

# Derivation of BGK models for mixtures.

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## Abstract

This paper is devoted to the construction of a BGK operator for gas mixtures. The construction is based as in ([12], [13]) on the introduction of relaxation coefficients and a principle of minimization of the entropy under constraints of moments. These free parameters are compared with the free parameters introduced in the Thermodynamics of Irreversible Processes approach of the Navier-Stokes system. At the end the BGK model is proved to satisfy Fick and Newton laws.

Key words: Kinetic theory, gas mixtures, BGK models, entropy minimization, hydrodynamic limit.

## 1 Introduction.

The BGK equation [8] is a seminal simplified model of the nonlinear Boltzmann equation of gas dynamics. Its features are to replace the complicated integral of collisions with a relaxation model while keeping some important physical and mathematical properties of the interaction term (conservation laws, H-theorem, equilibrium states,...). Thus it is very interesting from a numerical point of view. Its drawbacks rely upon a somewhat bad description of the distribution function far from equilibrium and closed to equilibrium in the sense that the Navier-Stokes limit might be not correct (Prandtl number). Though a correction can be brought to obtain this important ratio between viscosity and heat conductivity (see the Ellipsoidal Statistical Model by Holway [22]). In the case of gas mixtures things are less clear. The Boltzmann equation(s) is still considered to describe the true behavior of the distribution function but BGK models and their extensions meet fundamental difficulties. The first one is that conservations laws stand only for the whole set of particles; exchanges of momentum

and energy occur between each species. The second is that the hydrodynamical limit is much more complicated. Phenomena such as diffusion or thermal diffusion must be considered. Many of those problems have been widely studied by Japanese researchers (see for example [29, 2, 5, 6] and show great difference with the usual monatomic case. Finally theoretical aspects such as existence theorems [7, 9, 11] or study of a binary mixture closed to a local equilibrium [10] confirm the specificity of multi-component case.

Coming back to modeling there exists however a great variety of BGK models which traces back to the work of Gross and Krook [17] to the most recent model by Kosuge [26]. A first family of model has been proposed [17, 30, 20, 27] (often in the context of Maxwellian molecules). Those BGK models intend to mimic the Boltzmann equations for self and cross interaction and some of them give the right exchange of momentum and energy between each species [20, 27]. A second family adds to the previous properties the so-called indiffentiability principle that reduces the whole family of relaxation models to a single one when all masses and cross sections are equal [19, 1]. Finally Kosuge has generalized the model of Garzo & al [19] to relaxation terms that allow to approximate exchanges of momentum, energy, cross moments of order two and heat flux between each species. Though numerical results may be quite good for some models or may enjoy nice mathematical properties for others it is quite surprising that none of them has attempted to reach the right hydrodynamical limit. In general their authors rather study the hydrodynamical limit of their model and eventually compared it with the right one [21].

Our approach goes the other way. We first consider the right hydrodynamical limit and then construct a model that allows to recover the kinetic coefficients -in the present case the Fick law and the viscosity.

The paper is constructed as follows. In section 2 we recall the main properties of the Boltzmann equation and the linearized operator which lead us to propose a list of necessary properties that should satisfy any approximation of the interaction terms. We also introduce a space of moments denoted by  $\mathbb{C}$  (see (1) that features the non-conservation of momentum per species. Section 3 is the cornerstone of our paper. After recalling the Navier-Stokes equation for gas mixtures and how the thermodynamic of irreversible processes allow to define the fluxes and the different laws (Fick, Soret, Dufour) that do not exist in the case of a single specie, we revisit the way those fluxes can be computed starting from the kinetic theory. Though this connection has already been done in the celebrated book by De Groot and Mazur [18] and in a certain sense by Chapman and Cowling [14], we present a synthetic and clear computation of the kinetic coefficients that is based on one hand on the mathematical properties of the linearized Boltzmann operator and on the other hand on the space  $\mathbb{C}$ . Section 4 is devoted to the construction of our model. It leans on two ideas that were introduced by two of the authors [12, 13]: the operator must relax certain moments of the distribution functions so as to obtain the correct hydrodynamical limit and the model is constructed via a principle of minimization of entropy under moment constraints. In section 5 we prove that the whole set of properties

that were introduced in section 2 are satisfied and we easily derive from them and from the formalism of section 3 the hydrodynamical limit. We also address the properties of indifferentiability and correct hydrodynamical limit for BGK models. Finally section 6 is devoted to a discussion implying physics, modeling and mathematical aspects.

## 2 Notations and recall about the Boltzmann and other general kinetic equation for gas mixtures.

### 2.1 The Boltzmann operator for mixtures.

#### 2.1.1 Detailed expression.

Let us consider a gas mixtures with  $p$  components. The functions  $f_i(t, x, v)$  (or for short  $f_i, i \in [1, p]$  with  $\mathbf{f} := (f_1, \dots, f_p)$ ) associated to a given species  $i$  evolves according to the Boltzmann equation:

$$\forall i \in [1, p], \partial_t f_i + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = \sum_{k=1}^{k=p} Q_{ki}(f_k, f_i) := Q_i(\mathbf{f}, \mathbf{f}), \quad (1)$$

where

$$Q_{ki}(f_k, f_i) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} (f_k(\mathbf{w}_{ki}^*) f_i(\mathbf{v}_{ki}^*) - f_k(\mathbf{w}) f_i(\mathbf{v})) \sigma_{ik}(\boldsymbol{\omega}, \mathbf{V}, \|\mathbf{V}\|) \|\mathbf{V}\| d\mathbf{w} d\boldsymbol{\omega}.$$

Here  $Q_{ki}$  is the Boltzmann collision operator between molecules of species  $i$  and  $k$  and  $\sigma_{ik} = \sigma_{ki}$  is the differential cross section which depend on the interaction potential of the species  $i$  and  $k$ . Finally  $\mathbf{V} = \mathbf{w} - \mathbf{v}$  is the relative velocity. The post collisional velocities are given by

$$\begin{aligned} \mathbf{v}_{ki}^* &= \mathbf{v} - 2 \frac{m_k}{m_i + m_k} ((\mathbf{v} - \mathbf{w}) \cdot \boldsymbol{\omega}) \boldsymbol{\omega}, \\ \mathbf{w}_{ki}^* &= \mathbf{w} + 2 \frac{m_i}{m_i + m_k} ((\mathbf{v} - \mathbf{w}) \cdot \boldsymbol{\omega}) \boldsymbol{\omega}. \end{aligned}$$

Those equations satisfy the conservation of momentum and energy at a microscopic level

$$\begin{aligned} m_i \mathbf{v} + m_k \mathbf{w} &= m_i \mathbf{v}_{ki}^* + m_k \mathbf{w}_{ki}^*, \\ m_i \|\mathbf{v}\|^2 + m_k \|\mathbf{w}\|^2 &= m_i \|\mathbf{v}_{ki}^*\|^2 + m_k \|\mathbf{w}_{ki}^*\|^2. \end{aligned}$$

#### 2.1.2 Macroscopic quantities for the mixture.

We denote with  $n^i, \rho^i, u^i, E^i, T^i$  and  $\mathcal{E}^i$  the macroscopic quantities representing respectively the number density, density, average velocity, energy per unit

volume, energy per particle and finally temperature of a given specie  $i$ . They are defined by the following relations:

$$\begin{aligned} n^i &= \int_{\mathbb{R}^3} f_i d\mathbf{v}, & \rho^i &= m_i n^i, & n^i \mathbf{u}^i &= \int_{\mathbb{R}^3} \mathbf{v} f_i d\mathbf{v}, \\ E^i &= \frac{1}{2} \rho^i \|\mathbf{u}^i\|^2 + n^i \mathcal{E}^i, & \mathcal{E}^i &= \frac{3}{2} k_B T^i = \frac{m_i}{2n^i} \int_{\mathbb{R}^3} \|\mathbf{v} - \mathbf{u}^i\|^2 f_i d\mathbf{v}, \end{aligned}$$

where  $k_B$  is the Boltzmann constant. In the same way, we can introduce hydrodynamic quantities for the mixture

$$n = \sum_{k=1}^p n^k, \quad \rho = \sum_{k=1}^p \rho^k, \quad \rho \mathbf{u} = \sum_{k=1}^p \rho^k \mathbf{u}^k, \quad (2)$$

$$n \mathcal{E} + \frac{\rho}{2} \|\mathbf{u}\|^2 = E = \sum_{k=1}^p E^k, \quad \mathcal{E} = \frac{3}{2} k_B T. \quad (3)$$

