ij}(|\eta| + |v|) \quad \text{and} \quad \nabla_\eta \left( (\bar{R}\omega + \bar{O}) \cdot u_i \right) \leq C_{ij}|u_i|,$$

thus

$$\nabla_\eta M_i^\varepsilon(\bar{R}\omega + \bar{O}) \leq C_{ij}(\delta_5)c_i(|\eta| + |v| + \varepsilon|u_i|)\mathcal{M}_i^{\delta_5}(\bar{R}\omega + \bar{O}),$$

for any  $\delta_5 \in (0, 1)$ . Therefore, since  $\varepsilon \leq 1$ , we can upper bound the last term as

$$|I_{1,5}^S| \leq C(\delta_5)c_i|\eta|^\gamma (|\eta| + |v| + |u_i|) e^{-\delta_5\lambda(m_i, m_j)\left(|\eta|^2 + \frac{|\eta|^2 - 2(v \cdot \eta)|^2}{|\eta|^2}\right)} \sqrt{\frac{\mathcal{M}_i^{\delta_5}(v)}{\mathcal{M}_j^{\delta_5}(v - \eta)}}.$$

Gathering the estimates on  $I_{1,k}^S$ ,  $k \in \{1, \dots, 5\}$ , and, in particular, carefully choosing the parameter  $\delta_5 \in (0, 1)$  in order to control the term in  $|v|$ , the computations carried out in Chapter 2 directly apply and provide the uniform bound

$$\begin{aligned} & \left| \nabla_\eta \kappa_{ij}^{(1),S}(v, \eta) \right| \sqrt{\frac{\mu_j(v - \eta)}{\mu_i(v)}} \\ & \leq C_{ij}(\delta) \sqrt{\frac{\bar{c}_j}{\bar{c}_i}} \|\mathbf{c}\|_{L_t^\infty L_x^\infty} \left( 1 + \|\mathbf{u}\|_{L_t^\infty L_x^\infty} \right) (1 + |\eta|^{\gamma-1} + |\eta|^{\gamma+1} + |\eta|^\gamma) e^{-C(\delta)|\eta|^2}, \end{aligned} \quad (3.4.6)$$

holding for any  $v \in \mathbb{R}^3$  and any  $\delta \in (\bar{\delta}, 1)$ , where  $\bar{\delta} \in (0, 1)$  is fixed independently of  $\varepsilon$ .

In a similar way, we can estimate the  $v$ -derivatives of  $\kappa_{ij}^{(1),S}$  and  $\kappa_{ij}^{(1),R}$ . It is even simpler in this case, since the only dependence on  $v$  inside these operators appears in

the Maxwellian  $M_i^\varepsilon(\bar{R}\omega + \bar{O})$ . Looking at  $\nabla_v \kappa_{ij}^{(1),S}$  (for  $\nabla_v \kappa_{ij}^{(1),R}$  the same computations will apply), we easily get

$$\nabla_v \kappa_{ij}^{(1),S}(v, \eta) = C_{ij} \mathbb{1}_{\{|\eta| \geq \xi\}} |\eta|^\gamma \int_{\mathbb{S}^2} b_{ij} W_{ij}^{(1)} \nabla_v M_i^\varepsilon(\bar{R}\omega + \bar{O}) d\omega,$$

where this time

$$\nabla_v M_i^\varepsilon(\bar{R}\omega + \bar{O}) = -\frac{m_i}{2} M_i^\varepsilon(\bar{R}\omega + \bar{O}) \left( \frac{2m_j}{|m_i - m_j|} |\eta| \omega + 2v + \frac{2m_j}{m_i - m_j} \eta - 2\varepsilon u_i \right).$$

Therefore, repeating the previous considerations and thanks to the straightforward upper bound

$$\nabla_v M_i^\varepsilon(\bar{R}\omega + \bar{O}) \leq C_{ij}(\delta) c_i (|\eta| + |v| + |u_i|) \mathcal{M}_i^\delta(\bar{R}\omega + \bar{O}),$$

valid for any  $\delta \in (0, 1)$ , we recover the uniform estimate

$$\begin{aligned} & \left| \nabla_v \kappa_{ij}^{(1),S}(v, \eta) \right| \sqrt{\frac{\mu_j(v - \eta)}{\mu_i(v)}} \\ & \leq C_{ij}(\delta) \sqrt{\frac{\bar{c}_j}{\bar{c}_i}} \|\mathbf{c}\|_{L_t^\infty L_x^\infty} \left( 1 + \|\mathbf{u}\|_{L_t^\infty L_x^\infty} \right) (1 + |\eta|^\gamma + |\eta|^{\gamma+1}) e^{-C(\delta)|\eta|^2}, \end{aligned} \quad (3.4.7)$$

holding for all  $v \in \mathbb{R}^3$  and for any  $\delta \in (\bar{\delta}, 1)$ , where  $\bar{\delta} \in (0, 1)$  is fixed independently of  $\varepsilon$ , and can in particular be chosen in order to satisfy both (3.4.7) and (3.4.6). Using the same arguments in order to derive an upper bound for  $\nabla_v \kappa_{ij}^{(1),R}$ , estimates (3.4.6)–(3.4.7) finally imply that for all  $v \in \mathbb{R}^3$  we have

$$\begin{aligned} & \left\| \nabla_\eta \kappa_{ij}^{(1),S}(v, \eta) \sqrt{\frac{\mu_j(v - \eta)}{\mu_i(v)}} \right\|_{L_\eta^1} \leq C_{ij}^{(1)}(\delta, \xi), \\ & \left\| \nabla_v \kappa_{ij}^{(1),S}(v, \eta) \sqrt{\frac{\mu_j(v - \eta)}{\mu_i(v)}} \right\|_{L_\eta^1} \leq C_{ij}^{(1)}(\delta, \xi), \\ & \left\| \nabla_v \kappa_{ij}^{(1),R}(v, \eta) \sqrt{\frac{\mu_j(v - \eta)}{\mu_i(v)}} \right\|_{L_\eta^1} \leq C_{ij}^{(1)}(\delta, \xi). \end{aligned} \quad (3.4.8)$$

**Step 2 - Estimates for  $\kappa_{ij}^{(2)}$ .** We proceed in the same way as for  $\kappa_{ij}^{(1)}$ . We rename the relative velocity  $\eta = v - v_*$ , so that  $v_* = v - \eta$ , and the explicit form of  $\kappa_{ij}^{(2)}$  given by (B.2.1) reads in the new configuration

$$\begin{aligned} \kappa_{ij}^{(2)}(v, \eta) &= \mathcal{P}_{ij}(v, \eta) \int_{\mathbb{R}^2} b_{ij} \left( \frac{\left(\frac{m_i+m_j}{2m_j}\right)^2 |\eta|^2 - |X|^2}{\left(\frac{m_i+m_j}{2m_j}\right)^2 |\eta|^2 + |X|^2} \right) \left( \left(\frac{m_i+m_j}{2m_j}\right)^2 |\eta|^2 + |X|^2 \right)^{\frac{\gamma-1}{2}} \\ & \quad \times M_j^\varepsilon \left( R \left( \frac{\eta}{|\eta|}, \left( 0, X + \frac{1}{2} \bar{X} \right) \right) \right) dX, \end{aligned}$$

with

$$\mathcal{P}_{ij}(v, \eta) = \frac{C_{ji}}{|\eta|} e^{-\frac{m_i^2}{8m_j} |\eta|^2 - \frac{m_j}{8} \frac{|\eta|^2 - 2(v \cdot \eta)|^2}{|\eta|^2} + \varepsilon \frac{m_i}{2} (\eta \cdot u_j) - \varepsilon \frac{m_j}{2} \left( \frac{|\eta|^2 - 2(v \cdot \eta)}{|\eta|} \frac{\eta}{|\eta|} \right) \cdot u_j} \sqrt{\frac{\mu_i(v)}{\mu_i(v - \eta)}}.$$

Next, for some small parameter  $\xi > 0$ , introduce a mollified indicator function  $\mathbf{1}_{\{|\cdot| \geq \xi\}}$  and define the splitting

$$\kappa_{ij}^{(2)} = \kappa_{ij}^{(2),S} + \kappa_{ij}^{(2),R},$$

where again we have called the smooth part

$$\kappa_{ij}^{(2),S}(v, \eta) = \mathbf{1}_{\{|\eta| \geq \xi\}} \kappa_{ij}^{(2)}(v, \eta),$$

and  $\kappa_{ij}^{(2),R}$  is the remainder. Following again [45, Lemma 5.1] and our computations in Chapter 2, a similar analysis to the one carried out for  $\kappa_{ij}^{(1)}$  gives in this case

$$\kappa_{ij}^{(2),R}(v, \eta) \sqrt{\frac{\mu_i(v - \eta)}{\mu_i(v)}} \leq C_{ji}(\delta) |\eta|^{\gamma-2} e^{-C(\delta)|\eta|^2}, \quad \forall v \in \mathbb{R}^3,$$

for some positive explicit constants  $C_{ji}(\delta), C(\delta)$  depending on a parameter  $\delta \in (\bar{\delta}, 1)$ , where  $\bar{\delta} \in (0, 1)$ . This in turns means that we recover the needed control in  $L_\eta^1$ , which reads

$$\left\| \kappa_{ij}^{(2),R}(v, \eta) \sqrt{\frac{\mu_i(v - \eta)}{\mu_i(v)}} \right\|_{L_\eta^1} \leq C_{ji}^{(2)}(\delta) \xi^{\gamma+1}, \quad \forall v \in \mathbb{R}^3. \quad (3.4.9)$$

Next, we consider some  $\eta$ -derivatives of  $\kappa_{ij}^{(2),S}$ . Naming this time

$$W_{ij}^{(2)}(|\eta|^2, |X|^2) = \left( \left( \frac{m_i + m_j}{2m_j} \right)^2 |\eta|^2 + |X|^2 \right)^{\frac{\gamma-1}{2}},$$

direct computations show that

$$(1) \quad \nabla_\eta \mathcal{P}_{ij}(v, \eta) \leq C_{ji} \left( 1 + \|\mathbf{u}\|_{L_{t,x}^\infty} \right) \left( |v| + |v|^2 + |v|^4 + \sum_{k=-2}^1 |\eta|^k \right) \mathcal{P}_{ij}(v, \eta),$$

$$(2) \quad \nabla_\eta b_{ij}(|\eta|^2, |X|^2) \leq C_{ji} \frac{|\eta|^2 + |X|^4}{|\eta|^4},$$

$$(3) \quad W_{ij}^{(2)}(|\eta|^2, |X|^2) \leq C_{ji} |\eta|^{\gamma-1},$$

$$(4) \quad \nabla_\eta W_{ij}^{(2)}(|\eta|^2, |X|^2) \leq C_{ji} |\eta|^{\gamma-2},$$

and at last that

$$\nabla_\eta \left| R \left( \frac{\eta}{|\eta|}, \left( 0, X + \frac{1}{2} \bar{X} \right) \right) - \varepsilon u_j \right|^2 \leq C_{ji} \frac{1 + \|\mathbf{u}\|_{L_{t,x}^\infty}^2 + |X|^2}{|\eta|}.$$

By gathering these estimates together, we derive the following upper bound for  $\nabla_{\eta}\kappa_{ij}^{(2),S}$ :

$$\left| \nabla_{\eta}\kappa_{ij}^{(2),S}(v, \eta) \right| \sqrt{\frac{\mu_i(v-\eta)}{\mu_i(v)}} \leq C_{ji}(\delta) \|\mathbf{c}\|_{L_{t,x}^{\infty}} \left(1 + \|\mathbf{u}\|_{L_{t,x}^{\infty}}\right) \left(1 + \sum_{k=0}^4 |\eta|^{\gamma-k}\right) e^{-C(\delta)|\eta|^2},$$

holding for all  $v \in \mathbb{R}^3$  and for any  $\delta \in (\bar{\delta}, 1)$ , where  $\bar{\delta} \in (0, 1)$  is fixed independently of  $\varepsilon$ . Then, we can obtain a similar control for  $\nabla_v\kappa_{ij}^{(2),S}$ , which reads

$$\left| \nabla_v\kappa_{ij}^{(2),S}(v, \eta) \right| \sqrt{\frac{\mu_i(v-\eta)}{\mu_i(v)}} \leq C_{ji}(\delta) \|\mathbf{c}\|_{L_{t,x}^{\infty}} \left(1 + \varepsilon \|\mathbf{u}\|_{L_{t,x}^{\infty}}\right) (1 + |\eta|^{\gamma} + |\eta|^{\gamma-1}) e^{-C(\delta)|\eta|^2},$$

and the same holds for the remainder term  $\nabla_v\kappa_{ij}^{(2),R}$ . The collection of these inequalities finally ensure the expected bounds in  $L_{\eta}^1$

$$\begin{aligned} \left\| \nabla_{\eta}\kappa_{ij}^{(2),S}(v, \eta) \sqrt{\frac{\mu_i(v-\eta)}{\mu_i(v)}} \right\|_{L_{\eta}^1} &\leq C_{ij}^{(2)}(\delta, \xi), \\ \left\| \nabla_v\kappa_{ij}^{(2),S}(v, \eta) \sqrt{\frac{\mu_i(v-\eta)}{\mu_i(v)}} \right\|_{L_{\eta}^1} &\leq C_{ij}^{(2)}(\delta, \xi), \\ \left\| \nabla_v\kappa_{ij}^{(2),R}(v, \eta) \sqrt{\frac{\mu_i(v-\eta)}{\mu_i(v)}} \right\|_{L_{\eta}^1} &\leq C_{ij}^{(2)}(\delta, \xi). \end{aligned} \tag{3.4.10}$$

**Step 3 - Estimates for  $\kappa_{ij}^{(3)}$ .** The case of  $\kappa_{ij}^{(3)}$  is straightforward and we do not need any additional effort. Introducing as before the splitting  $\kappa_{ij}^{(3)} = \kappa_{ij}^{(3),S} + \kappa_{ij}^{(3),R}$  and renaming  $\eta = v - v_*$ ,  $v_* = v - \eta$ , very easy computations provide the bound for the remainder  $\kappa_{ij}^{(3),R}$

$$\left\| \kappa_{ij}^{(3),R}(v, \eta) \sqrt{\frac{\mu_j(v-\eta)}{\mu_i(v)}} \right\|_{L_{\eta}^1} \leq C_{ij}^{(3)}(\delta) \xi^{\gamma+3}, \tag{3.4.11}$$

and the estimates for the derivatives

$$\begin{aligned} \left\| \nabla_{\eta}\kappa_{ij}^{(3),S}(v, \eta) \sqrt{\frac{\mu_j(v-\eta)}{\mu_i(v)}} \right\|_{L_{\eta}^1} &\leq C_{ij}^{(3)}(\delta, \xi), \\ \left\| \nabla_v\kappa_{ij}^{(3),S}(v, \eta) \sqrt{\frac{\mu_j(v-\eta)}{\mu_i(v)}} \right\|_{L_{\eta}^1} &\leq C_{ij}^{(3)}(\delta, \xi), \\ \left\| \nabla_v\kappa_{ij}^{(3),R}(v, \eta) \sqrt{\frac{\mu_j(v-\eta)}{\mu_i(v)}} \right\|_{L_{\eta}^1} &\leq C_{ij}^{(3)}(\delta, \xi), \end{aligned} \tag{3.4.12}$$

for all  $v \in \mathbb{R}^3$ .



**Step 4 - Conclusion.** Now, we can successively write

$$\begin{aligned}
& \langle \nabla_v \mathbf{K}^\varepsilon(\mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\
&= \sum_{i,j=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} \left( \nabla_v \int_{\mathbb{R}^3} \left( \kappa_{ij}^{(1)}(v, v_*) f_j^* + \kappa_{ij}^{(2)}(v, v_*) f_i^* - \kappa_{ij}^{(3)}(v, v_*) f_j^* \right) dv_* \right) \nabla_v f_i \mu_i^{-1} dx dv \\
&= \sum_{i,j=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} \left( \nabla_v \int_{\mathbb{R}^3} \left( \kappa_{ij}^{(1),S}(v, \eta) + \kappa_{ij}^{(1),R}(v, \eta) \right) f_j(v - \eta) d\eta \right) \nabla_v f_i \mu_i^{-1} dx dv \\
&\quad + \sum_{i,j=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} \left( \nabla_v \int_{\mathbb{R}^3} \left( \kappa_{ij}^{(2),S}(v, \eta) + \kappa_{ij}^{(2),R}(v, \eta) \right) f_i(v - \eta) d\eta \right) \nabla_v f_i \mu_i^{-1} dx dv \\
&\quad + \sum_{i,j=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} \left( \nabla_v \int_{\mathbb{R}^3} \left( \kappa_{ij}^{(3),S}(v, \eta) + \kappa_{ij}^{(3),R}(v, \eta) \right) f_j(v - \eta) d\eta \right) \nabla_v f_i \mu_i^{-1} dx dv \\
&:= \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3.
\end{aligned}$$

The behaviour of the three terms is the same. We shall thus focus on the first one and the others will be estimated in an equivalent way. Since

$$\nabla_v f_j(v - \eta) = -\nabla_\eta f_j(v - \eta),$$

we initially apply integration by parts to deduce that

$$\begin{aligned}
& \nabla_v \int_{\mathbb{R}^3} \left( \kappa_{ij}^{(1),S}(v, \eta) + \kappa_{ij}^{(1),R}(v, \eta) \right) f_j(v - \eta) d\eta \\
&= \int_{\mathbb{R}^3} \left( \nabla_v \kappa_{ij}^{(1),S}(v, \eta) - \nabla_\eta \kappa_{ij}^{(1),S}(v, \eta) + \nabla_v \kappa_{ij}^{(1),R}(v, \eta) \right) f_j(v - \eta) d\eta \\
&\quad + \int_{\mathbb{R}^3} \kappa_{ij}^{(1),R}(v, \eta) \nabla_v f_j(v - \eta) d\eta.
\end{aligned}$$

Thus, if we multiply and divide inside the integral by the factor  $\sqrt{\mu_j(v - \eta)/\mu_i(v)}$ , we can apply Cauchy-Schwarz inequality and an  $L^1/L^2$  convolution inequality, together with estimates (3.4.5) and (3.4.8), to finally deduce that

$$\mathcal{I}_1 \leq C_1^{(1)}(\delta, \xi) \|\mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \xi C_2^{(1)}(\delta) \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2,$$

for any  $\xi \in (0, 1)$ .

As already mentioned, the same argument applies to  $\mathcal{I}_2$  and  $\mathcal{I}_3$  using estimates (3.4.9)–(3.4.12) and for some positive constants  $C_k^{(2)}, C_k^{(3)}$ ,  $k = 1, 2$ . Gathering the bounds for the three terms concludes the proof.

### 3.4.4 Proof of Lemma 3.3.6

The proof follows exactly the computations presented in Chapter 2, except for the final estimate where Young's inequality allows to refine the control on  $\pi_{\mathbf{L}}(\mathbf{f})$ . Let us sketch the idea.

We initially rewrite  $\mathbf{L}^\varepsilon$  componentwise as

$$\begin{aligned} L_i^\varepsilon(\mathbf{f}) &= \\ &\sum_{j=1}^N \int_{\mathbb{R}^3 \times \mathbb{S}^2} B_{ij}(v, v_*, \vartheta) \left( c_{i,\infty} \mathcal{M}_i^{\varepsilon'} f_j'^* + c_{j,\infty} \mathcal{M}_j^{\varepsilon' *} f_i' - c_{i,\infty} \mathcal{M}_i^\varepsilon f_j^* - c_{j,\infty} \mathcal{M}_j^{\varepsilon *} f_i \right) dv_* d\sigma \\ &\quad + \varepsilon \sum_{j=1}^N \int_{\mathbb{R}^3 \times \mathbb{S}^2} B_{ij}(v, v_*, \vartheta) \left( \tilde{c}_i \mathcal{M}_i^{\varepsilon'} f_j'^* + \tilde{c}_j \mathcal{M}_j^{\varepsilon' *} f_i' - \tilde{c}_i \mathcal{M}_i^\varepsilon f_j^* - \tilde{c}_j \mathcal{M}_j^{\varepsilon *} f_i \right) dv_* d\sigma \\ &:= L_{i,\infty}^\varepsilon(\mathbf{f}) + \varepsilon \tilde{L}_i^\varepsilon(\mathbf{f}). \end{aligned}$$

Now, following the method in Chapter 2, we can study the Dirichlet form of  $\mathbf{L}^\varepsilon$  by introducing the penalization with respect to  $\mathbf{L}$ . Recall the shorthand notation  $\mathbf{f}^\perp = \mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f})$ . Using the fact that  $\mathbf{L}^\varepsilon$  shares the conservation properties of the Boltzmann operator  $\mathbf{Q}$ , we can successively write

$$\begin{aligned} \langle \mathbf{L}^\varepsilon(\mathbf{f}), \mathbf{f} \rangle_{L_v^2(\mu^{-\frac{1}{2}})} &= \langle \mathbf{L}^\varepsilon(\mathbf{f}), \mathbf{f}^\perp \rangle_{L_v^2(\mu^{-\frac{1}{2}})} \\ &= \langle \mathbf{L}(\mathbf{f}), \mathbf{f}^\perp \rangle_{L_v^2(\mu^{-\frac{1}{2}})} + \langle \mathbf{L}_\infty^\varepsilon(\mathbf{f}) - \mathbf{L}(\mathbf{f}), \mathbf{f}^\perp \rangle_{L_v^2(\mu^{-\frac{1}{2}})} \\ &\quad + \varepsilon \langle \tilde{\mathbf{L}}^\varepsilon(\mathbf{f}), \mathbf{f}^\perp \rangle_{L_v^2(\mu^{-\frac{1}{2}})}. \end{aligned}$$

We estimate each term separately. Thanks to [45, Theorem 3.3], the first term provides the spectral gap for  $\mathbf{L}$

$$\langle \mathbf{L}(\mathbf{f}), \mathbf{f}^\perp \rangle_{L_v^2(\mu^{-\frac{1}{2}})} \leq -\lambda_{\mathbf{L}} \|\mathbf{f}^\perp\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2.$$

Recalling that  $\mathbf{L}_\infty^\varepsilon - \mathbf{L} = \mathcal{O}(\varepsilon)$ , the second term can be estimated following the strategy of Chapter 2. We split  $\mathbf{f} = \mathbf{f}^\perp + \pi_{\mathbf{L}}(\mathbf{f})$  and we then apply Young's inequality with a positive constant  $\eta_1/\varepsilon$  to recover

$$\begin{aligned} \langle (\mathbf{L}_\infty^\varepsilon - \mathbf{L})(\mathbf{f}), \mathbf{f}^\perp \rangle_{L_v^2(\mu^{-\frac{1}{2}})} &= \langle (\mathbf{L}_\infty^\varepsilon - \mathbf{L})(\mathbf{f}^\perp), \mathbf{f}^\perp \rangle_{L_v^2(\mu^{-\frac{1}{2}})} \\ &\quad + \langle (\mathbf{L}_\infty^\varepsilon - \mathbf{L})(\pi_{\mathbf{L}}(\mathbf{f})), \mathbf{f}^\perp \rangle_{L_v^2(\mu^{-\frac{1}{2}})} \\ &\leq (\varepsilon + \eta_1) C_2^{\mathbf{L}} \|\mathbf{f}^\perp\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 + \varepsilon^2 \|\mathbf{u}\|_{L_{t,x}^\infty} \frac{C_2^{\mathbf{L}}}{\eta_1} \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2. \end{aligned}$$

In a very similar way, using again Young's inequality with the same constant  $\eta_1/\varepsilon$  and increasing the constant  $C_2^{\mathbf{L}}$  if necessary, the third term provides

$$\begin{aligned} \langle \tilde{\mathbf{L}}^\varepsilon(\mathbf{f}), \mathbf{f}^\perp \rangle_{L_v^2(\mu^{-\frac{1}{2}})} &= \langle \tilde{\mathbf{L}}^\varepsilon(\mathbf{f}^\perp), \mathbf{f}^\perp \rangle_{L_v^2(\mu^{-\frac{1}{2}})} + \langle \tilde{\mathbf{L}}^\varepsilon(\pi_{\mathbf{L}}(\mathbf{f})), \mathbf{f}^\perp \rangle_{L_v^2(\mu^{-\frac{1}{2}})} \\ &\leq \frac{\eta_1 C_2^{\mathbf{L}}}{\varepsilon} \|\mathbf{f}^\perp\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2 + \varepsilon \|\tilde{\mathbf{c}}\|_{L_{t,x}^\infty} \frac{C_2^{\mathbf{L}}}{\eta_1} \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}^2. \end{aligned}$$

Gathering the three estimates, and using the Sobolev embedding of  $H_x^{s/2}$  in  $L_x^\infty$  to upper bound  $\|\mathbf{u}\|_{L_{t,x}^\infty}$  and  $\|\tilde{\mathbf{c}}\|_{L_{t,x}^\infty}$  by  $\delta_{\text{MS}}$ , we obtain the expected result. This ends the proof.

### 3.4.5 Proof of Lemma 3.3.7

The first part comes from the conservation properties of the Boltzmann operator. In fact, we have seen that

$$\sum_{i=1}^N \int_{\mathbb{R}^3} Q_i(\mathbf{g}, \mathbf{h})(v) \psi_i(v) dv = 0, \quad \forall \mathbf{g}, \mathbf{h} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}),$$

whenever  $\boldsymbol{\psi} \in \text{Span}(\mathbf{e}^{(1)}, \dots, \mathbf{e}^{(N)}, v_1 \mathbf{m}, v_2 \mathbf{m}, v_3 \mathbf{m}, |v|^2 \mathbf{m})$  is a collision invariant of the mixture. In particular the above equality rewrites

$$\langle \mathbf{Q}(\mathbf{g}, \mathbf{h}), \pi_{\mathbf{L}}(\mathbf{f}) \rangle_{L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = 0, \quad \forall \mathbf{f}, \mathbf{g}, \mathbf{h} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}),$$

which is exactly (3.3.13) for  $\mathbf{Q}$ . Then the property follows also for  $\mathbf{L}^\varepsilon$ , since by definition  $\mathbf{L}^\varepsilon(\mathbf{f}) = \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{f}) + \mathbf{Q}(\mathbf{f}, \mathbf{M}^\varepsilon)$  and both terms are orthogonal to  $\ker \mathbf{L}$ .

The second part is an extension of the same property satisfied by the Boltzmann operator in the mono-species case. Let  $s \in \mathbb{N}$  and  $\alpha, \beta$  be fixed such that  $|\alpha| + |\beta| = s$ . We initially note that

$$\langle \partial_v^\beta \partial_x^\alpha \mathbf{Q}(\mathbf{g}, \mathbf{h}), \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \sum_{i,j=1}^N \langle \partial_v^\beta \partial_x^\alpha Q_{ij}(g_i, h_j), f_i \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}.$$

Since each  $Q_{ij}$  acts like a mono-species Boltzmann operator, we can easily adapt the computations made in [43, Appendix A] to prove that, for any  $1 \leq i, j \leq N$ , there exist two nonnegative functionals  $\mathcal{G}_{ij}^{x,v,s}$  and  $\mathcal{G}_{ij}^{x,s}$  satisfying  $\mathcal{G}_{ij}^{x,v,s+1} \leq \mathcal{G}_{ij}^{x,v,s}$ ,  $\mathcal{G}_{ij}^{x,s+1} \leq \mathcal{G}_{ij}^{x,s}$  and such that

$$\langle \partial_v^\beta \partial_x^\alpha Q_{ij}(g_i, h_j), f_i \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \begin{cases} \mathcal{G}_{ij}^{x,s}(g_i, h_j) \|f_i\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} & \text{if } |\beta| = 0, \\ \mathcal{G}_{ij}^{x,v,s}(g_i, h_j) \|f_i\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} & \text{if } |\beta| \geq 1. \end{cases}$$

Moreover, there exists an integer  $s_0 > 0$  such that, for all  $s > s_0$ , there exists an explicit constant  $C_{ij}^Q > 0$  verifying

$$\begin{aligned} & \mathcal{G}_{ij}^{x,s}(g_i, h_j) \\ & \leq C_{ij}^Q \left( \|g_i\|_{H_x^s L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \|h_j\|_{H_x^s L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} + \|h_j\|_{H_x^s L_v^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \|g_i\|_{H_x^s L_v^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \right), \end{aligned}$$

and

$$\begin{aligned} & \mathcal{G}_{ij}^{x,v,s}(g_i, h_j) \\ & \leq C_{ij}^Q \left( \|g_i\|_{H_{x,v}^s(\boldsymbol{\mu}^{-\frac{1}{2}})} \|h_j\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} + \|h_j\|_{H_{x,v}^s(\boldsymbol{\mu}^{-\frac{1}{2}})} \|g_i\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \right). \end{aligned}$$

From this, we immediately deduce that

$$\langle \partial_v^\beta \partial_x^\alpha \mathbf{Q}(\mathbf{g}, \mathbf{h}), \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \begin{cases} \left( \sum_{i,j=1}^N \mathcal{G}_{ij}^{x,s}(g_i, h_j) \right) \|\mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} & \text{if } |\beta| = 0, \\ \left( \sum_{i,j=1}^N \mathcal{G}_{ij}^{x,v,s}(g_i, h_j) \right) \|\mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} & \text{if } |\beta| \geq 1, \end{cases}$$

and defining  $C_s^Q = N^2 \max_{1 \leq i,j \leq N} C_{ij}^Q$  finishes the proof of (3.3.14)–(3.3.15).

