DIFFUSION ASYMPTOTICS OF A KINETIC MODEL FOR GASEOUS MIXTURES

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ABSTRACT. In this work, we consider the non-reactive fully elastic Boltzmann equations for mixtures in the diffusive scaling. We mainly use a Hilbert expansion of the distribution functions. After briefly recalling the H-theorem, the lower-order non trivial equality obtained from the Boltzmann equations leads to a linear functional equation in the velocity variable. This equation is solved thanks to the Fredholm alternative. Since we consider multicomponent mixtures, the classical techniques introduced by Grad cannot be applied, and we propose a new method to treat the terms involving particles with different masses.

1. INTRODUCTION

The study of the asymptotic behaviour of the Boltzmann equation for small mean free path is known as *Hilbert's sixth problem*, after its formulation by Hilbert himself during the International Congress of Mathematicians held in Paris in 1900 [20]. Since then, it has been a very active field of research, and many results have been obtained, both at a formal level and in the context of rigorous limits.

The main tools are based on asymptotic (Hilbert, Chapman-Enskog) expansions with respect to the mean free path, see for instance [10]. The translation in a rigorous mathematical language has been performed in a series of pioneering papers by Bardos, Golse and Levermore [1, 2, 3], where the authors established the ground of the subsequent results concerning the rigorous asymptotic limits. They stated a program that led to many interesting results, such as [23]. This trail culminated in [15], where Golse and Saint-Raymond established a Navier-Stokes limit for the Boltzmann equation considered over the infinite spatial domain $\mathbb{R}^3$: appropriately scaled families of DiPerna-Lions renormalized solutions are shown to have fluctuations whose limit points are governed by Leray solutions of the limiting Navier-Stokes equations. We can also refer to [16], which extends the results of [15] for hard cutoff potentials in Grad's sense.

Apart from the research concerning with the classical Boltzmann equation (see [11] as a review article), which can be seen as a model describing a mono-species, monoatomic and ideal gas, one can focus on the study, at a kinetic level, of gaseous mixtures, without excluding the possibility of chemical reactions. In such a framework, the models are much more intricate. It is indeed necessary to treat systems of Boltzmann-like equations, rather than one single equation, with multi-species kernels and cross interactions between the different distribution functions describing each component of the mixture [28, 19, 25]. The complexity of the models grows dramatically if exchanges of internal energy and chemical reactions are allowed [26, 28, 8, 27].

The derivation of macroscopic equations from kinetic models remains crucial for mixtures, both at a mathematical level and for deducing relevant macroscopic equations based on the modelling of microscopic binary interactions. In this spirit, in [12], the authors propose a model describing a reacting mixture of polyatomic gases and recover in the limit, via the appropriate scaling $(t, x) \to (t/\varepsilon, x/\varepsilon)$ for $\varepsilon > 0$, the reactive Euler equations.

The diffusive scaling we investigate here, i.e. $(t, x) \to (t/\varepsilon^2, x/\varepsilon)$, is more complicated, and even the formal structure of the asymptotic hierarchy is not trivial at all. After the first attempts of Chapman and Cowling [10], in [4], the authors consider a binary mixture of red and blue particles which interact via strong short range (hard core) and weak long range pair potentials, and study the small free path limit

in various situations. Ref. [13] handles the same kind of model of binary mixture with a heavy species and a lighter one.

In this paper, we consider a mixture of several different non reactive gases, which evolves in time via the classical Boltzmann system for non-reacting multicomponent mixtures, and study the formal Hilbert expansion leading to the Navier-Stokes system for mixtures. Even if this strategy dates back to Grad [17, 18], who studied the formal small free path limit for the monatomic and monospecies Boltzmann equation, the development leading to write the Chapman-Enskog hierarchy owns some particular properties, which are inherited from the multispecies feature of the mixture.

First of all, we can observe that the structure of the small free-path asymptotics for mixtures, composed by three or more species, differs from the case of a mono-species gas or a binary mixture. The most apparent feature which is peculiar to a (at least) ternary mixture is the phenomenon of uphill diffusion, independently foreseen by Maxwell [24] and Stefan [29], and experimentally recovered by Duncan and Toor [14]. This kind of diffusion is described by second-order coupled terms, which make the asymptotics quite different from the limit related to a binary mixture [7].

A second important aspect is that we cannot apply Grad's methodology when we have to deal with different species, with different masses and different cross sections. We hence propose a new approach to the problem which only works when the binary collisions involve particles with different masses, and we then use Grad's procedure [18] when considering collisions between same mass particles. Note that both approaches are needed to give a complete answer to the question of resolvability of the first-order (in ε) equations of the hierarchy, obtained by means of the Fredholm alternative. We point out that our approach holds for generic cut-off cross sections, as those described in Section 2.

Note that this type of asymptotics is also numerically investigated, see, for instance, [5, 21], using BGK approaches.

The article is structured as follows. In the next section, we describe the model, its basic properties and the main results which are proved in the rest of the paper. Then Sections 3 and 4 are devoted to the proof of the mathematical results stated in Section 2. More precisely, Fredholm's alternative is applied in Section 3 (provided the compactness of some operator is known), and the proof of the compactness is treated in Section 4. As we already mentioned, the case of particles of same masses is treated following Grad's method [18] (see Section 4.1), whereas the case of different masses needs a new approach (see Section 4.2, in particular Lemma 3).

2. MODEL

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

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

We assume that the mixture only involves molecular elastic collisions. Let us consider two colliding molecules of species $\mathcal{A}_i$ and $\mathcal{A}_j$, $1 \leq i, j \leq I$. Their masses are m_i and m_j, and their pre-collisional velocities v' and v'_*. After a collision, the particles belong to the same species (no chemical reactions), so their masses remain as they were, and their velocities become v and v_*. Since the collisions are elastic, both momentum and kinetic energy are conserved, i.e.

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

Consequently, v' and v'_* can be written in terms of v and v_*:

$$(2) \qquad v' = \frac{m_i v + m_j v_*}{m_i + m_j} + \frac{m_j}{m_i + m_j} T_\omega(v - v_*), \qquad v'_* = \frac{m_i v + m_j v_*}{m_i + m_j} - \frac{m_i}{m_i + m_j} T_\omega(v - v_*),$$

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

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

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

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

where v' and v'_* are defined by (2), and f and g are two functions of the velocity variable. The cross-section $\check{\mathcal{B}}_{ij}(v, v_*, \omega)$ only depends on v, v_* and ω. In fact, $\check{\mathcal{B}}_{ij}$ is only a function of $|v - v_*|$ and the angle θ between ω and $V := v - v_*$, by Galilean invariance. Let us set

$$\mathcal{B}_{ij}(\omega, v - v_*) = \check{\mathcal{B}}_{ij}(v, v_*, \omega), \quad \forall \omega \in S^2, \quad \forall v, v_* \in \mathbb{R}^3.$$

The collisions are also supposed microreversible. That ensures that

$$(4) \qquad \mathcal{B}_{ij}(\omega, v - v_*) = \mathcal{B}_{ji}(\omega, v - v_*), \quad \mathcal{B}_{ij}(\omega, v - v_*) = \mathcal{B}_{ij}(\omega, v' - v'_*), \quad \forall \omega \in S^2, \, \forall v, v_* \in \mathbb{R}^3.$$

Moreover, we assume that $\mathcal{B}_{ij}$ satisfies a general condition

$$(5) \qquad \mathcal{B}_{ij}(\omega, V) \leq a \, |\sin\theta| \, |\cos\theta| \left(|V| + \frac{1}{|V|^{1-\delta}} \right), \quad \forall \omega \in S^2, \, \forall V \in \mathbb{R}^3,$$

where $a > 0$, $0 < \delta < 1$. As emphasized in [18], this corresponds to intermolecular potentials with finite range and it means that $\mathcal{B}_{ij}$ linearly approaches 0 near $\theta = 0$ and $\theta = \pi/2$, and is of restricted growth for both small and large $|V|$.

Condition (5) is, for instance, satisfied by hard spheres of diameter $\sigma_{ij} > 0$:

$$\mathcal{B}_{ij}(\omega, V) = \sigma_{ij}^2 \, |V| \, \sin\theta \, \cos\theta$$

and, by all cutoff power-law potentials:

$$\mathcal{B}_{ij}(\omega, V) = |V|^{\gamma_{ij}} \beta_{ij}(\theta), \quad \gamma_{ij} = \frac{s_{ij} - 5}{s_{ij} - 1},$$

where $\beta_{ij}(\theta)$ is a bounded function and linearly approaches 0 when θ tends to $\pi/2$, and $s_{ij} > 3$.