Given a mixture of  $p$  species featuring the parameters  $n^i, \mathbf{u}, T$ , an important list of functions are the Maxwellians of equilibrium reading as:

$$\forall i \in [1, p], \mathcal{M}_i = \frac{n^i}{(2\pi k_B T / m_i)^{\frac{3}{2}}} \exp\left(-\frac{m_i (\mathbf{v} - \mathbf{u})^2}{2k_B T}\right). \quad (4)$$

In the sequel we will denote by  $\mathbf{M} := (\mathcal{M}_1, \dots, \mathcal{M}_p)$  this list of functions. At last for any list of non negative functions  $\mathbf{f} := (f_1, \dots, f_p)$  we define the entropy function  $H$  as:

$$H(\mathbf{f}) := \sum_{i=1}^p \int_{\mathbb{R}^3} (f_i \ln(f_i) - f_i) d\mathbf{v}.$$

### 2.1.3 Spaces of interest.

Using the above notations we note as  $\mathbb{L}^2(\mathbf{M})$  the set of measurable functions  $\Psi = (\psi_1, \dots, \psi_p)$  such that:

$$\|\Psi\|^2 := \sum_{i=1}^p \int_{\mathbb{R}^3} \psi_i^2 \mathcal{M}_i < +\infty.$$

This space is equipped using its natural dot product:

$$\langle \Psi, \Phi \rangle = \sum_{i=1}^p \int_{\mathbb{R}^3} \psi_i \phi_i \mathcal{M}_i dv.$$

In the sequel, we will often use the dot product notation even if what lies in the bracket is not a list of  $p$  scalar functions but is a list of  $p$  tensorial functions. For

instance, if  $\Psi, \Phi$  are two lists of  $p$  (symmetrical) tensorial functions  $\psi_i, \phi_i, i \in [1, p]$ , then the dot product notation  $\langle \psi, \phi \rangle$  should be understood as

$$\langle \psi, \phi \rangle := \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \psi_i \otimes \phi_i \mathcal{M}_i d\mathbf{v},$$

where  $\otimes$  denotes the usual tensorial product. Note also the following convention: assume that  $\mathbf{V}$  is a list of  $p$  vectors and  $\mathbf{T}$  a list of  $p$  square matrixes. Then a notation like  $\alpha \mathbf{V}, \alpha \mathbf{T}$  (where  $\alpha$  is a scalar) means that the scalar  $\alpha$  is distributed on each line of the list of vectors or matrixes. Besides, if  $\boldsymbol{\beta}$  is a vector, then a notation like  $\boldsymbol{\beta} \cdot \mathbf{V}$  means that we distribute the dot product by  $\boldsymbol{\beta}$  on each line of the vector  $\mathbf{V}$ . The same way, if  $\boldsymbol{\gamma}$  is a square matrix, then a notation like  $\boldsymbol{\gamma} : \mathbf{T}$  means that we distribute the (total) dot product (between matrix) by  $\boldsymbol{\gamma}$  on each line of the line of  $\mathbf{T}$ . Finally, if  $\mathbf{s}$  is a tensor and  $\mathbf{S}$  a list of  $p$  tensors, then a notation like  $\mathbf{s} \otimes \mathbf{S}$  means that we distribute the tensor product by  $\mathbf{s}$  on the left on each line of the list  $\mathbf{S}$ .

Introduce now the following subspace  $\mathbb{K}$  of  $\mathbb{L}^2(\mathbf{M})$  of dimension  $p+4$  generated by the following list of functions:

$$\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \dots, \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}, \begin{pmatrix} m_1 v_x \\ m_2 v_x \\ \vdots \\ m_p v_x \end{pmatrix}, \begin{pmatrix} m_1 v_y \\ m_2 v_y \\ \vdots \\ m_p v_y \end{pmatrix}, \begin{pmatrix} m_1 v_z \\ m_2 v_z \\ \vdots \\ m_p v_z \end{pmatrix}, \begin{pmatrix} m_1 \mathbf{v}^2 \\ m_2 \mathbf{v}^2 \\ \vdots \\ m_p \mathbf{v}^2 \end{pmatrix}.$$

This space is of dimension  $p+4$  and the above list of functions is noted  $\boldsymbol{\phi}^l, l \in [1, p+4]$ .  $\mathbb{K}$  is the natural space of collisional invariants but contrarily to the case of monatomic gas there exists a "complementary" space  $\mathbb{C}$  of moments of degree 1 in velocity which is not conserved. Our purpose is now to exhibit a basis of  $\mathbb{C}$ .

**Definition 1.** Let  $\mathbf{C}_i$  be the vector having 0 everywhere except on its  $i^{\text{th}}$  line where it lies  $\mathbf{v} - \mathbf{u}$ . Note by  $\mathcal{P}_{\mathbb{K}}$  the orthogonal projection on  $\mathbb{K}$  and  $\mathcal{I}$  the identity operator. Then we define  $\mathbb{C}$  as the space generated by the vectors  $(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_i), i \in [1, p]$ .

We have the following lemma

**Lemma 1.** The family  $(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_i), i \in [1, p]$  is composed of  $p-1$  independant "vectors" and as a consequence the dimension of  $\mathbb{C}$  is  $3(p-1)$ .

We postpone the proof of this lemma in appendix.

## 2.2 Properties of the Boltzmann operator.

### 2.2.1 Collisional invariants, H-theorem and equilibrium states.

1. **Collisional invariants:** for all  $\mathbf{f} = (f_1, \dots, f_p)$  the following equation holds

$$\sum_{i=1}^{i=p} \sum_{j=1}^{j=p} \int_{\mathbb{R}^3} Q_{ji}(f_j, f_i) \phi_i d\mathbf{v} = 0$$

iff  $\phi \in \mathbb{K}$ .

2. **H-theorem:** for any list of nonnegative functions  $\mathbf{f} = (f_1, \dots, f_p)$  it holds that

$$\sum_{i=1}^{i=p} \sum_{j=1}^{j=p} \int_{\mathbb{R}^3} Q_{j,i}(f_j, f_i) \ln f_i d\mathbf{v} \leq 0. \quad (5)$$

3. **Equilibrium states:** the equality holds in the above equation if and only if  $\mathbf{f}$  is at thermodynamical equilibrium i.e there exists hydrodynamic values  $n_1, \dots, n_p, \mathbf{u}, T$  such that

$$\forall i \in [1, p], f_i = \mathcal{M}_i$$

In such a case we denote  $\mathbf{f} = \mathbf{M}$ . Moreover the equality in (5) holds if and only if

$$\sum_{i=1}^{i=p} \sum_{j=1}^{j=p} \int_{\mathbb{R}^3} Q_{j,i}(f_j, f_i) d\mathbf{v} = 0$$

that is iff  $f_i = \mathcal{M}_i$ .