### 3.4.6 Proof of Lemma 3.3.8

We divide the proof into two separated parts for the sake of clarity. The first one deals with inequalities (3.3.16)–(3.3.17), where at least one  $v$ -derivative is considered, since the proofs of the two estimates are almost the same. The second part treats pure spatial derivatives, which require a slightly different approach. Note that, throughout the proof, we shall carefully keep track of the parameter  $\delta_{\text{MS}}^2$  which uniformly bounds the quantities  $\|\tilde{\mathbf{c}}\|_{L_t^\infty H_x^s(\mathbf{c}_\infty^{-\frac{1}{2}})}^2$  and  $\|\mathbf{u}\|_{L_t^\infty H_x^s}^2$ . For simplicity, all the other factors multiplying the term of interest  $\delta_{\text{MS}}^2$  will always be hidden inside a suitable constant, even if a lower order (in  $\delta_{\text{MS}}$  or in  $\varepsilon$ ) appears. This choice will also help in enlightening the computations.

**Step 1 - Estimates with velocity derivatives.** The idea to recover the first estimate (3.3.18) is to show that  $\partial_v^\beta \partial_x^\alpha \mathbf{S}^\varepsilon = \mathcal{O}(\varepsilon^{-1})$ . For this, let us initially extract a power  $\varepsilon^{-1}$  from the source term and write

$$\begin{aligned} \left\langle \partial_v^\beta \partial_x^\alpha \mathbf{S}^\varepsilon, \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\mu^{-\frac{1}{2}})} &= \frac{1}{\varepsilon} \left( - \left\langle \partial_v^\beta \partial_x^\alpha (\partial_t \mathbf{M}^\varepsilon + \frac{1}{\varepsilon} v \cdot \nabla_x \mathbf{M}^\varepsilon), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\mu^{-\frac{1}{2}})} \right. \\ &\quad \left. + \frac{1}{\varepsilon^2} \left\langle \partial_v^\beta \partial_x^\alpha \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\mu^{-\frac{1}{2}})} \right). \end{aligned}$$

We shall treat the linear part and the nonlinear term separately.

Computing the time and space derivatives in the linear contribution, we note that, for any  $1 \leq i \leq N$ ,

$$\begin{aligned} \partial_t M_i^\varepsilon + \frac{1}{\varepsilon} v \cdot \nabla_x M_i^\varepsilon &= \left( \partial_t c_i + \varepsilon m_i c_i (v - \varepsilon u_i) \cdot \partial_t u_i \right. \\ &\quad \left. + \sum_{k=1}^3 v_k \left( \varepsilon \partial_{x_k} \tilde{c}_i + m_i c_i (v - \varepsilon u_i) \cdot \partial_{x_k} u_i \right) \right) \mathcal{M}_i^\varepsilon, \end{aligned} \quad (3.4.13)$$

and that the leading order seems to be  $\mathcal{O}(1)$ . Let us show that it is actually  $\mathcal{O}(\delta_{\text{MS}})$ . For this, recall that  $(\mathbf{c}, \mathbf{u})$  is the unique perturbative solution of the Maxwell-Stefan system (3.2.3)–(3.2.5). From the mass equation (3.2.3)

$$\partial_t \mathbf{c} = -\nabla_x \cdot (\mathbf{c}\mathbf{u}) = -\varepsilon \nabla_x \tilde{\mathbf{c}} \cdot \mathbf{u} - \mathbf{c} \nabla_x \cdot \mathbf{u}$$

we easily deduce a bound for  $\partial_t \mathbf{c}$ . In a similar way, we can derive an estimate for  $\partial_t \mathbf{u}$  by taking the time derivative on both sides of the momentum equation (3.2.4), to obtain

$$A(\mathbf{c}) \partial_t \mathbf{u} = -\partial_t A(\mathbf{c}) \mathbf{u} + \partial_t (\nabla_x \mathbf{c}).$$

It is then straightforward to check that the right-hand side of the above equality satisfies

$$-\partial_t A(\mathbf{c}) \mathbf{u} + \partial_t (\nabla_x \mathbf{c}) \in (\ker A)^\perp,$$

so that the relation can be inverted by applying  $A(\mathbf{c})^{-1}$ , and the equation governing  $\partial_t \mathbf{u}$  explicitly reads

$$\partial_t \mathbf{u} = -A(\mathbf{c})^{-1} \left( \partial_t A(\mathbf{c}) \mathbf{u} - \nabla_x (-\varepsilon \nabla_x \tilde{\mathbf{c}} \cdot \mathbf{u} - \mathbf{c} \nabla_x \cdot \mathbf{u}) \right).$$

Thanks to these considerations, we can copy the arguments used in order to deal with the tri- and bi-norm terms appearing in the proof of Proposition 3.2.12, establishing the *a priori* energy estimates for the Maxwell-Stefan system. Specifically, noticing that one of the macroscopic quantities  $\tilde{\mathbf{c}}$  and  $\mathbf{u}$  (or their derivatives) always appears as a factor in each term of (3.4.13), by means of the continuous Sobolev embedding of  $H_x^{s/2}$  in  $L_x^\infty$ ,  $s > 3$ , we can infer the existence of a polynomial  $P$ , such that, for any  $1 \leq i \leq N$  and for almost every  $(t, x, v) \in \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ ,

$$\left| \partial_t M_i^\varepsilon(t, x, v) + \frac{1}{\varepsilon} v \cdot \nabla_x M_i^\varepsilon(t, x, v) \right|^2 \leq \delta_{\text{MS}}^2 C(\delta) P(v) \mathcal{M}_i^{2\delta}(v),$$

for a positive constant  $C(\delta)$  only depending on an arbitrary parameter  $\delta \in (0, 1)$ , which is chosen independently of  $\varepsilon$ . Note in particular the factor 2 (simply coming from the square power) in the exponent of  $\mathcal{M}_i^{2\delta}$ , which is crucial in order to compensate the weight  $\mu_i^{-1}$  of the  $L_{x,v}^2(\mu^{-\frac{1}{2}})$  norm. Moreover, we again emphasize that the other terms containing the quantities  $\|\mathbf{c}\|_{L_t^\infty H_x^s(\mathbf{c}_\infty^{-\frac{1}{2}})}$  or  $\|\mathbf{u}\|_{L_t^\infty H_x^s}$  (for  $s \leq 4$ ) have been simply collected inside the constant  $C(\delta)$ .

Now, taking  $\alpha$  and  $\beta$  derivatives of the linear term only increases the number of factors depending on polynomials of  $v$ , and (at most)  $|\alpha| + 4$  derivatives of  $\mathbf{c}$  and  $\mathbf{u}$ . In particular it does not modify the leading order  $\mathcal{O}(\varepsilon^{-1})$ , nor the presence of the multiplicative constant  $\delta_{\text{MS}}^2$ . Therefore, the exact same arguments apply, and we deduce that there also exist a polynomial  $P_L$  and a constant  $C_L(\delta) > 0$  such that, for any  $1 \leq i \leq N$  and for almost every  $(t, x, v) \in \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ ,

$$\left| \partial_v^\beta \partial_x^\alpha \left( \partial_t M_i^\varepsilon(t, x, v) + \frac{1}{\varepsilon} v \cdot \nabla_x M_i^\varepsilon(t, x, v) \right) \right|^2 \leq \delta_{\text{MS}}^2 C_L(\delta) P_L(v) \mathcal{M}_i^{2\delta}(v), \quad (3.4.14)$$

where again  $\delta \in (0, 1)$  is arbitrarily chosen, and the other dependencies on  $\|\mathbf{c}\|_{L_t^\infty H_x^{|\alpha|+4}}$  and  $\|\mathbf{u}\|_{L_t^\infty H_x^{|\alpha|+4}}$  have been hidden inside  $C_L(\delta)$ .

If we now fix  $\delta \in (1/2, 1)$  in (3.4.14), applying Young's inequality with a positive constant  $\eta_2/\varepsilon$  and recalling that we use the notation  $\mu_i = c_{i,\infty} \mathcal{M}_i$  for any  $1 \leq i \leq N$ , we can finally estimate the linear part as

$$\begin{aligned} & \frac{1}{\varepsilon} \left| \left\langle \partial_v^\beta \partial_x^\alpha \left( \partial_t \mathbf{M}^\varepsilon + \frac{1}{\varepsilon} v \cdot \nabla_x \mathbf{M}^\varepsilon \right), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\mu^{-\frac{1}{2}})} \right| \\ & \leq \frac{1}{\eta_2} \left\| \partial_v^\beta \partial_x^\alpha \left( \partial_t \mathbf{M}^\varepsilon + \frac{1}{\varepsilon} v \cdot \nabla_x \mathbf{M}^\varepsilon \right) \right\|_{L_{x,v}^2(\mu^{-\frac{1}{2}})}^2 + \frac{\eta_2}{\varepsilon^2} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\mu^{-\frac{1}{2}})}^2 \\ & \leq \frac{\delta_{\text{MS}}^2 C_L(\delta)}{\eta_2} \sum_{i=1}^N \int_{\mathbb{T}^3 \times \mathbb{R}^3} c_{i,\infty}^{-1} P_L(v) \mathcal{M}_i^{2\delta-1}(v) dx dv + \frac{\eta_2}{\varepsilon^2} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\mu^{-\frac{1}{2}})}^2 \quad (3.4.15) \\ & \leq \frac{\delta_{\text{MS}}^2 C_L(\delta)}{\eta_2 \min_{1 \leq i \leq N} c_{i,\infty}} + \frac{\eta_2}{\varepsilon^2} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\mu^{-\frac{1}{2}})}^2, \end{aligned}$$

by simply increasing the constant  $C_L(\delta)$  in order to include the value of the sum of the integrals, which are clearly finite since  $2\delta - 1 > 0$  thanks to our choice of the parameter  $\delta$ .

Let us continue with the analysis of the nonlinear term  $\mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon)$ . For this, recall that the macroscopic velocity  $\mathbf{u}$  is defined componentwise as  $u_i = \bar{u} + \varepsilon \tilde{u}_i$ , and introduce the local Maxwellian distribution  $\mathcal{M}_{\bar{u}} = (\mathcal{M}_{\bar{u},1}, \dots, \mathcal{M}_{\bar{u},N})$ , given for any  $1 \leq i \leq N$  by

$$\mathcal{M}_{\bar{u},i}(t, x, v) = \left(\frac{m_i}{2\pi}\right)^{3/2} \exp\left\{-\frac{m_i}{2}|v - \varepsilon \bar{u}(t, x)|^2\right\}, \quad t \geq 0, \quad x \in \mathbb{T}^3, \quad v \in \mathbb{R}^3.$$

Since the bulk velocity  $\bar{u}$  is common to all the different species,  $\mathcal{M}_{\bar{u}}$  is a local equilibrium state of the mixture. This means in particular that  $\mathbf{Q}(\mathcal{M}_{\bar{u}}, \mathcal{M}_{\bar{u}}) = 0$ . We exploit this property by following the idea developed in Chapter 2 for the study of the linearized operator  $\mathbf{L}^\varepsilon$ . Namely, we split  $\mathbf{M}^\varepsilon = \mathbf{c}\mathcal{M}_{\bar{u}} + (\mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}})$  into a local equilibrium part which cancels the nonlinear term, plus a penalty which is close to this local equilibrium up to an order  $\varepsilon^2 \|\tilde{\mathbf{u}}\|_{L_{t,x}^\infty}$ . More precisely, since also  $\mathbf{Q}(\mathbf{c}\mathcal{M}_{\bar{u}}, \mathbf{c}\mathcal{M}_{\bar{u}}) = 0$ , we can rewrite

$$\begin{aligned} \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon) &= \mathbf{Q}(\mathbf{c}\mathcal{M}_{\bar{u}}, \mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}}) + \mathbf{Q}(\mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}}, \mathbf{c}\mathcal{M}_{\bar{u}}) \\ &\quad + \mathbf{Q}(\mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}}, \mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}}). \end{aligned}$$

Similarly to the case of the linear part, one can infer (see Lemma 2.4.1 of Chapter 2 for more details) the existence of some polynomials  $P_1$  and  $P_2$  in one variable, such that, for any  $1 \leq i \leq N$  and for almost every  $(t, x, v) \in \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ ,

$$\partial_v^\beta \partial_x^\alpha \left( c_i(t, x) (\mathcal{M}_i^\varepsilon(t, x, v) - \mathcal{M}_{\bar{u},i}(t, x, v)) \right) \leq \varepsilon^2 \delta_{\text{MS}} C_1(\delta) P_1(v) \mathcal{M}_i^\delta(v), \quad (3.4.16)$$

$$\partial_v^\beta \partial_x^\alpha (c_i(t, x) \mathcal{M}_{\bar{u},i}(t, x, v)) \leq C_2(\delta) P_2(v) \mathcal{M}_i^\delta(v),$$

for some positive constants  $C_1(\delta), C_2(\delta)$  depending on a parameter  $\delta \in (0, 1)$ , which can be chosen independently of  $\varepsilon$ . It is important to note that, for  $|\alpha| = 0$ , we can still recover the correct factor  $\delta_{\text{MS}}$  in the first inequality, but this is not the case for the second one. Indeed, when  $|\alpha| = 0$ , the computations carried out in the proof of Lemma 2.4.1 show that

$$\partial_v^\beta (c_i(\mathcal{M}_i^\varepsilon - \mathcal{M}_{\bar{u},i})) \leq \varepsilon^2 \|\tilde{\mathbf{u}}\|_{L_{t,x}^\infty} \tilde{C}_1(\delta) \tilde{P}_1(v) \mathcal{M}_i^\delta(v),$$

for some other polynomial  $\tilde{P}_1$  and a constant  $\tilde{C}_1(\delta) > 0$ . In particular, we immediately see that this does not represent an issue, since we always consider products of type  $\partial_v^\beta \partial_x^\alpha (c_i(\mathcal{M}_i^\varepsilon - \mathcal{M}_{\bar{u},i})) \times \partial_v^\beta \partial_x^\alpha (c_i \mathcal{M}_{\bar{u},i})$ , which preserve the expected  $\mathcal{O}(\delta_{\text{MS}}^2)$ .

Indeed, using estimate (3.3.15) from Lemma 3.3.7 applied to the decomposition of the term  $\mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon)$ , we deduce that

$$\begin{aligned} &\frac{1}{\varepsilon^3} \left| \left\langle \partial_v^\beta \partial_x^\alpha \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\mu^{-\frac{1}{2}})} \right| \\ &\leq \frac{2C_s^{\mathbf{Q}}}{\varepsilon} \left( \left\| \mathbf{c}\mathcal{M}_{\bar{u}} \right\|_{H_{x,v}^s(\mu^{-\frac{1}{2}})} \left\| \frac{\mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}}}{\varepsilon^2} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})} \right. \\ &\quad \left. + \left\| \frac{\mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}}}{\varepsilon^2} \right\|_{H_{x,v}^s(\mu^{-\frac{1}{2}})} \left\| \mathbf{c}\mathcal{M}_{\bar{u}} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})} \right) \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})} \\ &\quad + \frac{C_s^{\mathbf{Q}}}{\varepsilon} \left( \left\| \mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}} \right\|_{H_{x,v}^s(\mu^{-\frac{1}{2}})} \left\| \frac{\mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}}}{\varepsilon^2} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})} \right. \\ &\quad \left. + \left\| \frac{\mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}}}{\varepsilon^2} \right\|_{H_{x,v}^s(\mu^{-\frac{1}{2}})} \left\| \mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}} \right\|_{H_{x,v}^s(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})} \right) \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \mu^{-\frac{1}{2}})}. \end{aligned}$$

Now, each term inside the parentheses is dealt with by simply taking the square power in the inequalities (3.4.16). In particular, we recognize the same structure of (C.1.1), which allows to infer the boundedness of all the terms involving  $\mathbf{c}\mathcal{M}_{\bar{u}}$  and  $\mathbf{M}^\varepsilon - \mathbf{c}\mathcal{M}_{\bar{u}}$ , by some constant only depending on  $\|\mathbf{c}\|_{L_t^\infty H_x^{|\alpha|+4}}(\mathbf{c}_\infty^{-\frac{1}{2}})$  and  $\|\mathbf{u}\|_{L_t^\infty H_x^{|\alpha|+4}}$ . In this way we recover the correct leading order  $\mathcal{O}(\varepsilon^{-1})$ , and we can finally apply Young's inequality with the same constant  $\eta_2/\varepsilon$  used for the linear part, to get

$$\frac{1}{\varepsilon^3} \left\langle \partial_v^\beta \partial_x^\alpha \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{\delta_{\text{MS}}^2 C_Q(\delta)}{\eta_2} + \frac{\eta_2}{\varepsilon^2} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (3.4.17)$$

To conclude, since  $\langle v \rangle^\gamma \geq 1$ , it is straightforward that

$$\left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}, \quad \forall \mathbf{f} \in H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}}).$$

Thanks to this inequality, we can further bound the linear part (3.4.15) to finally ensure the validity of the first estimate (3.3.16), by gathering (3.4.15) and (3.4.17) with the choices  $C_{\alpha,\beta}^s = \max \left\{ \frac{C_L(\delta)}{\min_i c_{i,\infty}}, C_Q(\delta) \right\}$ .

The same arguments can be used to derive estimate (3.3.17). The only difference is that, in the  $\mathcal{H}_\varepsilon^s$  norm, we only have a factor  $\varepsilon$  multiplying the commutator. Therefore, in this case, we are constrained to preserve the order  $\varepsilon^{-1}$  in front of each term. This is easily achieved by choosing a general positive constant  $\eta_3$  (in place of  $\eta_2/\varepsilon$ ) each time Young's inequality is applied. In this way, estimate (3.3.17) for the commutator directly follows.

**Step 2 - Estimates for the spatial derivatives.** In order to prove estimate (3.3.18) for the  $x$ -derivatives, we first expand the scalar product by means of the orthogonal projection  $\pi_{\mathbf{L}}$ . We split

$$\langle \partial_x^\alpha \mathbf{S}^\varepsilon, \partial_x^\alpha \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \langle \pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{S}^\varepsilon), \pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{f}) \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} + \langle \partial_x^\alpha \mathbf{S}^{\varepsilon\perp}, \partial_x^\alpha \mathbf{f}^\perp \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}, \quad (3.4.18)$$

and we study both contributions separately. Regarding the first term, let us begin by making some considerations about  $\pi_{\mathbf{L}}(\mathbf{S}^\varepsilon)$ . Using the linearity of the orthogonal projection, together with the fact that  $\mathbf{Q}(\mathbf{f}, \mathbf{f}) \in (\ker \mathbf{L})^\perp$ , from Lemma 3.3.7, we obtain

$$\begin{aligned} \pi_{\mathbf{L}}(\mathbf{S}^\varepsilon) &= \pi_{\mathbf{L}} \left( -\frac{1}{\varepsilon} \partial_t \mathbf{M}^\varepsilon - \frac{1}{\varepsilon^2} v \cdot \nabla_x \mathbf{M}^\varepsilon \right) + \frac{1}{\varepsilon^3} \pi_{\mathbf{L}}(\mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{M}^\varepsilon)) \\ &= -\frac{1}{\varepsilon^2} \pi_{\mathbf{L}}(\varepsilon \partial_t \mathbf{M}^\varepsilon + v \cdot \nabla_x \mathbf{M}^\varepsilon). \end{aligned}$$

The idea is again to prove that this term is actually  $\mathcal{O}(\delta_{\text{MS}})$ . In fact,  $\pi_{\mathbf{L}}(\varepsilon \partial_t \mathbf{M}^\varepsilon + v \cdot \nabla_x \mathbf{M}^\varepsilon)$  is nothing but the projection onto the macroscopic equations governed by the Maxwell-Stefan system (3.1.7)–(3.1.9). Thus, following the computations in [39], it is easy to see that, for any  $1 \leq i \leq N$ ,

$$\int_{\mathbb{R}^3} M_i^\varepsilon(t, x, v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = \begin{pmatrix} c_i(t, x) \\ \varepsilon c_i(t, x) u_i(t, x) \\ \frac{3}{m_i} c_i(t, x) + \varepsilon^2 c_i(t, x) |u_i(t, x)|^2 \end{pmatrix}.$$

We can then deduce, for any  $1 \leq i \leq N$ , that

$$\begin{aligned} \int_{\mathbb{R}^3} (\varepsilon \partial_t M_i^\varepsilon + v \cdot \nabla_x M_i^\varepsilon) dv &= \varepsilon \left( \partial_t c_i + \nabla_x \cdot (c_i u_i) \right), \\ \int_{\mathbb{R}^3} m_i v (\varepsilon \partial_t M_i^\varepsilon + v \cdot \nabla_x M_i^\varepsilon) dv &= \varepsilon^2 m_i \left( \partial_t (c_i u_i) + \nabla_x \cdot (c_i u_i \otimes u_i) \right) + \nabla_x c_i, \\ \int_{\mathbb{R}^3} \frac{m_i |v|^2 - 3}{\sqrt{6}} (\varepsilon \partial_t M_i^\varepsilon + v \cdot \nabla_x M_i^\varepsilon) dv &= \\ &= \frac{2\varepsilon}{\sqrt{6}} \nabla_x \cdot (c_i u_i) + \frac{\varepsilon^3}{\sqrt{6}} \left( m_i \partial_t (c_i |u_i|^2) + 3 \nabla_x \cdot (c_i |u_i|^2 u_i) \right), \end{aligned}$$

since

$$\int_{\mathbb{R}^3} |v|^2 v \cdot \nabla_x M_i^\varepsilon dv = \varepsilon \frac{5}{m_i} \nabla_x \cdot (c_i u_i) + \varepsilon^3 \frac{3}{m_i} \nabla_x \cdot (c_i |u_i|^2 u_i).$$

The fact that  $(\mathbf{c}, \mathbf{u})$  is a solution of the system (3.1.7)–(3.1.9) ensures that, for any  $1 \leq i \leq N$ ,

$$\partial_t c_i + \nabla_x \cdot (c_i u_i) = 0,$$

with

$$\sum_{i=1}^N \nabla_x c_i = 0, \quad \partial_t \left( \sum_{i=1}^N c_i \right) = 0, \quad \nabla_x \cdot \left( \sum_{i=1}^N c_i u_i \right) = 0.$$

This allows to conclude from (3.3.4) that the orthogonal projection of  $\mathbf{S}^\varepsilon$  onto  $\ker \mathbf{L}$  explicitly writes

$$\begin{aligned} \pi_{\mathbf{L}}(\mathbf{S}^\varepsilon) &= \\ &= - \frac{v}{\sum_{i=1}^N m_i c_{i,\infty}} \cdot \left[ \sum_{i=1}^N m_i \left( \partial_t (c_i u_i) + \nabla_x \cdot (c_i u_i \otimes u_i) \right) \right] (m_i \mu_i)_{1 \leq i \leq N} \\ &= - \frac{\varepsilon}{\sqrt{6} \sum_{i=1}^N c_{i,\infty}} \left[ \sum_{i=1}^N \left( m_i \partial_t (c_i |u_i|^2) + 3 \nabla_x \cdot (c_i |u_i|^2 u_i) \right) \right] \left( \frac{m_i |v|^2 - 3}{\sqrt{6}} \mu_i \right)_{1 \leq i \leq N}. \end{aligned}$$

Supposing that we have all the required regularity on the solution  $(\mathbf{c}, \mathbf{u})$ , as done in the previous step, we now note that either  $\tilde{c}_i$  or  $u_i$  always appear in each term of the sums in the left-hand side. Therefore, we can infer the existence of two constants  $C_1, C_2 > 0$  such that

$$\begin{aligned} \left\| \sum_{i=1}^N \left( \partial_t (c_i u_i) + \nabla_x \cdot (c_i u_i \otimes u_i) \right) \right\|_{L_x^2}^2 &\leq C_1 \delta_{\text{MS}}^2, \\ \left\| \sum_{i=1}^N \left( m_i \partial_t (c_i |u_i|^2) + 3 \nabla_x \cdot (c_i |u_i|^2 u_i) \right) \right\|_{L_x^2}^2 &\leq C_2 \delta_{\text{MS}}^2, \end{aligned}$$



which in turn ensures that it is possible to control  $\pi_{\mathbf{L}}(\mathbf{S}^\varepsilon)$  in the  $L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm as

$$\begin{aligned} \|\pi_{\mathbf{L}}(\mathbf{S}^\varepsilon)\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &\leq C_{\pi_{\mathbf{L}}} \delta_{\text{MS}}^2 \|(1 + |v| + |v|^2)\boldsymbol{\mu}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\leq C_{\pi_{\mathbf{L}}} \delta_{\text{MS}}^2, \end{aligned}$$

since the integral is clearly finite (we have also used that  $\varepsilon \in (0, 1]$ ).

Moreover, because the orthogonal projection only acts on the velocity variable, it commutes with the  $x$ -derivatives. Note that this property was not at hand in the previous step, when dealing with  $v$ -derivatives. Therefore, in the case  $|\beta| = 0$  we are looking at here, the arguments used for  $\pi_{\mathbf{L}}(\mathbf{S}^\varepsilon)$  apply in the exact same way to  $\pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{S}^\varepsilon)$ , allowing to deduce that

$$\|\pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{S}^\varepsilon)\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 = \|\partial_x^\alpha \pi_{\mathbf{L}}(\mathbf{S}^\varepsilon)\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq C_\alpha^{(1)} \delta_{\text{MS}}^2.$$

We conclude that the first contribution can easily be estimated applying Young's inequality with a constant  $\eta_4 > 0$ , to get

$$\begin{aligned} \langle \pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{S}^\varepsilon), \pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{f}) \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} &\leq \frac{1}{\eta_4} \|\pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{S}^\varepsilon)\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \eta_4 \|\pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{f})\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\leq \frac{\delta_{\text{MS}}^2 C_\alpha^{(1)}}{\eta_4} + \eta_4 \|\pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{f})\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2. \end{aligned} \tag{3.4.19}$$

The second contribution in (3.4.18) is handled in a very similar way, by explicitly writing the definition of the orthogonal part. It gives

$$\begin{aligned} \langle \partial_x^\alpha \mathbf{S}^{\varepsilon\perp}, \partial_x^\alpha \mathbf{f}^\perp \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} &= \langle \partial_x^\alpha \mathbf{S}^\varepsilon - \pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{S}^\varepsilon), \partial_x^\alpha \mathbf{f}^\perp \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &= \langle \partial_x^\alpha \mathbf{S}^\varepsilon, \partial_x^\alpha \mathbf{f}^\perp \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} - \langle \pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{S}^\varepsilon), \partial_x^\alpha \mathbf{f}^\perp \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}. \end{aligned}$$

Looking at these two terms, we recognize the same structure of the scalar products that led to estimates (3.4.15), (3.4.17) and (3.4.19). In fact, all the computations carried out until now only depend on the particular form of the source term, and not on the scalar product in itself (the final upper bounds have been always obtained thanks to an application of Young's inequality). Using Young's inequality with two positive constants  $\eta_5/\varepsilon$  and  $\eta_5$ , we can thus repeat the previous considerations to recover (increasing the values of the constants if necessary)

$$\langle \partial_x^\alpha \mathbf{S}^\varepsilon, \partial_x^\alpha \mathbf{f}^\perp \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{\delta_{\text{MS}}^2 (C_{\mathbf{L}}(\delta) + C_{\mathbf{Q}}(\delta))}{\eta_5} + \frac{\eta_5}{\varepsilon^2} \left\| \partial_x^\alpha \mathbf{f}^\perp \right\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2,$$

from (3.4.15)–(3.4.17), and

$$\langle \pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{S}^\varepsilon), \partial_x^\alpha \mathbf{f}^\perp \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{\delta_{\text{MS}}^2 C_\alpha^{(1)}}{\eta_5} + \eta_5 \left\| \partial_x^\alpha \mathbf{f}^\perp \right\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2,$$

from (3.4.19). Therefore, since the  $L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})$  norm controls the  $L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm, we obtain

$$\langle \partial_x^\alpha \mathbf{S}^{\varepsilon\perp}, \partial_x^\alpha \mathbf{f}^\perp \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{\delta_{\text{MS}}^2 C_\alpha^{(2)}}{\eta_5} + \frac{\eta_5}{\varepsilon^2} \left\| \partial_x^\alpha \mathbf{f}^\perp \right\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \tag{3.4.20}$$

We finally infer the validity of the last estimate (3.3.18), by gathering (3.4.19)–(3.4.20) with the choice  $C_\alpha^{\mathfrak{S}} = \max \left\{ \eta_5 C_\alpha^{(1)}, \eta_4 C_\alpha^{(2)} \right\}$ . This concludes the proof of Lemma 3.3.8.