The collision operators can be also written under weak forms, obtained from (3) using the changes of variables $(v, v_*) \mapsto (v_*, v)$ and $(v, v_*) \mapsto (v', v'_*)$ for a fixed $\omega \in S^2$. Weak forms in the cases $i = j$ and $i \neq j$ are intrinsically different, and are explained in detail in [12, 7]. Mention that, if we choose suitable test-functions, the weak forms of (3) allow to formally write, for any i and j, and any functions f and g for which the following equations make sense:

$$(6) \qquad \int_{\mathbb{R}^3} Q_{ij}(f, g)(v) \, dv = 0,$$

$$(7) \qquad \int_{\mathbb{R}^3} Q_{ij}(f, g)(v) \begin{pmatrix} m_i \, v \\ m_i \, v^2/2 \end{pmatrix} dv + \int_{\mathbb{R}^3} Q_{ji}(g, f)(v) \begin{pmatrix} m_j \, v \\ m_j \, v^2/2 \end{pmatrix} dv = 0.$$

2.2. **H-theorem.** Let us now write down the H-theorem corresponding to the collisional operators we defined in the previous subsection, and discuss the mechanical equilibrium. The main tool is the *entropy production functional*, whose explicit form is given by

$$D(f_1, \ldots, f_I) := \sum_{i=1}^{I} \sum_{j=1}^{I} \int_{\mathbb{R}^3} Q_{ij}(f_i, f_j)(v) \log\left(\frac{f_i(v)}{m_i^3}\right) dv.$$

It is well defined when all f_i are non-negative and satisfy some suitable assumptions of regularity and decay to infinity, which we will not discuss here since our purpose consists in finding formal results.

The following properties hold [7] (see also [12]).

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

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

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

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

    i. *For any $1 \leq i, j \leq I$ and $v \in \mathbb{R}^3$*

(8)
$$Q_{ij}(f_i, f_j)(v) = 0.$$

    ii. *The entropy production vanishes, that is*

$$D(f_1, \ldots, f_I) = \sum_{i=1}^{I} \sum_{j=1}^{I} \int_{\mathbb{R}^3} Q_{ij}(f_i, f_j)(v) \, \log \left(\frac{f_i(v)}{m_i^3} \right) \, \mathrm{d}v = 0.$$

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

(9)
$$f_i(v) = n_i \left(\frac{m_i}{2 \, \pi \, k \, T} \right)^{3/2} e^{-\frac{m_i}{2kT}|v-u|^2}.$$

2.3. **Statement of the problem.** In this work, we focus on the diffusion limit of the Boltzmann equations for mixtures. That limit is obtained from the framework of the classical diffusive scaling, where the scaling parameter is the mean free path. Let us choose $\varepsilon > 0$ as the mean free path. Hence, for any i, each distribution function f_i^ε must solve the following scaled Boltzmann equation, that is

(10)
$$\varepsilon \, \partial_t f_i^\varepsilon + v \cdot \nabla_x f_i^\varepsilon = \frac{1}{\varepsilon} \sum_{j=1}^{I} Q_{ij}(f_i^\varepsilon, f_j^\varepsilon), \quad t > 0, \, x \in \mathbb{R}^3, \, v \in \mathbb{R}^3.$$

We look for f_i^ε as a formal power series in ε, replace f_i^ε in (10) and identify the same order terms. We only focus on the first two orders. Thanks to Proposition 1, the order -1 of (10) allows to find the zero-th order term of the series: Maxwell functions (9). Therefore, each distribution function f_i^ε, $1 \leq i \leq I$, can be seen as a perturbation of the equilibrium (9). Without any loss of generality, we set $u = 0$ (diffusion limit) and $kT = 1$. Thus we can write f_i^ε as

(11)
$$f_i^\varepsilon(t, x, v) = M_i(v) \, n_i(t, x) + \varepsilon \, M_i(v)^{1/2} \, g_i(t, x, v) + ..., \quad \forall t \geq 0, \, \forall x, v \in \mathbb{R}^3,$$

where $M_i(v)$ is the normalized, centred Maxwell function

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

In (11), we choose to put $M_i(v)^{1/2}$ within the first-order term of f_i^ε. As a matter of fact, it allows us to work in a plain L^2 framework in the variable v for g_i.

We then focus on the zero-th order in ε coming from (10). Taking (8) into account, we obtain the following equation, holding for any $1 \leq i \leq I$,

(12)
$$M_i^{-1/2} \sum_{j=1}^{I} \left(n_i \, Q_{ij}(M_i, M_j^{1/2} g_j) + n_j \, Q_{ij}(M_i^{1/2} g_i, M_j) \right) = M_i^{1/2} \, (v \cdot \nabla_x n_i).$$

In this work, we investigate the existence of $g = (g_1, \ldots, g_I)$ with respect to a given $(n_1, \ldots, n_I)$ satisfying (12). Note that the dependence of (12) on t and x is not crucial, in the sense that t, x, (n_i) and $(\nabla_x n_i)$ can be seen as parameters.

The role of the first-order in ε coming from (10) is briefly discussed at the end of this article, in Section 5.

For any function $g \in L^2(\mathbb{R}^3)^I$ of v, we shall write the L^2 norm of g:

$$\|g\|_{L^2}^2 = \sum_{j=1}^{I} \|g_j\|_{L^2}^2 = \sum_{j=1}^{I} \int_{\mathbb{R}^3} g_j(t,x,v)^2 \, \mathrm{d}v.$$

We can write the left-hand side of (12) in a more suitable form if we introduce the operator $\mathcal{K}$, where the i-th component of $\mathcal{K}g$ is given by

$$(13) \quad [\mathcal{K}g]_i(v) = \sum_{j=1}^{I} \left(\frac{m_j}{2\pi}\right)^{3/4} \iint_{\mathbb{R}^3 \times S^2} \mathcal{B}_{ij}(\omega, v - v_*) \, e^{-\frac{1}{4}m_i v^2} \, e^{-\frac{1}{2}m_j v_*^2}$$
$$\left[n_i \left(\frac{m_i}{2\pi}\right)^{3/4} \left(e^{\frac{1}{4}m_j v_*'^2} g_j(v_*') - e^{\frac{1}{4}m_j v_*^2} g_j(v_*) \right) + n_j \left(\frac{m_j}{2\pi}\right)^{3/4} e^{\frac{1}{4}m_i v'^2} g_i(v') \right] \mathrm{d}\omega \, \mathrm{d}v_*,$$

for any i, and the positive function $\nu = \nu(v)$, whose i-th component is

$$(14) \qquad \nu_i(v) = \sum_{j=1}^{I} n_j \left(\frac{m_j}{2\pi}\right)^{3/2} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{2}m_j v_*^2} \mathcal{B}_{ij}(\omega, v - v_*) \, \mathrm{d}\omega \, \mathrm{d}v_*.$$

Consequently, (12) can be written as a functional equation in the variable v:

$$(15) \qquad (\mathcal{K} - \nu \, \mathrm{Id}) \, g = \left(M_i^{1/2} \left(v \cdot \nabla_x n_i \right) \right)_{1 \leq i \leq I}.$$

Let us now state the main result of this work.

Theorem 1. *Suppose that the cross sections* $(\mathcal{B}_{ij})_{1 \leq i,j \leq I}$ *are positive functions satisfying* (5). *If we assume that*

$$(16) \qquad \sum_{i=1}^{I} n_i(t,x) \text{ does not depend on } x,$$

then, for any t, x, *there exists* $g(t,x,\cdot) \in L^2(\mathbb{R}_v^3)^I$ *satisfying* (15), *where* $\mathcal{K}$ *and* ν *are given by* (13)–(14).

Condition (16) means that we consider a situation where the total number density of gaseous particles is uniform in space, see Section 5 for further discussions. Let us briefly draw the sketch of the proof of this theorem. We shall first need the following proposition.

Proposition 2. *The operator* $\mathcal{K}$, *defined by* (13), *is compact from* $L^2(\mathbb{R}_v^3)^I$ *to* $L^2(\mathbb{R}_v^3)^I$.

The proof of Proposition 2 is given in Section 4. Let us emphasize again that, in Proposition 2, t, x and (n_i) are considered as parameters and the compactness is only related to the variable v. Since $\mathcal{K}$ is compact, we can apply the Fredholm alternative to the operator $\mathcal{K} - \nu \, \mathrm{Id}$. This is explained in the next section.

3. Proof of Theorem 1

This section is devoted to the proof of the main result of our article. We here assume that the compactness of the operator $\mathcal{K}$ is known. Let us denote $\mathcal{L} = \mathcal{K} - \nu \, \mathrm{Id}$, and study the null space of $\mathcal{L}$, as required by the Fredholm alternative.