### 2.2.2 Linearized operator.

Define now the linearized Boltzmann operator  $\mathcal{L}_B := (\mathcal{L}_{B,1}, \dots, \mathcal{L}_{B,p})$  operating on  $\mathbf{g} = (g_1, \dots, g_p) \in \mathbb{L}^2(\mathbf{M})$  as

$$\forall i \in [1, p], \mathcal{L}_{B,i}(\mathbf{g}) := \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon \mathcal{M}_i} \sum_{j=1}^{j=p} Q_{ji}(\mathcal{M}_j(1 + \epsilon g_j), \mathcal{M}_i(1 + \epsilon g_i)).$$

Basically, such an operator may be computed as:

$$\mathcal{L}_{B,i}(\mathbf{g}) = \frac{1}{\mathcal{M}_i} \left( \sum_{j=1}^p Q_{ji}(\mathcal{M}_j, \mathcal{M}_i g_i) + Q_{ji}(\mathcal{M}_j g_j, \mathcal{M}_i) \right). \quad (6)$$

**Property 1.** *The operator  $\mathcal{L}_B$  is self-adjoint and non-negative and its kernel is exactly  $\mathbb{K}$ .*

Another important property of the linearized operator is the following:

**Property 2.**  *$\mathcal{L}_B$  is the sum of a diagonal operator  $f \mapsto \nu f$ , such that  $(\nu f)_i = \nu_i(\mathbf{v}) f^i$  and a compact operator  $\mathcal{K}$  (for regular enough differential cross sections) such that for any  $i \in \{1, \dots, p\}$ ,*

$$(\mathcal{K}f)_i = \sum_{j=1}^p \left( \int_{\mathbb{R}^3 \times \mathcal{S}^2} \mathcal{M}_j f^i(\mathbf{v}_{ji}^*) \sigma_{ji}(\mathbf{V} \cdot \boldsymbol{\omega}, \|\mathbf{V}\|) \|\mathbf{V}\| d\boldsymbol{\omega} d\mathbf{w} + \frac{1}{\mathcal{M}_j} Q_{ji}(\mathcal{M}_j f^j, \mathcal{M}_i) \right).$$

*As a consequence  $\mathcal{L}_B$  is a Fredholm operator and  $\mathcal{L}_B : \mathbb{K}^\perp \rightarrow \mathbb{K}^\perp$  is continuous and invertible. For the sequel, we note as  $\mathcal{L}_B^{-1}$  the pseudo inverse of  $\mathcal{L}_B$ . It is an obvious self adjoint positive operator on  $\mathbb{K}^\perp$ .*

*Proof.* This proof is given in details in [3] in the context of a two component gas and can be easily generalized to a given number of components.  $\square$

### 2.3 The Boltzmann operator as a model for other kinetic operators: minimum properties for a BGK operator.

In many practical situations the computation of the full Boltzmann operator is expansive. This is the reason why one looks for BGK ones which will be denoted as  $\mathcal{R} := (\mathcal{R}_1, \dots, \mathcal{R}_p)$  in the sequel. For mono-specie system such operators exist already and an abundant literature may be found on the subject. However for multi-species systems things are less clear even if there exist already different models. Our framework is that of the classical Boltzmann operator, that is  $\mathcal{R}$  must satisfy the following list of properties. The first ones read

$$\mathcal{R}_i(\mathbf{f}) = 0 \Leftrightarrow \exists n^i, \mathbf{u}, T \text{ s.t. } \forall i \in [1, p], f_i = \mathcal{M}_i \quad (7)$$

while the other are those of section 2.2.1

$$\forall \mathbf{f}, f_i \geq 0, \forall \phi, \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathcal{R}_i(\mathbf{f}) \phi_i d\mathbf{v} = 0 \Leftrightarrow \phi \in \mathbb{K}, \quad (8)$$

$$\forall \mathbf{f}, f_i \geq 0, \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathcal{R}_i(\mathbf{f}) \ln(f_i) d\mathbf{v} \leq 0, \quad (9)$$

$$\int_{\mathbb{R}^3} \mathcal{R}_i(\mathbf{f}) \ln(f_i) d\mathbf{v} = 0 \Leftrightarrow \exists n^i, \mathbf{u}, T \text{ s.t. } \forall i \in [1, p], f_i = \mathcal{M}_i. \quad (10)$$

If these properties are satisfied we define the linearized BGK operator  $\mathcal{L} := (\mathcal{L}_1, \dots, \mathcal{L}_p)$  acting on  $\mathbf{g} \in \mathbb{L}^2(\mathcal{M})$  with

$$\forall i \in [1, p], \mathcal{L}_i(\mathbf{g}) = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon \mathcal{M}_i} \mathcal{R}_i(\mathcal{M}_1(1 + \epsilon g_1), \dots, \mathcal{M}_p(1 + \epsilon g_p)).$$

Then the second list of properties concerns the linear operator.

$$\text{Ker}(\mathcal{L}) = \mathbb{K} \text{ and } \mathcal{L} \text{ is Fredholm on } \mathbb{K}^\perp, \quad (11)$$

$$\mathcal{L} \text{ is self adjoint negative on } \mathbb{K}^\perp. \quad (12)$$

As a consequence of the Fredholm property the operator  $\mathcal{L}$  is continuous and one to one on  $\mathbb{K}^\perp$  as well as its pseudo inverse  $\mathcal{L}^{-1} : \mathbb{K}^\perp \mapsto \mathbb{K}^\perp$  which is also self adjoint and negative on  $\mathbb{K}^\perp$ .

**Definition 2.** Any kinetic operator satisfying all above properties (7, 8, 10, 11, 12) is said to be properly defined.

### 3 The Navier-Stokes equations for mixtures and the Boltzmann expansion: importance of the linearized operator.

In this section we aim firstly at introducing the hydrodynamic equations that lead the behaviour of gas mixtures. We recall how the "new" terms appearing in the Navier-Stokes equations are interpreted from a physical point of view using the thermodynamics of irreversibility processes (TIP). Yet the measurements of the kinetic or hydrodynamic coefficients is a hard task and it is of interest to look at the hydrodynamical limit of the Boltzmann equation to approximate them. Following the path of Chapman and Cowling for binary gas mixtures we secondly perform a Chapman-Enskog expansion of the Boltzmann equation in the case of more than two species. Though the previous physically correct Navier-Stokes equations are necessary to make some conclusions concerning the linearized Boltzmann operator. This comparison between the two theories also allows to derive some conditions on the hydrodynamical coefficients. In particular we are going to see that the computation of those coefficients and their properties only depends on the linearized kinetic operator  $\mathcal{L}$ .

#### 3.1 The Navier-Stokes equations.

The Navier-Stokes system for a mixture of  $p$  components reads

$$\forall i \in [1, p], \partial_t n^i + \nabla \cdot (n^i \mathbf{u} + \mathbf{J}_i) = 0, \quad (13)$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\mathbb{P} + \rho \mathbf{u} \otimes \mathbf{u} + \mathbb{J}_{\mathbf{u}}) = 0, \quad (14)$$

$$\partial_t E + \nabla \cdot (E \mathbf{u} + \mathbb{P}[\mathbf{u}] + \mathbb{J}_{\mathbf{u}}[\mathbf{u}] + \mathbf{J}_q) = 0, \quad (15)$$

where  $\mathbf{J}_i$ ,  $\mathbb{J}_{\mathbf{u}}$   $\mathbf{J}_q$  are respectively the mass, momentum and heat fluxes. Such fluxes have been observed experimentally since a long time. From a phenomenological point of view they have been linked to the gradients of macroscopic variables like density, velocity and temperature through coefficients or tensors. One of the challenge of the transport theory consists in finding models to compute these coefficients. Technically this can be achieved from at least two ways: one by using the general construction of the thermodynamic of irreversible processes (TIP), the other by considering the hydrodynamical limit of the Boltzmann equation. The second method will be detailed in this article. But we first need to give few words about the first one.