## Chapitre 4

# A numerical scheme for a kinetic model for mixtures in the diffusive limit using the moment method

Ce chapitre fait l'objet de la publication [31], en collaboration avec Laurent Boudin et B er enice Grec.

### 4.1 Introduction

The derivation and mathematical analysis of models describing gaseous mixtures raise many questions, from the theoretical as well as from the numerical point of view. A wide variety of models can be considered, depending on both the scale and the setting where the model is derived. In this article, we focus on describing mixtures in a diffusive setting at a macroscopic scale. Such models arise in various fields of physics and medicine, for example in the context of respiration, in order to describe the diffusive flow of air in the lower part of the lungs, or for the modelling of polluting particles. The first macroscopic diffusion models for mixtures have been introduced on the one hand by Maxwell and Stefan [153, 180], and by Fick on the other hand [88]. Both models lie in the family of cross-diffusion models [62, 68, 137, 69], coupling the molar fluxes and the mole fractions of each species of the mixture. The Maxwell-Stefan equations have been derived at the macroscopic level from mechanical considerations [141, 164], whereas the Fick equations are obtained from Onsager's contributions from the thermodynamic of irreversible processes. Fick and Maxwell-Stefan formulations have a strong formal analogy, and both models can surely be linked in some regimes [96, 97, 33].

In this work, we shall focus on the Maxwell-Stefan equations, in the setting of a non-reactive mixture of  $N \geq 2$  ideal gases in an open bounded subset  $\Omega$  of  $\mathbb{R}^d$ ,  $d \geq 1$ . For any species  $\mathcal{E}_i$ ,  $1 \leq i \leq N$ , we denote by  $c_i$  its concentration in the mixture and  $u_i$  the associated velocity, which both depend on time  $t \geq 0$  and position  $x \in \Omega$ . Mass conservation is written on  $\mathbb{R}_+ \times \Omega$ , for any  $1 \leq i \leq N$ , as

$$\partial_t c_i + \nabla_x \cdot (c_i u_i) = 0. \quad (4.1.1)$$

Now, defining the total concentration  $c = \sum_i c_i$ , the Maxwell-Stefan diffusion equations

are written on  $\mathbb{R}_+ \times \Omega$ , for any  $1 \leq i \leq N$ ,

$$-\nabla_x \left( \frac{c_i}{c} \right) = \frac{1}{c} \sum_{k \neq i} \frac{c_k c_i u_i - c_i c_k u_k}{c D_{ik}}, \quad (4.1.2)$$

where  $D_{ik} = D_{ki} > 0$  is the binary diffusion coefficient between species  $\mathcal{E}_i$  and  $\mathcal{E}_k$ . The model is supplied with initial conditions  $c_i(0, \cdot) = c_i^{\text{in}}$ ,  $u_i(0, \cdot) = u_i^{\text{in}}$  and boundary conditions on the fluxes  $u_i \cdot \mathbf{n}|_{\partial\Omega} = 0$ , where  $\mathbf{n}$  denotes the exterior normal to the boundary.

Because of the symmetry of the binary diffusion coefficients, the  $N$  equations (4.1.2) are not linearly independent. Therefore, an additional relationship is needed in order to close the system, for example the equimolar diffusion assumption, which means that the total flux of the mixture  $\sum_i c_i u_i$  equals zero for any time and anywhere in  $\Omega$ . In this equimolar diffusion setting, if, in addition, the total concentration  $c$  of the mixture is uniform in space at initial time, it remains constant for all time, and we can assume  $c$  to be equal to 1 without loss of generality. Thus, assuming  $c(t, x) = 1$  for any  $(t, x) \in \mathbb{R}_+ \times \Omega$ , equations (4.1.2) become, for any  $1 \leq i \leq N$ ,

$$-\nabla_x c_i = \sum_{k \neq i} \frac{c_k c_i u_i - c_i c_k u_k}{D_{ik}}. \quad (4.1.3)$$

The Maxwell-Stefan equations have been studied recently from both mathematical [97, 33, 38, 138] and numerical [97] viewpoints (see also the review [141]).

A natural question is to justify such macroscopic diffusion models from a kinetic description at the mesoscopic level, mainly the Boltzmann equation. This falls into the wide literature about hydrodynamic limits, beginning with the pioneering works of Bardos, Golse and Levermore [13, 14], which lead to other works on the Navier-Stokes or Euler hydrodynamic limit (see [66, 102, 103, 124, 125, 195]) for a single monoatomic gas.

For mixtures, suitable kinetic models have been introduced in the middle of the 20th century [179, 158]. Further, consistent BGK-models for mixtures were derived [95, 4, 47], and a generalization of Boltzmann equations for mixtures was introduced in [70] for polyatomic gases with chemical reactions.

For our study, consider a non-reactive mixture of  $N$  monoatomic gases, where each species  $\mathcal{E}_i$  is described by its distribution function  $f_i$  depending on time  $t \geq 0$ , position  $x \in \mathbb{R}^d$  and velocity  $v \in \mathbb{R}^d$ . Assuming the only interactions between molecules at the microscopic level to be elastic collisions, two molecules of species  $\mathcal{E}_i$  and  $\mathcal{E}_k$ ,  $1 \leq i, k \leq p$ , of respective masses  $m_i$ ,  $m_k$  and post-collisional velocities  $v$  and  $v_*$ , have pre-collisional velocities  $v'$  and  $v'_*$  given by

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

where  $\sigma \in \mathbb{S}^{d-1}$ , because of momentum and energy conservations. The Boltzmann collision operator is then defined, for  $v \in \mathbb{R}^d$ , by

$$Q_{ik}(f_i, f_k)(v) = \int_{\mathbb{R}^d \times \mathbb{S}^{d-1}} \mathcal{B}_{ik}(v, v_*, \sigma) \left( f_i(v') f_k(v'_*) - f_i(v) f_k(v_*) \right) dv_* d\sigma,$$

with cross sections  $\mathcal{B}_{ik} = \mathcal{B}_{ki} > 0$ . We restrict our study to Maxwellian molecules, meaning that for any  $1 \leq i, k \leq N$ , there exist even functions  $b_{ik} : [-1, 1] \rightarrow \mathbb{R}_+ \in L^1(-1, 1)$  such that the cross sections  $\mathcal{B}_{ik}$  are written

$$\mathcal{B}_{ik}(v, v_*, \sigma) = b_{ik} \left( \frac{v - v_*}{|v - v_*|} \cdot \sigma \right) = b_{ik}(\cos \vartheta),$$

where  $\vartheta \in [0, \pi]$  is the deviation angle between  $v - v_*$  and  $\sigma$ .

This collision operator satisfies conservation properties [70]

$$\int_{\mathbb{R}^d} Q_{ik}(f_i, f_k)(v) m_i dv = 0, \quad 1 \leq i, k \leq N, \quad (4.1.4)$$

$$\int_{\mathbb{R}^d} Q_{ii}(f_i, f_i)(v) m_i v dv = 0, \quad 1 \leq i \leq N. \quad (4.1.5)$$

The Boltzmann equations for mixtures are then written, for  $1 \leq i \leq N$ ,

$$\partial_t f_i + v \cdot \nabla_x f_i = \sum_{k=1}^N Q_{ik}(f_i, f_k) \quad \text{on } \mathbb{R}_+ \times \Omega \times \mathbb{R}^d. \quad (4.1.6)$$

In the context of mixtures, formal hydrodynamic limits have been performed in several regimes. We here focus on the diffusive scaling (small Knudsen and Mach numbers). Euler and Navier-Stokes equations, coupled or not with a Vlasov equation, were obtained as the fluid-dynamic limit of the Boltzmann equations for a binary mixture [16, 19], as well as the incompressible Euler and Navier-Stokes equations for general mixtures [22]. It has also been shown in [39] that Maxwell-Stefan's equations can be seen as the limit in the small Mach and Knudsen number regime of the Boltzmann equations for mixtures in the case of Maxwellian molecules. This result has been extended to some analytical cross sections in [127], and generalized to general cross sections in [35], as well as in a non-isothermal setting in [126].

In this article, we are concerned with the same diffusive scaling as in [39], assuming Mach and Knudsen numbers to be of the same order of magnitude  $\varepsilon \ll 1$ . Then equations (4.1.6) are written, for  $1 \leq i \leq N$ ,

$$\varepsilon \partial_t f_i^\varepsilon + v \cdot \nabla_x f_i^\varepsilon = \frac{1}{\varepsilon} \sum_{k=1}^N Q_{ik}(f_i^\varepsilon, f_k^\varepsilon) \quad \text{on } \mathbb{R}_+ \times \Omega \times \mathbb{R}^d. \quad (4.1.7)$$

Their formal hydrodynamic limit obtained thanks to a moment method are the Maxwell-Stefan equations (4.1.3) on  $c_i$  and  $c_i u_i$ ,  $1 \leq i \leq N$ ,  $c_i$  and  $c_i u_i$  being the limits, when  $\varepsilon$  vanishes, of the zeroth- and first-order moments of the distribution functions  $f_i^\varepsilon$ ,  $1 \leq i \leq N$ .

We here aim to write a numerical scheme which could both capture the behaviour of physical solutions to the Boltzmann equations in a rarefied regime and describe the solutions of the Maxwell-Stefan equations in the fluid regime. However, this induces some difficulties, due to the fact that the collision term (and, in a lesser way, the transport term) becomes stiffer when the parameter  $\varepsilon$  tends to zero. In particular, a satisfactory numerical scheme needs to use time and space steps independent of the parameter  $\varepsilon$ , which falls into the class of asymptotic-preserving (AP) schemes. Such AP schemes have been derived for many equations in several regimes [89], and we refer the reader to the review [132] treating AP schemes for kinetic and hyperbolic equations. In the context of kinetic equations for mixtures, AP schemes capturing the Euler and Navier-Stokes hydrodynamic limit from the Boltzmann equation for mixtures are derived in [136, 133].

In the following, in order to describe numerical schemes, let us introduce a time discretization  $(t^n)_{n \in \mathbb{N}}$  with a time step  $\Delta t > 0$ , such that  $t^n = n \Delta t$ .

A reasonable attempt to derive an AP numerical scheme for Boltzmann equations for mixtures is to use a penalty method by a linear BGK-operator as in [89], which has been extended to the multi-species case in [133]. This operator would then be defined for each

species  $1 \leq i \leq N$  as  $P_i : f_i \mapsto \beta_i(M_i - f_i)$ , where  $M_i$  is the global Maxwellian equilibrium state defined by

$$M_i(t, x, v) = c_i(t, x) \left( \frac{m_i}{2\pi K_B T} \right)^{d/2} \exp \left\{ -\frac{m_i v^2}{2K_B T} \right\}, \quad t \geq 0, \quad x \in \Omega, \quad v \in \mathbb{R}^d,$$

and  $\beta_i$  is some positive constant to be specified. The semi-discretized scheme is then written, for  $1 \leq i \leq N$ ,

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} + \frac{1}{\varepsilon} v \cdot \nabla_x f_i^n = \frac{Q_i^n - P_i^n}{\varepsilon^2} + \frac{P_i^{n+1}}{\varepsilon^2},$$

where  $f_i^n \simeq f_i^\varepsilon(t^n, x, v)$ ,  $P_i^n = P_i(f_i^n)$ , and  $Q_i^n = \sum_{k=1}^N Q_{ik}(f_i^n, f_k^n)$ .

However, such a scheme leads to a transport term of order  $1/\varepsilon$ , which imposes a very fine discretization for the velocity variable, and a growing support in the velocity variable, since the velocity domain is unbounded. Therefore, we had to choose another method.

Our approach is to mimic the analytical method used to obtain the Maxwell-Stefan equations in the low Mach and Knudsen numbers limit from the Boltzmann equations for mixtures. Whereas the Fick equations are naturally obtained from the kinetic equations by a perturbative method, the Maxwell-Stefan ones are obtained, as we already stated, by a moment method [35]. Thus the scheme we propose relies on the computation of the moments of the distribution functions  $f_i^\varepsilon$ ,  $1 \leq i \leq N$ , under the ansatz that these distributions functions are at local Maxwellian states. Following this idea, we derive a numerical scheme for the Boltzmann kinetic model for mixtures, which nicely converges to the Maxwell-Stefan equations in the small Mach and Knudsen numbers limit. In particular, henceforth we shall assume that  $d = 1$  in order to prove numerical properties of the scheme (the extension of the proofs is not clear in the case  $d \geq 2$ ).

The chapter is organized as follows. In Section 4.2, we briefly recall the moment method for the Boltzmann equations for mixtures and describe the chosen numerical scheme. A priori estimates for this scheme are proved in Section 4.3, in particular the positivity of the concentrations. In Section 4.4, these estimates are used to prove the existence of a solution to the numerical scheme. Last, in Section 4.5, we present numerical simulations illustrating the asymptotic-preserving behaviour of the scheme, and its capacity to describe uphill diffusion phenomena for mixtures.

## 4.2 Derivation of a numerical scheme for Boltzmann equations for mixtures

We choose a one-dimensional space domain  $\Omega \subset \mathbb{R}$  ( $d = 1$ ).

### 4.2.1 Moment method

Since formal theoretical asymptotic results [39, 35] are obtained by a moment method [147], assuming that the distribution function of each species  $i$  is at a local Maxwellian state with a small velocity for any  $(t, x) \in \mathbb{R}_+ \times \Omega$ , we apply the same approach in order to derive a numerical scheme which nicely behaves when  $\varepsilon$  tends to 0. More precisely, the results are obtained under the following ansatz, for any  $1 \leq i \leq N$ ,

$$f_i^\varepsilon(t, x, v) = c_i^\varepsilon(t, x) \left( \frac{m_i}{2\pi K_B T} \right)^{1/2} \exp \left\{ -\frac{m_i (v - \varepsilon u_i^\varepsilon(t, x))^2}{2K_B T} \right\}, \quad t \geq 0, \quad x \in \Omega, \quad v \in \mathbb{R}. \quad (4.2.1)$$

The same ansatz is also made on the the initial condition  $f_i^{\text{in}}(x, v) = f_i^\varepsilon(0, x, v)$ . In order for the scheme to be consistent with the possible closure relation of equimolar diffusion, we assume that the macroscopic quantities  $c_i^{\text{in}}(x) = c_i(0, x)$  and  $u_i^{\text{in}}(x) = u_i(0, x)$  satisfy the compatibility conditions

$$\sum_{i=1}^N c_i^{\text{in}} = 1 \quad \text{and} \quad \sum_{i=1}^N c_i^{\text{in}} u_i^{\text{in}} = 0. \quad (4.2.2)$$

When integrating with respect to  $v$  equations (4.1.7) and using (4.1.4), we obtain, for any  $1 \leq i \leq N$ ,

$$\varepsilon \partial_t c_i^\varepsilon + \int_{\mathbb{R}} v \partial_x f_i^\varepsilon dv = 0,$$

which, using ansatz (4.2.1), becomes the usual mass conservation for any species  $1 \leq i \leq N$

$$\partial_t c_i^\varepsilon + \partial_x (c_i^\varepsilon u_i^\varepsilon) = 0. \quad (4.2.3)$$

Now, we integrate with respect to  $v$  equations (4.1.7) multiplied by  $m_i v$  to obtain, for any  $1 \leq i \leq N$

$$\varepsilon^2 m_i \partial_t (c_i^\varepsilon u_i^\varepsilon) + m_i \int_{\mathbb{R}} v^2 \partial_x f_i^\varepsilon dv = \frac{m_i}{\varepsilon} \sum_{k=1}^N \int_{\mathbb{R}} Q_{ik}(f_i^\varepsilon, f_k^\varepsilon) v dv,$$

which becomes, using (4.1.5) and again ansatz (4.2.1) as in [39],

$$\varepsilon^2 m_i \partial_t (c_i^\varepsilon u_i^\varepsilon) + \varepsilon^2 m_i \partial_x (c_i^\varepsilon (u_i^\varepsilon)^2) + K_B T \partial_x c_i^\varepsilon = \sum_{k \neq i} \mu_{ik} B_{ik} c_i c_k (u_k - u_i), \quad (4.2.4)$$

where  $\mu_{ik} = \frac{2m_i m_k}{m_i + m_k}$  is the reduced mass corresponding to species  $\mathcal{E}_i$  and  $\mathcal{E}_k$ , and we have denoted  $B_{ik} = \frac{1}{2} \|b_{ik}\|_{L^1(-1,1)} > 0$  the constant cross-section for Maxwellian molecules in dimension 1. This equation can be written in a matrix form introducing the coefficients  $(A_{ik}^\varepsilon)_{1 \leq i, k \leq N}$

$$A_{ik}^\varepsilon = \begin{cases} -\mu_{ik} B_{ik} c_i^\varepsilon & \text{if } i \neq k, \\ \sum_{\ell \neq i} \mu_{i\ell} B_{i\ell} c_\ell^\varepsilon & \text{if } i = k. \end{cases} \quad (4.2.5)$$

Let us denote  $\mathcal{F}^\varepsilon = (c_i^\varepsilon u_i^\varepsilon)_{1 \leq i \leq N}$  the vector of the fluxes, and  $[A^\varepsilon \mathcal{F}^\varepsilon]_i = \sum_{k=1}^N A_{ik}^\varepsilon c_k^\varepsilon u_k^\varepsilon$  the  $i$ -th coordinate of the product vector  $A^\varepsilon \mathcal{F}^\varepsilon$ . Equation (4.2.4) is then written

$$\varepsilon^2 m_i \partial_t (c_i^\varepsilon u_i^\varepsilon) + \varepsilon^2 m_i \partial_x (c_i^\varepsilon (u_i^\varepsilon)^2) + K_B T \partial_x c_i^\varepsilon = -[A^\varepsilon \mathcal{F}^\varepsilon]_i. \quad (4.2.6)$$

Now, denoting  $F_i^\varepsilon = c_i^\varepsilon u_i^\varepsilon$ , we obtain the following system

$$\begin{cases} \partial_t c_i^\varepsilon + \partial_x F_i^\varepsilon = 0, \\ \varepsilon^2 m_i \partial_t F_i^\varepsilon + \varepsilon^2 m_i \partial_x (c_i^\varepsilon (u_i^\varepsilon)^2) + K_B T \partial_x c_i^\varepsilon = -[A^\varepsilon \mathcal{F}^\varepsilon]_i. \end{cases} \quad (4.2.7)$$

This system is supplemented with initial conditions on the concentrations and fluxes, as well as boundary conditions on the fluxes, for any  $1 \leq i \leq N$ ,

$$c_i^\varepsilon(0, \cdot) = c_i^{\text{in}} \geq 0 \quad \text{and} \quad F_i^\varepsilon(0, \cdot) = F_i^{\text{in}}, \quad \text{in } \Omega, \quad (4.2.8)$$

$$F_i^\varepsilon(t, \cdot)|_{\partial\Omega} = 0, \quad \forall t > 0. \quad (4.2.9)$$



### 4.2.2 Description of the numerical scheme

Consider a space discretization  $(x_j)_{0 \leq j \leq J}$  of the domain  $\Omega$ , with a space step  $\Delta x > 0$ , such that  $x_j = j\Delta x$ . The scheme is obtained thanks to a discretization of system (4.2.7) using a staggered dual grid. For each species  $1 \leq i \leq N$ , its concentration  $c_i$  is evaluated at the points  $x_j$ ,  $0 \leq j \leq J$ , whereas its flux  $F_i$  is evaluated at  $x_{j+\frac{1}{2}} = (j + \frac{1}{2})\Delta x$ , for  $0 \leq j \leq J - 1$ . Therefore, we denote  $c_{i,j}^n \simeq c_i^\varepsilon(t^n, x_j)$  and  $F_{i,j+\frac{1}{2}}^n \simeq F_i^\varepsilon(t^n, x_{j+\frac{1}{2}})$  the numerical approximations of the unknowns at the discretization points. Introducing the ratio  $\lambda = \Delta t / \Delta x$ , the first equation of system (4.2.7) can then be discretized as follows, for any  $1 \leq i \leq N$  and  $0 \leq j \leq J$

$$c_{i,j}^{n+1} + \lambda \left( F_{i,j+\frac{1}{2}}^{n+1} - F_{i,j-\frac{1}{2}}^{n+1} \right) = c_{i,j}^n. \quad (4.2.10)$$

For the second one, we observe that the matrix  $A$  contains concentrations, which have to be evaluated at the same points as the fluxes. In order to prove nonnegativity of the concentrations (Proposition 4.3.4), we shall see that a relevant choice [3] for the quantities  $c_{i,j+\frac{1}{2}}^{n+1}$  is the following:

$$c_{i,j+\frac{1}{2}}^{n+1} = \min \left\{ c_{i,j}^{n+1}, c_{i,j+1}^{n+1} \right\}. \quad (4.2.11)$$

Moreover, we have to discretize the nonlinear term  $c_i u_i^2$ . Let us introduce the following quantities, for  $1 \leq i \leq N$  and  $0 \leq j \leq J - 1$ ,

$$r_{i,j}^n = \begin{cases} \frac{1}{4c_{i,j}^n} \left( F_{i,j+\frac{1}{2}}^n + F_{i,j-\frac{1}{2}}^n \right)^2 & \text{if } c_{i,j}^n \neq 0, \\ 0 & \text{if } c_{i,j}^n = 0. \end{cases}$$

We denote by  $R_{i,j+\frac{1}{2}}^n / \Delta x$  a discretization of  $\partial_x(c_i u_i^2)$  at  $x_{j+\frac{1}{2}}$  and time  $t^n$ , chosen such that

$$R_{i,j+\frac{1}{2}}^n = r_{i,j+1}^n - r_{i,j}^n.$$

This leads to the following discretization of the second equation of system (4.2.7), for any  $1 \leq i \leq N$  and  $0 \leq j \leq J - 1$ ,

$$\begin{aligned} & \left( -\Delta t \sum_{k \neq i} \mu_{ik} B_{ik} c_{k,j+\frac{1}{2}}^{n+1} - \varepsilon^2 m_i \right) F_{i,j+\frac{1}{2}}^{n+1} + \Delta t c_{i,j+\frac{1}{2}}^{n+1} \sum_{k \neq i} \mu_{ik} B_{ik} F_{k,j+\frac{1}{2}}^{n+1} \\ & = K_B T \lambda \left( c_{i,j+1}^{n+1} - c_{i,j}^{n+1} \right) + \varepsilon^2 m_i \lambda R_{i,j+\frac{1}{2}}^n - \varepsilon^2 m_i F_{i,j+\frac{1}{2}}^n. \end{aligned} \quad (4.2.12)$$

In order for this discretization to be well-defined, we need to supplement it with boundary conditions on the fluxes in ghost cells  $F_{i,-\frac{1}{2}}^{n+1}$  and  $F_{i,J+\frac{1}{2}}^{n+1}$ . In accordance with (4.2.9), we choose, for  $1 \leq i \leq N$ ,

$$F_{i,-\frac{1}{2}}^{n+1} = F_{i,J+\frac{1}{2}}^{n+1} = 0, \quad (4.2.13)$$

which allows the scheme to satisfy mass conservation (Proposition 4.3.1). The scheme is thus written, for  $1 \leq i \leq N$ ,

$$\begin{cases} c_{i,j}^{n+1} + \lambda \left( F_{i,j+\frac{1}{2}}^{n+1} - F_{i,j-\frac{1}{2}}^{n+1} \right) = c_{i,j}^n, & 0 \leq j \leq J, \\ \left( -\Delta t \sum_{k \neq i} \mu_{ik} B_{ik} c_{k,j+\frac{1}{2}}^{n+1} - \varepsilon^2 m_i \right) F_{i,j+\frac{1}{2}}^{n+1} + \Delta t c_{i,j+\frac{1}{2}}^{n+1} \sum_{k \neq i} \mu_{ik} B_{ik} F_{k,j+\frac{1}{2}}^{n+1} \\ \quad = K_B T \lambda \left( c_{i,j+1}^{n+1} - c_{i,j}^{n+1} \right) + \varepsilon^2 m_i \lambda R_{i,j+\frac{1}{2}}^n - \varepsilon^2 m_i F_{i,j+\frac{1}{2}}^n, & 0 \leq j \leq J-1, \end{cases} \quad (4.2.14)$$

and it can be written for all species simultaneously in a matrix form, introducing the following vector of unknowns  $\mathbf{y}^n = \begin{pmatrix} \mathbf{y}_1^n \\ \mathbf{y}_2^n \end{pmatrix} \in \mathbb{R}^{N(2J+1)}$ , where

$$\begin{aligned} \mathbf{y}_1^n &= (c_{1,0}^n, \dots, c_{1,J}^n, \dots, c_{N,0}^n, \dots, c_{N,J}^n)^\top \in \mathbb{R}^{N(J+1)}, \\ \mathbf{y}_2^n &= (F_{1,\frac{1}{2}}^n, \dots, F_{1,J-\frac{1}{2}}^n, \dots, F_{N,\frac{1}{2}}^n, \dots, F_{N,J-\frac{1}{2}}^n)^\top \in \mathbb{R}^{NJ}. \end{aligned}$$

In a similar way, we define

$$\begin{aligned} \mathbf{m}\mathbf{y}_2^n &= (m_1 F_{1,\frac{1}{2}}^n, \dots, m_1 F_{1,J-\frac{1}{2}}^n, \dots, m_N F_{N,\frac{1}{2}}^n, \dots, m_N F_{N,J-\frac{1}{2}}^n)^\top \in \mathbb{R}^{NJ}, \\ \mathbf{m}\mathbf{R}^n &= (m_1 R_{1,\frac{1}{2}}^n, \dots, m_1 R_{1,J-\frac{1}{2}}^n, \dots, m_N R_{N,\frac{1}{2}}^n, \dots, m_N R_{N,J-\frac{1}{2}}^n)^\top \in \mathbb{R}^{NJ}. \end{aligned}$$

Indeed, system (4.2.14) then becomes

$$\mathbb{S}^\varepsilon(\mathbf{y}_1^{n+1})\mathbf{y}^{n+1} = \mathbf{b}^n, \quad (4.2.15)$$

where we have denoted

$$\mathbf{b}^n = \left( \mathbf{y}_1^n, \varepsilon^2 (\lambda \mathbf{m}\mathbf{R}^n - \mathbf{m}\mathbf{y}_2^n) \right)^\top \in \mathbb{R}^{N(2J+1)}. \quad (4.2.16)$$

The matrix  $\mathbb{S}^\varepsilon$  depends on the vector of concentrations  $\mathbf{y}_1$  and is given by

$$\mathbb{S}^\varepsilon(\mathbf{y}_1) = \begin{bmatrix} \mathbb{S}_{11} & \mathbb{S}_{12} \\ \mathbb{S}_{21} & \mathbb{S}_{22}^\varepsilon(\mathbf{y}_1) \end{bmatrix},$$

where  $\mathbb{S}_{11} = \mathbb{I}_{N(J+1)}$  is the identity matrix of size  $N(J+1)$ . The other blocks are defined using the following notation.

**Notation 4.2.1.** For any  $q, r, s \in \mathbb{N}^*$  and any matrices  $M_\ell \in \mathbb{R}^{r \times s}$ ,  $1 \leq \ell \leq q$ , we define the block matrix

$$\text{Diag}_{qr \times qs}(M_\ell) = \begin{bmatrix} M_1 & & & \\ & M_2 & & \\ & & \ddots & \\ & & & M_q \end{bmatrix} \in \mathbb{R}^{qr \times qs},$$

where the matrices which do not appear in the block writing are all zero.