Step 1 − Study of ker $\mathcal{L}$. Writing down the i-th component of $\mathcal{L}g$ and performing the change of variable $(v, v_*) \mapsto (v', v'_*)$ while ω remains fixed, we obtain

$$[\mathcal{L}g]_i(v) = \sum_{j=1}^{I} \iint_{\mathbb{R}^3 \times S^2} M_i(v)^{1/2} M_j(v_*) \Big[n_j M_i(v')^{-1/2} g_i(v') + n_i M_j(v'_*)^{-1/2} g_j(v'_*)$$
$$- n_j M_i(v)^{-1/2} g_i(v) - n_i M_j(v_*)^{-1/2} g_j(v_*) \Big] \mathcal{B}_{ij}(\omega, v - v_*) \, \mathrm{d}\omega \, \mathrm{d}v_*.$$

Thanks to the H-theorem, $g \in \ker \mathcal{L}$ if and only if there exist $\alpha \in \mathbb{R}^I$, $\beta \in \mathbb{R}^3$, $\gamma \in \mathbb{R}$ such that, for any i,

$$g_i(t, x, v) = n_i(t, x) \, M_i(v)^{1/2} \left(\alpha_i + m_i \beta \cdot v + \gamma \frac{m_i}{2} v^2 \right), \quad \forall \, t > 0, \, x, \, v \in \mathbb{R}^3.$$

Consequently, $\ker \mathcal{L} \neq \{0\}$, and the Fredholm alternative allows to state that (15) has a solution if and only if

$$(17) \qquad \left(M_i^{1/2} (v \cdot \nabla_x n_i) \right)_{i=1,\ldots,I} \in (\ker \mathcal{L}^*)^\perp, \quad \forall \, t > 0, \, x \in \mathbb{R}^3.$$

Step 2 − Computation of $\mathcal{L}^*$. Let us compute the adjoint operator $\mathcal{L}^*$ by studying the inner product between $\mathcal{L}g$ and a vector $h \in L^2(\mathbb{R}_v^3)^I$. We successively write, using the change of variables $(v, v_*) \mapsto (v', v'_*)$ and $(v, v_*) \mapsto (v_*, v)$

$$\sum_{i=1}^{I} \int_{\mathbb{R}^3} [\mathcal{L}g]_i(v) \, h_i(v) \mathrm{d}v$$
$$= \sum_{i,j=1}^{I} \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times S^2} h_i(v) \, M_i(v)^{-1/2} \Big[n_i \, M_i(v') M_j^{1/2}(v'_*) g_j(v'_*) - n_i M_i(v) M_j(v_*)^{1/2} g_j(v_*)$$
$$+ n_j M_j(v'_*) M_i(v')^{1/2} g_i(v') - n_j M_j(v_*) M_i(v)^{1/2} g_i(v) \Big] \mathcal{B}_{ij}(\omega, v - v_*) \, \mathrm{d}\omega \, \mathrm{d}v_* \mathrm{d}v$$
$$= \sum_{i,j=1}^{I} \iiint_{\mathbb{R}^3 \times \mathbb{R}^3 \times S^2} g_i(v) \, n_j \, M_i(v)^{-1/2} \Big[M_i(v') M_j^{1/2}(v'_*) h_j(v'_*) - M_i(v) M_j(v_*)^{1/2} h_j(v_*)$$
$$+ M_j(v'_*) M_i(v')^{1/2} h_i(v') - M_j(v_*) M_i(v)^{1/2} h_i(v) \Big] \mathcal{B}_{ij}(\omega, v - v_*) \, \mathrm{d}\omega \, \mathrm{d}v_* \mathrm{d}v.$$

Consequently, we have

$$[\mathcal{L}^* h]_i = M_i^{-1/2} \sum_{j=1}^{I} n_j \left(Q_{ij}(M_i, M_j^{1/2} h_j) + Q_{ij}(M_i^{1/2} h_i, M_j) \right).$$

Thanks to the H-theorem, $h \in \ker \mathcal{L}^*$ if and only if there exist $a \in \mathbb{R}^I$, $b \in \mathbb{R}^3$, $c \in \mathbb{R}$ such that, for any i,

$$(18) \qquad h_i(v) = M_i(v)^{1/2} \left(a_i + m_i \, b \cdot v + c \frac{m_i}{2} v^2 \right), \quad \forall \, v \in \mathbb{R}^3.$$

Step 3 − Conclusion. Now, taking (18) into account, condition (17) can be rewritten as

$$\sum_{i=1}^{I} \sum_{k=1}^{3} \frac{\partial n_i}{\partial x_k} \int_{\mathbb{R}^3} \begin{pmatrix} v_k \\ m_i v_k \, v_j \\ m_i v_k \, v^2/2 \end{pmatrix} M_i(v) \, \mathrm{d}v = 0, \quad 1 \le j \le 3.$$

Using parity arguments, the first and third integrals are immediately satisfied, as well as the second ones if $k \neq j$. In the case when $k = j$, the condition $\nabla_x \sum n_i = 0$, which is assumed in (16), allows to complete the proof.

4. Proof of Proposition 2

We still have to prove that $\mathcal{K}$ is compact. In this section, $(n_i)_{1 \le i \le I}$ are assumed to be nonnegative constants. Let $g \in L^2(\mathbb{R}^3)^I$. Note that we do not need g to be the function defined in (11). First, we write $\mathcal{K}$ as the sum of four operators $\mathcal{K}_1,..., \mathcal{K}_4$. For any i, the i-th component of each $\mathcal{K}_\ell g$, $1 \le \ell \le 4$, is given by

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

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

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

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

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

We denoted, for any i,

$$\mathcal{M}_i := \{1 \le j \le I \mid m_j = m_i\},$$

which is non empty since $i \in \mathcal{M}_i$. It is crucial to dissociate the cases when $m_i \ne m_j$ or $m_i = m_j$, because the proofs are quite different.

We successively prove that $\mathcal{K}_\ell$, $1 \le \ell \le 4$, is compact. To this end, we shall use the following property. An operator $\mathcal{J}$ is compact if it satisfies

- a uniform decay at infinity

(19)
$$\|\mathcal{J}g\|_{L^2(B(0,R)^c)} \le \sigma(R) \|g\|_{L^2(\mathbb{R}^3)}, \qquad \forall R > 0,$$

where $B(0, R)$ denotes the open ball of $\mathbb{R}_v^3$ centred at 0 and of radius R, and $\sigma(R)$ goes to 0 when R goes to $+\infty$;
- an equicontinuity property, i.e., for any $\varepsilon > 0$, there exists $\varrho > 0$ such that, for all $w \in B(0, \varrho)$,

(20)
$$\|(\tau_w - I)\mathcal{J}g\|_{L^2(\mathbb{R}^3)} \le \varepsilon \|g\|_{L^2(\mathbb{R}^3)},$$

where τ_w denotes the translation operator, i.e.

$$\tau_w \mathcal{J}g(v) = \mathcal{J}g(v + w), \qquad \forall v, w \in \mathbb{R}^3.$$

4.1. **Compactness of $\mathcal{K}_1$.** Let us denote, for any i, j,

$$k_1^{ij}(v, v_*) = \int_{S^2} e^{-\frac{1}{4}m_i v^2} e^{-\frac{1}{4}m_j v_*^2} \mathcal{B}_{ij}(\omega, v - v_*) \, d\omega, \quad \forall v, v_* \in \mathbb{R}^3.$$

We immediately have, for any i,

$$[\mathcal{K}_1 g]_i(v) = -n_i \sum_{j=1}^{I} \left(\frac{m_i m_j}{4\pi^2}\right)^{3/4} \int_{\mathbb{R}^3} g_j(v_*) k_1^{ij}(v, v_*) \, dv_*, \quad \forall v \in \mathbb{R}^3.$$

4.1.1. *Properties of k_1^{ij}.* First of all, note that $k_1^{ij}(v, v_*) = k_1^{ji}(v_*, v)$, for any i, j and v, v_*, thanks to (4).

In order to prove the uniform decay to infinity and the equicontinuity for $\mathcal{K}_1$ (i.e. the inequalities (19) and (20)), we need to establish some preliminary properties of k_1^{ij}.