#### 3.2 The Thermodynamic of Irreversible Processes.

The classical reference concerning the thermodynamics of irreversibility processes (TIP) for gas mixtures is the book of De Groot and Mazur [18]. In this book it is shown how to define the different fluxes  $\mathbf{J}_i$ ,  $\mathbf{J}_u$  and  $\mathbf{J}_q$  basing on the second principle of thermodynamic. Though the structure of those fluxes are



expressed in a slightly different form and one can show that they can be written as

$$\begin{aligned}\mathbf{J}_i &= \sum_{j=1}^{j=p} L_{ij} \nabla \left( \frac{-\mu_j}{T} \right) + L_{i\mathbf{q}} \nabla \left( \frac{1}{T} \right) \\ \mathbf{J}_{\mathbf{q}} &= \sum_{j=1}^{j=p} L_{\mathbf{q}j} \nabla \left( \frac{-\mu_j}{T} \right) + L_{\mathbf{q}\mathbf{q}} \nabla \left( \frac{1}{T} \right) \\ \mathbb{J}_{\mathbf{u}} &= L_{\mathbf{u}\mathbf{u}} \mathbb{D}(\mathbf{u}),\end{aligned}\tag{16}$$

where  $\mu_i$  is the chemical potential of the species  $i$  in the mixture and  $\mathbb{D}(\mathbf{u})$  the traceless part of the deformation tensor. In a mixture of ideal gases the chemical potential by species is known (up to some additional constant) through the relation:

$$-\frac{\mu_i}{T} = k_B \left( \ln(n_i) - \frac{3}{2} \ln \left( \frac{2\pi k_B T}{m_i} \right) \right).\tag{17}$$

Moreover if one assumes that the Casimir-Onsager relations are satisfied for kinetic coefficients then the following matrix:

$$\mathbf{L} := \begin{bmatrix} L_{ij} & L_{i\mathbf{q}} & 0 \\ L_{\mathbf{q}i} & L_{\mathbf{q}\mathbf{q}} & 0 \\ 0 & 0 & L_{\mathbf{u}\mathbf{u}} \end{bmatrix}\tag{18}$$

must be symmetrical non positive<sup>1</sup>. On top of that it must be added the mass conservation equation stating that

$$\sum_{i=1}^{i=p} m_i \mathbf{J}_i = 0 \Rightarrow \forall j \in [1, p], \sum_{i=1}^{i=p} m_i L_{ij} = 0.\tag{19}$$

As a consequence the rank of the matrix  $L_{ij}$  is at most  $p - 1$ . However the TIP is not capable anymore in whole generality to say more things about  $\mathbf{L}$ . In particular if one uses the relation (19) and the symmetry of the matrix  $\mathbf{L}$  (18) then we can only infer that there are  $p(p + 1)/2 + 1$  unknowns to search for. Using the phenomenological point of view such fluxes are preferentially expressed as gradient of density, temperature and velocity. They read

$$\mathbf{J}_i = \sum_{j=1}^{j=p} D_{ij} \nabla n_j + D_{iT} \nabla T, \quad \mathbf{J}_{\mathbf{q}} = \sum_{j=1}^{j=p} D_{\mathbf{q}j} \nabla n_j - D_{\mathbf{q}\mathbf{q}} \nabla T,$$

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<sup>1</sup>Following precisely the TIP, such a matrix must be actually symmetrical *non negative*. This discrepancy is simply linked to the definition one uses for the entropy. To perfectly match the thermodynamical approach, we should have defined

$$H(\mathbf{f}) := -k_B \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} (f_i \ln(f_i) - f_i) d\mathbf{v}$$

where  $k_B$  is the Boltzmann constant. The choice we have made for the entropy is however the most usual for mathematical reasons as it enables to consider the minimization of a convex functions rather than maximization of concave functions. As a consequence of this definition, the corresponding Onsager matrix must be symmetrical non positive rather than symmetrical non negative

where  $D_{ij}$  and  $D_{iT}$ ,  $D_{\mathbf{q}j}$  and  $D_{\mathbf{q}\mathbf{q}}$  respectively denote the Fick, Soret, Duffour and Fourier coefficients. The main reason for introducing such coefficients lies on the possibility to measure them conveniently from experimental data while kinetic coefficients cannot be obtained directly. There drawback are the lost of symmetry -Casimir-Onsager relations- on the phenomenological coefficients. Remark however that for mixture of ideal gases the one to one correspondance between those coefficients and the matrix  $\mathbf{L}$  is straightforward. As we will see in the next section, writing the different fluxes in term of the kinetic coefficients (16) is the most natural choice not only for the TIP but also to express them starting from the kinetic theory.

### 3.3 Basic recalls on the Chapman-Enskog theory.

The Chapman-Enskog theory begins with performing a change in scale in the time and space coordinates and considers the rescaled kinetic equation:

$$\forall i \in [1, p], \partial_t f_i^\epsilon + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i^\epsilon = \frac{1}{\epsilon} \sum_{k=1}^{k=p} Q_{ki}(f_k^\epsilon, f_i^\epsilon). \quad (20)$$

By letting then  $\epsilon \rightarrow 0$  one searches for an asymptotical expansion of  $f_i^\epsilon$  as  $f_i^0 + \epsilon f_i^1 + \dots$  such that (20) remains bounded. As a consequence, at order  $\epsilon^{-1}$  one must choose  $f_i^0$  such that the collision operator vanishes, meaning then

$$\forall i \in [1, p], f_i^0 = \mathcal{M}_i, \quad (21)$$

where the hydrodynamical parameters  $n^i, T, \mathbf{u}$  defining the  $\mathcal{M}_i$  depend on space and time. Then setting  $f_i^1 = \mathcal{M}_i g_i$  and considering the order  $\epsilon^0$ , one must solve the equation:

$$\forall i \in [1, p], (\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}}) [\mathcal{M}_i] = \mathcal{M}_i \mathcal{L}_{B,i}(g_1, \dots, g_p), \quad (22)$$

where  $\mathcal{L}_B := (\mathcal{L}_{B,1}, \dots, \mathcal{L}_{B,p})$  is the linearized collision operator as it as been defined in the former section. Next we aime to calculate the left-hand side of (22) in such a way that the expression of  $g$  can be easily computed. Following the path of Levermore ([25]), the equation (22) may be written as follows:

**Lemma 2.** *The linearized operator defined in (22) is given by the expression*

$$\mathcal{L}_B(g) = \sum_{j=1}^{j=p} k_B^{-1} (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_j) \cdot \nabla \left( \frac{-\mu_j}{T} \right) + \mathbb{A} : \mathbb{D}(\mathbf{u}) + \mathbf{B} \cdot \nabla \left( \frac{1}{T} \right) \quad (23)$$

where  $\mathcal{I}$  refers to the identity operator on  $\mathbb{L}^2(\mathbf{M})$ ,  $\mathcal{P}_{\mathbb{K}}$  the orthogonal projection on  $\mathbb{K}$ , while the list of tensors  $\mathbb{A}, \mathbf{B}$  (that belong to  $\mathbb{K}^\perp$ ) feature on their  $i^{\text{th}}$  line the tensors:

$$\begin{aligned} (\mathbb{A})_i &= m_i \left[ (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) - \frac{1}{3} \|\mathbf{v} - \mathbf{u}\|^2 \mathbb{I} \right], \\ (\mathbf{B})_i &= (\mathbf{v} - \mathbf{u}) \left[ \frac{1}{2} m_i (\mathbf{v} - \mathbf{u})^2 - \frac{5}{2} k_B T \right] \end{aligned}$$

while the tensor  $\mathbb{D}(\mathbf{u})$  reads as:

$$\mathbb{D}(\mathbf{u}) = \frac{1}{2} \left[ \nabla_{\mathbf{x}} \mathbf{u} + (\nabla_{\mathbf{x}} \mathbf{u})^T \right] - \frac{1}{3} (\nabla_{\mathbf{x}} \cdot \mathbf{u}) \mathbb{I}.$$

The proof of Lemma 2 is left to appendix.