The block  $\mathbb{S}_{12} \in \mathbb{R}^{N(J+1) \times NJ}$  is given by  $\mathbb{S}_{12} = \lambda \text{Diag}_{N(J+1) \times NJ}(\mathbb{S}_{12})$ . The matrices  $\mathbb{S}_{21}$  and  $\mathbb{S}_{12}$  are linked by  $\mathbb{S}_{21} = K_B T \mathbb{S}_{12}^\top \in \mathbb{R}^{NJ \times N(J+1)}$ , and  $\mathbb{S}_{12} \in \mathbb{R}^{(J+1) \times J}$  is defined by  $(\mathbb{S}_{12})_{i,j} = \delta_{ij} - \delta_{i,j+1}$ ,  $1 \leq i \leq J+1$ ,  $1 \leq j \leq J$ . The last block  $\mathbb{S}_{22}^\varepsilon$  is given by

$$\mathbb{S}_{22}^\varepsilon(\mathbf{y}_1) = \begin{bmatrix} \mathbb{B}_{11}^\varepsilon(\mathbf{y}_1) & \cdots & \mathbb{B}_{1N}(\mathbf{y}_1) \\ \vdots & \ddots & \vdots \\ \mathbb{B}_{N1}(\mathbf{y}_1) & \cdots & \mathbb{B}_{NN}^\varepsilon(\mathbf{y}_1) \end{bmatrix},$$

where the blocks  $\mathbb{B}_{ij}(\mathbf{y}_1)$  are defined by

$$\begin{cases} \mathbb{B}_{ij}(\mathbf{y}_1) = \Delta t \mu_{ij} B_{ij} \text{Diag}_{J \times J} \left( c_{i,\ell+\frac{1}{2}}^{n+1} \right) & \text{if } i \neq j, \\ \mathbb{B}_{ij}^\varepsilon(\mathbf{y}_1) = -\Delta t \text{Diag}_{N \times N}(\kappa_\ell) & \text{if } i = j, \end{cases}$$

where  $\kappa_\ell = \sum_{k \neq i} \mu_{ik} B_{ik} c_{k,\ell+\frac{1}{2}}^{n+1} + \varepsilon^2 \frac{m_i}{\Delta t}$ , for any  $0 \leq \ell \leq J-1$ . System (4.2.15) with boundary conditions (4.2.13) is then solved by a Newton fixed-point method, with initial conditions satisfying the compatibility conditions (4.2.2).

### 4.3 *A priori* estimates for the numerical scheme

In this section, we prove that, for each species and all time, the scheme satisfies mass conservation, and the concentrations remain nonnegative if they are initially nonnegative.

**Proposition 4.3.1.** *System (4.2.14) with boundary conditions (4.2.13) satisfies mass conservation for each species  $\mathcal{E}_i$ ,  $1 \leq i \leq N$ , i.e.*

$$\sum_{j=0}^J c_{i,j}^{n+1} = \sum_{j=0}^J c_{i,j}^n, \quad \forall n \in \mathbb{N}.$$

*Proof.* For each species  $\mathcal{E}_i$ ,  $1 \leq i \leq N$ , we sum equations (4.2.10) over  $0 \leq j \leq J$ , we obtain

$$\sum_{j=0}^J c_{i,j}^{n+1} = F_{i,J+\frac{1}{2}}^{n+1} - F_{i,-\frac{1}{2}}^{n+1} + \sum_{j=0}^J c_{i,j}^n, \quad \forall n \in \mathbb{N}.$$

Boundary conditions (4.2.13) ensure the claimed result.  $\square$

In order to prove nonnegativity of the solutions, we apply the method used in [3] and introduce the following auxiliary scheme

$$\begin{aligned} & \left( -\Delta t \sum_{k \neq i} \mu_{ik} B_{ik} \left[ c_{k,j+\frac{1}{2}}^{n+1} \right]^+ - \varepsilon^2 m_i \right) F_{i,j+\frac{1}{2}}^{n+1} + \Delta t \left[ c_{i,j+\frac{1}{2}}^{n+1} \right]^+ \sum_{k \neq i} \mu_{ik} B_{ik} F_{k,j+\frac{1}{2}}^{n+1} \\ & = K_B T \lambda \left( c_{i,j+1}^{n+1} - c_{i,j}^{n+1} \right) + \varepsilon^2 m_i \lambda R_{i,j+\frac{1}{2}}^n - \varepsilon^2 m_i F_{i,j+\frac{1}{2}}^n, \end{aligned} \quad (4.3.1)$$

with the notation  $[c]^+ = \max(c, 0)$  for any  $c \in \mathbb{R}$ . In the same way as for (4.2.6), we can write these equations in a matrix form, introducing a modified matrix  $\tilde{A} = ([\tilde{A}]_{ik})_{1 \leq i,k \leq N}$  defined by

$$[\tilde{A}]_{ik} = \begin{cases} -\Delta t \mu_{ik} B_{ij} [c_i]^+ & \text{if } i \neq k, \\ \Delta t \sum_{\ell \neq i} \mu_{i\ell} B_{i\ell} [c_\ell]^+ + \varepsilon^2 m_i & \text{if } i = k. \end{cases} \quad (4.3.2)$$

Observe that this matrix depends on the concentrations of each species, and can therefore vary for any discrete time  $t^n$ ,  $n \geq 0$  and any point  $x_j$ ,  $j \in \{0, \frac{1}{2}, \dots, N - \frac{1}{2}, N\}$ . When needed, we shall denote this dependence in the following straightforward way, for the same  $j \in \{0, \frac{1}{2}, \dots, N - \frac{1}{2}, N\}$ ,

$$\tilde{A}_j^n = \left( [\tilde{A}_j^n]_{ik} \right)_{1 \leq i, k \leq N} \quad \text{with} \quad [\tilde{A}_j^n]_{ik} = \begin{cases} -\Delta t \mu_{ik} B_{ij} [c_{i,j}^n]^+ & \text{if } i \neq k, \\ \Delta t \sum_{\ell \neq i} \mu_{i\ell} B_{i\ell} [c_{\ell,j}^n]^+ + \varepsilon^2 m_i & \text{if } i = k. \end{cases}$$

In this perspective, we can define, for any  $n \geq 0$ , the vectors of unknowns of all species

$$\mathcal{C}_j^n = (c_{1,j}^n, \dots, c_{N,j}^n)^\top \in \mathbb{R}^N, \quad 0 \leq j \leq J,$$

$$\mathcal{F}_{j+\frac{1}{2}}^n = (F_{1,j+\frac{1}{2}}^n, \dots, F_{N,j+\frac{1}{2}}^n)^\top \in \mathbb{R}^N, \quad 0 \leq j \leq J-1.$$

The continuity equations (4.2.10) can be written for any  $n \in \mathbb{N}$  and any  $1 \leq j \leq J-1$  as

$$\frac{\mathcal{C}_j^{n+1} - \mathcal{C}_j^n}{\lambda} + \left( \mathcal{F}_{j+\frac{1}{2}}^{n+1} - \mathcal{F}_{j-\frac{1}{2}}^{n+1} \right) = 0. \quad (4.3.3)$$

Equation (4.3.1) can also be written in a vectorial form for any  $n \in \mathbb{N}$  and any  $0 \leq j \leq J-1$

$$-\tilde{A}_{j+\frac{1}{2}}^{n+1} \mathcal{F}_{j+\frac{1}{2}}^{n+1} = K_B T \lambda \left( \mathcal{C}_{j+1}^{n+1} - \mathcal{C}_j^{n+1} \right) + \varepsilon^2 \mathcal{S}_{j+\frac{1}{2}}^n, \quad (4.3.4)$$

where the vectorial source term is defined by

$$\mathcal{S}_{j+\frac{1}{2}}^n = \left( m_1 \left( \lambda R_{1,j+\frac{1}{2}}^n - F_{1,j+\frac{1}{2}}^n \right), \dots, m_N \left( \lambda R_{N,j+\frac{1}{2}}^n - F_{N,j+\frac{1}{2}}^n \right) \right)^\top \in \mathbb{R}^N.$$

As we noted,  $\tilde{A}$  is defined point-wise in time and space, and the proof of nonnegativity of the concentrations relies on some particular properties of this matrix  $\tilde{A}$  (Lemmata 4.3.2 and 4.3.3), which are true for any time and any space point.

**Lemma 4.3.2.** *The matrix  $\tilde{A}$  defined by (4.3.2) is invertible for any  $\varepsilon > 0$ , and its eigenvalues are positive.*

*Proof.* We first observe that the matrix  $\tilde{A}$  is diagonally dominant, since, for any  $\varepsilon > 0$  and  $1 \leq i \leq N$ ,

$$\left| [\tilde{A}]_{ii} \right| = \Delta t \sum_{\ell \neq i} \mu_{i\ell} B_{i\ell} [c_\ell]^+ + \varepsilon^2 m_i > \Delta t \sum_{\ell \neq i} \mu_{i\ell} B_{i\ell} [c_\ell]^+ = \sum_{\ell \neq i} \left| [\tilde{A}]_{i\ell} \right|,$$

which ensures the invertibility. Furthermore, in order to prove the positivity of the eigenvalues, let us assume in a first step that  $[c_i]^+ > 0$ , for all  $1 \leq i \leq N$ . Then the matrix  $\tilde{A}$  can be written under the following form  $\tilde{A} = \Delta S \Delta^{-1} + D$ , where  $D$  and  $\Delta$  are diagonal matrices defined by

$$D = \varepsilon^2 \text{diag}(m_1, \dots, m_N), \quad \Delta = \text{diag} \left( \sqrt{[c_1]^+}, \dots, \sqrt{[c_N]^+} \right),$$

and matrix  $S = (S_{ik})_{1 \leq i, k \leq N}$  is defined by

$$S_{ik} = \begin{cases} -\Delta t \mu_{ik} B_{ij} \sqrt{[c_i]^+ [c_k]^+} & \text{if } i \neq k, \\ \Delta t \sum_{\ell \neq i} \mu_{i\ell} B_{i\ell} [c_\ell]^+ & \text{if } i = k. \end{cases}$$

This matrix  $S$  is obviously symmetric and is also positive semidefinite, since for any  $v \in \mathbb{R}^N$ ,

$$v^\top S v = \Delta t \sum_{i,k=1}^N \mu_{ik} B_{ik} \left( \sqrt{[c_i]^+} v_k - \sqrt{[c_k]^+} v_i \right)^2 \geq 0.$$

Thus, it follows that  $\tilde{A}$  is similar to a symmetric matrix  $S + D = \Delta^{-1} \tilde{A} \Delta$ , which is positive definite for any  $\varepsilon > 0$ , thus all its eigenvalues are positive.

Now, let us prove that the result also holds if only one of the  $[c_i]^+$  equals 0. Without loss of generality, renumbering the species if necessary, we can assume that  $[c_N]^+ = 0$ , and  $[c_i]^+ > 0$  for  $1 \leq i \leq N-1$ . Then  $[\tilde{A}]_{Nk} = 0$ , for any  $1 \leq k \leq N-1$ . In order to compute the eigenvalues of  $\tilde{A}$ , we can thus compute  $\det(\tilde{A} - \sigma \mathbb{I}_N)$  using the cofactor expansion for this determinant with respect to the last row

$$\det(\tilde{A} - \sigma \mathbb{I}_N) = \left( \Delta t \sum_{k \neq N} \mu_{Nk} B_{Nk} [c_k]^+ + \varepsilon^2 m_N - \sigma \right) \pi(\sigma),$$

where  $\pi(\sigma)$  is the characteristic polynomial of the  $(N-1) \times (N-1)$  matrix coming from the first  $N-1$  lines and columns of  $\tilde{A}$ . For this  $(N-1) \times (N-1)$  matrix, we can apply the result of the previous step, since all  $[c_i]^+ > 0$  for  $1 \leq i \leq N-1$ , which means that all its eigenvalues are positive, and thus all eigenvalues of  $\tilde{A}$  are also positive. A backward induction reasoning allows to treat in a same way the case when more than one  $[c_i]^+$  is equal to zero, which concludes the proof.  $\square$

We also need some properties on the elements of the inverse matrix  $\tilde{A}^{-1}$ , which are summed up in the following lemma.

**Lemma 4.3.3.** *The coefficients of the matrix  $\tilde{A}^{-1}$  are nonnegative. Moreover, all its extra-diagonal terms of row  $i$ ,  $1 \leq i \leq N$ , contain a factor  $[c_i]^+$ .*

*Proof.* The nonnegativity of the matrix  $\tilde{A}^{-1}$  comes from the  $M$ -matrices theory. Indeed, since all extra-diagonal terms of  $\tilde{A}$  are nonpositive, and since all eigenvalues of  $\tilde{A}$  are positive (Lemma 4.3.2), matrix  $\tilde{A}^{-1}$  is nonnegative [171, by Thm. 1, equivalence of  $C_9$  and  $F_{15}$  for matrices in  $Z^{n,n}$ ].

Consider now an extra-diagonal term  $[\tilde{A}^{-1}]_{ik}$  of  $\tilde{A}^{-1}$ ,  $1 \leq i, k \leq N$ ,  $i \neq k$ . The determinant formula for inversion gives  $[\tilde{A}^{-1}]_{ik} = \tilde{A}_{ki} / \det(\tilde{A})$ ,  $\tilde{A}_{ki}$  being the cofactor of the matrix  $\tilde{A}$  associated with the  $k$ -th row and  $i$ -th column. This cofactor equals the determinant of a matrix that is obtained from  $\tilde{A}$  by deleting its  $i$ -th column, and therefore all elements of the  $i$ -th row contain a factor  $[c_i]^+$ . Since obviously  $\det(\tilde{A})$  cannot be factorized by  $[c_i]^+$ , this concludes the proof.  $\square$

Let us now state an *a priori* positivity result on the concentrations for our scheme (4.2.10)–(4.2.12) with boundary conditions (4.2.13). The existence of solutions to this scheme will be proved in the next section (Theorem 4.4.1). As mentioned earlier, the proof relies on the introduction of an auxiliary system:

$$\begin{cases} c_{i,j}^{n+1} + \lambda \left( F_{i,j+\frac{1}{2}}^{n+1} - F_{i,j-\frac{1}{2}}^{n+1} \right) = c_{i,j}^n, \\ \left( -\Delta t \sum_{k \neq i} \mu_{ik} B_{ik} [c_{k,j+\frac{1}{2}}^{n+1}]^+ - \varepsilon^2 m_i \right) F_{i,j+\frac{1}{2}}^{n+1} + \Delta t [c_{i,j+\frac{1}{2}}^{n+1}]^+ \sum_{k \neq i} \mu_{ik} B_{ik} F_{k,j+\frac{1}{2}}^{n+1} \\ = K_B T \lambda \left( c_{i,j+1}^{n+1} - c_{i,j}^{n+1} \right) + \varepsilon^2 m_i \lambda R_{i,j+\frac{1}{2}}^n - \varepsilon^2 m_i F_{i,j+\frac{1}{2}}^n. \end{cases} \quad (4.3.5)$$

In order to precisely state the boundedness assumption needed on the source terms in Proposition 4.3.4, let us define the quantity

$$M_\varepsilon = \varepsilon^2 \max_{1 \leq i \leq N} \max_{n \geq 0} \max_{0 \leq j \leq J-1} \left| \mathcal{S}_{i,j+\frac{1}{2}}^n \right|. \quad (4.3.6)$$

We need the source terms to be uniformly bounded, which is guaranteed by

$$\lim_{\varepsilon \rightarrow 0} M_\varepsilon = 0. \quad (4.3.7)$$

**Proposition 4.3.4.** *Assume that for any  $1 \leq i \leq N$  and any  $n \geq 0$ , there exist solutions  $(c_{i,j}^n)_{0 \leq j \leq J}$ ,  $(F_{i,j+\frac{1}{2}}^n)_{0 \leq j \leq J-1}$  of the auxiliary system (4.3.5) with boundary conditions (4.2.13). Assume also that (4.3.7) holds. If, for any  $1 \leq i \leq N$ ,  $0 \leq j \leq J$ ,  $c_{i,j}^{\text{in}} \geq 0$ , then for any  $n \in \mathbb{N}$  and  $\varepsilon$  small enough,  $c_{i,j}^n \geq 0$ . Moreover,  $(c_{i,j}^n)_{0 \leq j \leq J}$ ,  $(F_{i,j+\frac{1}{2}}^n)_{0 \leq j \leq J-1}$  are also solutions of the initial system (4.2.14) with boundary conditions (4.2.13).*

*Proof.* Let us prove this result by induction. The base case is obviously true by assumption. Assume that  $c_{i,j}^n \geq 0$ , for any  $1 \leq i \leq N$ ,  $0 \leq j \leq J$ . Since  $\tilde{A}_{j+\frac{1}{2}}^{n+1}$  is invertible for any  $0 \leq j \leq J-1$  and  $n \in \mathbb{N}$ , we can rewrite (4.3.4) as

$$\mathcal{F}_{j+\frac{1}{2}}^{n+1} = - \left( \tilde{A}_{j+\frac{1}{2}}^{n+1} \right)^{-1} \left( K_B T \lambda \left( \mathcal{C}_{j+1}^{n+1} - \mathcal{C}_j^{n+1} \right) + \varepsilon^2 \mathcal{S}_{j+\frac{1}{2}}^n \right).$$

Injecting this expression in the continuity equations (4.3.3), we obtain multi-species diffusion equations for  $1 \leq j \leq J-1$ ,

$$\begin{aligned} \frac{\mathcal{C}_j^{n+1} - \mathcal{C}_j^n}{\lambda} &= \left( \tilde{A}_{j+\frac{1}{2}}^{n+1} \right)^{-1} \left( K_B T \lambda \left( \mathcal{C}_{j+1}^{n+1} - \mathcal{C}_j^{n+1} \right) + \varepsilon^2 \mathcal{S}_{j+\frac{1}{2}}^n \right) \\ &\quad - \left( \tilde{A}_{j-\frac{1}{2}}^{n+1} \right)^{-1} \left( K_B T \lambda \left( \mathcal{C}_j^{n+1} - \mathcal{C}_{j-1}^{n+1} \right) + \varepsilon^2 \mathcal{S}_{j-\frac{1}{2}}^n \right), \end{aligned} \quad (4.3.8)$$

and using boundary conditions (4.2.13), we obtain the two additional equations

$$\begin{aligned} \frac{\mathcal{C}_0^{n+1} - \mathcal{C}_0^n}{\lambda} &= \left( \tilde{A}_{\frac{1}{2}}^{n+1} \right)^{-1} \left( K_B T \lambda \left( \mathcal{C}_1^{n+1} - \mathcal{C}_0^{n+1} \right) + \varepsilon^2 \mathcal{S}_{\frac{1}{2}}^n \right), \\ \frac{\mathcal{C}_J^{n+1} - \mathcal{C}_J^n}{\lambda} &= - \left( \tilde{A}_{J-\frac{1}{2}}^{n+1} \right)^{-1} \left( K_B T \lambda \left( \mathcal{C}_J^{n+1} - \mathcal{C}_{J-1}^{n+1} \right) + \varepsilon^2 \mathcal{S}_{J-\frac{1}{2}}^n \right). \end{aligned} \quad (4.3.9)$$

It is then possible to apply the same approach as in [3] to these multi-species diffusion equations. Let us denote by  $\langle u, v \rangle_N = \sum_{i=1}^N u_i v_i$ , for  $u, v \in \mathbb{R}^N$  the usual scalar product in  $\mathbb{R}^N$ , and define  $[\mathcal{C}_j^n]^- = ([c_{1,j}^n]^- , \dots , [c_{N,j}^n]^-)^\top \in \mathbb{R}^N$ ,  $0 \leq j \leq J$ , the vectorial negative part of the concentrations, with the notation  $[c]^- = \max(-c, 0)$  for any  $c \in \mathbb{R}$ . Now, we sum equations (4.3.8) for  $1 \leq j \leq J-1$  and both equations in (4.3.9), we compute the scalar product in  $\mathbb{R}^N$  with  $[\mathcal{C}_j^{n+1}]^-$ , and perform a discrete integration by parts to obtain

$$\begin{aligned} &\sum_{j=0}^J \left\langle \frac{\mathcal{C}_j^{n+1} - \mathcal{C}_j^n}{\lambda}, [\mathcal{C}_j^{n+1}]^- \right\rangle_N \\ &\quad + K_B T \lambda \sum_{j=0}^J \left\langle \left( \tilde{A}_{j+\frac{1}{2}}^{n+1} \right)^{-1} \left( \mathcal{C}_{j+1}^{n+1} - \mathcal{C}_j^{n+1} \right), \left( [\mathcal{C}_{j+1}^{n+1}]^- - [\mathcal{C}_j^{n+1}]^- \right) \right\rangle_N \\ &\quad + \varepsilon^2 \sum_{j=0}^J \left\langle \left( \tilde{A}_{j+\frac{1}{2}}^{n+1} \right)^{-1} \mathcal{S}_{j+\frac{1}{2}}^n, \left( [\mathcal{C}_{j+1}^{n+1}]^- - [\mathcal{C}_j^{n+1}]^- \right) \right\rangle_N = 0. \end{aligned}$$

Let us momentarily fix  $0 \leq j \leq J$  and consider the terms involving the product with the matrix  $(\tilde{A}_{j+\frac{1}{2}}^{n+1})^{-1}$ . Expanding the product, there are terms involving the extra-diagonal terms of the matrix, which are written, for any  $1 \leq i, k \leq N$ ,  $k \neq i$ ,

$$T_{ik} = \left[ \left( \tilde{A}_{j+\frac{1}{2}}^{n+1} \right)^{-1} \right]_{ik} \left( K_B T \lambda \left( c_{k,j+1}^{n+1} - c_{k,j}^{n+1} \right) + \varepsilon^2 \mathcal{S}_{k,j+\frac{1}{2}}^n \right) \left( [c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^- \right),$$

and terms involving the diagonal terms of  $(\tilde{A}_{j+\frac{1}{2}}^{n+1})^{-1}$ , which are written for any  $1 \leq i \leq N$

$$T_{ii} = \left[ \left( \tilde{A}_{j+\frac{1}{2}}^{n+1} \right)^{-1} \right]_{ii} \left( K_B T \lambda \left( c_{i,j+1}^{n+1} - c_{i,j}^{n+1} \right) + \varepsilon^2 \mathcal{S}_{i,j+\frac{1}{2}}^n \right) \left( [c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^- \right).$$

Thanks to Lemma 4.3.3, we know that all terms  $T_{ik}$  contain a factor  $[c_{i,j+\frac{1}{2}}^{n+1}]^+$ . Using the definition (4.2.11) of  $c_{i,j+\frac{1}{2}}$ , we deduce that all  $T_{ik}$  contain a factor

$$\min \left\{ [c_{i,j}^{n+1}]^+, [c_{i,j+1}^{n+1}]^+ \right\} \left( [c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^- \right)$$

which always equals 0, since  $\min(a^+, b^+)(a^- - b^-) = 0$  for any  $a, b \in \mathbb{R}$ . This ensures that  $T_{ik} = 0$ .

As far as the diagonal terms  $T_{ii}$  are concerned, we know from Lemma 4.3.3 that the quantities  $[(\tilde{A}_{j+\frac{1}{2}}^{n+1})^{-1}]_{ii}$  are positive. Moreover, observe that

$$\left( c_{i,j+1}^{n+1} - c_{i,j}^{n+1} \right) \left( [c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^- \right) \leq 0$$

for any values of the concentrations, since  $(a - b)(a^- - b^-) \leq 0$  for any  $a, b \in \mathbb{R}$ . Instead, the term involving  $\mathcal{S}_{i,j+\frac{1}{2}}^n$  has an undefined sign, but the assumption of  $\mathcal{S}_{i,j+\frac{1}{2}}^n$  ensures that it remains controlled, for  $\varepsilon$  small enough, by the first term. Thus, if the case when  $(c_{i,j+1}^{n+1} - c_{i,j}^{n+1})([c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^-) < 0$ , for  $\varepsilon$  small enough, we can ensure that  $T_{ii}$  remains negative. Moreover, it is obvious that if  $(c_{i,j+1}^{n+1} - c_{i,j}^{n+1})([c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^-) = 0$ , then  $[c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^- = 0$ , which ensures that  $T_{ii} = 0$ . Finally, it follows that

$$\sum_{j=0}^J \left\langle \mathcal{C}_j^{n+1} - \mathcal{C}_j^n, [\mathcal{C}_j^{n+1}]^- \right\rangle_N \geq 0.$$

Using that  $\mathcal{C}_j^{n+1} = [\mathcal{C}_j^{n+1}]^+ - [\mathcal{C}_j^{n+1}]^-$ , and that  $\langle [\mathcal{C}_j^{n+1}]^+, [\mathcal{C}_j^{n+1}]^- \rangle_N = 0$ , we deduce that

$$- \sum_{j=0}^J \left\langle [\mathcal{C}_j^{n+1}]^-, [\mathcal{C}_j^{n+1}]^- \right\rangle_N \geq \sum_{j=0}^J \left\langle \mathcal{C}_j^n, [\mathcal{C}_j^{n+1}]^- \right\rangle_N.$$

Since  $c_{i,j}^n \geq 0$  for any  $1 \leq i \leq N$ ,  $0 \leq j \leq J$  by induction hypothesis, this implies that  $\sum_{j=0}^J \left\| [\mathcal{C}_j^{n+1}]^- \right\|_N^2 \leq 0$ , where  $\|\cdot\|_N$  is the norm associated to the scalar product  $\langle \cdot, \cdot \rangle_N$ . Therefore,  $[\mathcal{C}_{i,j}^{n+1}]^- = 0$  for any  $1 \leq i \leq N$ ,  $0 \leq j \leq J$ , which means that  $c_{i,j}^{n+1} \geq 0$ , and concludes the proof by induction.

Last, we note that any solution  $(c_{i,j}^n)_{0 \leq j \leq J}$ ,  $(F_{i,j+\frac{1}{2}}^n)_{0 \leq j \leq J-1}$  of the auxiliary system (4.3.5) is also solution of (4.2.14) because of the nonnegativity of  $(c_{i,j}^n)_{0 \leq j \leq J}$ , which implies that  $[c_{i,j}^{n+1}]^+ = c_{i,j}^{n+1}$ .  $\square$

**Remark 4.3.5.** Assumption (4.3.7), stating that the source term  $\mathcal{S}_{i,j+\frac{1}{2}}^n$  is bounded for any  $1 \leq i \leq N$ ,  $0 \leq j \leq J-1$ ,  $n \in \mathbb{N}$  uniformly with respect to  $\varepsilon$ , is satisfied if the nonlinear terms (discretization of  $\partial_x(cu^2)$ ) and the fluxes remain uniformly bounded. This assumption will be numerically checked a posteriori in Section 4.5 for the numerical tests.

**Remark 4.3.6.** It is worth noting that (4.2.14) is consistent with the continuous problem (4.2.7) for any  $\varepsilon \geq 0$ . In particular, the scheme is only first order accurate in space, because of (4.2.11). This choice is crucial to establish positivity of solutions to the discretized system and we did not tackle the design of higher order schemes able to preserve this property.