Lemma 1. *There exists $C > 0$ such that, for any i, j,*

$$(21) \qquad \int_{\mathbb{R}^3} k_1^{ij}(v, v_*) \mathrm{d}v_* \leq C\, e^{-\frac{1}{4} m_i v^2} \left(1 + |v|\right), \quad \forall v \in \mathbb{R}^3.$$

Proof. Thanks to (5) and using the change of variables $v_* \mapsto V_* = v_* - v$, we can write

$$\int_{\mathbb{R}^3} k_1^{ij}(v, v_*) \mathrm{d}v_* \leq C \int_{\mathbb{R}^3} e^{-\frac{1}{4} m_i v^2}\, e^{-\frac{1}{4} m_j (V_* + v)^2} \left(|V_*| + |V_*|^{\delta-1} \right) \mathrm{d}V_*$$

$$\leq C\, e^{-\frac{1}{4} m_i v^2} \left[\int_{|V_*| \leq 1} \left(|V_*| + |V_*|^{\delta-1} \right) \mathrm{d}V_* + \int_{|V_*| \geq 1} \left(1 + |V_*|\right) e^{-\frac{1}{4} m_j (V_* + v)^2} \mathrm{d}V_* \right].$$

This inequality allows us to get (21). $\qquad \square$

Lemma 2. *For any i, j, k_1^{ij} belongs to $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$.*

Proof. The proof follows the same strategy as the previous one, using (5) and the same change of variables. We can write

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} k_1^{ij}(v, v_*)^2 \mathrm{d}v_*\, \mathrm{d}v \leq C \iint_{\mathbb{R}^3 \times \mathbb{R}^3} e^{-\frac{1}{2} m_i v^2}\, e^{-\frac{1}{2} m_j v_*^2} \left(|v - v_*|^2 + |v - v_*|^{2\delta-2} \right) \mathrm{d}v_*$$

$$\leq C \int_{\mathbb{R}^3} e^{-\frac{1}{2} m_i v^2} \left(1 + v^2\right) \mathrm{d}v,$$

which is clearly finite. $\qquad \square$

4.1.2. *Uniform decay.* The L^2 norm of $\mathcal{K}_1 g$ decreases at infinity. More precisely, the following proposition holds.

Proposition 3. *Let $g \in L^2(\mathbb{R}^3)^I$. For any $R > 0$ and any i, we have*

$$(22) \qquad \| \left[\mathcal{K}_1 g \right]_i \|_{L^2(B(0,R)^c)} \leq \frac{C\, n_i}{R} \|g\|_{L^2(\mathbb{R}^3)},$$

where $C > 0$ is a constant.

Proof. Let $1 \leq i \leq I$ and write

$$\int_{\mathbb{R}^3} v^2 \left[\mathcal{K}_1 g \right]_i (v)^2 \mathrm{d}v \leq C n_i^2 \sum_{j=1}^{I} \int_{\mathbb{R}^3} v^2 \left[\int_{\mathbb{R}^3} k_1^{ij}(v, v_*)\, g_j(v_*)\, \mathrm{d}v_* \right]^2 \mathrm{d}v.$$

Thanks to the Cauchy-Schwarz inequality, the previous inequality becomes

$$\int_{\mathbb{R}^3} v^2 \left[\mathcal{K}_1 g \right]_i (v)^2 \mathrm{d}v \leq C n_i^2 \sum_{j=1}^{I} \int_{\mathbb{R}^3} v^2 \left[\int_{v_* \in \mathbb{R}^3} g_j(v_*)^2\, k_1^{ij}(v, v_*) \mathrm{d}v_* \right] \left[\int_{\mathbb{R}^3} k_1^{ij}(v, v_*) \mathrm{d}v_* \right] \mathrm{d}v.$$

Using Lemma 1 and Fubini's theorem, we get

$$\int_{\mathbb{R}^3} v^2 \left[\mathcal{K}_1 g \right]_i (v)^2 \mathrm{d}v \leq C n_i^2 \sum_{j=1}^{I} \int_{\mathbb{R}^3} g_j(v_*)^2 \left[\int_{\mathbb{R}^3} k_1^{ij}(v, v_*) \phi_i(v) \mathrm{d}v \right] \mathrm{d}v_*,$$

where $\phi_i(v) = v^2 \left(1 + |v|\right) e^{-\frac{1}{4} m_i v^2}$ is clearly bounded. Consequently, since $k_1^{ij}(v, v_*) = k_1^{ji}(v_*, v)$, we have

$$\int_{\mathbb{R}^3} v^2 \left[\mathcal{K}_1 g \right]_i (v)^2 \mathrm{d}v \leq C n_i^2 \sum_{j=1}^{I} \int_{\mathbb{R}^3} g_j(v_*)^2 \left(\int_{\mathbb{R}^3} k_1^{ji}(v_*, v) \mathrm{d}v \right) \mathrm{d}v_*.$$

Eventually, using Lemma 1 again, we obtain

$$\int_{\mathbb{R}^3} v^2 \left[\mathcal{K}_1 g\right]_i (v)^2 \mathrm{d}v \leq C n_i^2 \|g\|_{L^2}^2.$$

Besides, we can deduce, for any $R > 0$,

$$\int_{\mathbb{R}^3} v^2 \left[\mathcal{K}_1 g\right]_i (v)^2 \mathrm{d}v \geq \int_{|v| \geq R} v^2 \left[\mathcal{K}_1 g\right]_i (v)^2 \mathrm{d}v \geq R^2 \int_{|v| \geq R} \left[\mathcal{K}_1 g\right]_i (v)^2 \mathrm{d}v.$$

It is then easy to recover (22). $\qquad\square$

4.1.3. *Equicontinuity.* The following property of equicontinuity of $\mathcal{K}_1$ holds.

Proposition 4. *For any $w \in \mathbb{R}^3$, set*

$$\varrho_1(w) = C \max_{i,j} \left[n_i \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \left(k_1^{ij}(v + w, v_*) - k_1^{ij}(v, v_*) \right)^2 \mathrm{d}v_* \mathrm{d}v \right]^{1/2},$$

where C is a suitable nonnegative constant. Then, for any i, we have

(23) $$\left\| \left[(\tau_w - \mathrm{Id})\mathcal{K}_1 g\right]_i \right\|_{L^2(\mathbb{R}_v^3)} \leq \varrho_1(w) \|g\|_{L^2(\mathbb{R}_v^3)}, \quad \forall w \in \mathbb{R}^3,$$

and $\varrho_1(w)$ tends to 0 when w tends to 0.

Proof. First, thanks to Lemma 2, it is clear that ϱ_1 is a continuous function of w, and goes to 0 when w goes to zero. Let us now focus on (23). For any i, using the Cauchy-Schwarz inequality, we have

$$\left\| \left[(\tau_w - \mathrm{Id})\mathcal{K}_1 g\right]_i \right\|_{L^2(\mathbb{R}^3)}^2 \leq C n_i^2 \sum_{j=1}^{I} \|g_j\|_{L^2}^2 \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \left(k_1^{ij}(v + w, v_*) - k_1^{ij}(v, v_*) \right)^2 \mathrm{d}v_* \mathrm{d}v.$$

Estimate (23) is an immediate consequence of the previous inequality. $\qquad\square$

4.2. **Compactness of $\mathcal{K}_2$.** As in section 4.1, we first write $\mathcal{K}_2$ in a more convenient form. Indeed, thanks to (1), we have

$$-\frac{1}{4}m_i v^2 - \frac{1}{2}m_j v_*^2 + \frac{1}{4}m_j v_*'^2 = -\frac{1}{4}m_j v_*^2 - \frac{1}{4}m_i v'^2.$$

Hence, $[\mathcal{K}_2]_i$ becomes

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

The next step consists in writing (24) in a form that allows to apply the same strategy used for $\mathcal{K}_1$.

In order to get this particular form, we need the following lemma.

Lemma 3. *There exists $b > 0$ such that, for any i, j satisfying $m_i \neq m_j$,*

(25) $$m_i v'^2 + m_j v_*^2 \geq b \left(m_i v^2 + m_j v_*'^2 \right)$$

for any $v, v_* \in \mathbb{R}^3$ and v', v_*' given by (2).

Remark. The assumption on the masses is here crucial, as we shall see in the proof. Indeed, (25) somehow gives a property of norm equivalence in $\mathbb{R}^3 \times \mathbb{R}^3$, linking (v, v_*') and (v', v_*). Such a property does not hold when we deal with molecules of the same mass.