Thanks to Properties 1 and 2, such an equation has one unique solution in  $\mathbf{g} \in \mathbb{K}^\perp$ .

### 3.4 Link between the Boltzmann equation and the Thermodynamic of Irreversible Processes.

While this theory has already been set in [18] and in some way in [14] we present here a concise formalism based on the mathematical properties of the linearized operator  $\mathcal{L}_B$  and on the space  $\mathbb{C}$ . Once the perturbative function  $\mathbf{g}$  has been computed, one can recover the formal expressions of the different fluxes as

**Lemma 3.** For  $g$  defined by relation 23 the fluxes  $\mathbf{J}_i$ ,  $\mathbb{J}_u$  and  $\mathbf{J}_q$  are given by

$$\mathbf{J}_i = \langle \mathbf{g}, (\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_i) \rangle, \quad \mathbb{J}_u = \langle \mathbf{g}, \mathbb{A} \rangle, \quad \mathbf{J}_q = \langle \mathbf{g}, \mathbf{B} \rangle.$$

Thanks to Lemma 2, this enables to recover the expression of the kinetic coefficients. Indeed  $L_{ij}$ ,  $L_{iq}$ ,  $L_{qi}$ ,  $L_{uu}$  and  $L_{qq}$  can be respectively obtained from

$$L_{ij} \mathbf{I} = k_B^{-1} \langle \mathcal{L}_B^{-1} [(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_i)], (\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_j) \rangle, \quad (24)$$

$$L_{iq} \mathbf{I} = L_{qi} \mathbf{I} = \langle \mathcal{L}_B^{-1}(\mathbf{B}), (\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_i) \rangle, \quad (25)$$

$$L_{uu} \mathbf{I} \otimes \mathbf{I} = \langle \mathcal{L}_B^{-1}(\mathbb{A}), \mathbb{A} \rangle, \quad (26)$$

$$L_{qq} \mathbf{I} = \langle \mathcal{L}_B^{-1}(\mathbf{B}), \mathbf{B} \rangle. \quad (27)$$

When using the linearized Boltzmann operator, the fact that tensors finally reduce to scalar coefficients (meaning that they are spherical) is linked to the Galilean invariance of the differential cross section in the full Boltzmann collision operator. Here we see immediately that the Onsager-Casimir properties  $\mathbf{L}$  (18) are derived from the properties of symmetry and non positiveness of the linearized operator  $\mathcal{L}_B^{-1}$ . It is interesting to note here, that the kinetic coefficients  $L_{ij}$  are known as soon as we know the vectors  $(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_j)$ ,  $j \in [1, p]$ . In short this means that the Fick coefficients form a family  $p-1$  degree of freedom. For example in the case of two species they can be computed from a single one.

**Remark 1.** All properly defined operator in the sense of definition 2 gives a Navier-Stokes equation at the hydrodynamical limit with kinetic coefficients given by (24, 25, 26, 27) replacing  $\mathcal{L}_B$  by the proper linearized operator  $\mathcal{L}$

## 4 Definition of a Fick-Relaxation operator.

### 4.1 The idea of the relaxation: link with the BGK operator.

The main idea to construct our model is to reproduce the above connections between the thermodynamic forces (and associated kinetic repeat coefficients) and the kinetic theory in a simplest way. We have seen that every **linear** small perturbations around local equilibrium states are moments of the perturbation around the local Maxwellian states and kinetic coefficients are only connected to the properties of the linear interaction operator. Kinetic coefficients can be interpreted as (functions of) relaxation rates associated to those moments and any simple model should reproduce this in the hydrodynamical limit. This is the principle that was shed in light in [12, 13]. Then if one thinks of relaxation models the second principle is that the corresponding relaxation function(s) must satisfy an entropy minimization under constraints that are exactly the relaxation of the moments under consideration. This has permitted to recover the ES-BGK operators for monatomic ([22]) and polyatomic gases ([4]). Remark that if one just takes into account the conservation laws in the second principle one falls on the classical BGK model ([8]).

In the present work we restrict our approach to *the Fick and Newton laws*. Fick laws must actually be obtained from the kinetic theory using moments of the distribution functions in  $\mathbb{K}^\perp$  (see (24)). Let  $\mathbf{w}_r \in \mathbb{K}^\perp$  and consider the moment  $\sum_{j=1}^p \int_{\mathbb{R}^3} f_j \mathbf{w}_{r,j}$ . Then replacing the Boltzmann collision operator with a relaxation operator

$$\mathcal{R}(\mathbf{f}) = \nu(\mathbf{G} - \mathbf{f}), \quad (28)$$

the above interpretation amounts to set

$$\nu \sum_{j=1}^{j=p} \int_{\mathbb{R}^3} (G_j - f_j) \mathbf{w}_{r,j} = -\lambda_r \sum_{j=1}^{j=p} \int_{\mathbb{R}^3} f_j \mathbf{w}_{r,j}, \quad (29)$$

where  $\lambda_r$  is a relaxation coefficient. The choice of a basis  $(\mathbf{w}_r)_{r=1,\dots,p-1}$  of  $\mathbb{K}^\perp$  is crucial as well as that of the relaxation coefficients  $(\lambda_r)_{r=1,\dots,p-1}$  to obtain the Fick laws at the hydrodynamical limit ( $\mu$  is a free parameter that will be adjusted later on to fit the viscosity). We proceed as follows. We firstly compute the relaxation coefficients  $\lambda_r$  and corresponding moments  $\mathbf{w}_r$  such as to obtain the above coefficients. This computation is essentially based on two arguments (theorem 1):

1. the mass fluxes must depend on the moments  $\int \mathcal{M}_j \mathbf{g}_j \mathbf{w}_{r,j}$  of a small perturbation  $\mathbf{g}$  around a local thermodynamical equilibrium  $\mathbf{M}$ ,
2. the relaxation coefficients  $\lambda_r$  and corresponding moments  $\mathbf{w}_r$  are only connected to the property of the Fick coefficients matrix  $L_{ij}$ .

Secondly  $\mathbf{G}$  is obtained through the minimization of entropy principle under the above constraints plus the conservation laws (theorem 2).

## 4.2 Computation of the relaxation coefficients and moments.

Before we set the main result it is important to examine the properties of the Fick coefficients matrix  $L_{ij}$  obtained from the linearization of the true Boltzmann operator.

**Lemma 4.** *If it is computed thanks to the Boltzmann linearized operator, the matrix  $L_{ij}, (i, j) \in [1, p]^2$  of the kinetic coefficient has a rank  $p - 1$  and for any  $k \in [1, p - 1]$  the matrix  $L_{ij}, (i, j) \in [1, k]^2$  has a full rank.*

We postpone the proof of this lemma to appendix. An important consequence of this lemma is the following result.