## 4.4 Existence of a solution to the numerical scheme

It remains to prove the existence of a solution to our scheme. To this end, we use a matrix form similar to (4.2.15) of a new auxiliary system, inspired from (4.3.5). Let

$$\tilde{\mathbf{y}} = (\tilde{\mathbf{y}}_1, \mathbf{y}_2)^\top = ([c_{1,0}]^+, \dots, [c_{1,J}]^+, \dots, [c_{N,0}]^+, \dots, [c_{N,J}]^+, \mathbf{y}_2)^\top \in \mathbb{R}^{N(2J+1)}.$$

Then we prove the existence of a solution to the following new auxiliary system

$$\begin{cases} [c_{i,j}^{n+1}]^+ + \lambda \left( F_{i,j+\frac{1}{2}}^{n+1} - F_{i,j-\frac{1}{2}}^{n+1} \right) = c_{i,j}^n, \\ \left( -\Delta t \sum_{k \neq i} \mu_{ik} B_{ik} [c_{k,j+\frac{1}{2}}^{n+1}]^+ - \varepsilon^2 m_i \right) F_{i,j+\frac{1}{2}}^{n+1} + \Delta t [c_{i,j+\frac{1}{2}}^{n+1}]^+ \sum_{k \neq i} \mu_{ik} B_{ik} F_{k,j+\frac{1}{2}}^{n+1} \\ = K_B T \lambda \left( [c_{i,j+1}^{n+1}]^+ - [c_{i,j}^{n+1}]^+ \right) + \varepsilon^2 m_i \lambda R_{i,j+\frac{1}{2}}^n - \varepsilon^2 m_i F_{i,j+\frac{1}{2}}^n. \end{cases} \quad (4.4.1)$$

This system (4.4.1) can be written as

$$\tilde{\mathbb{S}}^\varepsilon (\tilde{\mathbf{y}}_1^{n+1}) \tilde{\mathbf{y}}^{n+1} = \mathbf{b}^n, \quad \text{where} \quad \tilde{\mathbb{S}}^\varepsilon (\tilde{\mathbf{y}}_1) = \begin{bmatrix} \mathbb{S}_{11} & \mathbb{S}_{12} \\ \mathbb{S}_{21} & \tilde{\mathbb{S}}_{22}^\varepsilon (\tilde{\mathbf{y}}_1) \end{bmatrix},$$

and  $\tilde{\mathbb{S}}_{22}^\varepsilon$  is given by

$$\tilde{\mathbb{S}}_{22}^\varepsilon (\tilde{\mathbf{y}}_1) = \begin{bmatrix} \tilde{\mathbb{B}}_{11}^\varepsilon (\tilde{\mathbf{y}}_1) & \cdots & \tilde{\mathbb{B}}_{1p} (\tilde{\mathbf{y}}_1) \\ \vdots & \ddots & \vdots \\ \tilde{\mathbb{B}}_{p1} (\tilde{\mathbf{y}}_1) & \cdots & \tilde{\mathbb{B}}_{pp}^\varepsilon (\tilde{\mathbf{y}}_1) \end{bmatrix},$$

where the blocks  $\tilde{\mathbb{B}}_{ij} (\tilde{\mathbf{y}}_1)$  are defined by

$$\begin{cases} \tilde{\mathbb{B}}_{ij} (\tilde{\mathbf{y}}_1) = \Delta t \mu_{ij} B_{ij} \text{Diag}_{J \times J} \left( [c_{i,\ell-\frac{1}{2}}^{n+1}]^+ \right) & \text{if } i \neq j, \\ \tilde{\mathbb{B}}_{ii}^\varepsilon (\tilde{\mathbf{y}}_1) = -\Delta t \text{Diag}_{J \times J} (\bar{\kappa}_\ell), \end{cases}$$

where  $\bar{\kappa}_\ell = \sum_{k \neq i} \mu_{ik} B_{ik} [c_{k,\ell-\frac{1}{2}}^{n+1}]^+ + \varepsilon^2 \frac{m_i}{\Delta t}$ , for any  $1 \leq \ell \leq J$ .

**Theorem 4.4.1.** For any  $\varepsilon > 0$ , there exists a solution  $(c_{i,j}^n)_{0 \leq j \leq J}$ ,  $(F_{i,j+\frac{1}{2}}^n)_{0 \leq j \leq J-1}$  of the system (4.4.1) with boundary conditions (4.2.13), which also solves (4.3.5). Moreover, thanks to Proposition 4.3.4, for  $\varepsilon > 0$  small enough, it is also a solution of system (4.2.14) with boundary conditions (4.2.13).



*Proof.* First, let us prove that  $\tilde{\mathbb{S}}^\varepsilon(\tilde{\mathbf{y}}_1)$  is invertible for any  $\tilde{\mathbf{y}}_1$  and any  $\varepsilon > 0$ . Since the block  $\mathbb{S}_{11} = \mathbb{I}_{N(J+1)}$  is obviously invertible of determinant 1, and block determinant computation using the Schur complement leads to

$$\det\left(\tilde{\mathbb{S}}^\varepsilon(\tilde{\mathbf{y}}_1)\right) = \det\left(\tilde{\mathbb{S}}_{22}^\varepsilon(\tilde{\mathbf{y}}_1) - \mathbb{S}_{21}\mathbb{S}_{12}\right).$$

Let us denote  $\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1) = \tilde{\mathbb{S}}_{22}^\varepsilon(\tilde{\mathbf{y}}_1) - \mathbb{S}_{21}\mathbb{S}_{12}$ . Obviously, proving that  $\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1)$  is invertible is enough to prove that  $\tilde{\mathbb{S}}^\varepsilon(\tilde{\mathbf{y}}_1)$  also is. We compute

$$\mathbb{S}_{21}\mathbb{S}_{12} = K_B T \lambda^2 \begin{pmatrix} 2 & -1 & \cdots & 0 \\ -1 & 2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots \\ 0 & \cdots & \cdots & -1 & 2 \end{pmatrix} \in \mathbb{R}^{NJ \times NJ}.$$

It follows that the diagonal terms of  $\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1)$  are negative, whereas its extra-diagonal terms are nonnegative. Moreover, the transpose of matrix  $\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1)$  is also diagonally dominant, since for any  $\varepsilon > 0$ ,  $n \geq 0$  and any  $1 \leq q \leq NJ$

$$\begin{aligned} \left|[\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1)^\top]_{qq}\right| &= \sum_{k \neq i} \Delta t \mu_{ik} B_{ik} [c_{k,\ell-\frac{1}{2}}^{n+1}]^+ + m_i \varepsilon^2 + 2K_B T \lambda^2 \\ &> \sum_{k \neq i} \Delta t \mu_{ik} B_{ik} [c_{k,\ell-\frac{1}{2}}^{n+1}]^+ + 2K_B T \lambda^2 \geq \sum_{r \neq q} \left|[\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1)^\top]_{qr}\right| \end{aligned}$$

where  $i = \lfloor \frac{q-1}{J} \rfloor + 1$ , and  $\ell = q - J \lfloor \frac{q-1}{J} \rfloor$ . This proves the invertibility of  $\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1)$ , and thus the one of  $\tilde{\mathbb{S}}^\varepsilon(\tilde{\mathbf{y}}_1)$ . Since  $\tilde{\mathbb{S}}^\varepsilon(\tilde{\mathbf{y}}_1)$  is invertible for any  $\tilde{\mathbf{y}}_1$  and any  $\varepsilon > 0$ , the new auxiliary system (4.4.1) can be written under the form

$$\tilde{\mathbf{y}}^{n+1} = \left(\tilde{\mathbb{S}}^\varepsilon(\tilde{\mathbf{y}}_1^{n+1})\right)^{-1} \mathbf{b}^n,$$

where  $\mathbf{b}^n = (\mathbf{b}_1^n, \mathbf{b}_2^n)^\top$  is defined by (4.2.16). The existence of a solution to this system is then proved using Schaefer's fixed-point theorem. To apply this fixed-point theorem, we compute, again thanks to the Schur complement,

$$\left(\tilde{\mathbb{S}}^\varepsilon(\tilde{\mathbf{y}}_1^{n+1})\right)^{-1} = \begin{bmatrix} \mathbb{I}_{N(J+1)} + \mathbb{S}_{12} \left(\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1^{n+1})\right)^{-1} \mathbb{S}_{21} & -\mathbb{S}_{12} \left(\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1^{n+1})\right)^{-1} \\ -\left(\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1^{n+1})\right)^{-1} \mathbb{S}_{21} & \left(\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1^{n+1})\right)^{-1} \end{bmatrix},$$

which means that we can define two functions  $f$  and  $g$  so that the system can also be written as

$$\begin{cases} \tilde{\mathbf{y}}_1^{n+1} = f(\tilde{\mathbf{y}}_1^{n+1}) = \mathbf{b}_1^n + \mathbb{S}_{12} \left(\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1^{n+1})\right)^{-1} \mathbb{S}_{21} \mathbf{b}_1^n - \mathbb{S}_{12} \left(\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1^{n+1})\right)^{-1} \mathbf{b}_2^n, \\ \mathbf{y}_2^{n+1} = g(\tilde{\mathbf{y}}_1^{n+1}) = -\left(\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1^{n+1})\right)^{-1} \mathbb{S}_{21} \mathbf{b}_1^n + \left(\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1^{n+1})\right)^{-1} \mathbf{b}_2^n. \end{cases}$$

The proof principle is the following: we prove that there exists a solution to the first equation  $\tilde{\mathbf{y}}_1^{n+1} = f(\tilde{\mathbf{y}}_1^{n+1})$ , then the existence of  $\mathbf{y}_2$  immediately follows, in view of the second equation.

First, observe that the application  $f$  maps  $(\mathbb{R}_+)^{N(J+1)}$  to  $(\mathbb{R}_+)^{N(J+1)}$ , thanks to Proposition 4.3.4. Moreover, it is continuous, since  $(\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathbf{y}}_1^{n+1}))^{-1}$  is the inverse of an affine function. Since we work in a finite-dimensional setting,  $f$  is also compact. Endow  $\mathbb{R}^{N(J+1)}$  with the discrete  $L^1$ -norm  $\|v\|_1 = \sum_{k=1}^{N(J+1)} |v_k|$ , for any  $v \in \mathbb{R}^{N(J+1)}$ . The set

$$E = \left\{ \tilde{\mathbf{y}}_1 \in (\mathbb{R}_+)^{N(J+1)} \mid \exists \xi \in [0, 1] \text{ such that } \tilde{\mathbf{y}}_1 = \xi f(\tilde{\mathbf{y}}_1) \right\}$$

is bounded. Indeed, let  $\tilde{\mathbf{y}}_1 \in E$ , and  $\xi \in [0, 1]$  such that  $\tilde{\mathbf{y}}_1 = \xi f(\tilde{\mathbf{y}}_1)$ . Define  $\mathbf{y}_2 = \xi g(\tilde{\mathbf{y}}_1)$ , and  $\tilde{\mathbf{y}} = (\tilde{\mathbf{y}}_1, \mathbf{y}_2)^\top$ . Then  $\tilde{\mathbf{y}}$  is solution of the equation

$$\tilde{\mathbb{S}}^\varepsilon(\tilde{\mathbf{y}}_1)\tilde{\mathbf{y}} = \xi \mathbf{b}. \quad (4.4.2)$$

Now, observe that as for recovering mass conservation (Proposition 4.3.1), if we sum the first equations of (4.4.1) over  $i$  and  $j$ , we obtain

$$\sum_{\substack{1 \leq i \leq N \\ 0 \leq j \leq J}} [c_{i,j}^{n+1}]^+ = \sum_{\substack{1 \leq i \leq N \\ 0 \leq j \leq J}} c_{i,j}^n,$$

which means that  $\|\tilde{\mathbf{y}}_1^{n+1}\|_1 = \|\mathbf{b}_1^n\|_1$  by definition of  $\mathbf{b}_1$ . With the same reasoning, a solution  $\tilde{\mathbf{y}}_1$  of (4.4.2) satisfies

$$\|\tilde{\mathbf{y}}_1^{n+1}\|_1 = \xi \|\mathbf{b}_1^n\|_1 \leq \|\mathbf{b}_1^n\|_1, \quad \forall \xi \in [0, 1].$$

This proves that the set  $E$  is bounded. Therefore, Schaefer's fixed point theorem [87, Thm. 4, p. 509] ensures that  $f$  has a fixed point  $\tilde{\mathbf{y}}_1^{n+1}$ , and  $\tilde{\mathbf{y}}^{n+1} = (\tilde{\mathbf{y}}_1^{n+1}, \mathbf{y}_2^{n+1})^\top$  is thus a solution of the new auxiliary system (4.4.1). By construction, since we added positive parts on every concentration in this new auxiliary system, all components of  $\tilde{\mathbf{y}}_1$  are nonnegative, which means that it is also a solution to the auxiliary system (4.3.5). Finally, Proposition 4.3.4 ensures that it is also a solution to (4.2.14).  $\square$

## 4.5 Numerical experiments

In this section, we illustrate the good behaviour of the scheme on some numerical examples.

### 4.5.1 Parameters of the scheme, validation

The numerical values of the different constants involved in the equations are the following.

- The temperature  $T$  is given by  $T = 300\text{K}$ , and  $K_B = \mathcal{N}_A R$ , where  $\mathcal{N}_A$  is the Avogadro constant and  $R = 8.314\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ . The equations for the fluxes are actually multiplied by  $\mathcal{N}_A$ , so that we can use the molar masses of each species.
- Species 1, 2 and 3 have respective molar masses  $M_1 = 2\text{g} \cdot \text{mol}^{-1}$ ,  $M_2 = 28\text{g} \cdot \text{mol}^{-1}$  and  $M_3 = 44\text{g} \cdot \text{mol}^{-1}$ . These values respectively correspond to hydrogen, nitrogen and carbon dioxide.
- The cross sections are computed from the binary diffusion coefficients  $D_{ij}$  through the formula  $B_{ij} = \frac{(m_i + m_j)K_B T}{4\pi m_i m_j D_{ij}}$ , with

$$D_{12} = 0.833\text{cm}^2 \cdot \text{s}^{-1}, \quad D_{13} = 0.68\text{cm}^2 \cdot \text{s}^{-1}, \quad D_{23} = 0.168\text{cm}^2 \cdot \text{s}^{-1}.$$

In the computations, we chose to rescale the actual values of the cross sections by a factor  $10^5$  (which corresponds to accelerating time) to get

$$B_{12} = 0.802 \times 10^3 \text{ s}^{-1}, \quad B_{13} = 0.958 \times 10^3 \text{ s}^{-1}, \quad B_{23} = 0.433 \times 10^3 \text{ s}^{-1}.$$

This choice is made to prevent situations where the matrix  $\mathbb{S}^\varepsilon(y_1^{n+1})$  in (4.2.15) could be ill-conditioned. The rescaling can thus be seen as a pre-conditioning technique which allows the Newton iteration to rapidly converge for any value of the parameter  $\varepsilon \geq 0$ .

- The spatial domain  $\Omega$  is chosen as  $\Omega = [-1, 1]$ , with a space step  $\Delta x = 10^{-2}$  and a time step  $\Delta t = \Delta x^2 = 10^{-4}$  (obtained after performing the scaling). Observe that the discretization parameters are constant for all simulations we performed, and in particular that they are chosen *a priori*, not depending on  $\varepsilon$ .

**Remark 4.5.1.** *The kinetic model (4.1.7) we use actually holds only for monoatomic gases. However, the macroscopic diffusion model (4.1.3) is valid for more general gases, including polyatomic ones. Since we aim to mimic Duncan and Toor's experiment [82], and in particular to observe uphill diffusion, we chose to simulate the behaviour of hydrogen, nitrogen and carbon dioxide, which are not monoatomic gases.*

First, we numerically check that constant solutions are preserved by the discretization, since constant states are exact solutions of our scheme. Indeed, for constant initial concentrations and zero initial fluxes, the scheme preserves the initial state and the mixture does not move from its equilibrium.

#### 4.5.2 Two-species diffusion

The first test case we consider consists in a two-species mixture (species 1 and 3). In this case, the limit model (4.1.3) reduces to a simple heat equation on each species, since the cross-diffusion effects cancel due to the symmetry of the diffusion coefficients. We consider the following initial conditions

$$c_1^{\text{in}}(x) = \mathbb{1}_{[-1,0]}, \quad c_3^{\text{in}}(x) = \mathbb{1}_{[0,1]}, \quad F_1^{\text{in}}(x) = F_3^{\text{in}}(x) = 0.$$

For  $\varepsilon = 10^{-2}$ , we plot on Figure 4.1 the evolution of the concentrations of each species for various times ( $t = 0$ ,  $t = 10^{-2}$ ,  $t = 10^{-1}$ ,  $t = 1$  and  $t = 10$ , since  $\Delta t = 10^{-4}$ ). Both species have the expected behaviour and diffuse until reaching the equilibrium.

#### Discussion about the closure relation for the Maxwell-Stefan equations

As mentioned earlier, Maxwell-Stefan equations (4.1.3) need an additional closure relation to be solved, and a possible one is the equimolar diffusion setting, in which  $c$  is identically equal to 1. The initial conditions in our scheme are chosen in (4.2.2) in order to be compatible with this condition. However, the evolution in space and time of the total concentration is not imposed. In order to be consistent with the closure relation in the Maxwell-Stefan equations, we a posteriori check, at least numerically, that the total concentration remains close to 1 for any time and space. This is shown in Figure 4.2.

We observe that  $c = 1 + O(\varepsilon^2)$ , and in particular, for small values of  $\varepsilon$ , the closure relation is completely consistent with Boltzmann equations for mixtures.

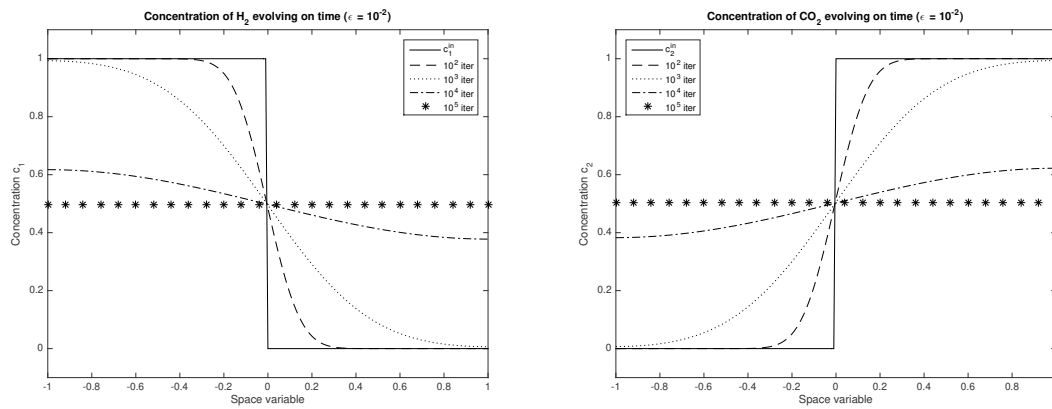


Figure 4.1 – Evolution of the concentrations of species 1 and 2 in time in the two-species test case

### Numerical checking of Assumption (4.3.7) on the source terms

As stated in Remark 4.3.5, the proof of Proposition 4.3.4 relies on the assumption that the source terms  $\mathcal{S}_{i,j+\frac{1}{2}}^n$  are bounded for any  $1 \leq i \leq N$ ,  $0 \leq j \leq J - 1$ ,  $n \in \mathbb{N}$ , uniformly with respect to  $\varepsilon$ . This assumption is a posteriori numerically checked in each test case. More precisely, if we recall the quantity  $M_\varepsilon$  defined by (4.3.6), we need  $M_\varepsilon$  to become smaller when  $\varepsilon$  vanishes, which is the case, as shown on Figure 4.3.

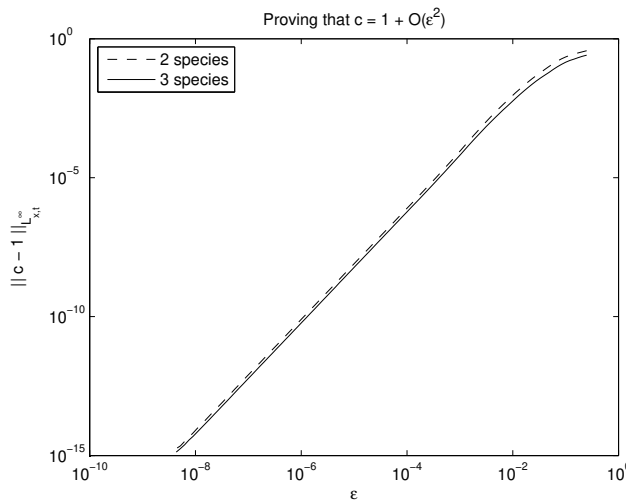


Figure 4.2 –  $L^\infty$ -norm of  $c - 1$  with respect to  $\varepsilon$

### 4.5.3 Three-species diffusion

We focus now on the three-species case, which shows a much richer behaviour. Consider the following initial conditions

$$c_1^{\text{in}}(x) = 0.8 \times \mathbb{1}_{[-1,0]}, \quad c_2^{\text{in}}(x) = 0.2, \quad c_3^{\text{in}}(x) = 0.8 \times \mathbb{1}_{[0,1]},$$

$$F_1^{\text{in}}(x) = F_2^{\text{in}}(x) = F_3^{\text{in}}(x) = 0.$$

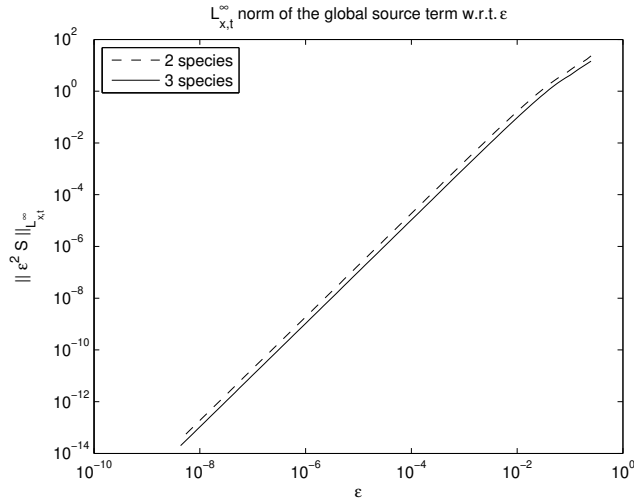


Figure 4.3 – Maximum  $M_\epsilon$  of the source terms with respect to  $\epsilon$

**Uphill diffusion rising**

Duncan and Toor’s experiment [82] shows that this configuration enables the so-called uphill diffusion phenomenon, meaning that nitrogen, although being already at equilibrium, moves because of the movement of other species and their particular friction properties, due to their different mass ratios. This behaviour is indeed observed, for  $\epsilon = 10^{-2}$ , as shown in Figure 4.4. After some time (corresponding to the diffusion barrier), the classical diffusion takes over and all species diffuse towards equilibrium.

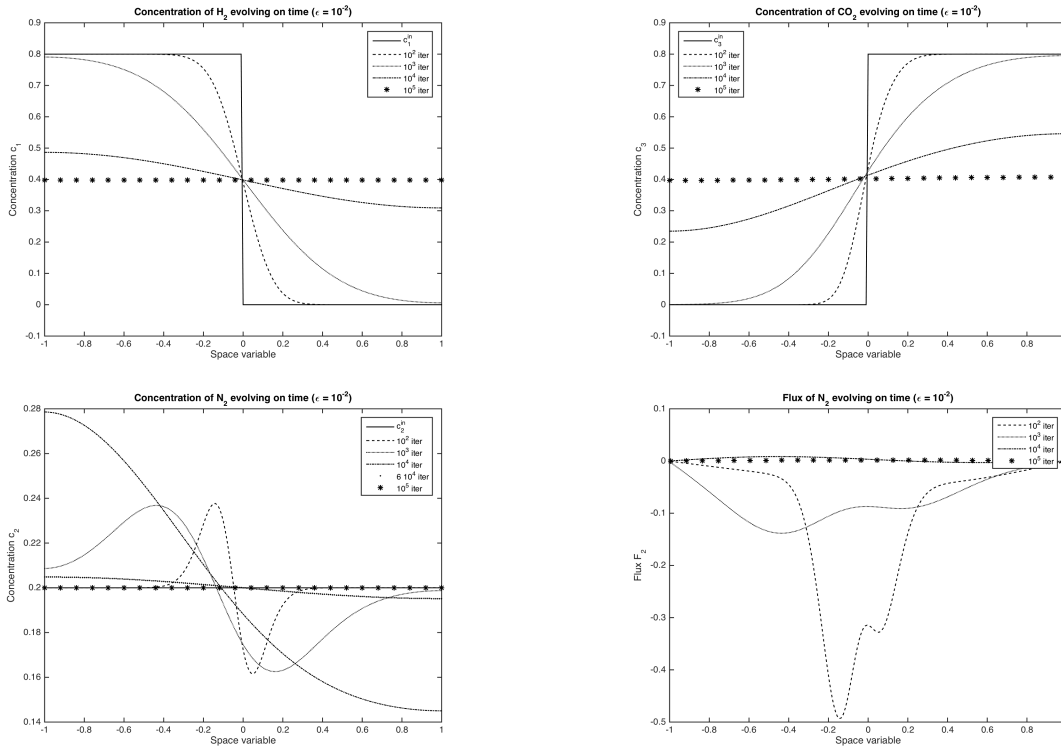


Figure 4.4 – Evolution of the concentrations of species 1, 2 and 3, as well as the flux of species 2 in time in the three-species test case

As similarly done the two-species case, we then check the consistency with the closure relation  $c = 1$  (see Figure 4.2), and the assumption on the source terms ( $M_\varepsilon$  tends to zero when  $\varepsilon$  tends to zero, see Figure 4.3).

### Asymptotic behaviour of the scheme and convergence towards the Maxwell-Stefan equations

The numerical scheme described in this paper has been especially designed in order to nicely degenerate for arbitrary small values of  $\varepsilon$ . Moreover, it has been proved, at least formally [39, 35], that the Boltzmann equations for mixtures tend to the Maxwell-Stefan equations when  $\varepsilon$  vanishes. Therefore, for each species, we compute the  $L^\infty$ -norm in both  $x$  and  $t$  of the difference between its concentration and the concentration computed by Maxwell-Stefan equations. The computation of the solution to the Maxwell-Stefan equations is done as in [38], in particular using the closure relation corresponding to equimolar diffusion (*i.e.* the total flux of the mixture is identically equal to 0). This is done for several values of  $\varepsilon$ , and shown in Figure 4.5. The apparent order of convergence of the scheme is better than 1 with respect to  $\varepsilon$ .

We observe the expected behaviour: the smaller  $\varepsilon$  is, the closer to Maxwell-Stefan equations we are. Let us emphasize that these results are obtained for fixed  $\Delta x$  and  $\Delta t$ , as given at the beginning of the section. Therefore, the scheme does not need any restrictive condition on the parameters in order to remain accurate for small values of  $\varepsilon$ . We were not able to theoretically prove that the scheme is asymptotic-preserving. Indeed, even if the discretization (4.2.14) is consistent with the continuous problem (4.2.7) for any  $\varepsilon \geq 0$ , it appears very hard to establish a stability property with respect to  $\varepsilon$ . Nevertheless, numerical experiments suggest that the scheme is stable under a mixed convection-diffusive CFL condition of type  $\Delta t \leq \varepsilon C_1 \Delta x + C_2 \Delta x^2$ , which shows that the scheme should actually be asymptotic-preserving in the small limit of  $\varepsilon$ .

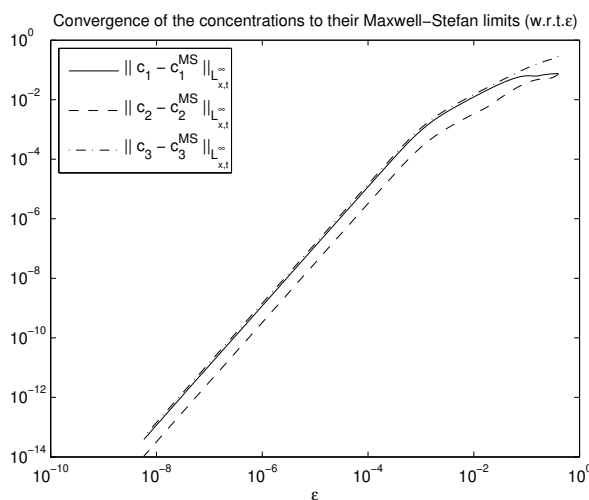


Figure 4.5 –  $L^\infty_{x,t}$ -norm of the difference between the computed concentrations and the solutions of Maxwell-Stefan equations for species 1, 2 and 3 with respect to  $\varepsilon$

### Influence of the parameter $\varepsilon$ on the diffusion process

We can also observe the influence of  $\varepsilon$  on the diffusion process (see Figure 4.6). As we already observed, for small values of  $\varepsilon$ , the diffusion is very similar to the Maxwell-Stefan's

one. However, for larger values of  $\varepsilon$  we observe some variations in the diffusion process. Although the diffusion process is quite different, the concentrations still converge in time to the same equilibrium as for smaller values of  $\varepsilon$ .