Proof. Choose $j \notin \mathcal{M}_i$. Equation (2) can be rewritten as

$$(26) \qquad v' = \left(I_3 - 2 \frac{m_j}{m_i + m_j} \omega\, \omega^T \right) v + 2 \frac{m_j}{m_i + m_j} \omega\, \omega^T v_*,$$

$$(27) \qquad v'_* = \left(I_3 - 2 \frac{m_i}{m_i + m_j} \omega\, \omega^T \right) v_* + 2 \frac{m_i}{m_i + m_j} \omega\, \omega^T v,$$

where I_3 is the identity matrix of $\mathbb{R}^3$. Then, from (27), we get

$$\left(I_3 - 2 \frac{m_i}{m_i + m_j} \omega\, \omega^T \right) v_* = v'_* - 2 \frac{m_i}{m_i + m_j} \omega\, \omega^T v.$$

Let us now set

$$A = I_3 - 2 \frac{m_i}{m_i + m_j} \omega\, \omega^T.$$

This matrix A is invertible, since $\det A = (m_j - m_i)/(m_i + m_j)$ and $j \notin \mathcal{M}_i$. Consequently, we can write

$$(28) \qquad v_* = \left(I_3 - A^{-1} \right) v + A^{-1} v'_*,$$

where we used the equality

$$-2 \frac{m_i}{m_i + m_j} A^{-1} \omega\, \omega^T = I_3 - A^{-1}.$$

Then we put (28) in (26) to obtain

$$v' = \left(\frac{m_i + m_j}{m_i} I_3 - \frac{m_j}{m_i} A^{-1} \right) v - \frac{m_j}{m_i} \left(I_3 - A^{-1} \right) v'_*.$$

Consider now the following block matrix

$$\mathbb{A} = \begin{bmatrix} \frac{m_i+m_j}{m_i} I_3 - \frac{m_j}{m_i} A^{-1} & -\sqrt{\frac{m_j}{m_i}} \left(I_3 - A^{-1} \right) \\ \sqrt{\frac{m_j}{m_i}} \left(I_3 - A^{-1} \right) & A^{-1} \end{bmatrix},$$

which is invertible: $\det \mathbb{A} = -1$ and $\mathbb{A}^{-1} = \mathbb{A}$. The following vector equality holds:

$$\begin{bmatrix} \sqrt{m_i}\, v' \\ \sqrt{m_j}\, v_* \end{bmatrix} = \mathbb{A} \begin{bmatrix} \sqrt{m_i}\, v \\ \sqrt{m_j}\, v'_* \end{bmatrix}.$$

In fact, (25) is obtained by finding a lower bound of

$$\frac{\left| \mathbb{A} \begin{bmatrix} \sqrt{m_i}\, v & \sqrt{m_j}\, v'_* \end{bmatrix}^T \right|^2}{\left| \begin{bmatrix} \sqrt{m_i}\, v & \sqrt{m_j}\, v'_* \end{bmatrix}^T \right|^2},$$

which is $\|\mathbb{A}^{-1}\|_2^{-2} = \|\mathbb{A}\|_2^{-2}$. Since $\mathbb{A}$ is clearly a continuous function of ω, we may conclude that the matrix norm $\|\mathbb{A}\|_2$ is a positive continuous function of ω on S^2, which is compact. Therefore, it reaches its minimum, which of course remains positive. Choosing

$$b = \min_{\omega \in S^2} \|\mathbb{A}\|_2^{-2} > 0$$

leads to the required estimate (25). $\qquad \square$

Using (5) and Lemma 3, we obtain the upper bound

$$[\mathcal{K}_2 g]_i (v) \le C\, n_i \sum_{j \notin \mathcal{M}_i} e^{-\frac{1}{4} m_j v^2} \int_{\mathbb{R}^3} e^{-\frac{1}{4} m_i v'^2_*}\, g_j(v'_*) \left(|v - v_*| + |v - v_*|^{\delta-1} \right) \mathrm{d}v_*.$$

Let us then perform the change of variable $v_* \mapsto v'_*$, whose Jacobian is $1/\det A$. Since

$$v - v_* = A^{-1} \left(v - v'_* \right) \quad \text{and} \quad \|A\|_2^{-1} \le \frac{\left| A^{-1} \left(v - v'_* \right) \right|}{\left| (v - v'_*) \right|} \le \|A^{-1}\|_2,$$

we can write
$$|v - v_*| + |v - v_*|^{\delta-1} \leq \|A^{-1}\|_2 \, |v - v'_*| + \|A\|_2^{1-\delta} \, |v - v'_*|^{\delta-1}.$$
Eventually, we obtain
$$[\mathcal{K}_2 g]_i (v) \leq C \, n_i \sum_{j \notin \mathcal{M}_i} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4} m_i v^2} \, e^{-\frac{1}{4} m_j v'^2_*} \, g_j(v'_*) \left(|v - v'_*| + |v - v'_*|^{\delta-1} \right) d\omega \, dv'_*.$$

The upper bound in the previous equality has exactly a kernel form, which allows us to conclude on the compactness of $\mathcal{K}_2$ in the same way as in section 4.1.

4.3. **Compactness of $\mathcal{K}_3$.** This operator describes interactions between molecules with the same mass. Note that it does not mean that species $\mathcal{A}_i$ and $\mathcal{A}_j$ are the same, since $\mathcal{B}_{ii}$, $\mathcal{B}_{ij}$ and $\mathcal{B}_{jj}$ can be different. We only have to adapt ideas from [18] and [9] used in the monospecies case.

4.3.1. *Obtaining a kernel form.* Note that if $m_i = m_j$, (2) becomes
$$(29) \qquad v' = v - (\omega \cdot (v - v_*)) \, \omega, \quad v'_* = v_* + (\omega \cdot (v - v_*)) \, \omega.$$

Symmetry properties allow us to write $[\mathcal{K}_3 g]_i$ in terms of v, v_* and v', and not v'_* anymore. More precisely, we have the following lemma.

Lemma 4. *For any i, there exist nonnegative functions $\left(\tilde{\mathcal{B}}_{ij} \right)_{1 \leq j \leq I}$ satisfying (5), such that*
$$(30) \qquad [\mathcal{K}_3 g]_i (v) = \sum_{j \in \mathcal{M}_i} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4} m_i v^2 - \frac{1}{2} m_j v^2_* + \frac{1}{4} m_i v'^2} \, g_j(v') \, \tilde{\mathcal{B}}_{ij}(\omega, v - v_*) \, d\omega \, dv_*, \quad \forall v \in \mathbb{R}^3.$$

Proof. The key idea of the proof lies in (29). Indeed, if we consider the relative velocity $V = v - v_*$, we can choose one unit vector $\omega^\perp \in \text{Span}(V, \omega)$ orthogonal to ω (the choice of either $\omega^\perp$ or $-\omega^\perp$ is relevant, but must be performed in a continuous way with respect to ω, and not randomly). Consequently, we can write
$$V = \omega(\omega \cdot V) + \omega^\perp(\omega^\perp \cdot V),$$
from which we immediately get
$$(31) \qquad v - (\omega \cdot V)\omega = v_* + (\omega^\perp \cdot V)\omega^\perp, \qquad v_* + (\omega \cdot V)\omega = v - (\omega^\perp \cdot V)\omega^\perp.$$
We can see that, if we look for the post-collision relative velocity for the same pre-collisional V, but with respect to $\omega^\perp$, we just exchange the velocities v' and v'_*: for instance, the new v'_*, depending on $\omega^\perp$, will be the old v', depending on ω. Hence, it is clear that $\omega \mapsto \omega^\perp$ implies $v' \mapsto v'_*$ and $v'_* \mapsto v'$.

Consequently, if we replace ω by $\omega^\perp$ in the integral
$$\iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{2} m_i v^2_*} e^{\frac{1}{4} m_i (v_* + (\omega \cdot V)\omega)^2} \, g_j(v_* + (\omega \cdot V)\omega) \, \mathcal{B}_{ij}(\omega, V) \, d\omega \, dv_*,$$
it becomes
$$\iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{2} m_i v^2_*} e^{\frac{1}{4} m_i (v_* + (\omega^\perp \cdot V)\omega^\perp)^2} \, g_j(v_* + (\omega^\perp \cdot V)\omega^\perp) \, \mathcal{B}_{ij}(\omega^\perp, V) \, d\omega^\perp \, dv_*.$$

Changing the variable ω into $\omega^\perp$ is obtained thanks to a rotation, so $d\omega^\perp = d\omega$. Hence, using (31), the previous integral becomes
$$\iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{2} m_i v^2_*} e^{\frac{1}{4} m_i v'^2} \, g_j(v') \, \mathcal{B}_{ij}(\omega^\perp, V) \, d\omega^\perp \, dv_* = \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{2} m_i v^2_*} e^{\frac{1}{4} m_i v'^2} \, g_j(v') \, \mathcal{B}_{ij}(\omega^\perp, V) \, d\omega \, dv_*.$$
Let us set
$$\tilde{\mathcal{B}}_{ij}(\omega, V) = \left(\frac{m_i}{2\pi} \right)^{3/2} \begin{cases} n_i \, \mathcal{B}_{ij}(\omega^\perp, V) & \text{if } i \neq j, \\ \displaystyle\sum_{k \in \mathcal{M}_i} n_k \, \mathcal{B}_{ik}(\omega, V) + n_i \, \mathcal{B}_{ii}(\omega^\perp, V) & \text{if } i = j. \end{cases}$$