**Lemma 5.** *The symmetric non positive matrix  $L_{ij}^*$  defined by*

$$L_{ij}^* := \frac{k_B L_{ij}}{\|\mathbf{C}_i\| \|\mathbf{C}_j\|} = k_B L_{ij} \sqrt{\frac{m_i}{n_i k_B T}} \sqrt{\frac{m_j}{n_j k_B T}}, \quad \forall i, j \in [1, p] \quad (30)$$

*always diagonalizes in an orthonormal basis as:*

$$L^* = W^T D^* W$$

*so that the corresponding eigenvalues  $(d_r^*)_r$  are non null for  $r = 1, \dots, p - 1$  while  $d_p^* = 0$ . Moreover the vectors defined by*

$$\mathbf{w}_r = \sum_{s=1}^p W_{rs} \frac{\mathbf{C}_s}{\|\mathbf{C}_s\|}, \quad r = 1, \dots, p - 1 \quad (31)$$

*form an orthonormal basis of  $\mathbb{C}$  while the vector*

$$\mathbf{w}_p = \sum_s \sqrt{\frac{\rho_s}{\rho}} \frac{\mathbf{C}_s}{\|\mathbf{C}_s\|} = \pm \sum_{s=1}^{s=p} W_{ps} \frac{\mathbf{C}_s}{\|\mathbf{C}_s\|} \quad (32)$$

*is orthogonal to  $\mathbb{C}$  (in fact belongs to  $\mathbb{K}$ ) and normalized.*

*Proof.* Since  $L^*$  is symmetrical, it may be diagonalized. The fact that it has exactly one vanishing eigenvalue is linked to its rank which is  $p - 1$ . Finally, we can always permute indexes so that  $d_p^* = 0$ . Consider the vector  $\varpi$  whose components are  $\sqrt{\rho_j}/\sqrt{\rho}$ . Then a direct computation shows that:

$$(L^* \varpi)_i = \sum_{j=1}^{j=p} \frac{k_B L_{ij}}{\|\mathbf{C}_i\| \|\mathbf{C}_j\|} \sqrt{\frac{\rho_j}{\rho}} = \frac{k_B}{\|\mathbf{C}_i\| \sqrt{\rho k_B T}} \sum_{j=1}^{j=p} L_{ij} m_j = 0$$

the last equality being obtained thanks to (19). Besides, the vector  $\varpi$  is normalized for the usual vector norm. As a consequence, when diagonalizing the matrix  $L^*$  in a orthonormalized basis, then the normalized eigenvector associated to  $d_p^* = 0$  is necessary equal to  $\pm \varpi$ . Then we have  $W_{ps} = \pm \sqrt{\rho_s}/\sqrt{\rho}$ . At

last, as  $\|\mathbf{C}_s\| = \sqrt{n^s k_B T} / \sqrt{m_s}$ , a direct computation shows that the vector  $\mathbf{w}_p$  has  $m_i (\mathbf{v} - \mathbf{u}) / \sqrt{\rho k_B T}$  on its  $i^{\text{th}}$  line, so belongs to  $\mathbb{K}$ .

Now, since the matrix  $W^T$  is orthogonal and since the family  $\mathbf{C}_i / \|\mathbf{C}_i\|$ ,  $i \in [1, p]$  is orthonormalized for the  $\mathbb{L}^2(\mathbf{M})$  dot product, then the family  $\mathbf{w}_s$ ,  $s \in [1, p]$  is also orthonormalized for the  $\mathbb{L}^2(\mathbf{M})$  dot product.

Finally, in the family  $\mathbf{w}_s$ ,  $s \in [1, p-1]$ , every vector is a linear combination of the  $\mathbf{C}_i$ ,  $i \in [1, p]$  but does not belong to  $\mathbb{K}$  so it is in  $\mathbb{C}$  and finally constitutes an orthonormalized basis of it.  $\square$

Now we can set our main result which relies the eigenvalues of the matrix  $L^*$  to the relaxation coefficients.

**Theorem 1.** *Let  $\mathcal{L}$  be the linearized operator of  $\mathcal{R}$  (see section 2.3). Assume that (10) holds and that  $\mathcal{L}^{-1}(\mathbf{B})$  and  $\mathcal{L}^{-1}(\mathbb{A})$  are orthogonal to  $\mathbb{C}$ . Let  $d_r^*$  and  $\mathbf{w}_r$  ( $r \in [1, p]$ ) be defined as in lemma 5, then setting*

$$\lambda_r = d_r^{*-1}, \quad \lambda_p = 0 \quad (33)$$

the BGK model that satisfies relaxation equations (29) allows to recover at the hydrodynamic limit the Fick laws meaning that the corresponding mass fluxes are given by

$$\mathbf{J}_i = \sum_{j=1}^{j=p} L_{ij} \nabla \left( \frac{-\mu_j}{T} \right).$$

*Proof. Step 1* Let us consider the rescaled equation

$$\partial_t \mathbf{f}^\epsilon + \mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{f}^\epsilon = \frac{1}{\epsilon} \mathcal{R}(\mathbf{f}^\epsilon) \quad (34)$$

and perform a Chapman-Enskog expansion. Assume that (10) holds then the zeroth order equation satisfied by  $\mathbf{f}^0 = \mathbf{M}$  yields as usual the Euler equation. As a consequence lemma 2 remains valid and we have

$$\mathcal{L}(\mathbf{g}) = \sum_{j=1}^{j=p} k_B^{-1} (\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_j) \cdot \nabla \left( \frac{-\mu_j}{T} \right) + \mathbb{A} : \mathbb{D}(\mathbf{u}) + \mathbf{B} \cdot \nabla \left( \frac{1}{T} \right). \quad (35)$$

Next assuming that  $\mathcal{L}^{-1}(\mathbf{B})$  and  $\mathcal{L}^{-1}(\mathbb{A})$  are orthogonal to  $\mathbb{C}$  (see definition 1) then equation (23) implies that mass fluxes defined by

$$\mathbf{J}_i = \langle \mathbf{g}, \mathbf{C}_i \rangle$$

depend only on the values of  $(\nabla \mu_j / T)$ . Our aim is to obtain at the hydrodynamic limit the Fick coefficients  $L_{ij}$  computed from the true Boltzmann equations (1), that is

$$\mathbf{J}_i = \langle \mathbf{g}, \mathbf{C}_i \rangle = \sum_{j=1}^p L_{sj} \nabla \left( \frac{-\mu_j}{T} \right). \quad (36)$$

**Step 2** Consider now the first order expansion of relaxation equations (29)

$$\langle \mathcal{L}(\mathbf{g}), \mathbf{w}_r \rangle = -\lambda_r \langle \mathbf{g}, \mathbf{w}_r \rangle, \quad r \in [1, p], \quad (37)$$

If we choose the moments  $\mathbf{w}_r$  as linear combinations of the basis  $(\mathbf{C}_i)_i$  then the right hand sides of the above equations can be written in terms of the required mass fluxes (36) while the left hand sides are determined thanks to (35). So we need to find relaxation coefficients and moments such that both sides of equations (37) fit. Let us compute those terms with our choice of moments  $(\mathbf{w}_r)_r$  (lemma 5). The right hand sides read

$$\langle \mathbf{g}, \mathbf{w}_r \rangle = \sum_{s=1}^p \frac{W_{rs}}{\|\mathbf{C}_s\|} \mathbf{J}_s = \sum_{s,j=1}^p \frac{W_{rs}}{\|\mathbf{C}_s\|} L_{sj} \nabla \left( \frac{-\mu_j}{T} \right), \quad (38)$$

where  $W$  is the matrix of eigenvectors defined in lemma 5. Next the left hand sides can be computed thanks to (23)

$$\begin{aligned} \langle \mathcal{L}(\mathbf{g}), \mathbf{w}_r \rangle &= \sum_{j,s=1}^p k_B^{-1} \frac{W_{rs}}{\|\mathbf{C}_s\|} \langle \mathbf{C}_j, \mathbf{C}_s \rangle \nabla \left( \frac{-\mu_j}{T} \right) \\ &= k_B^{-1} \sum_{j=1}^p W_{rj} \|\mathbf{C}_j\| \nabla \left( \frac{-\mu_j}{T} \right), \quad r = 1, \dots, p-1 \end{aligned}$$

since  $\langle (\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_j), \mathbf{w}_r \rangle = \langle \mathbf{C}_j, \mathbf{w}_r \rangle \forall \mathbf{w}_r \in \mathbb{C}$ . As concerns the case  $r = p$  it is obvious that

$$\frac{1}{\sqrt{\rho k_B T}} \sum_j \langle \mathcal{L}(\mathbf{g}), m_j \mathbf{C}_j \rangle = 0.$$