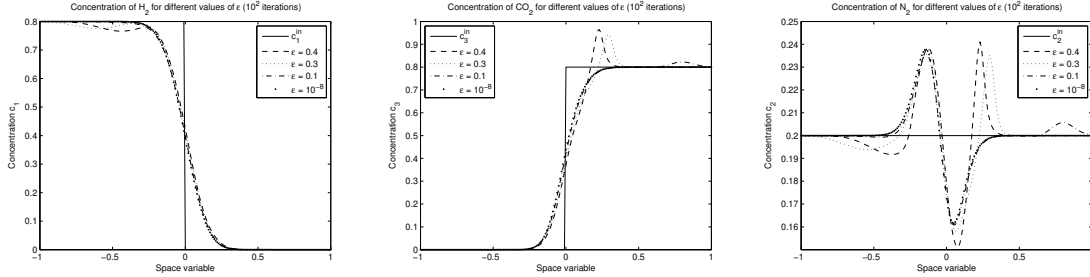


Figure 4.6 – Concentrations of species 1, 2 and 3 at time  $t = 10^{-2}$  with respect to  $\varepsilon$

### Velocity distributions

As stated before, the numerical scheme presented here relies on the moment method to treat the kinetic equation (4.1.7). More precisely, by using ansatz (4.2.1) stating that the distribution functions are at local Maxwellian states, we compute the zero-th and first order moments in velocity of  $f_i^\varepsilon(t, x, v)$ . On Figure 4.7, we plot the distribution function  $f_1^\varepsilon(t, x, v)$  with respect to  $v$  for  $\varepsilon = 10^{-2}$ ,  $x = -0.21$  and several times  $t$  (for the same values as before  $t = 0$ ,  $t = 10^{-2}$ ,  $t = 10^{-1}$ ,  $t = 1$  and  $t = 10$ ). The amplitude of the Maxwellian is of course decreasing, since  $c_1(t, x)$  decreases with time at the chosen value of  $x$ . In our configuration, the fluxes remain of order  $10^{-1}$ , which corresponds to velocities  $u_i$  of order 1 (see Figure 4.4). Therefore, the Maxwellian are centered around  $\varepsilon u_1 \simeq 10^{-2}$ , and the shift cannot be seen on the plot.

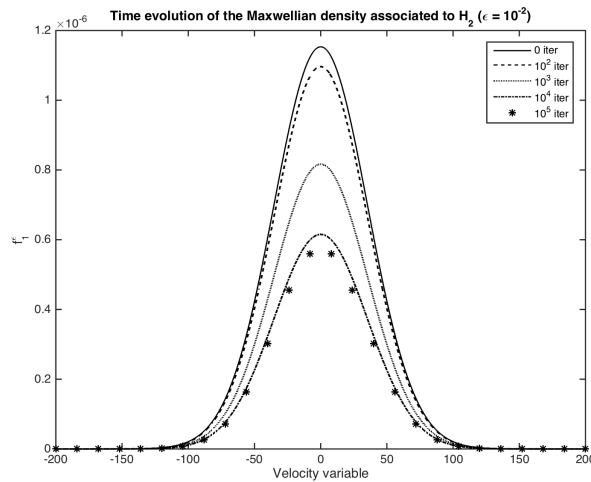


Figure 4.7 – Evolution of the velocity distribution of species 1 at  $x = -0.21$  in the three-species case

## Annexe A

# Properties of the Maxwell-Stefan matrix

We prove some properties of the Maxwell-Stefan matrix  $A$ , as well as some estimates on its derivatives. We conclude with properties and estimates on the pseudoinverse of  $A$  on its image.

**Lemma A.1.1.** *For any  $\mathbf{c} \geq 0$  the matrix  $A(\mathbf{c})$  is nonpositive, in the sense that there exist two positive constants  $\lambda_A$  and  $\mu_A$  such that, for any  $\mathbf{X} \in \mathbb{R}^N$ ,*

$$\|A(\mathbf{c})\mathbf{X}\| \leq \mu_A \langle \mathbf{c}, \mathbf{1} \rangle^2 \|\mathbf{X}\|,$$

$$\langle \mathbf{X}, A(\mathbf{c})\mathbf{X} \rangle \leq -\lambda_A \left( \min_{1 \leq i \leq N} c_i \right)^2 \left[ \|\mathbf{X}\|^2 - \langle \mathbf{X}, \mathbf{1} \rangle^2 \right] \leq 0.$$

*Proof.* Let us consider two  $N$ -vectors  $\mathbf{c} \geq 0$  and  $\mathbf{X}$ . First, the boundedness of  $A(\mathbf{c})$  can be showed in the supremum norm, since all norms are equivalent in  $\mathbb{R}^N$ . It is straightforward that, for any  $1 \leq i \leq N$ ,

$$\left| \sum_{j=1}^N \frac{c_i c_j}{\Delta_{ij}} (X_j - X_i) \right| \leq \frac{2 \max_{1 \leq i \leq N} c_i}{\min_{1 \leq i, j \leq N} \Delta_{ij}} \left( \sum_{j=1}^N c_j \right) \max_{1 \leq j \leq N} |X_j|,$$

from which the first inequality directly follows since  $\max_{1 \leq i \leq N} c_i \leq \sum_{j=1}^N c_j$ , and we can thus choose  $\mu_A = 2 / \min_{1 \leq i, j \leq N} \Delta_{ij}$ .

We then compute

$$\langle \mathbf{X}, A(\mathbf{c})\mathbf{X} \rangle = - \sum_{i=1}^N \sum_{j=1}^N \frac{c_i c_j}{\Delta_{ij}} (X_i - X_j) X_i = - \sum_{i=1}^N \sum_{j=1}^N \frac{c_i c_j}{\Delta_{ij}} (X_i - X_j)^2 \leq 0.$$

Note in particular that, since  $c_i \geq 0$  and  $\Delta_{ij} > 0$  for any  $1 \leq i, j \leq N$ , the relation  $A(\mathbf{c})\mathbf{X} = 0$  implies  $X_i = X_j$  for all  $i$  and  $j$ , and so  $\ker A = \text{Span}(\mathbf{1})$ . If we now set  $\lambda_A = 2 / \max_{1 \leq i, j \leq N} \Delta_{ij}$ , we deduce the bound

$$\langle \mathbf{X}, A(\mathbf{c})\mathbf{X} \rangle \leq -\frac{\lambda_A}{2} \left( \min_{1 \leq i \leq N} c_i \right)^2 \sum_{i=1}^N \sum_{j=1}^N (X_i - X_j)^2,$$

and conclude the proof.  $\square$



**Lemma A.1.2.** Consider a multi-index  $\alpha \in \mathbb{N}^3$  and let  $\mathbf{c}, \tilde{\mathbf{U}} \in H^{|\alpha|}(\mathbb{T}^3)$ , with  $\mathbf{c} \geq 0$ . Then, for any  $\mathbf{X} \in \mathbb{R}^N$ ,

$$\begin{aligned} \langle \partial_x^\alpha [A(\mathbf{c})\mathbf{U}], \mathbf{X} \rangle &\leq \langle A(\mathbf{c}) (\partial_x^\alpha \mathbf{U}), \mathbf{X} \rangle \\ &+ 2N^2 \mu_A \langle \mathbf{c}, \mathbf{1} \rangle \|\mathbf{X}\| \sum_{\substack{\alpha_1 + \alpha_3 = \alpha \\ |\alpha_1| \geq 1}} \|\partial_x^{\alpha_1} \mathbf{c}\| \|\partial_x^{\alpha_3} \mathbf{U}\| \\ &+ N^2 \mu_A \|\mathbf{X}\| \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1}} \|\partial_x^{\alpha_1} \mathbf{c}\| \|\partial_x^{\alpha_2} \mathbf{c}\| \|\partial_x^{\alpha_3} \mathbf{U}\|, \end{aligned}$$

where  $\mu_A$  is defined in Lemma A.1.1.

*Proof.* Let  $\mathbf{X}$  be in  $\mathbb{R}^N$ . We can explicitly compute

$$\begin{aligned} \langle \partial_x^\alpha [A(\mathbf{c})\mathbf{U}], \mathbf{X} \rangle &= \sum_{i=1}^N \partial_x^\alpha \left( \sum_{j=1}^N \frac{c_i c_j}{\Delta_{ij}} (U_j - U_i) \right) X_i \\ &= \sum_{1 \leq i, j \leq N} X_i \sum_{\alpha_1 + \alpha_2 + \alpha_3 = \alpha} \frac{\partial_x^{\alpha_1} c_i \partial_x^{\alpha_2} c_j}{\Delta_{ij}} (\partial_x^{\alpha_3} U_j - \partial_x^{\alpha_3} U_i) \\ &= \langle A(\mathbf{c}) \partial_x^\alpha \mathbf{U}, \mathbf{X} \rangle \\ &+ \sum_{1 \leq i, j \leq N} X_i \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1}} \frac{\partial_x^{\alpha_1} c_i \partial_x^{\alpha_2} c_j}{\Delta_{ij}} (\partial_x^{\alpha_3} U_j - \partial_x^{\alpha_3} U_i) \\ &+ \sum_{1 \leq i, j \leq N} X_i \sum_{\substack{\alpha_2 + \alpha_3 = \alpha \\ |\alpha_2| \geq 1}} \frac{c_i \partial_x^{\alpha_2} c_j}{\Delta_{ij}} (\partial_x^{\alpha_3} U_j - \partial_x^{\alpha_3} U_i) \\ &+ \sum_{1 \leq i, j \leq N} X_i \sum_{\substack{\alpha_1 + \alpha_3 = \alpha \\ |\alpha_1| \geq 1}} \frac{c_j \partial_x^{\alpha_1} c_i}{\Delta_{ij}} (\partial_x^{\alpha_3} U_j - \partial_x^{\alpha_3} U_i). \end{aligned}$$

We then use Cauchy-Schwarz inequality and the fact that  $\Delta = \min \Delta_{ij} > 0$ , together with the straightforward controls  $0 \leq c_i \leq \sum_{j=1}^N c_j$  and  $|c_i| \leq \|\mathbf{c}\|$ , to finally get

$$\begin{aligned} \langle \partial_x^\alpha [A(\mathbf{c})\mathbf{U}], \mathbf{X} \rangle &\leq \langle A(\mathbf{c}) \partial_x^\alpha \mathbf{U}, \mathbf{X} \rangle + \frac{4N^2}{\Delta} \left[ \left( \sum_{j=1}^N c_j \right) \sum_{\substack{\alpha_1 + \alpha_2 = \alpha \\ |\alpha_1| \geq 1}} \|\partial_x^{\alpha_1} \mathbf{c}\| \|\partial_x^{\alpha_2} \mathbf{U}\| \right] \|\mathbf{X}\| \\ &+ \frac{2N^2}{\Delta} \left[ \sum_{\substack{\alpha_1 + \alpha_2 + \alpha_3 = \alpha \\ |\alpha_1|, |\alpha_2| \geq 1}} \|\partial_x^{\alpha_1} \mathbf{c}\| \|\partial_x^{\alpha_2} \mathbf{c}\| \|\partial_x^{\alpha_3} \mathbf{U}\| \right] \|\mathbf{X}\|, \end{aligned}$$

which is the expected result.  $\square$

**Lemma A.1.3.** For any  $\mathbf{c} \in (\mathbb{R}_+^*)^N$  and any  $\mathbf{U} \in (\text{Span}(\mathbf{1}))^\perp$ , the following estimates hold:

$$\|A(\mathbf{c})^{-1}\mathbf{U}\| \leq \frac{1}{\lambda_A \left( \min_{1 \leq i \leq N} c_i \right)^2} \|\mathbf{U}\|,$$

$$\langle A(\mathbf{c})^{-1}\mathbf{U}, \mathbf{U} \rangle \leq -\frac{\lambda_A \left( \min_{1 \leq i \leq N} c_i \right)^2}{\mu_A^2 \langle \mathbf{c}, \mathbf{1} \rangle^4} \|\mathbf{U}\|^2,$$

where  $\lambda_A$  and  $\mu_A$  are defined in Lemma A.1.1.

*Proof.* The proof is a direct application of Proposition 3.2.8. Indeed, Cauchy-Schwarz inequality yields, for all  $\mathbf{X} \in (\text{Span}(\mathbf{1}))^\perp$ ,

$$-\|\mathbf{X}\| \|A(\mathbf{c})\mathbf{X}\| \leq -\lambda_A \left( \min_{1 \leq i \leq N} c_i \right)^2 \|\mathbf{X}\|^2,$$

so that

$$\|\mathbf{X}\| \leq \frac{1}{\lambda_A \left( \min_{1 \leq i \leq N} c_i \right)^2} \|A(\mathbf{c})\mathbf{X}\|,$$

which proves the first estimate by simply taking  $\mathbf{X} = A(\mathbf{c})^{-1}\mathbf{U}$ .

The second property comes from the boundedness of  $A(\mathbf{c})$  given by Lemma A.1.1 for  $\mathbf{X} = A(\mathbf{c})^{-1}\mathbf{U}$ , which translates into a coercivity estimate

$$\|\mathbf{U}\|^2 \leq \left( \mu_A \langle \mathbf{c}, \mathbf{1} \rangle^2 \right)^2 \|A(\mathbf{c})^{-1}(\mathbf{U})\|^2,$$

that we plug into the spectral gap inequality satisfied by  $A(\mathbf{c})$ . □



## Annexe B

# Explicit Carleman representation of the operator $\mathbf{K}^\varepsilon$

We here provide the basic tools that are used in Lemma 3.3.5 to prove the regularizing effect of  $\partial_v^\beta \partial_x^\alpha \mathbf{K}^\varepsilon$ . Looking at the work of Mouhot and Neumann [161] in the mono-species context, the authors recover this property by transferring to the kernel of the compact operator  $K$  all the derivatives, which are then computed and estimated explicitly. This analysis is possible mainly because the kernel of  $K$  has itself an explicit expression. Ideally, one may want to apply a similar strategy in our multi-species framework, but this would require knowing the structure of the kernel of  $\mathbf{K}^\varepsilon$ .

In this first appendix we derive an explicit expression of the kernel of  $\mathbf{K}^\varepsilon$ , following the methods of [45] where a Carleman representation of the Boltzmann multi-species operator was obtained. In particular, we shall rework the pointwise estimates established by the authors, replacing them by a series of pointwise equalities where all the technical computations are made fully explicit.

Let us begin by recalling that  $\mathbf{K}^\varepsilon = (K_1^\varepsilon, \dots, K_N^\varepsilon)$  can be written componentwise, for any  $\mathbf{f} \in L^2(\mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$ , under the kernel form [45, Lemma 5.1]

$$\begin{aligned} K_i^\varepsilon(\mathbf{f})(v) = & \\ & \sum_{j=1}^N C_{ij} \int_{\mathbb{R}^3} \left( \frac{1}{|v - v_*|} \int_{\tilde{E}_{vv_*}^{ij}} \frac{B_{ij} \left( v - V(w, v_*), \frac{v_* - w}{|w - v_*|} \right)}{|w - v_*|} M_i^\varepsilon(w) \, d\tilde{E}(w) \right) f_j^* \, dv_* \\ & + \sum_{j=1}^N C_{ji} \int_{\mathbb{R}^3} \left( \frac{1}{|v - v_*|} \int_{E_{vv_*}^{ij}} \frac{B_{ij} \left( v - V(v_*, w), \frac{w - v_*}{|w - v_*|} \right)}{|w - v_*|} M_j^\varepsilon(w) \, dE(w) \right) f_i^* \, dv_* \\ & - \sum_{j=1}^N \int_{\mathbb{R}^3} \left( \int_{\mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) M_i^\varepsilon \, d\sigma \right) f_j^* \, dv_*, \end{aligned}$$

where we have defined  $V(w, v_*) = v_* + m_i m_j^{-1} w - m_i m_j^{-1} v$  and called  $C_{ij}, C_{ji} > 0$  some explicit constants which only depend on the masses  $m_i, m_j$ . Moreover, we have denoted by  $dE$  the Lebesgue measure on the hyperplane  $E_{vv_*}^{ij}$ , orthogonal to  $v - v_*$  and passing through

$$V_E(v, v_*) = \frac{m_i + m_j}{2m_j} v - \frac{m_i - m_j}{2m_j} v_*,$$

and by  $d\tilde{E}$  the Lebesgue measure on the space  $\tilde{E}_{vv_*}^{ij}$  which corresponds to the hyperplane  $E_{vv_*}^{ij}$  whenever  $m_i = m_j$ , and to the sphere of radius  $R = R(v, v_*)$

$$R = \frac{m_j}{|m_i - m_j|} |v - v_*|$$

and centred at  $O = O(v, v_*)$

$$O = \frac{m_i}{m_i - m_j} v - \frac{m_j}{m_i - m_j} v_*,$$

whenever  $m_i \neq m_j$ .

We can thus define, for any  $1 \leq i, j \leq N$ , the kernels

$$\kappa_{ij}^{(1)}(v, v_*) = \frac{C_{ij}}{|v - v_*|} \int_{\tilde{E}_{vv_*}^{ij}} \frac{B_{ij}\left(v - V(w, v_*), \frac{v_* - w}{|w - v_*|}\right)}{|w - v_*|} M_i^\varepsilon(w) d\tilde{E}(w),$$

$$\kappa_{ij}^{(2)}(v, v_*) = \frac{C_{ji}}{|v - v_*|} \int_{E_{vv_*}^{ij}} \frac{B_{ij}\left(v - V(v_*, w), \frac{w - v_*}{|w - v_*|}\right)}{|w - v_*|} M_j^\varepsilon(w) dE(w),$$

$$\kappa_{ij}^{(3)}(v, v_*) = \int_{\mathbb{S}^2} B_{ij}(|v - v_*|, \cos \vartheta) M_i^\varepsilon d\sigma,$$

where we have dropped the parameter  $\varepsilon$  in order to enlighten our notations. In this way, each  $K_i^\varepsilon$  can be rewritten as

$$K_i^\varepsilon(\mathbf{f})(v) = \sum_{j=1}^N \left\{ \int_{\mathbb{R}^3} \kappa_{ij}^{(1)}(v, v_*) f_j^* dv_* + \int_{\mathbb{R}^3} \kappa_{ij}^{(2)}(v, v_*) f_i^* dv_* - \int_{\mathbb{R}^3} \kappa_{ij}^{(3)}(v, v_*) f_j^* dv_* \right\}.$$

Let us now fix two indices  $i, j \in \{1, \dots, N\}$  and study each of the three kernels separately.

## B.1 Explicit form of $\kappa_{ij}^{(1)}$

The first kernel is easy to make explicit, since the domain of integration  $\tilde{E}_{vv_*}^{ij}$  is a sphere. We thus perform an initial change of variables consisting on a translation of its centre and a dilation of its radius, in order to end up on  $\mathbb{S}^2$ . In this new coordinate system,  $\kappa_{ij}^{(1)}$  reads

$$\kappa_{ij}^{(1)}(v, v_*) = \frac{C_{ij} m_j^2}{(m_i - m_j)^2} |v - v_*| \int_{\mathbb{S}^2} \frac{b_{ij}(v, v_*, \omega)}{|R\omega + O - v_*|^{1-\gamma}} M_i^\varepsilon(R\omega + O) d\omega$$

where the angular part  $b_{ij}$  explicitly writes

$$b_{ij}(v, v_*, \omega) = b_{ij} \left( \frac{(v - V(R\omega + O, v_*)) \cdot (v_* - (R\omega + O))}{|v - V(R\omega + O, v_*)| |R\omega + O - v_*|} \right),$$

recalling that we have defined  $V(w, v_*) = v_* + m_i m_j^{-1} w - m_i m_j^{-1} v$ . Simple algebraic manipulations show that

$$\begin{aligned} v - V(R\omega + O, v_*) &= v - v_* - \frac{m_i}{m_j} (R\omega + O) + \frac{m_i}{m_j} v \\ &\quad - \frac{m_i}{|m_i - m_j|} |v - v_*| \omega - \frac{m_j}{m_i - m_j} (v - v_*), \end{aligned}$$

and similarly

$$v_* - (R\omega + O) = -\frac{m_j}{|m_i - m_j|} |v - v_*| \omega - \frac{m_i}{m_i - m_j} (v - v_*).$$

It is then easy to check that

$$\begin{aligned} & (v - V(R\omega + O, v_*)) \cdot (v_* - (R\omega + O)) \\ &= \frac{2m_i m_j}{(m_i - m_j)^2} |v - v_*|^2 + \frac{m_i^2 + m_j^2}{(m_i - m_j)|m_i - m_j|} |v - v_*| (v - v_*) \cdot \omega \\ &= |v - v_*|^2 \left( \frac{2m_i m_j}{(m_i - m_j)^2} + \frac{m_i^2 + m_j^2}{(m_i - m_j)|m_i - m_j|} \frac{(v - v_*) \cdot \omega}{|v - v_*|} \right) \end{aligned}$$

and

$$\begin{aligned} |v - V(R\omega + O, v_*)|^2 &= |R\omega + O - v_*|^2 \\ &= \frac{m_i^2 + m_j^2}{(m_i - m_j)^2} |v - v_*|^2 + \frac{2m_i m_j}{(m_i - m_j)|m_i - m_j|} |v - v_*| (v - v_*) \cdot \omega \\ &= |v - v_*|^2 \left( \frac{m_i^2 + m_j^2}{(m_i - m_j)^2} + \frac{2m_i m_j}{(m_i - m_j)|m_i - m_j|} \frac{(v - v_*) \cdot \omega}{|v - v_*|} \right). \end{aligned}$$

Thus, the angular part depends on  $v$  only through the cosine of the deviation angle between  $\frac{v - v_*}{|v - v_*|}$  and  $\omega \in \mathbb{S}^2$ , and finally reads

$$b_{ij} \left( \omega \cdot \frac{v - v_*}{|v - v_*|} \right) = b_{ij} \left( \frac{\frac{2m_i m_j}{(m_i - m_j)^2} + \frac{m_i^2 + m_j^2}{(m_i - m_j)|m_i - m_j|} \frac{(v - v_*) \cdot \omega}{|v - v_*|}}{\frac{m_i^2 + m_j^2}{(m_i - m_j)^2} + \frac{2m_i m_j}{(m_i - m_j)|m_i - m_j|} \frac{(v - v_*) \cdot \omega}{|v - v_*|}} \right).$$

We can then rewrite our integral term  $\kappa_{ij}^{(1)}$  as

$$\begin{aligned} \kappa_{ij}^{(1)}(v, v_*) &= C_{ij} c_i |v - v_*|^\gamma \int_{\mathbb{S}^2} \frac{b_{ij} \left( \omega \cdot \frac{v - v_*}{|v - v_*|} \right) c_i}{\left| \frac{m_i^2 + m_j^2}{(m_i - m_j)^2} + \frac{2m_i m_j}{(m_i - m_j)|m_i - m_j|} \frac{(v - v_*) \cdot \omega}{|v - v_*|} \right|^{1-\gamma}} \\ &\quad \times e^{-\frac{m_i}{2} |R\omega + O|^2 + \varepsilon m_i (R\omega + O) \cdot u_i - \varepsilon^2 \frac{m_i}{2} |u_i|^2} d\omega, \quad (\text{B.1.1}) \end{aligned}$$

where we have renamed for simplicity

$$C_{ij} = \frac{C_{ij} m_j^2}{(m_i - m_j)^2} \left( \frac{m_i}{2\pi} \right)^{3/2}$$

and the exponent explicitly reads

$$\begin{aligned} |R\omega + O|^2 &= \frac{m_j^2}{(m_i - m_j)^2} |v - v_*|^2 + \frac{2m_j |v - v_*|}{(m_i - m_j)|m_i - m_j|} (m_i v - m_j v_*) \cdot \omega \\ &\quad + \frac{1}{(m_i - m_j)^2} |m_i v - m_j v_*|^2, \end{aligned}$$

$$(R\omega + O) \cdot u_i = \frac{m_j}{|m_i - m_j|} |v - v_*| \omega \cdot u_i + \frac{(m_i v - m_j v_*) \cdot u_i}{m_i - m_j}.$$

This concludes the study for  $\kappa_{ij}^{(1)}$ .

## B.2 Explicit form of $\kappa_{ij}^{(2)}$

Recovering the explicit expression of  $\kappa_{ij}^{(2)}$  is more subtle. We recall that the domain of integration  $E_{vv_*}^{ij}$  is the hyperplane orthogonal to  $v - v_*$  and passing through

$$V_E(v, v_*) = \frac{m_i + m_j}{2m_j}v - \frac{m_i - m_j}{2m_j}v_*.$$

Let us consider  $\omega \in (\text{Span}(v - v_*))^\perp$  and perform the change of variables  $w = V_E(v, v_*) + \omega$  which translates  $E_{vv_*}^{ij}$  to the parallel hyperplane passing through the origin of  $\mathbb{R}^3$ . Thus  $\kappa_{ij}^{(2)}$  transforms into

$$\begin{aligned} \kappa_{ij}^{(2)}(v, v_*) &= \frac{C_{ji}}{|v - v_*|} \int_{E_{vv_*}^{ij}} \frac{B_{ij}\left(v - V(v_*, w), \frac{w - v_*}{|w - v_*|}\right)}{|w - v_*|} M_j^\varepsilon(w) \, dE(w) \\ &= \frac{C_{ji}}{|v - v_*|} \int_{(v - v_*)^\perp} \frac{b_{ij}(v, v_*, \omega)}{|v - V(v_*, V_E(v, v_*) + \omega)|^{1-\gamma}} M_j^\varepsilon(V_E(v, v_*) + \omega) \, d\omega, \end{aligned}$$

where the angular part writes

$$b_{ij}(v, v_*, \omega) = b_{ij} \left( \frac{(v - V(v_*, V_E(v, v_*) + \omega)) \cdot (V_E(v, v_*) + \omega - v_*)}{|v - V(v_*, V_E(v, v_*) + \omega)| |V_E(v, v_*) + \omega - v_*|} \right).$$

Easy calculations show that

$$\begin{aligned} V_E(v, v_*) + \omega - v_* &= \frac{m_i + m_j}{2m_j}(v - v_*) + \omega, \\ v - V(v_*, V_E(v, v_*) + \omega) &= \frac{m_i + m_j}{2m_j}(v - v_*) - \omega, \end{aligned}$$

and

$$\begin{aligned} (v - V(v_*, V_E(v, v_*) + \omega)) \cdot (V_E(v, v_*) + \omega - v_*) &= \left( \frac{m_i + m_j}{2m_j} \right)^2 |v - v_*|^2 - |\omega|^2, \\ |v - V(v_*, V_E(v, v_*) + \omega)|^2 &= |V_E(v, v_*) + \omega - v_*|^2 = \left( \frac{m_i + m_j}{2m_j} \right)^2 |v - v_*|^2 + |\omega|^2. \end{aligned}$$

Moreover, the exponent of the Maxwellian can be computed as follows. We initially develop the square to get

$$|V_E(v, v_*) + \omega - \varepsilon u_j|^2 = |V_E(v, v_*) + \omega|^2 - 2\varepsilon(V_E(v, v_*) + \omega) \cdot u_j + \varepsilon^2 |u_j|^2.$$

The first term can be rewritten as

$$\begin{aligned} |V_E(v, v_*) + \omega|^2 &= \left| \omega + \frac{1}{2}(v + v_*) + \frac{m_i}{2m_j}(v - v_*) \right|^2 \\ &= \left| \omega + \frac{1}{2}(v + v_*) \right|^2 + \frac{m_i^2}{4m_j^2} |v - v_*|^2 + \frac{m_i}{2m_j} (|v|^2 - |v_*|^2) \\ &= \left| \omega + \frac{1}{2}V^\perp \right|^2 + \frac{1}{4} \|V\|^2 + \frac{m_i^2}{4m_j^2} |v - v_*|^2 + \frac{m_i}{2m_j} (|v|^2 - |v_*|^2), \end{aligned}$$

where we have decomposed  $v+v_* = V^\parallel + V^\perp$ , with  $V^\parallel$  being the projection onto  $\text{Span}(v-v_*)$  and  $V^\perp$  being the orthogonal part. In the same way, the second term reads

$$(V_E(v, v_*) + \omega) \cdot u_j = \left( \frac{1}{2}V^\parallel + \frac{m_i}{2m_j}(v - v_*) \right) \cdot u_j + \left( \frac{1}{2}V^\perp + \omega \right) \cdot u_j.$$

Since by the definition of  $V^\parallel$

$$\left| V^\parallel \right|^2 = \frac{((v + v_*) \cdot (v - v_*))^2}{|v - v_*|^2} = \frac{||v|^2 - |v_*|^2|^2}{|v - v_*|^2},$$

the kernel  $\kappa_{ij}^{(2)}$  becomes

$$\kappa_{ij}^{(2)}(v, v_*) = \mathcal{P}_{ij}(v, v_*) \int_{(v-v_*)^\perp} b_{ij}(v, v_*, \omega) W_{ij}(v, v_*, \omega) M_j^\varepsilon \left( \omega + \frac{1}{2}V^\perp \right) dE(\omega),$$

where

$$\begin{aligned} \mathcal{P}_{ij}(v, v_*) &= \frac{C_{ji}}{|v - v_*|} e^{-\frac{m_i^2}{8m_j}|v-v_*|^2 - \frac{m_j}{8} \frac{||v|^2 - |v_*|^2|^2}{|v-v_*|^2} + \varepsilon \frac{m_i}{2}(v-v_*) \cdot u_j + \varepsilon \frac{m_j}{2} \frac{|v|^2 - |v_*|^2}{|v-v_*|} \frac{(v-v_*) \cdot u_j}{|v-v_*|}} \sqrt{\frac{\mu_i}{\mu_i^*}}, \\ b_{ij}(v, v_*, \omega) &= b_{ij} \left( \frac{\left( \frac{m_i+m_j}{2m_j} \right)^2 |v - v_*|^2 - |\omega|^2}{\left( \frac{m_i+m_j}{2m_j} \right)^2 |v - v_*|^2 + |\omega|^2} \right), \\ W_{ij}(v, v_*, \omega) &= \left( \left( \frac{m_i + m_j}{2m_j} \right)^2 |v - v_*|^2 + |\omega|^2 \right)^{\frac{\gamma-1}{2}}. \end{aligned}$$

Finally, it remains to take care of the domain of integration which still depends on  $(v, v_*)$ . The idea is to transform the hyperplane defined by  $(v - v_*)^\perp$  to end up on  $\mathbb{R}^2$ . Proceeding as in [160, Proposition 2.4], we first observe that the integral is even with respect to  $v - v_*$ , since it only depends on its modulus. Thus, we focus on the set of relative velocities  $v - v_*$  such that the first coordinate is nonnegative. Call  $e_1$  the first unit vector of the corresponding orthonormal basis and, for any fixed  $\frac{v-v_*}{|v-v_*|}$ , introduce the linear transformation

$$\mathcal{L} \left( \frac{v - v_*}{|v - v_*|}, \mathcal{X} \right) = 2 \frac{\left( e_1 + \frac{v-v_*}{|v-v_*|} \right) \cdot \mathcal{X}}{\left| e_1 + \frac{v-v_*}{|v-v_*|} \right|^2} \left( e_1 + \frac{v - v_*}{|v - v_*|} \right) - \mathcal{X}, \quad \forall \mathcal{X} \in \mathbb{R}^3,$$

which corresponds to the specular reflection through the axis defined by  $e_1 + \frac{v-v_*}{|v-v_*|}$ . Now,  $\mathcal{L}$  is a diffeomorphism from  $\{\mathcal{X} = (0, X), X \in \mathbb{R}^2\}$  onto  $(v - v_*)^\perp$ , with unitary Jacobian matrix. Thus, we can use this linear transformation to pass from  $(v - v_*)^\perp$  to  $\mathbb{R}^2$  into the integral of  $\kappa_{ij}^{(2)}$ , which can be finally explicitly written as

$$\begin{aligned} \kappa_{ij}^{(2)}(v, v_*) &= \\ \mathcal{P}_{ij}(v, v_*) &\int_{\mathbb{R}^2} b_{ij} \left( \frac{\left( \frac{m_i+m_j}{2m_j} \right)^2 |v - v_*|^2 - |X|^2}{\left( \frac{m_i+m_j}{2m_j} \right)^2 |v - v_*|^2 + |X|^2} \right) \left( \left( \frac{m_i + m_j}{2m_j} \right)^2 |v - v_*|^2 + |X|^2 \right)^{\frac{\gamma-1}{2}} \\ &\times M_j^\varepsilon \left( \mathcal{L} \left( \frac{v - v_*}{|v - v_*|}, \left( 0, X + \frac{1}{2}\bar{X} \right) \right) \right) dX, \quad (\text{B.2.1}) \end{aligned}$$



where we have called  $\bar{X} \in \mathbb{R}^2$  the preimage of  $V^\perp \in (v-v_*)^\perp$  through the transformation  $\mathcal{L}$ , and we have used the straightforward identity

$$\left| \mathcal{L} \left( \frac{v-v_*}{|v-v_*|}, (0, X) \right) \right| = |X|, \quad \forall X \in \mathbb{R}^2, \forall v, v_* \in \mathbb{R}^3.$$

This concludes the study for  $\kappa_{ij}^{(2)}$ .