Assumption (5) on both $\mathcal{B}_{ij}(\omega, V)$ and $\mathcal{B}_{ij}(\omega^\perp, V)$ ensures that, for any i, j

$$(32) \qquad \tilde{\mathcal{B}}_{ij}(\omega, V) \le 2\, a \left(\frac{m_i}{2\pi}\right)^{3/2} \left(\max_{k \in \mathcal{M}_i} n_k\right) |\sin\theta|\,|\cos\theta| \left(|V| + |V|^{\delta - 1}\right),$$

as well as (30). $\qquad\qquad\square$

Lemma 4 allows to obtain the kernel form of $\mathcal{K}_3$. More precisely, we have

Proposition 5. *Denote, for any i, j,*

$$(33) \qquad k_3^{ij}(\eta, v) = e^{-\frac{1}{8}m_i(\eta - v)^2 - \frac{1}{8}m_i \frac{(\eta^2 - v^2)^2}{(\eta - v)^2}} |\eta - v|^{-1} \varphi_3^{ij}(\eta - v), \quad \forall \, \eta, v \in \mathbb{R}^3,$$

where

$$(34) \qquad \varphi_3^{ij}(p) = \frac{2}{|p|} \int_{\{p\}^\perp} e^{-\frac{1}{2}m_i(q + z_2)^2} \tilde{\mathcal{B}}_{ij}(p, q) \, |\sin(p, p + q)|^{-1} \, \mathrm{d}q, \quad \forall \, p \in \mathbb{R}^3.$$

Then we have

$$[\mathcal{K}_3 g]_i(v) = \sum_{j \in \mathcal{M}_i} \int_{\mathbb{R}^3} g_j(\eta) \, k_3^{ij}(\eta, v) \mathrm{d}\eta, \quad \forall \, v \in \mathbb{R}^3.$$

Proof. We perform the change of variable $v_* \mapsto V_* = v_* - v$ in (30), whose Jacobian equals 1, and get

$$(35) \qquad [\mathcal{K}_3 g]_i(v) = \sum_{j \in \mathcal{M}_i} \iint_{\mathbb{R}^3 \times S^2} e^{-\frac{1}{4}m_i v^2} e^{-\frac{1}{2}m_i(V_* + v)^2} e^{\frac{1}{4}m_i v'^2} g_j(v') \tilde{\mathcal{B}}_{ij}(\omega, V_*) \, \mathrm{d}\omega \, \mathrm{d}V_*.$$

Next, we consider the components of V_* respectively parallel and orthogonal to ω, i.e. we write $V_* = p + q$, where $p = \omega(\omega \cdot V_*)$, $q = V_* - \omega(\omega \cdot V_*)$. The component q which is orthogonal to ω belongs to the plane $\Pi = \{\omega\}^\perp = \{p\}^\perp$.
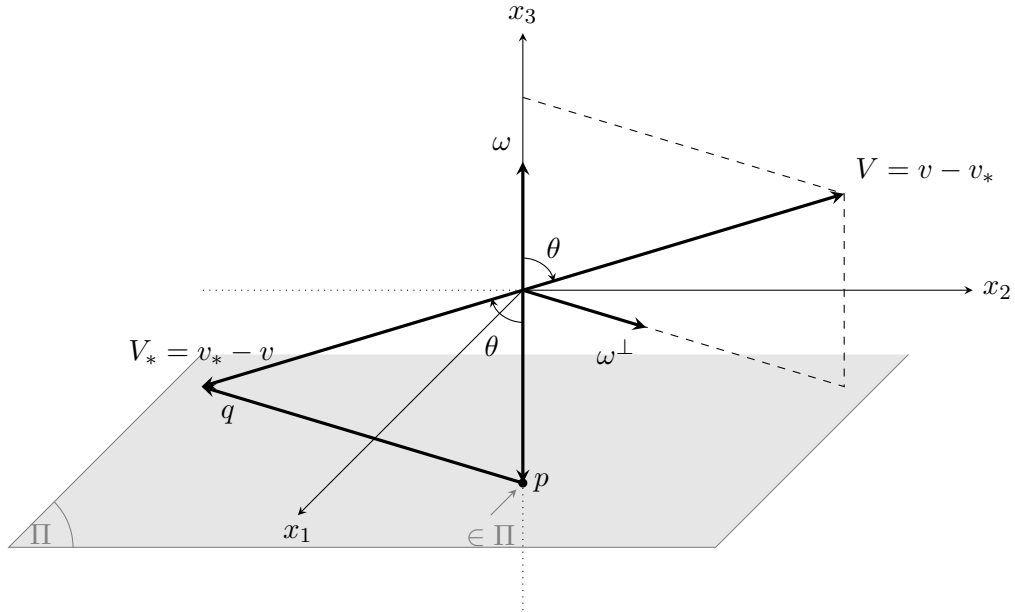

FIGURE 1. Geometrical situation for the change of variables (36)

We now perform the change of variables (see Figure 1)

$$(36) \qquad\qquad (V_*, \omega) \mapsto (p, q), \qquad \mathbb{R}^3 \times S^2 \to \mathbb{R}^3 \times \Pi.$$

Let us compute its Jacobian. For ω fixed, the replacement of V_* by p and q has unit Jacobian. Note that V_* and ω are independent of each other, which is not the case with p and q. Therefore, the integration

order is crucial. Hence we first integrate with respect to q since $\Pi = \{p\}^\perp$. Then we combine the one-dimensional integration in the direction ω with the integral of ω over the unit sphere to give a three-dimensional integration over the three rectangular components of $|p|\omega$. We have to introduce the factor 2, since $p = \pm|p|\omega$. The Jacobian from p to $(|p|,\omega)$ (Cartesian to spherical coordinates) is $p^2 \sin(p, p+q)$. Consequently, we can write

$$\mathrm{d}V_* \, \mathrm{d}\omega = \frac{2}{p^2 \sin(p, p+q)} \mathrm{d}p \, \mathrm{d}q.$$

Eventually, it is clear that

$$v' = v - \omega(\omega \cdot (v - v_*)) = v + \omega(\omega \cdot V_*) = v + p.$$

Hence, (35) becomes

$$(37) \quad [\mathcal{K}_3 g]_i (v) = 2 \sum_{j \in \mathcal{M}_i} \int_{\mathbb{R}^3} \int_\Pi e^{-\frac{1}{4} m_i v^2 - \frac{1}{2} m_i (p+q+v)^2 + \frac{1}{4} m_i (v+p)^2} \, g_j(v+p)$$

$$\tilde{\mathcal{B}}_{ij}(p,q) \, |p|^{-2} \, |\sin(p, p+q)|^{-1} \, \mathrm{d}q \, \mathrm{d}p.$$

Since $p \cdot q = 0$, we can deduce

$$-\frac{1}{4} v^2 + \frac{1}{4} (v+p)^2 - \frac{1}{2} (p+q+v)^2 = -\frac{1}{8} p^2 - \frac{1}{2} \left[q + \frac{1}{2}(2v+p) \right]^2.$$

Consequently, we obtain

$$[\mathcal{K}_3 g]_i (v) = 2 \sum_{j \in \mathcal{M}_i} \int_{\mathbb{R}^3} \int_\Pi e^{-\frac{1}{8} m_i p^2 - \frac{1}{2} m_i \left[q + \frac{1}{2}(2v+p) \right]^2} \, g_j(v+p) \tilde{\mathcal{B}}_{ij}(p,q) \, |p|^{-2} \, |\sin(p, p+q)|^{-1} \, \mathrm{d}q \, \mathrm{d}p.$$

Furthermore, let us set

$$z = \frac{1}{2} (2v + p),$$

and denote by z_1 the component of z which is parallel to ω and $z_2 = z - z_1 \in \Pi$. Then we can write

$$\left[q + \frac{1}{2} (2v+p) \right]^2 = (q + z_1 + z_2)^2 = z_1^2 + (q + z_2)^2,$$

and $[\mathcal{K}_3 g]_i$ becomes

$$[\mathcal{K}_3 g]_i = 2 \sum_{j \in \mathcal{M}_i} \int_{\mathbb{R}^3} e^{-\frac{1}{8} m_i p^2 - \frac{1}{2} m_i z_1^2} \, g_j(v+p) \, |p|^{-2} \int_\Pi e^{-\frac{1}{2} m_i (q+z_2)^2} \, \tilde{\mathcal{B}}_{ij}(p,q) \, |\sin(p, p+q)|^{-1} \, \mathrm{d}q \, \mathrm{d}p.$$

Finally, we perform the change of variable $p \mapsto \eta = p + v$, and write

$$z_1^2 = \left(z \cdot \frac{\eta - v}{|\eta - v|} \right)^2 = \left(\frac{1}{2}(\eta + v) \cdot \frac{(\eta - v)}{|\eta - v|} \right)^2 = \frac{1}{4} \frac{(\eta^2 - v^2)^2}{|\eta - v|^2}.$$

This completes the proof. $\qquad\qquad\square$

4.3.2. *Properties of k_3^{ij}.* Let us first prove the following lemma, and then investigate some properties of k_3^{ij}.