To summarize (37) reads

$$k_B^{-1} \sum_{j=1}^p W_{rj} \|\mathbf{C}_j\| \nabla \left( \frac{-\mu_j}{T} \right) = -\lambda_r \sum_{s,j=1}^p \frac{W_{rs}}{\|\mathbf{C}_s\|} L_{sj} \nabla \left( \frac{-\mu_j}{T} \right), \quad r = 1, \dots, p-1,$$

and since those equations must be valid for all values of  $(\nabla \mu_j / T)_j$  we have

$$W_{rj} = -\lambda_r \sum_{s=1}^p W_{rs} L_{sj}^*, \quad \forall r = 1, \dots, p-1, \quad j = 1, \dots, p$$

where  $L_{sj}^*$  is defined in equation 30. We can also complete this set of equations with

$$0 = \sum_{s=1}^p W_{ps} L_{sj}^*, \quad j = 1, \dots, p$$

thanks to (19) and the symmetry of  $L_{sj}^*$ . Multiplying both side of the above equations with  $W_{tj}$  and summing over  $j$  we obtain

$$\begin{aligned}\delta_{rt} &= -\lambda_r \sum_{s,j=1}^p W_{rs} L_{sj}^* W_{tj}, \quad \forall r = 1, \dots, p-1, t = 1, \dots, p \\ 0 &= \sum_{s,j=1}^p W_{ps} L_{sj}^* W_{pj}, \quad \forall t = 1, \dots, p\end{aligned}$$

which amounts to diagonalize  $L^*$  and thus define  $\lambda_r = -d_r^{*-1}$ ,  $r = 1, \dots, p-1$  and  $\lambda_p = 0$  in a unique way (see lemma 5).  $\square$

### 4.3 Definition Fick-Relaxation operator.

**Theorem 2.** Let  $\phi^l, l \in [1, p+4]$  be the natural basis for  $\mathbb{K}$  and  $\mathbf{w}_r, r \in [1, p-1]$  be the orthonormalized basis for  $\mathbb{C}$  to which we associate the relaxation values  $\lambda_r, r \in [1, p-1]$ . For  $\mathbf{f}$  a list non negative non null functions with suitable integration properties, consider the set  $\mathbf{K}(\mathbf{f})$  defined as

$$\mathbf{g} \in \mathbf{K}(\mathbf{f}) \Leftrightarrow \begin{cases} \forall l \in [1, p+4], \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \phi_i^l (g_i - f_i) d\mathbf{v} = 0, \\ \forall r \in [1, p-1], \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathbf{w}_{r,i} (g_i - (1 - \frac{\lambda_r}{\nu}) f_i) d\mathbf{v} = \mathbf{0}. \end{cases} \quad (39)$$

Then there exist a unique minimizer  $\mathbf{G}$  of the entropy function  $H$  under the constraint that  $\mathbf{G}$  should belong to  $\mathbf{K}(\mathbf{f})$ . Moreover, if we note by  $n^i, \mathbf{u}^i, T$  the hydrodynamic parameters associated to the function  $\mathbf{f}$ , then such a minimizer reads as:

$$\forall i \in [1, p], G_i = \frac{n^i}{(2\pi k_B T / m_i)^{3/2}} \exp\left(-\frac{m_i (\mathbf{v} - \mathbf{u}_i)^2}{2k_B T}\right), \quad (40)$$

where the velocities  $\mathbf{u}_i$  are defined by the relations

$$\underline{\mathbf{U}} - \mathbf{U} = N^{-1} W^T \left( \mathbf{I} - \frac{1}{\nu} \Lambda \right) W \mathbf{N} (\overline{\mathbf{U}} - \mathbf{U}). \quad (41)$$

Here  $\overline{\mathbf{U}} = (\mathbf{u}^1, \dots, \mathbf{u}^p)^T$ ,  $\underline{\mathbf{U}} = (\mathbf{u}_1, \dots, \mathbf{u}_p)^T$  and  $\mathbf{U} = (\mathbf{u}, \dots, \mathbf{u})^T$ .  $\mathbf{N}$  and  $\Lambda$  denote respectively the diagonal matrix with diagonal terms  $(\sqrt{\rho_1}, \dots, \sqrt{\rho_p})$  and  $(\lambda_1, \dots, \lambda_p)$ .

*Proof.* The first set of constraints amounts to impose the conservation of densities for each species and the global conservation of momentum and energy. Let us now perform the computation of velocities  $(u_i)_i$ . The set of constraints related to the velocities are firstly those involving moments  $(\mathbf{w}_r)_{r=1, \dots, p-1}$  and secondly those expressing conservation of momentum (moments  $\phi^{i=p+1, p+2, p+3}$ ). Remark that the later can be written as

$$\sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathbf{w}_{p,i} (g_i - f_i) d\mathbf{v} = \mathbf{0}$$



thanks to the definition of  $\mathbf{w}_p$  (32). Then the whole set of constraints on the moments  $(\mathbf{w}_r)_r$  reads

$$\begin{aligned} & \sum_{j=1}^p W_{rj} \frac{1}{\|\mathbf{C}_j\|} \int G_j(\mathbf{v} - \mathbf{u}) dv = \left(1 - \frac{\lambda_r}{\nu}\right) \sum_{j=1}^p W_{rj} \frac{1}{\|\mathbf{C}_j\|} \int f_j(\mathbf{v} - \mathbf{u}) dv \\ \Leftrightarrow & \sum_{j=1}^p W_{rj} \frac{n^j}{\|\mathbf{C}_j\|} (\mathbf{u}_j - \mathbf{u}) = \left(1 - \frac{\lambda_r}{\nu}\right) \sum_{j=1}^p W_{rj} \frac{n^j}{\|\mathbf{C}_j\|} (\mathbf{u}^j - \mathbf{u}), \quad r = 1, \dots, p \\ \Leftrightarrow & \sum_{j=1}^p W_{rj} \sqrt{\rho_j} (\mathbf{u}_j - \mathbf{u}) = \left(1 - \frac{\lambda_r}{\nu}\right) \sum_{j=1}^p W_{rj} \sqrt{\rho_j} (\mathbf{u}^j - \mathbf{u}), \quad r = 1, \dots, p. \end{aligned}$$

This system of equations can be written

$$W \mathbf{N} (\underline{\mathbf{U}} - \mathbf{U}) = \left( \mathbf{I} - \frac{1}{\nu} \Lambda \right) W \mathbf{N} (\overline{\mathbf{U}} - \mathbf{U})$$

which gives exactly the result of the theorem.

Next we must prove the existence of a (unique) minimizer of the entropy in the set  $\mathbf{K}(\mathbf{f})$ . Roughly speaking this is a generalization of the complex problem of minimization of the entropy under moment constraints (see [23, 28]). For example we can follow the approach Junk ([23]) which consists in examining the set

$$\{(\alpha_l)_l, (\beta_r)_r / \int \exp \left( \sum_{l=1}^{l=p+4} \alpha_l \phi_i^l + \sum_{r=1}^{p-1} \beta_r w_{r,i} \right) dv < +\infty\}.$$

Then Junk proved that if this set is open then the minimization problem has a unique solution as soon as the set of constraints is realizable in the sense that there exists a nonnegative function in  $\mathbf{K}(\mathbf{f})$ . Here the existence of such a function is obtained simply by exhibiting the function (40). Moreover the solution to the minimization problem must be of the exponential form and so it is  $\mathbf{G}$  itself which ends the proof.  $\square$

This result enables us to define our Fick-Relaxation operator.

**Definition 3.** We define the Fick-Relaxation operator  $\mathcal{R}(\mathbf{f})$  by the relation

$$\mathcal{R}(\mathbf{f}) = \nu (\mathbf{G} - \mathbf{f}), \quad (42)$$

where  $\nu > 0$  and

$$\mathbf{G} = \min\{H(g), \text{ s.t. } g \in \mathbf{K}(\mathbf{f})\}.$$

**Remark 2.** In the definition of  $\mathbf{K}(\mathbf{f})$  given in equation (39), the first constraint leads to conservation laws whereas the second one gives the Fick law through the determination of  $\lambda_r$ .