### B.3 Explicit form of $\kappa_{ij}^{(3)}$

The analysis of  $\kappa_{ij}^{(3)}$  is the easiest one, since it is already fully explicit. It simply reads

$$\begin{aligned} \kappa_{ij}^{(3)}(v, v_*) &= \int_{\mathbb{S}^2} B_{ij}(|v-v_*|, \cos \vartheta) M_i^\varepsilon d\sigma \\ &= \int_{\mathbb{S}^2} b_{ij} \left( \sigma \cdot \frac{v-v_*}{|v-v_*|} \right) |v-v_*|^\gamma M_i^\varepsilon(v) d\sigma. \end{aligned}$$

This concludes its study.

## Annexe C

# Proofs of the *a priori* energy estimates for the Boltzmann equation

We shall follow the computations in [43, Appendix B], in order to show that we recover very similar *a priori* estimates for the quantities in  $H_{x,v}^s(\boldsymbol{\mu}^{-\frac{1}{2}})$ .

Let us thus consider an integer  $s \in \mathbb{N}^*$  and a function  $\mathbf{f} \in H^s(\mathbb{T}^3 \times \mathbb{R}^3, \boldsymbol{\mu}^{-\frac{1}{2}})$  which solves the perturbed Boltzmann equation

$$\partial_t \mathbf{f} + \frac{1}{\varepsilon} v \cdot \nabla_x \mathbf{f} = \frac{1}{\varepsilon^2} \mathbf{L}^\varepsilon(\mathbf{f}) + \frac{1}{\varepsilon} \mathbf{Q}(\mathbf{f}, \mathbf{f}) + \mathbf{S}^\varepsilon, \quad (\text{C.0.1})$$

and satisfies initially  $\|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \mathcal{O}(\delta_{\text{MS}})$ . In particular, we suppose from now on that  $\delta_{\text{MS}} \leq 1$ . Indeed, even if not optimal, this choice helps in enlightening the presentation.

To simplify the computations, we recall that we denote  $\mathbf{f}^\perp = \mathbf{f} - \pi_{\mathbf{L}}(\mathbf{f})$  the projection onto  $(\ker \mathbf{L})^\perp$ .

### C.1 Time evolution of $\|\mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2$

We initially take the scalar product of (C.0.1) against  $\mathbf{f}\boldsymbol{\mu}^{-1}$  and we integrate in  $x$  and  $v$  to get

$$\begin{aligned} \frac{d}{dt} \|\mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &= \frac{2}{\varepsilon^2} \langle \mathbf{L}^\varepsilon(\mathbf{f}), \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} - \frac{2}{\varepsilon} \langle v \cdot \nabla_x \mathbf{f}, \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &\quad + \frac{2}{\varepsilon} \langle \mathbf{Q}(\mathbf{f}, \mathbf{f}), \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} + 2 \langle \mathbf{S}^\varepsilon, \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}. \end{aligned}$$

Thanks to the anti-symmetry of  $v \cdot \nabla_x$ , the term containing the transport operator vanishes. In order to bound the linear term, we exploit the spectral gap estimate (3.3.12) satisfied

by  $\mathbf{L}^\varepsilon$ . We successively obtain

$$\begin{aligned} \frac{2}{\varepsilon^2} \langle \mathbf{L}^\varepsilon(\mathbf{f}), \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} &\leq -\frac{2}{\varepsilon^2} \left( \lambda_{\mathbf{L}} - (\varepsilon + \eta_1) C_2^{\mathbf{L}} \right) \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \frac{2\delta_{\text{MS}} C_2^{\mathbf{L}}}{\eta_1} \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\leq -\frac{2}{\varepsilon^2} \left( \lambda_{\mathbf{L}} - (\varepsilon + \eta_1) C_2^{\mathbf{L}} \right) \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \delta_{\text{MS}} \frac{4C_2^{\mathbf{L}} C_\pi C_{\mathbb{T}^3}}{\eta_1} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \delta_{\text{MS}}^3 \frac{2C_2^{\mathbf{L}} C_\pi C^{\mathbf{T}}}{\eta_1}, \quad (\text{C.1.1}) \end{aligned}$$

where we have also used the equivalence between the  $L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})$  and  $L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})$  norms on  $\ker \mathbf{L}$  from Lemma 3.3.10, and the Poincaré inequality (3.3.21).

The bilinear term is handled thanks to properties (3.3.13)–(3.3.14). Applying Young's inequality with a positive constant  $\eta/\varepsilon$ , we recover

$$\frac{2}{\varepsilon} \langle \mathbf{Q}(\mathbf{f}, \mathbf{f}), \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2}{\eta} \mathcal{G}_x^0(\mathbf{f}, \mathbf{f})^2 + \frac{2\eta}{\varepsilon^2} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.1.2})$$

Finally, the source term is dealt with using estimate (3.3.18) for the  $x$ -derivatives, which also holds when  $|\alpha| = 0$ , with some positive constant  $C_0^{\mathbf{S}}$ . Applying again the Poincaré inequality (3.3.21), we compute

$$\begin{aligned} 2\langle \mathbf{S}^\varepsilon, \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} &\leq \frac{2\delta_{\text{MS}}^2 C_0^{\mathbf{S}}}{\eta_4 \eta_5} + 2\eta_4 \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2\eta_5}{\varepsilon^2} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\leq \frac{2\delta_{\text{MS}}^2 C_0^{\mathbf{S}}}{\eta_4 \eta_5} + \frac{2\eta_5}{\varepsilon^2} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + 4\eta_4 C_{\mathbb{T}^3} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + 2\eta_4 \delta_{\text{MS}}^2 C^{\mathbf{T}}. \end{aligned} \quad (\text{C.1.3})$$

Gathering inequalities (C.1.1)–(C.1.3), with the choices  $\eta = \eta_1 = \eta_5 = \frac{\lambda_{\mathbf{L}}}{4(C_2^{\mathbf{L}}+1)}$  and also  $\eta_4 = \delta_{\text{MS}}$  and  $\varepsilon \leq \eta$ , we obtain

$$\begin{aligned} \frac{d}{dt} \|\mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &\leq -\frac{\lambda_{\mathbf{L}}}{\varepsilon^2} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{8(C_2^{\mathbf{L}}+1)}{\lambda_{\mathbf{L}}} \mathcal{G}_x^0(\mathbf{f}, \mathbf{f})^2 \\ &\quad + \delta_{\text{MS}} \left( 8C_{\mathbb{T}^3} + \frac{32C_2^{\mathbf{L}} C_\pi C_{\mathbb{T}^3} (C_2^{\mathbf{L}}+1)}{\lambda_{\mathbf{L}}} \right) \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \delta_{\text{MS}} \left( 2C^{\mathbf{T}} + \frac{8C_2^{\mathbf{L}} C_\pi C^{\mathbf{T}} (C_2^{\mathbf{L}}+1)}{\lambda_{\mathbf{L}}} + \frac{8C_0^{\mathbf{S}} (C_2^{\mathbf{L}}+1)}{\lambda_{\mathbf{L}}} \right), \end{aligned} \quad (\text{C.1.4})$$

holding for any  $\delta_{\text{MS}} \in [0, 1]$ . By choosing

$$\begin{aligned} C^{(1)} &= 8C_{\mathbb{T}^3} + \frac{32C_2^{\mathbf{L}} C_\pi C_{\mathbb{T}^3} (C_2^{\mathbf{L}}+1)}{\lambda_{\mathbf{L}}}, \\ \tilde{C}_0^{\mathbf{S}} &= 2C^{\mathbf{T}} + \frac{8C_2^{\mathbf{L}} C_\pi C^{\mathbf{T}} (C_2^{\mathbf{L}}+1)}{\lambda_{\mathbf{L}}} + \frac{8C_0^{\mathbf{S}} (C_2^{\mathbf{L}}+1)}{\lambda_{\mathbf{L}}}, \end{aligned}$$

we thus recover the first estimate (3.3.24).

## C.2 Time evolution of $\|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2$

The time evolution of the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm of  $\nabla_x \mathbf{f}$  is given by

$$\begin{aligned} \frac{d}{dt} \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &= \frac{2}{\varepsilon^2} \langle \nabla_x \mathbf{L}^\varepsilon(\mathbf{f}), \nabla_x \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} - \frac{2}{\varepsilon} \langle \nabla_x (v \cdot \nabla_x \mathbf{f}), \nabla_x \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &\quad + \frac{2}{\varepsilon} \langle \nabla_x \mathbf{Q}(\mathbf{f}, \mathbf{f}), \nabla_x \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} + 2 \langle \nabla_x \mathbf{S}^\varepsilon, \nabla_x \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}. \end{aligned}$$

First of all, since the transport operator commutes with  $x$ -derivatives, the anti-symmetry property allows again to get rid of it. We then study the linearized operator  $\mathbf{L}^\varepsilon$ . Applying the Leibniz derivation rule and using the orthogonality of  $\mathbf{Q}$  to  $\ker \mathbf{L}$  given by (3.3.13), we initially observe that

$$\begin{aligned} \langle \nabla_x \mathbf{L}^\varepsilon(\mathbf{f}), \nabla_x \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} &= \langle \mathbf{Q}(\nabla_x \mathbf{M}^\varepsilon, \mathbf{f}) + \mathbf{Q}(\mathbf{f}, \nabla_x \mathbf{M}^\varepsilon), \nabla_x \mathbf{f}^\perp \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &\quad + \langle \mathbf{L}^\varepsilon(\nabla_x \mathbf{f}), \nabla_x \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}. \end{aligned} \tag{C.2.1}$$

The addends involving the derivative of  $\mathbf{M}^\varepsilon$  are controlled by a factor of order  $\mathcal{O}(\varepsilon \delta_{\text{MS}})$ . Using estimate (3.3.9) we thus get

$$\begin{aligned} \langle \mathbf{Q}(\nabla_x \mathbf{M}^\varepsilon, \mathbf{f}) + \mathbf{Q}(\mathbf{f}, \nabla_x \mathbf{M}^\varepsilon), \nabla_x \mathbf{f}^\perp \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ \leq \varepsilon \delta_{\text{MS}} C_1^{\text{L}} K_x \|\mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \|\nabla_x \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}. \end{aligned}$$

Using the fact that  $\mathbf{f} = \pi_{\mathbf{L}}(\mathbf{f}) + \mathbf{f}^\perp$  and the equivalence of the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  and  $L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})$  norms for  $\pi_{\mathbf{L}}(\mathbf{f})$ , we can then apply Young's inequality with a positive constant  $\eta/\varepsilon$  (and increment  $K_x$  if necessary) to recover the upper bound

$$\begin{aligned} \langle \mathbf{Q}(\nabla_x \mathbf{M}^\varepsilon, \mathbf{f}) + \mathbf{Q}(\mathbf{f}, \nabla_x \mathbf{M}^\varepsilon), \nabla_x \mathbf{f}^\perp \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ \leq \eta \delta_{\text{MS}} C_1^{\text{L}} K_x \|\nabla_x \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2\varepsilon \delta_{\text{MS}} C_1^{\text{L}} K_x}{\eta} \|\mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ + \frac{2\varepsilon^2 \delta_{\text{MS}} C_\pi C_1^{\text{L}} K_x}{\eta} \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2, \end{aligned}$$

where we have also used that  $\varepsilon \leq 1$ . Moreover, the second term of (C.2.1) is handled thanks to estimate (3.3.12) on the spectral gap of  $\mathbf{L}^\varepsilon$ , and can be bounded as

$$\begin{aligned} \langle \mathbf{L}^\varepsilon(\nabla_x \mathbf{f}), \nabla_x \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} &\leq -\left(\lambda_{\mathbf{L}} - (\varepsilon + \eta_1) C_2^{\text{L}}\right) \|\nabla_x \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \varepsilon^2 \delta_{\text{MS}} \frac{C_2^{\text{L}}}{\eta_1} \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \end{aligned}$$

Choosing  $\eta = \eta_1$ , we can finally apply the Poincaré inequality (3.3.21) to obtain

$$\begin{aligned}
& \frac{2}{\varepsilon^2} \langle \nabla_x \mathbf{L}^\varepsilon(\mathbf{f}), \nabla_x \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\
& \leq -\frac{2}{\varepsilon^2} \left( \lambda_{\mathbf{L}} - \varepsilon C_2^{\mathbf{L}} - \eta_1 (C_2^{\mathbf{L}} + \delta_{\text{MS}} C_1^{\mathbf{L}} K_x) \right) \|\nabla_x \mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \quad + \frac{4\delta_{\text{MS}} C_1^{\mathbf{L}} K_x}{\varepsilon \eta_1} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{8\delta_{\text{MS}} C_\pi C_{\text{T}^3} (C_2^{\mathbf{L}} + 2C_1^{\mathbf{L}} K_x)}{\eta_1} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \quad + \frac{4\delta_{\text{MS}}^3 C_\pi C^{\text{T}} (C_2^{\mathbf{L}} + 2C_1^{\mathbf{L}} K_x)}{\eta_1}. \quad (\text{C.2.2})
\end{aligned}$$

The non-linear term is easily handled thanks to properties (3.3.13)–(3.3.14). Applying Young's inequality with a positive constant  $\eta_1/\varepsilon$  we successively get

$$\begin{aligned}
\frac{2}{\varepsilon} \langle \nabla_x \mathbf{Q}(\mathbf{f}, \mathbf{f}), \nabla_x \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} &= \frac{2}{\varepsilon} \langle \nabla_x \mathbf{Q}(\mathbf{f}, \mathbf{f}), \nabla_x \mathbf{f}^\perp \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\
&\leq \frac{2}{\eta_1} \mathcal{G}_x^1(\mathbf{f}, \mathbf{f})^2 + \frac{2\eta_1}{\varepsilon^2} \|\nabla_x \mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.2.3})
\end{aligned}$$

Finally, the source term is dealt with using estimate (3.3.18) on  $x$ -derivatives as before, to get

$$2 \langle \nabla_x \mathbf{S}^\varepsilon, \nabla_x \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2\delta_{\text{MS}}^2 C_x^{\text{S}}}{\eta_4 \eta_5} + 2\eta_4 \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2\eta_5}{\varepsilon^2} \|\nabla_x \mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2, \quad (\text{C.2.4})$$

where we have also used that  $\|\pi_{\mathbf{L}}(\nabla_x \mathbf{f})\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2$ .

To conclude, summing equations (C.2.2)–(C.2.4) and recalling that  $\delta_{\text{MS}} \leq 1$ , we recover the estimate

$$\begin{aligned}
\frac{d}{dt} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &\leq -\frac{2}{\varepsilon^2} \left( \lambda_{\mathbf{L}} - \varepsilon C_2^{\mathbf{L}} - \eta_1 (1 + C_2^{\mathbf{L}} + C_1^{\mathbf{L}} K_x) - \eta_5 \right) \|\nabla_x \mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
&\quad + \frac{4\delta_{\text{MS}} C_1^{\mathbf{L}} K_x}{\varepsilon \eta_1} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2}{\eta_1} \mathcal{G}_x^1(\mathbf{f}, \mathbf{f})^2 \\
&\quad + \left( 2\eta_4 + \frac{8\delta_{\text{MS}} C_\pi C_{\text{T}^3} (C_2^{\mathbf{L}} + 2C_1^{\mathbf{L}} K_x)}{\eta_1} \right) \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
&\quad + \frac{2\delta_{\text{MS}}^2 C_x^{\text{S}}}{\eta_4 \eta_5} + \frac{4\delta_{\text{MS}} C_\pi C^{\text{T}} (C_2^{\mathbf{L}} + 2C_1^{\mathbf{L}} K_x)}{\eta_1}.
\end{aligned}$$

By choosing

$$\eta_1 = \eta_5 = \frac{\lambda_{\mathbf{L}}}{2(2 + 2C_2^{\mathbf{L}} + C_1^{\mathbf{L}} K_x)}, \quad \eta_4 = \delta_{\text{MS}}, \quad \varepsilon \leq \eta_1,$$

we finally obtain

$$\begin{aligned} \frac{d}{dt} \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &\leq -\frac{\lambda_{\mathbf{L}}}{\varepsilon^2} \|\nabla_x \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &+ \frac{\delta_{\text{MS}}}{\varepsilon} \frac{8K_x(2 + 2C_2^{\mathbf{L}} + C_1^{\mathbf{L}}K_x)}{\lambda_{\mathbf{L}}} \|\mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{8(2 + 2C_2^{\mathbf{L}} + C_1^{\mathbf{L}}K_x)}{\lambda_{\mathbf{L}}} \mathcal{G}_x^1(\mathbf{f}, \mathbf{f})^2 \\ &+ \delta_{\text{MS}} \left( 2 + \frac{16C_\pi C_{\mathbb{T}^3}(C_2^{\mathbf{L}} + 2K_x)(2 + 2C_2^{\mathbf{L}} + C_1^{\mathbf{L}}K_x)}{\lambda_{\mathbf{L}}} \right) \|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &+ \delta_{\text{MS}} (4C_x^{\mathbf{S}} + 8C_\pi C^{\mathbf{T}}(C_2^{\mathbf{L}} + 2C_1^{\mathbf{L}}K_x)) \frac{2 + 2C_2^{\mathbf{L}} + C_1^{\mathbf{L}}K_x}{\lambda_{\mathbf{L}}}, \end{aligned}$$

which is exactly (3.3.25), with

$$\begin{aligned} C^{(2)} &= 2 + \frac{16C_\pi C_{\mathbb{T}^3}(C_2^{\mathbf{L}} + 2C_1^{\mathbf{L}}K_x)(2 + 2C_2^{\mathbf{L}} + C_1^{\mathbf{L}}K_x)}{\lambda_{\mathbf{L}}}, \\ C^{(3)} &= \frac{8K_x(2 + 2C_2^{\mathbf{L}} + K_x)}{\lambda_{\mathbf{L}}}, \\ \tilde{C}_x &= (4C_x^{\mathbf{S}} + 8C_\pi C^{\mathbf{T}}(C_2^{\mathbf{L}} + 2C_1^{\mathbf{L}}K_x)) \frac{2 + 2C_2^{\mathbf{L}} + C_1^{\mathbf{L}}K_x}{\lambda_{\mathbf{L}}}. \end{aligned}$$

### C.3 Time evolution of $\|\nabla_v \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2$

The evolution equation for the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm of  $\nabla_v \mathbf{f}$  writes

$$\begin{aligned} \frac{d}{dt} \|\nabla_v \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &= \frac{2}{\varepsilon^2} \langle \nabla_v \mathbf{L}^\varepsilon(\mathbf{f}), \nabla_v \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} - \frac{2}{\varepsilon} \langle \nabla_v (v \cdot \nabla_x \mathbf{f}), \nabla_v \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &+ \frac{2}{\varepsilon} \langle \nabla_v \mathbf{Q}(\mathbf{f}, \mathbf{f}), \nabla_v \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} + 2 \langle \nabla_v \mathbf{S}^\varepsilon, \nabla_v \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}. \end{aligned}$$

The first term can be rewritten using the operators  $\mathbf{K}^\varepsilon$  and  $\boldsymbol{\nu}^\varepsilon$  and is then dealt with thanks to estimates (3.3.10)–(3.3.11). We have, for any  $\xi > 0$ ,

$$\begin{aligned} \frac{2}{\varepsilon^2} \langle \nabla_v \mathbf{L}^\varepsilon(\mathbf{f}), \nabla_v \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} &= \frac{2}{\varepsilon^2} \langle \nabla_v \mathbf{K}^\varepsilon(\mathbf{f}), \nabla_v \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} - \frac{2}{\varepsilon^2} \langle \nabla_v \boldsymbol{\nu}^\varepsilon(\mathbf{f}), \nabla_v \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &\leq \frac{2(C_1^{\mathbf{K}}(\xi) + C_5^{\boldsymbol{\nu}})}{\varepsilon^2} \|\mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 - \frac{2C_3^{\boldsymbol{\nu}}}{\varepsilon^2} \|\nabla_v \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &+ \frac{2\xi C_2^{\mathbf{K}}}{\varepsilon^2} \|\nabla_v \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2. \end{aligned}$$

Now, we use the identity

$$\|\mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 = \|\mathbf{f}^\perp\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \|\pi_{\mathbf{L}}(\mathbf{f})\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2,$$

and the fact that the  $L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})$  norm controls the  $L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm to deduce the first upper bound

$$\begin{aligned} & \frac{2}{\varepsilon^2} \langle \nabla_v \mathbf{L}^\varepsilon(\mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ & \leq \frac{2(C_1^{\mathbf{K}}(\xi) + C_5^\nu)}{\varepsilon^2} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 - \frac{2}{\varepsilon^2} (C_3^\nu - \xi C_2^{\mathbf{K}}) \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ & \quad + \frac{4C_{\mathbb{T}^3}(C_1^{\mathbf{K}}(\xi) + C_5^\nu)}{\varepsilon^2} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2\delta_{\text{MS}}^2 C^{\mathbf{T}}(C_1^{\mathbf{K}}(\xi) + C_5^\nu)}{\varepsilon^2}, \end{aligned} \quad (\text{C.3.1})$$

where we also applied the Poincaré inequality (3.3.21). Next, the transport term is easily estimated thanks to Young's inequality as

$$\begin{aligned} -\frac{2}{\varepsilon} \langle \nabla_v (v \cdot \nabla_x \mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} &= -\frac{2}{\varepsilon} \langle \nabla_x \mathbf{f}, \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &\leq \frac{2}{\eta} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2\eta}{\varepsilon^2} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2, \end{aligned} \quad (\text{C.3.2})$$

holding for any  $\eta > 0$ . The non-linear term is handled in a similar way, using Young's inequality with the same constant  $\eta/\varepsilon$  to recover

$$\frac{2}{\varepsilon} \langle \nabla_v \mathbf{Q}(\mathbf{f}, \mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2}{\eta} \mathcal{G}_{x,v}^1(\mathbf{f}, \mathbf{f})^2 + \frac{2\eta}{\varepsilon^2} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.3.3})$$

Finally, the source term is dealt with using estimate (3.3.16), which gives

$$2 \langle \nabla_v \mathbf{S}^\varepsilon, \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2\delta_{\text{MS}}^2 C_v^{\mathbf{S}}}{\eta_2} + \frac{2\eta_2}{\varepsilon^2} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.3.4})$$

Therefore, summing (C.3.1)–(C.3.4) with the choices  $\xi = \eta = \eta_2 = \frac{C_3^\nu}{6 + 2C_2^{\mathbf{K}}}$ , we can finally recover

$$\begin{aligned} \frac{d}{dt} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 &\leq \frac{2(C_1^{\mathbf{K}}(\xi) + C_5^\nu)}{\varepsilon^2} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 - \frac{C_3^\nu}{\varepsilon^2} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \frac{1}{\varepsilon^2} \left( 4C_{\mathbb{T}^3}(C_1^{\mathbf{K}}(\xi) + C_5^\nu) + \frac{\varepsilon^2(12 + 4C_2^{\mathbf{K}})}{C_3^\nu} \right) \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{12 + 4C_2^{\mathbf{K}}}{C_3^\nu} \mathcal{G}_{x,v}^1(\mathbf{f}, \mathbf{f})^2 \\ &\quad + \frac{\delta_{\text{MS}}}{\varepsilon^2} \left( 2\delta_{\text{MS}} C^{\mathbf{T}}(C_1^{\mathbf{K}}(\xi) + C_5^\nu) + \frac{\delta_{\text{MS}} \varepsilon^2 C_v^{\mathbf{S}}(12 + 4C_2^{\mathbf{K}})}{C_3^\nu} \right) \end{aligned} \quad (\text{C.3.5})$$

which is estimate (3.3.26) with the choices

$$\begin{aligned} K_1 &= 2(C_1^{\mathbf{K}}(\xi) + C_5^\nu), \\ K_{dx} &= 4C_{\mathbb{T}^3}(C_1^{\mathbf{K}}(\xi) + C_5^\nu) + \frac{4(3 + C_2^{\mathbf{K}})}{C_3^\nu}, \\ \tilde{C}_v^{\mathbf{S}} &= 2C^{\mathbf{T}}(C_1^{\mathbf{K}}(\xi) + C_5^\nu) + \frac{4C_v^{\mathbf{S}}(3 + C_2^{\mathbf{K}})}{C_3^\nu}, \end{aligned}$$

where we have also used that both  $\varepsilon \leq 1$  and  $\delta_{\text{MS}} \leq 1$ .