Lemma 5. *The function $\varphi_3^{ij} : \mathbb{R}^3 \to \mathbb{R}$, defined by (34) for any i, j, belongs to $L^\infty(\mathbb{R}^3)$.*

Proof. Let $1 \le i, j \le I$, and choose $p \in \mathbb{R}^3$ and $q \in \{p\}^\perp$. From (32), we obtain

$$0 \le \frac{\tilde{\mathcal{B}}_{ij}(p,q)}{|\sin(p, p+q)|} \le 2 \, a \left(\frac{m_i}{2\pi} \right)^{3/2} \left(\max_{k \in \mathcal{M}_i} n_k \right) |\cos(p, p+q)| \left(|p+q| + |p+q|^{\delta-1} \right).$$

Since $|\tan(p, p+q)| = |q|/|p|$, we can write

$$0 \le \frac{\tilde{\mathcal{B}}_{ij}(p,q)}{|\sin(p, p+q)|} \le C_i \Big(\max_{k \in \mathcal{M}_i} n_k \Big) \left(1 + \frac{q^2}{p^2} \right)^{-\frac{1}{2}} \left[(p^2+q^2)^{\frac{1}{2}} + (p^2+q^2)^{\frac{\delta-1}{2}} \right],$$

where $C_i = 2 a \, (m_i/2\pi)^{3/2} > 0$. In what follows, C_i will denote any nonnegative constant only depending on m_i. This implies

$$0 \le \frac{\tilde{\mathcal{B}}_{ij}(p,q)}{|p| \, |\sin(p, p+q)|} \le C_i \Big(\max_{k \in \mathcal{M}_i} n_k \Big) \left[1 + (p^2+q^2)^{\frac{\delta}{2}-1} \right] \le C_i \Big(\max_{k \in \mathcal{M}_i} n_k \Big) \left[1 + |q|^{\delta-2} \right],$$

using the fact that $\delta < 1$. Now, we split the range of integration in (34) into $|q| \le 1$ and $|q| \ge 1$, and finally get

$$0 \le \varphi_3^{ij}(p) \le C_i \max_{k \in \mathcal{M}_i} n_k \left(\int_{|q| \le 1} (1 + |q|^{\delta-2}) \mathrm{d}q + \int_{|q| \ge 1} e^{-\frac{1}{2}(q+z_2)^2} \mathrm{d}q \right) \le C_i \max_{k \in \mathcal{M}_i} n_k.$$

This ends the proof of Lemma 5. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad$ $\square$

Let us now investigate two properties of k_3^{ij}, which are related to Lemmas 1 and 2 for k_1^{ij}.

Lemma 6. *There exists $C > 0$ such that, for any i, j,*

$$\int_{\mathbb{R}^3} k_3^{ij}(\eta, v) \, \mathrm{d}\eta \le \frac{C}{|v|}, \quad \forall \, v \in \mathbb{R}^3 \setminus \{0\}, \qquad \int_{\mathbb{R}^3} k_3^{ij}(\eta, v) \, \mathrm{d}\eta \le C, \quad \forall \, v \in \mathbb{R}^3.$$

Proof. Let $1 \le i, j \le I$. We integrate (33) with respect to η and perform the change of variable $\eta \mapsto p = \eta - v$. Using Lemma 5, we get

$$\int_{\mathbb{R}^3} k_3^{ij}(\eta, v) \, \mathrm{d}\eta \le C \int_{\mathbb{R}^3} e^{-\frac{1}{8}m_i p^2 - \frac{1}{8}m_i \frac{(p^2+2p\cdot v)^2}{p^2}} \frac{1}{|p|} \, \mathrm{d}p, \quad \forall \, v \in \mathbb{R}^3.$$

We split the right-hand integral into $I_1 + I_2$, where I_1 refers to $|p| \ge |v|$ and I_2 to $|p| \le |v|$. On the one hand, we have

$$I_1 \le \int_{|p| \ge |v|} e^{-\frac{1}{8}m_i p^2} \frac{1}{|p|} \, \mathrm{d}p \le C \, e^{-\frac{1}{8}m_i v^2}.$$

On the other hand, for the second integral, with spherical coordinates, we have

$$I_2 = \int_0^{|v|} \int_0^{2\pi} \int_0^{\pi} e^{-\frac{1}{8}m_i r^2 - \frac{1}{8}m_i (r + 2|v| \cos \psi_1)^2} r \sin \psi_1 \, \mathrm{d}\psi_1 \, \mathrm{d}\psi_2 \, \mathrm{d}r$$

$$= 2\pi \int_0^{|v|} r e^{-\frac{1}{8}m_i r^2} \int_0^{\pi} e^{-\frac{1}{8}m_i (r + 2|v| \cos \psi_1)^2} \sin \psi_1 \, \mathrm{d}\psi_1 \, \mathrm{d}r,$$

where ψ_1 corresponds to the angle between p and v. We then have to consider two situations for I_2: $|v| \ge 1$ and $|v| \le 1$. Simple changes of variables give, if $v \ne 0$,

$$\int_0^{\pi} e^{-\frac{1}{8}m_i (r + 2|v| \cos \psi_1)^2} \sin \psi_1 \, \mathrm{d}\psi_1 = \frac{1}{2|v|} \int_{r-2|v|}^{r+2|v|} e^{-\frac{1}{8}m_i s^2} \mathrm{d}s.$$

If $|v| \ge 1$,

$$I_2 \le \frac{C}{|v|} \int_0^{+\infty} r \, e^{-\frac{1}{8}m_i r^2} \mathrm{d}r \int_{-\infty}^{+\infty} e^{-\frac{1}{8}m_i s^2} \mathrm{d}s = \frac{C_i}{|v|} \le C_i.$$

On the contrary, if $|v| \le 1$,

$$I_2 \le \frac{C_i}{|v|} \int_{r-2|v|}^{r+2|v|} \mathrm{d}s = C_i, \qquad \text{if } v \ne 0.$$

Consequently, we get the required estimates. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad$ $\square$

Using the same strategy as above, the following lemma can also be proved.

Lemma 7. *For any i, j, k_3^{ij} belongs to $L_{loc}^2\left(\mathbb{R}_v^3; L^2\left(\mathbb{R}_\eta^3\right)\right)$.*

4.3.3. *Uniform decay.* Let us now prove the uniform decay property at infinity.

Proposition 6. *Let $g \in L^2(\mathbb{R}^3)^I$. For any $R > 0$ and any i, we have*

$$\|\,[\mathcal{K}_3 g]_i\,\|_{L^2(B(0,R)^c)} \leq \frac{C}{\sqrt{R}}\,\|g\|_{L^2(\mathbb{R}^3)},$$

where $C > 0$ is a constant.

Proof. Using the Cauchy-Schwarz inequality and Lemma 6, we can write

$$\|\,[\mathcal{K}_3 g]_i\,\|_{L^2(B(0,R)^c)}^2 \leq C \int_{|v| \geq R} \sum_{j \in \mathcal{M}_i} \left[\int_{\mathbb{R}^3} g_j(\eta)^2 k_3^{ij}(\eta, v)\,\mathrm{d}\eta\right]\left[\int_{\mathbb{R}^3} k_3^{ij}(\eta, v)\,\mathrm{d}\eta\right]\,\mathrm{d}v$$

$$\leq \frac{C}{R} \sum_{j \in \mathcal{M}_i} \int_{\mathbb{R}^3} \left[\int_{\mathbb{R}^3} k_3^{ij}(v, \eta)\,\mathrm{d}v\right] g_j(\eta)^2 \mathrm{d}\eta = \frac{C}{R}\|g\|_{L^2(\mathbb{R}^3)}^2,$$

where we also used the fact that $k_3^{ij}(\eta, v) = k_3^{ij}(v, \eta)$. This ends the proof. $\qquad\square$

4.3.4. *Equicontinuity.* This property is described in the following proposition.