### C.4 Time evolution of $\langle \nabla_x \mathbf{f}, \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}$

The equation describing the time evolution of the  $L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm of the commutator is given by

$$\begin{aligned} \frac{d}{dt} \langle \nabla_x \mathbf{f}, \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} &= \frac{2}{\varepsilon^2} \langle \nabla_x \mathbf{L}^\varepsilon(\mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} - \frac{2}{\varepsilon} \langle \nabla_x(v \cdot \nabla_x \mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &\quad + \frac{2}{\varepsilon} \langle \nabla_x \mathbf{Q}(\mathbf{f}, \mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} + \langle \nabla_x \mathbf{S}^\varepsilon, \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}. \end{aligned}$$

For the linear term we shall successively apply the Leibniz derivation rule and the decomposition  $\nabla_x \mathbf{f} = \nabla_x \mathbf{f}^\perp + \pi_{\mathbf{L}}(\nabla_x \mathbf{f})$  to obtain

$$\begin{aligned} \frac{2}{\varepsilon^2} \langle \nabla_x \mathbf{L}^\varepsilon(\mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} &= \frac{2}{\varepsilon^2} \langle \mathbf{L}^\varepsilon(\nabla_x \mathbf{f}^\perp), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &\quad + \frac{2}{\varepsilon^2} \langle (\mathbf{L}^\varepsilon - \mathbf{L})(\pi_{\mathbf{L}}(\nabla_x \mathbf{f})), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &\quad + \frac{2}{\varepsilon^2} \langle \mathbf{Q}(\nabla_x \mathbf{M}^\varepsilon, \mathbf{f}) + \mathbf{Q}(\mathbf{f}, \nabla_x \mathbf{M}^\varepsilon), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}, \end{aligned}$$

where we have used that  $\mathbf{L}(\pi_{\mathbf{L}}(\nabla_x \mathbf{f})) = 0$ . Now, the first term is handled thanks to estimate (3.3.9) as

$$\frac{2}{\varepsilon^2} \langle \mathbf{L}^\varepsilon(\nabla_x \mathbf{f}^\perp), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2C_1^{\mathbf{L}}}{\varepsilon^2} \|\nabla_x \mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})},$$

and can be bounded using Young's inequality with a positive constant  $e/\varepsilon$ , which gives

$$\frac{2}{\varepsilon^2} \langle \mathbf{L}^\varepsilon(\nabla_x \mathbf{f}^\perp), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2C_1^{\mathbf{L}}e}{\varepsilon^3} \|\nabla_x \mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2C_1^{\mathbf{L}}}{\varepsilon e} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2.$$

The second term is of order  $\mathcal{O}(\varepsilon \delta_{\text{MS}})$  and can be handled more easily. We again use estimate (3.3.9) and Young's inequality with a positive constant  $\eta$ , together with the equivalence of the  $L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})$  and  $L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})$  norms on  $\ker \mathbf{L}$ , to get

$$\begin{aligned} \frac{2}{\varepsilon^2} \langle (\mathbf{L}^\varepsilon - \mathbf{L})(\pi_{\mathbf{L}}(\nabla_x \mathbf{f})), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} &\leq \frac{2\eta \delta_{\text{MS}} C_1^{\mathbf{L}} C_\pi}{\varepsilon} \|\pi_{\mathbf{L}}(\nabla_x \mathbf{f})\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2C_1^{\mathbf{L}}}{\eta \varepsilon} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\leq \frac{2\eta \delta_{\text{MS}} C_1^{\mathbf{L}} C_\pi}{\varepsilon} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2C_1^{\mathbf{L}}}{\eta \varepsilon} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \end{aligned}$$

At last, we have already seen how to treat the third term. Skipping the details, we obtain

$$\begin{aligned} \frac{2}{\varepsilon^2} \langle \mathbf{Q}(\nabla_x \mathbf{M}^\varepsilon, \mathbf{f}) + \mathbf{Q}(\mathbf{f}, \nabla_x \mathbf{M}^\varepsilon), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} &\leq \frac{2\delta_{\text{MS}} C_1^{\mathbf{L}} K_x}{\eta \varepsilon} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{4\eta \delta_{\text{MS}} C_1^{\mathbf{L}} K_x}{\varepsilon} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &\quad + \frac{8\eta \delta_{\text{MS}} C_1^{\mathbf{L}} K_x C_\pi C_{\mathbb{T}^3}}{\varepsilon} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{4\eta \delta_{\text{MS}}^3 C_1^{\mathbf{L}} K_x C_\pi C_{\mathbb{T}^3}}{\varepsilon}. \end{aligned}$$



using again Young's inequality with  $\eta > 0$ , and the Poincaré inequality (3.3.21). Collecting these upper bounds, we finally derive the estimate for the linear term

$$\begin{aligned}
& \frac{2}{\varepsilon^2} \langle \nabla_x \mathbf{L}^\varepsilon(\mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\
& \leq \frac{2C_1^L e}{\varepsilon^3} \|\nabla_x \mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \left( \frac{2 + 2\delta_{\text{MS}} C_1^L K_x}{\eta \varepsilon} + \frac{2C_1^L}{\varepsilon e} \right) \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \quad + \frac{4\eta \delta_{\text{MS}} C_1^L K_x}{\varepsilon} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2\eta \delta_{\text{MS}} (1 + 4C_1^L K_x C_\pi C_{\mathbb{T}^3})}{\varepsilon} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \quad + \frac{4\eta \delta_{\text{MS}}^3 C_1^L K_x C_\pi C^{\mathbf{T}}}{\varepsilon}. \quad (\text{C.4.1})
\end{aligned}$$

For the transport term we successively integrate by parts, first in  $x$  and then in  $v$ . Direct calculations allows to recover

$$\begin{aligned}
-\frac{2}{\varepsilon} \langle \nabla_x (v \cdot \nabla_x \mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} &= -\frac{1}{\varepsilon} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 - \frac{1}{\varepsilon} \|v \cdot \nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
&\leq -\frac{1}{\varepsilon} \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.4.2})
\end{aligned}$$

The non-linear term is treated thanks to Young's inequality with the usual positive constant  $\eta$ , and we get

$$\frac{2}{\varepsilon} \langle \nabla_x \mathbf{Q}(\mathbf{f}, \mathbf{f}), \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2\eta}{\varepsilon} \mathcal{G}_{x,v}^1(\mathbf{f}, \mathbf{f})^2 + \frac{2}{\eta \varepsilon} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.4.3})$$

The source term is then treated using estimate (3.3.17), which gives

$$2 \langle \nabla_x \mathbf{S}^\varepsilon, \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2\delta_{\text{MS}}^2 C_{x,v}^{\mathbf{S}}}{\varepsilon \eta_3} + \frac{2\eta_3}{\varepsilon} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.4.4})$$

Gathering inequalities (C.4.1)–(C.4.4) with the choices  $\eta = e$  and  $\eta_3 = 1/e$ , we then recover the following estimate

$$\begin{aligned}
& \frac{d}{dt} \langle \nabla_x \mathbf{f}, \nabla_v \mathbf{f} \rangle_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})} \\
& \leq -\frac{1}{\varepsilon} \left( 1 - 2e\delta_{\text{MS}}(1 + 4C_1^L K_x C_\pi C_{\mathbb{T}^3}) \right) \|\nabla_x \mathbf{f}\|_{L^2_{x,v}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2e}{\varepsilon} \mathcal{G}_{x,v}^1(\mathbf{f}, \mathbf{f})^2 \\
& \quad + \frac{4eC_1^L K_x}{\varepsilon} \|\mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{5 + 2C_1^L(1 + K_x)}{\varepsilon e} \|\nabla_v \mathbf{f}\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \quad + \frac{2C_1^L e}{\varepsilon^3} \|\nabla_x \mathbf{f}^\perp\|_{L^2_{x,v}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2e\delta_{\text{MS}}^2 (2C_1^L K_x C_\pi C^{\mathbf{T}} + C_{x,v}^{\mathbf{S}})}{\varepsilon}, \quad (\text{C.4.5})
\end{aligned}$$

where we have also used that  $\delta_{\text{MS}} \leq 1$ . The choices

$$C^{(4)} = 5 + 2C_1^L(1 + K_x), \quad C^{(5)} = 2(1 + 4C_1^L K_x C_\pi C_{\mathbb{T}^3}),$$

$$C^{(6)} = 4C_1^L K_x, \quad \tilde{C}_{x,v}^{\mathbf{S}} = 2(2C_1^L K_x C_\pi C^{\mathbf{T}} + C_{x,v}^{\mathbf{S}})$$

finally lead to estimate (3.3.27).

## C.5 Time evolution of $\|\partial_x^\alpha \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2$

Consider now  $\alpha \in \mathbb{N}^3$  such that  $|\alpha| \leq s$ . Using the Leibniz derivation rule for multi-indices, a direct iteration of the computations that we have made for  $\|\nabla_x \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2$  immediately gives estimate (3.3.28), for some constants  $C^{(7)}$ ,  $K_\alpha$ ,  $C^{(8)}$  and  $\tilde{C}_\alpha^s$  which only depend on the constants of the problem  $\lambda_{\mathbf{L}}$ ,  $C_2^{\mathbf{L}}$ ,  $C_\pi$ ,  $C_{\mathbb{T}^3}$ ,  $C^{\mathbf{T}}$  and  $C_\alpha^s$ .

## C.6 Time evolution of $\partial_v^\beta \partial_x^\alpha \mathbf{f}$

Let  $\alpha, \beta \in \mathbb{N}^3$  be two multi-indices such that  $|\alpha| + |\beta| \leq s$ . The estimate for the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm of  $\partial_v^\beta \partial_x^\alpha \mathbf{f}$  is obtained in a very similar way to the the one derived for the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm of  $\nabla_v \mathbf{f}$ , therefore we shall skip some passages. Initially, the evolution equation reads

$$\begin{aligned} & \frac{d}{dt} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ &= \frac{2}{\varepsilon^2} \left\langle \partial_v^\beta \partial_x^\alpha \mathbf{L}^\varepsilon(\mathbf{f}), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} - \frac{2}{\varepsilon} \left\langle \partial_v^\beta \partial_x^\alpha (v \cdot \nabla_x \mathbf{f}), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ & \quad + \frac{2}{\varepsilon} \left\langle \partial_v^\beta \partial_x^\alpha \mathbf{Q}(\mathbf{f}, \mathbf{f}), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} + 2 \left\langle \partial_v^\beta \partial_x^\alpha \mathbf{S}^\varepsilon, \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}. \end{aligned}$$

Thanks to estimates (3.3.10)-(3.3.11) on  $\mathbf{K}^\varepsilon$  and  $\boldsymbol{\nu}^\varepsilon$ , the linear term can be bounded as already seen in the case of  $\nabla_v \mathbf{f}$ . We get

$$\begin{aligned} & \frac{2}{\varepsilon^2} \left\langle \partial_v^\beta \partial_x^\alpha \mathbf{L}^\varepsilon(\mathbf{f}), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ & \leq -\frac{2}{\varepsilon^2} \left( C_3^\nu - \varepsilon \mathbf{1}_{\{|\alpha| \geq 1\}} C_4^\nu - \xi C_2^K \right) \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ & \quad + \frac{2}{\varepsilon^2} \left( C_5^\nu + \varepsilon \mathbf{1}_{\{|\alpha| \geq 1\}} C_6^\nu + C_1^K(\xi) \right) \|\mathbf{f}\|_{H_{x,v}^{s-1}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ & \quad + \mathbf{1}_{\{|\alpha| \geq 1\}} \frac{C_7^\nu}{\varepsilon} \sum_{0 < |\alpha'| + |\beta'| \leq s-1} \left\| \partial_v^{\beta'} \partial_x^{\alpha'} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.6.1}) \end{aligned}$$

Next, direct calculations and the anti-symmetry of the transport term show that

$$\left\langle \partial_v^\beta \partial_x^\alpha (v \cdot \nabla_x \mathbf{f}), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = \sum_{k, \beta_k > 0} \beta_k \left\langle \partial_v^{\beta - e_k} \partial_x^{\alpha + e_k} \mathbf{f}, \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}.$$

Since  $k \leq 3$  and  $\beta_k \leq s$ , using Young's inequality with a positive constant  $\eta/\varepsilon > 0$  we can recover the estimate

$$\begin{aligned} & -\frac{2}{\varepsilon} \left\langle \partial_v^\beta \partial_x^\alpha (v \cdot \nabla_x \mathbf{f}), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ & \leq \frac{6\eta}{\varepsilon^2} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2s}{\eta} \sum_{k, \beta_k > 0} \left\| \partial_v^{\beta - e_k} \partial_x^{\alpha + e_k} \mathbf{f} \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.6.2}) \end{aligned}$$

We again apply Young's inequality with the same constant  $\eta/\varepsilon$  to control the non-linear term

$$\frac{2}{\varepsilon} \left\langle \partial_v^\beta \partial_x^\alpha \mathbf{Q}(\mathbf{f}, \mathbf{f}), \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2\eta}{\varepsilon^2} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2}{\eta} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2, \quad (\text{C.6.3})$$

while the source term is dealt with thanks to estimate (3.3.16)

$$2 \left\langle \partial_v^\beta \partial_x^\alpha \mathbf{S}^\varepsilon, \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2\delta_{\text{MS}}^2 C_{\alpha,\beta}^{\text{S}}}{\eta_2} + \frac{2\eta_2}{\varepsilon^2} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.6.4})$$

We now collect estimates (C.6.1)–(C.6.4) with the choice  $\eta_2 = \eta$ , to recover

$$\begin{aligned} & \frac{d}{dt} \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ & \leq -\frac{2}{\varepsilon^2} \left( C_3^\nu - \varepsilon \mathbf{1}_{\{|\alpha| \geq 1\}} C_4^\nu - \xi C_2^\mathbf{K} - 5\eta \right) \left\| \partial_v^\beta \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ & \quad + \frac{2}{\varepsilon^2} \left( C_5^\nu + \varepsilon \mathbf{1}_{\{|\alpha| \geq 1\}} C_6^\nu + C_1^\mathbf{K}(\xi) \right) \left\| \mathbf{f} \right\|_{H_{x,v}^{s-1}(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ & \quad + \mathbf{1}_{\{|\alpha| \geq 1\}} \frac{C_7^\nu}{\varepsilon} \sum_{0 < |\alpha'| + |\beta'| \leq s-1} \left\| \partial_v^{\beta'} \partial_x^{\alpha'} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\ & \quad + \frac{2s}{\eta} \sum_{k, \beta_k > 0} \left\| \partial_v^{\beta - e_k} \partial_x^{\alpha + e_k} \mathbf{f} \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2}{\eta} \mathcal{G}_{x,v}^s(\mathbf{f}, \mathbf{f})^2 + \frac{2\delta_{\text{MS}}^2 C_{\alpha,\beta}^{\text{S}}}{\eta}. \end{aligned}$$

Recalling that both  $\varepsilon \leq 1$  and  $\delta_{\text{MS}} \leq 1$ , and using the upper bound

$$\mathbf{1}_{\{|\alpha| \geq 1\}} \sum_{0 < |\alpha'| + |\beta'| \leq s-1} \left\| \partial_v^{\beta'} \partial_x^{\alpha'} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq \left\| \mathbf{f} \right\|_{H_{x,v}^{s-1}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2,$$

together with  $\mathbf{1}_{\{|\alpha| \geq 1\}} \leq 1$ , so that we finally obtain estimate (3.3.29) by choosing

$$\xi = \eta = \frac{C_3^\nu}{2(5 + C_2^\mathbf{K} + C_4^\nu)}, \quad \varepsilon \leq \eta,$$

$$K_{s-1} = 2(C_5^\nu + C_6^\nu + C_1^\mathbf{K}(\xi)),$$

$$C^{(9)} = \frac{4s(5 + C_2^\mathbf{K} + C_4^\nu)}{C_3^\nu},$$

$$\tilde{C}_{\alpha,\beta}^{\text{S}} = \frac{4C_{\alpha,\beta}^{\text{S}}(5 + C_2^\mathbf{K} + C_4^\nu)}{C_3^\nu}.$$

### C.7 Time evolution of $\langle \partial_x^\alpha \mathbf{f}, \partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}$

At last, consider a multi-index  $\alpha \in \mathbb{N}^3$ , with  $|\alpha| \leq s$  and  $\alpha_k > 0$ . The equation satisfied by the  $L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})$  norm of the commutator for higher derivatives is

$$\begin{aligned} & \frac{d}{dt} \langle \partial_x^\alpha \mathbf{f}, \partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ &= \frac{2}{\varepsilon^2} \langle \partial_x \mathbf{L}^\varepsilon(\mathbf{f}), \partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} - \frac{2}{\varepsilon} \langle \partial_x^\alpha (v \cdot \nabla_x \mathbf{f}), \partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ & \quad + \frac{2}{\varepsilon} \langle \partial_x^\alpha \mathbf{Q}(\mathbf{f}, \mathbf{f}), \partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} + 2 \langle \partial_x^\alpha \mathbf{S}^\varepsilon, \partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}. \end{aligned}$$

Thanks to Leibniz derivation rule, the linear operator can be split as

$$\begin{aligned} \partial_x^\alpha \mathbf{L}^\varepsilon(\mathbf{f}) &= \partial_x^\alpha \mathbf{Q}(\mathbf{M}^\varepsilon, \mathbf{f}) + \partial_x^\alpha \mathbf{Q}(\mathbf{f}, \mathbf{M}^\varepsilon) \\ &= \mathbf{L}^\varepsilon(\partial_x^\alpha \mathbf{f}) + \sum_{\substack{\gamma \leq \alpha \\ |\gamma| < |\alpha|}} \binom{\alpha}{\gamma} \left( \mathbf{Q}(\partial_x^\gamma \mathbf{M}^\varepsilon, \partial_x^{\alpha-\gamma} \mathbf{f}) + \mathbf{Q}(\partial_x^\gamma \mathbf{f}, \partial_x^{\alpha-\gamma} \mathbf{M}^\varepsilon) \right) \\ &= \mathbf{L}^\varepsilon(\partial_x^\alpha \mathbf{f}^\perp) + (\mathbf{L}^\varepsilon - \mathbf{L})(\pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{f})) \\ & \quad + \sum_{\substack{\gamma \leq \alpha \\ |\gamma| < |\alpha|}} \binom{\alpha}{\gamma} \left( \mathbf{Q}(\partial_x^\gamma \mathbf{M}^\varepsilon, \partial_x^{\alpha-\gamma} \mathbf{f}) + \mathbf{Q}(\partial_x^\gamma \mathbf{f}, \partial_x^{\alpha-\gamma} \mathbf{M}^\varepsilon) \right) \end{aligned}$$

where the second and third terms are of order  $\mathcal{O}(\varepsilon \delta_{\text{MS}})$ . Using estimate (3.3.9) we can thus initially bound the linear term as

$$\begin{aligned} & \frac{2}{\varepsilon^2} \langle \partial_x^\alpha \mathbf{L}^\varepsilon(\mathbf{f}), \partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\ & \leq \frac{2C_1^{\text{L}}}{\varepsilon^2} \left\| \partial_x^\alpha \mathbf{f}^\perp \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \left\| \partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \\ & \quad + \frac{2\delta_{\text{MS}} C_1^{\text{L}} K'_{\text{dx}}}{\varepsilon} \left\| \pi_{\mathbf{L}}(\partial_x^\alpha \mathbf{f}) \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \left\| \partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \\ & \quad + \frac{2\delta_{\text{MS}} C_1^{\text{L}} \tilde{K}_{\text{dx}}}{\varepsilon} \sum_{|\alpha'| < |\alpha|} \left\| \partial_x^{\alpha'} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})} \left\| \partial_v^{e_k} \partial_x^{\alpha-e_k} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}, \end{aligned}$$

for some positive (explicitly computable) constants  $K'_{\text{dx}}$  and  $\tilde{K}_{\text{dx}}$ . We then apply Young's inequality to the first term with a positive constant  $e/\varepsilon$  and to the second and third ones

with the constant  $e > 0$ , to recover

$$\begin{aligned}
& \frac{2}{\varepsilon^2} \langle \partial_x^\alpha \mathbf{L}^\varepsilon(\mathbf{f}), \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\
& \leq \frac{2C_1^L e}{\varepsilon^3} \left\| \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2\delta_{\text{MS}} e C_1^L K'_{\text{dx}} C_\pi}{\varepsilon} \left\| \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \quad + \frac{2C_1^L}{\varepsilon e} \left( 1 + \delta_{\text{MS}} (K'_{\text{dx}} C_\pi + 2\tilde{K}_{\text{dx}} (1 + C_\pi)) \right) \left\| \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
& \quad + \frac{2\delta_{\text{MS}} e C_1^L \tilde{K}_{\text{dx}}}{\varepsilon} \sum_{|\alpha'| < |\alpha|} \left\| \partial_x^{\alpha'} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.7.1})
\end{aligned}$$

The transport term is more tricky in this case. Indeed, integrating by parts in  $x_k$  and then in  $v_k$ , we get the identity

$$\begin{aligned}
& -\frac{2}{\varepsilon} \langle \partial_x^\alpha (v \cdot \nabla_x \mathbf{f}), \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\
& = -\frac{1}{\varepsilon} \left\| \partial_x^\alpha \mathbf{f} \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 - \frac{1}{\varepsilon} \langle \partial_x^{\alpha - e_k} (v \cdot \nabla_x \mathbf{f}), v_k \partial_x^\alpha \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}, \quad (\text{C.7.2})
\end{aligned}$$

where the second term comes from the integration by parts when one derives the maxwellian weight  $\boldsymbol{\mu}^{-1}$  with respect to the variable  $v_k$ . Note that this term does not have an explicit sign and could therefore create a problem when trying to close the estimates. However, it is important to recall that we are not interested in the estimate of each single  $|\alpha| = s$  with  $\alpha_k > 0$ , but we only care about controlling the sum of all these terms. In particular, one can prove that when summing over  $|\alpha| \leq s$  and  $\alpha_k > 0$  with  $k = 1, 2, 3$ , we get

$$-\sum_{\substack{|\alpha|=s \\ k, \alpha_k > 0}} \langle \partial_x^{\alpha - e_k} (v \cdot \nabla_x \mathbf{f}), v_k \partial_x^\alpha \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} = -\sum_{|\alpha|=s-1} \left\| v \cdot \nabla_x (\partial_x^{\alpha'} \mathbf{f}) \right\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq 0,$$

so that the problematic term actually exhibits an explicit sign and we can get rid of it.

Finally, thanks to Young's inequality applied with the positive constant  $e/C_1^L$ , we can control the non-linear term as

$$\frac{2}{\varepsilon} \langle \partial_x^\alpha \mathbf{Q}(\mathbf{f}, \mathbf{f}), \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2e}{\varepsilon C_1^L} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 + \frac{2C_1^L}{\varepsilon e} \left\| \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2, \quad (\text{C.7.3})$$

while the source term is handled thanks to estimate (3.3.17), and writes

$$2 \langle \partial_x^\alpha \mathbf{S}^\varepsilon, \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \leq \frac{2\delta_{\text{MS}}^2 C_{\alpha,k}^S}{\varepsilon \eta_3} + \frac{2\eta_3}{\varepsilon} \left\| \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2. \quad (\text{C.7.4})$$

Gathering estimates (C.7.1)–(C.7.4), together with the use of the upper bound

$$\sum_{|\alpha'| < |\alpha|} \left\| \partial_x^{\alpha'} \mathbf{f} \right\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \leq \left\| \mathbf{f} \right\|_{H_{x,v}^{s-1}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2,$$

choosing  $\eta_3 = C_1^{\mathbf{L}}/e$  and recalling that  $\delta_{\text{MS}} \leq 1$ , we finally obtain

$$\begin{aligned}
 & \frac{d}{dt} \langle \partial_x^\alpha \mathbf{f}, \partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})} \\
 & \leq -\frac{1}{\varepsilon} \left( 1 - 2\delta_{\text{MS}} e C_1^{\mathbf{L}} K'_{\text{dx}} C_\pi \right) \|\partial_x^\alpha \mathbf{f}\|_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2C_1^{\mathbf{L}} e}{\varepsilon^3} \|\partial_x^\alpha \mathbf{f}^\perp\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
 & \quad + \frac{2C_1^{\mathbf{L}}}{\varepsilon e} \left( 3 + K'_{\text{dx}} C_\pi + 2\tilde{K}_{\text{dx}}(1 + C_\pi) \right) \|\partial_v^{e_k} \partial_x^{\alpha - e_k} \mathbf{f}\|_{L_{x,v}^2(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 \\
 & \quad + \frac{2\delta_{\text{MS}} e C_1^{\mathbf{L}} \tilde{K}_{\text{dx}}}{\varepsilon} \|\mathbf{f}\|_{H_{x,v}^{s-1}(\langle v \rangle^{\frac{\gamma}{2}} \boldsymbol{\mu}^{-\frac{1}{2}})}^2 + \frac{2e}{\varepsilon C_1^{\mathbf{L}}} \mathcal{G}_x^s(\mathbf{f}, \mathbf{f})^2 + \frac{2\delta_{\text{MS}}^2 e C_{\alpha,k}^{\mathbf{S}}}{\varepsilon C_1^{\mathbf{L}}} \\
 & \quad - \frac{1}{\varepsilon} \langle \partial_x^{\alpha - e_k} (v \cdot \nabla_x \mathbf{f}), v_k \partial_x^\alpha \mathbf{f} \rangle_{L_{x,v}^2(\boldsymbol{\mu}^{-\frac{1}{2}})}, \quad (\text{C.7.5})
 \end{aligned}$$

which is estimate (3.3.31) with the choices

$$\begin{aligned}
 C^{(10)} &= 3 + K'_{\text{dx}} C_\pi + 2\tilde{K}_{\text{dx}}(1 + C_\pi), & C^{(11)} &= 2C_1^{\mathbf{L}} K'_{\text{dx}} C_\pi, \\
 K_{\alpha,k} &= 2C_1^{\mathbf{L}} \tilde{K}_{\text{dx}}, & \tilde{C}_{\alpha,k}^{\mathbf{S}} &= \frac{2C_{\alpha,k}^{\mathbf{S}}}{C_1^{\mathbf{L}}}.
 \end{aligned}$$



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# Asymptotique diffusive de l'équation de Boltzmann pour les mélanges gazeux, étude mathématique et numérique

**Résumé.** Cette thèse est consacrée à plusieurs études reliant l'équation de Boltzmann pour les mélanges gazeux aux équations de Maxwell-Stefan décrivant la diffusion gazeuse. Notre analyse est construite sur une linéarisation de la solution de l'équation cinétique autour d'un état maxwellien local ayant des vitesses différentes pour chaque espèce du mélange, mais de l'ordre du paramètre d'échelle qui prescrit l'asymptotique diffusive. Dans une première partie, nous montrons que l'opérateur de Boltzmann linéarisé autour d'une telle maxwellienne, ne constituant pourtant pas un état d'équilibre pour le gaz, satisfait une propriété de quasi-stabilité de son trou spectral : le trou spectral obtenu en linéarisant l'opérateur de collision autour d'un état d'équilibre global est préservé à une correction du même ordre que le paramètre d'échelle. Ainsi, nous sommes ensuite en mesure de prouver que le système de Maxwell-Stefan peut être dérivé rigoureusement à partir de l'équation de Boltzmann multi-espèce. Cette dérivation est obtenue en montrant existence et unicité des solutions perturbatives des modèles cinétique et macroscopique, grâce en particulier à des estimations d'hypocoercivité. Dans une deuxième partie du manuscrit, par le biais de la méthode des moments, nous construisons un schéma numérique capable de décrire le comportement des solutions aux différentes échelles de l'asymptotique diffusive. Pour ce schéma, nous prouvons un résultat d'existence et de positivité des solutions, et un caractère préservant l'asymptotique est montré à travers plusieurs tests numériques.

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## Diffusive asymptotics of the Boltzmann multi-species equation for gaseous mixtures, mathematical and numerical study

**Abstract.** This thesis is devoted to several studies which aim at investigating the link between the Boltzmann equation for gaseous mixtures and the Maxwell-Stefan equations, modelling purely diffusive phenomena inside a gas. Our analysis is built on a linearization of the solution of the kinetic equation around a local Maxwellian state characterized by different bulk velocities for each species of the mixture, but having the same order of magnitude of the scaling parameter which prescribes the diffusive asymptotic. In a first part, we start by showing that the Boltzmann operator linearized around such a Maxwellian, which does not constitute an equilibrium for the gas, exhibits a quasi-stability property on its spectral gap : the spectral gap known to exist for the collision operator linearized a global equilibrium state is preserved up to a correction which is of the same order of the scaling parameter. Thanks to this feature and *via* the derivation of suitable hypocoercivity estimates, we are then able to prove that the Maxwell-Stefan system can be rigorously obtained from the Boltzmann multi-species equation, by showing that the solutions of the kinetic and macroscopic models exist uniquely in a perturbative sense. In a second part of the manuscript, using the moment method, we design a numerical scheme which captures the correct behaviour of the solutions at different scales of the diffusive asymptotic. We prove that our scheme possesses at least one solution with positive concentrations, and we show numerically that it is asymptotic preserving in the vanishing limit of the scaling parameter.