Proposition 7. *For all $\varepsilon > 0$, there exists $\alpha > 0$ (not depending on g or i) such that*

$$(38) \qquad \|\,[(\tau_w - \mathrm{Id})\mathcal{K}_3 g]_i\,\|_{L^2(\mathbb{R}^3)} \leq \varepsilon\|g\|_{L^2(\mathbb{R}^3)}, \quad \forall\, w \in B(0, \alpha).$$

Proof. Let $R > 0$. We obviously have, for any $w \in B(0, R)$,

$$(39) \qquad \|\,[(\tau_w - \mathrm{Id})\,\mathcal{K}_3 g]_i\,\|_{L^2(\mathbb{R}^3)}^2 \leq \int_{B(0,2R)} ([\mathcal{K}_3 g]_i\,(v + w) - [\mathcal{K}_3 g]_i\,(v))^2\,\mathrm{d}v + \int_{B(0,R)^c} [\mathcal{K}_3 g]_i\,(v)^2 \mathrm{d}v.$$

Proposition 6 ensures that the second integral is upper-bounded by $\|g\|_{L^2}^2/R$. The first one can also be upper-estimated by

$$\sum_{j \in \mathcal{M}_i} \|g_j\|_{L^2}^2 \int_{B(0,2R)} \int_{\mathbb{R}^3} \left(k_3^{ij}(\eta, v + w) - k_3^{ij}(\eta, v)\right)^2 \mathrm{d}\eta\,\mathrm{d}v.$$

We can now choose $R \geq 2/\varepsilon^2 > 0$. Thanks to Lemma 7, there exists $\alpha > 0$ such that

$$|w| < \alpha \quad \Rightarrow \quad \int_{B(0,2R)} \int_{\mathbb{R}^3} \left(k_3^{ij}(\eta, v + w) - k_3^{ij}(\eta, v)\right)^2 \mathrm{d}\eta\,\mathrm{d}v \leq \frac{\varepsilon^2}{2}.$$

It is then immediate to recover (38) from (39). $\qquad\square$

4.4. **Compactness of $\mathcal{K}_4$.** The proof of the compactness of $\mathcal{K}_4$ is very similar to the final part of the proof for $\mathcal{K}_3$. The main difficulty is to obtain a kernel form of $\mathcal{K}_4$. Once it is done, (19)–(20) can easily be proven as in section 4.3. Using the same change of variables as to obtain (37), we can write

$$[\mathcal{K}_4 g]_i\,(v) = 2 \sum_{j \notin \mathcal{M}_i} n_j \left(\frac{m_j}{2\pi}\right)^{3/2} \int_{\mathbb{R}^3} \int_\Pi e^{-\frac{1}{4}m_i v^2 - \frac{1}{2}m_j(p+q+v)^2 + \frac{1}{4}m_i\left(v + 2\frac{m_j}{m_i+m_j}p\right)^2}$$

$$g_i\left(v + 2\frac{m_j}{m_i + m_j}p\right) \mathcal{B}_{ij}(p, q)\,|p|^{-2}\,|\sin(p, p + q)|^{-1}\,\mathrm{d}q\,\mathrm{d}p.$$

The exponential term can be modified thanks to the following relation

$$-\frac{1}{4}m_i v^2 - \frac{1}{2}m_j\,(p+q+v)^2 + \frac{1}{4}m_i\left(v + 2\frac{m_j}{m_i + m_j}p\right)^2 = -\frac{m_j\,m_i^2}{2\,(m_i + m_j)^2}\,p^2 - \frac{m_j}{2}\left(q + v + \frac{m_j}{m_i + m_j}p\right)^2.$$

If we denote

$$z = v + \frac{m_j}{m_i + m_j} \, p,$$

and decompose it into the component z_1 parallel to ω and the component z_2 orthogonal to ω ($z_2 \in \Pi$), we obtain the new form of $[\mathcal{K}_4 g]_i$:

$$[\mathcal{K}_4 g]_i (v) = 2 \sum_{j \notin \mathcal{M}_i} n_j \left(\frac{m_j}{2\pi}\right)^{3/2} \int_{\mathbb{R}^3} e^{-\frac{m_j \, m_i^2}{2(m_i + m_j)^2} \, p^2 - \frac{1}{2} m_j z_1{}^2} \, g_i \left(v + 2 \frac{m_j}{m_i + m_j} p\right) |p|^{-2}$$

$$\int_{\Pi} e^{-\frac{1}{2} m_j (q + z_2)^2} \, \mathcal{B}_{ij}(p, q) \, |\sin(p, p + q)|^{-1} \, \mathrm{d}q \, \mathrm{d}p.$$

Next, we perform the change of variables

$$p \mapsto \eta = v + 2 \frac{m_j}{m_i + m_j} p, \text{ whose Jacobian equals } \left(2 \frac{m_j}{m_i + m_j}\right)^3,$$

and write z_1^2 in the following form

$$z_1^2 = \left(z \cdot \frac{\eta - v}{|\eta - v|}\right)^2 = \frac{1}{4} \frac{(\eta^2 - v^2)^2}{(\eta - v)^2}.$$

Thus $[\mathcal{K}_4 g]_i$ becomes

$$[\mathcal{K}_4 g]_i (v) = \frac{1}{4} \sum_{j \notin \mathcal{M}_i} n_j \left(\frac{m_j}{2\pi}\right)^{3/2} \left(\frac{m_i + m_j}{m_j}\right) \int_{\eta \in \mathbb{R}^3} e^{-\frac{1}{8} \frac{m_i^2}{m_j} (\eta - v)^2 - \frac{1}{8} m_j \frac{(\eta^2 - v^2)^2}{(\eta - v)^2}} \, g_i(\eta) \, |\eta - v|^{-2}$$

$$\int_{\Pi} e^{-\frac{1}{2} m_j (q + z_2)^2} \, \mathcal{B}_{ij} \left(\frac{m_i + m_j}{2 m_j} (\eta - v), q\right) \left| \sin \left(\frac{m_i + m_j}{2 m_j} (\eta - v), \frac{m_i + m_j}{2 m_j} (\eta - v) + q\right) \right|^{-1} \, \mathrm{d}q \, \mathrm{d}\eta.$$

To write $[\mathcal{K}_4 g]_i$ into the convenient kernel form, we introduce the function

$$\varphi_4^{ij}(p) = \left(\frac{m_j}{2\pi}\right)^{3/2} \frac{m_i + m_j}{2 m_j |p|} \int_{q \in \Pi} e^{-m_j \frac{1}{2}(q + z_2)^2} \, \mathcal{B}_{ij}(p, q) \, |\sin(p, p + q)|^{-1} \, \mathrm{d}q.$$

It is easy to prove, in the same way as in Lemma 5, that there exists $C > 0$ such that $\|\varphi_4^{ij}\|_{L^\infty(\mathbb{R}^3)} \leq C$ for any i, j. The i-th component of $\mathcal{K}_4 g$ can be written in the kernel form

$$[\mathcal{K}_4 g]_i (v) = \sum_{j \notin \mathcal{M}_i} n_j \int_{\mathbb{R}^3} k_4^{ij}(\eta, v) g_i(\eta) \, \mathrm{d}\eta,$$

where $k_4^{ij}(\eta, v)$ is given by

$$k_4^{ij}(\eta, v) = \frac{1}{4} e^{-\frac{1}{8} \frac{m_i^2}{m_j} (\eta - v)^2 - \frac{1}{8} m_j \frac{(\eta^2 - v^2)^2}{(\eta - v)^2}} \, |\eta - v|^{-1} \, \varphi_4^{ij} \left(\frac{m_i + m_j}{2 m_j} (\eta - v)\right).$$

The form of each k_4^{ij} is exactly the same as in (33). Consequently, k_4^{ij} inherits the same properties as k_3^{ij} (see Lemmas 5 and 6), which allows to obtain (19)–(20) as in Propositions 6 and 7, and the compactness of $\mathcal{K}_4$.

5. Diffusion limit

To conclude this work, let us add a few words about the diffusion limit itself. Theorem 1 ensures the existence of $g = (g_i)_{1 \leq i \leq I}$, in the expansion (11), with respect to (n_i). Let us then write the first order in ε coming from (10), that is

$$M_i \partial_t n_i + M_i^{1/2} v \cdot \nabla_x g_i = \sum_{j=1}^{I} Q_{ij}(M_i^{1/2} g_i, M_j^{1/2} g_j).$$

Integrating the previous equality with respect to v, and using (6)–(7), we can write the usual continuity equation

$$(40) \qquad \partial_t n_i + \nabla_x \cdot N_i = 0,$$

where the flux N_i of species $\mathcal{A}_i$ is given by

$$(41) \qquad N_i(t, x) = \int_{\mathbb{R}^3} v \, g_i(t, x, v) \, M_i(v)^{1/2} \, \mathrm{d}v, \qquad \forall x, v \qquad 1 \leq i \leq I.$$

Since g_i only depends on (n_j), the flux N_i shares the same property thanks to (41). Consequently, the continuity equations give a system, which only involves (n_j). The existence of (n_j) was not investigated here. The reader can refer to [6, 7] for more details about the related macroscopic equations.

The expression of the flux (41) allows to clarify Assumption (16) of Theorem 1: the equimolar diffusion situation, which means $\sum N_i = 0$, is common in closed experimental settings [14, 22]. This property clearly implies that $\sum n_i$ equals its initial value (sum (40) over i). Hence, if we suppose that the initial value does not depend on x, assumption (16) is fulfilled.

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