**Remark 3.** Remark that

$$\mathbf{H}(\mathbf{G}) = \sum_i \left( n^i \ln n^i - \frac{3}{2} \ln \left( \frac{m_i}{2\pi k_B T} \right) \right) - n$$

depends only on  $n^i$ ,  $m^i$  and the temperature  $T$  of the mixture which is defined in (2). This value does not depend on each velocity  $\mathbf{u}_i$  as long as  $\sum_i \rho_i \mathbf{u}_i = \rho \mathbf{u}$ . This means that it is also the minimizer of the entropy in the broader set  $\tilde{\mathbf{K}}(\mathbf{f})$  defined by

$$\tilde{\mathbf{K}}(\mathbf{f}) = \{ \mathbf{g} \geq 0 \text{ a.e.} / \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \phi_i^l (g_i - f_i) d\mathbf{v} = 0 \quad \forall l \in [1, p+4] \} \quad (43)$$

where there is no unicity of the solution. All the minimizers are function of the form (40) with  $\sum_i \rho_i \mathbf{u}_i = \rho \mathbf{u}$ . So the unicity of the solution is only the sake of specifying the set of velocity  $(\mathbf{u}_i)_i$ .

## 5 Properties of the Fick-Relaxation operator.

In this part we firstly prove the fundamental properties of the Fick-Relaxation operator. Next we establish that the Fick-Relaxation operator is properly defined and we compute the linearized operator. From this we easily deduce all fluxes or kinetic coefficients. The end of the section is devoted to a discussion about the indifferentiability property. More precisely Proposition 3 shows an alternative property for a BGK model between fitting Fick coefficients at the hydrodynamic limit and satisfying an indifferentiability property.

### 5.1 Conserved moments and H-theorem.

Here we want to establish the physical properties (7,10,9,8) of the Fick relaxation operator  $\mathcal{R}(\mathbf{f})$ .

**Theorem 3.** *The Fick-Relaxation operator satisfies the general properties*

1. **Equilibrium states:**

$$\mathcal{R}(\mathbf{f}) = 0 \Leftrightarrow \exists n^i, \mathbf{u}, T \text{ s.t. } \forall i \in [1, p], f_i = \mathcal{M}_i.$$

2. **H-theorem:**

$$\forall \mathbf{f}, f_i \geq 0, \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathcal{R}_i(\mathbf{f}) \ln(f_i) d\mathbf{v} \leq 0.$$

3. **Characterization of equilibrium:**

$$\int_{\mathbb{R}^3} \mathcal{R}_i(\mathbf{f}) \ln(f_i) d\mathbf{v} = 0 \Leftrightarrow \exists n^i, \mathbf{u}, T \text{ s.t. } \forall i \in [1, p], f_i = \mathcal{M}_i.$$

4. *Conservation laws:*

$$\forall \mathbf{f}, f_i \geq 0, \forall \Phi, \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathcal{R}_i(\mathbf{f}) \Phi_i d\mathbf{v} = 0 \Leftrightarrow \Phi \in \mathbb{K}.$$

*Proof. Property 1: Equilibrium states* Taking into account the Maxwellian form of  $\mathbf{f} = \mathbf{G}$  we are let to prove that  $\underline{\mathbf{U}} = \overline{\mathbf{U}} \implies \overline{\mathbf{U}} = \mathbf{U}$ . Coming back to the definition of  $\underline{\mathbf{U}}$  (41) we have

$$\underline{\mathbf{U}} = \overline{\mathbf{U}} \implies 0 = W^T \mathbf{N}^{-1} \Lambda W \mathbf{N} (\overline{\mathbf{U}} - \mathbf{U}).$$

The second equation reduces to

$$0 = \Lambda W \mathbf{N} (\overline{\mathbf{U}} - \mathbf{U})$$

since the matrix  $\mathbf{N}^{-1} W^T$  is of rank  $p$ . Remark that  $\lambda_r \neq 0$  for all  $r \in [1, p-1]$  so the above equation reads

$$0 = \sum_i W_{ri} \sqrt{\rho_i} (\mathbf{u}^i - \mathbf{u}), \quad \forall r \in [1, p-1].$$

As concerns the case  $r = p$  recall that (32)

$$\sum_i W_{pi} \sqrt{\rho_i} (\mathbf{u}^i - \mathbf{u}) = \frac{1}{\sqrt{\rho}} \sum_i \rho_i (\mathbf{u}^i - \mathbf{u}) = 0$$

since  $\mathbf{u}$  is the mean velocity of  $\mathbf{f}$ . Gathering the two set of equations we have

$$W \mathbf{N} (\overline{\mathbf{U}} - \mathbf{U}) = 0$$

which implies that  $\overline{\mathbf{U}} - \mathbf{U} = 0$  since  $W \mathbf{N}$  is of rank  $p$ .

**Property 2: H theorem:** The convexity of the function  $x \rightarrow x \ln x$  implies

$$\sum_{i=1}^{i=p} \int_{\mathbb{R}^3} (G_i - f_i) \ln f_i d\mathbf{v} \leq \mathbf{H}(\mathbf{G}) - \mathbf{H}(\mathbf{f}). \quad (44)$$

Now since we have  $\sum_i \rho_i \mathbf{u}^i = \rho \mathbf{u}$  (which is self-evident), Remark 3 tells us that the function  $\mathbf{G}_{\mathbf{f}}$  defined by

$$G_{\mathbf{f},i} = \frac{n^i}{(2\pi k_B T / m_i)^{3/2}} \exp\left(-\frac{m_i (\mathbf{v} - \mathbf{u}^i)^2}{2k_B T}\right), \quad \forall i \in [1, p] \quad (45)$$

is a minimizer of the entropy in the set  $\tilde{\mathbf{K}}(\mathbf{f})$  (43) but also in the set  $\mathbf{K}(\mathbf{f})$  defined as

$$\mathbf{g} \in \mathbf{K}(\mathbf{f}) \Leftrightarrow \begin{cases} \forall l \in [1, p+4], \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \phi_i^l (g_i - f_i) d\mathbf{v} = 0, \\ \forall r \in [1, p], \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} (g_i - f_i) \mathbf{v} d\mathbf{v} = \mathbf{0}. \end{cases}$$

Thus

$$\sum_{i=1}^{i=p} \int_{\mathbb{R}^3} (G_i - f_i) \ln f_i d\mathbf{v} \leq \mathbf{H}(\mathbf{G}) - \mathbf{H}(\mathbf{G}_{\mathbf{f}}) = 0. \quad (46)$$

**Property 3: Characterization of Equilibrium:** The nullity of entropy flux implies

$$0 = \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} (G_i - f_i) \ln f_i d\mathbf{v} \leq \mathbf{H}(\mathbf{G}) - \mathbf{H}(\mathbf{f}) \leq 0.$$

Next the second inequality is strict unless  $\mathbf{f} = \mathbf{G}_{\mathbf{f}}$  (see above) so that we have

$$\sum_{i=1}^{i=p} \int_{\mathbb{R}^3} (G_i - G_{\mathbf{f},i}) \ln G_{\mathbf{f},i} d\mathbf{v} = 0.$$

A simple computation of this term gives

$$\sum_{i=1}^{i=p} \left( \int_{\mathbb{R}^3} G_i (\mathbf{v} - \mathbf{u}^i)^2 d\mathbf{v} - \frac{2n^i k_B T}{m_i} \right) = \sum_{i=1}^{i=p} n^i (\mathbf{u}_i - \mathbf{u}^i)^2 = 0,$$

where we have used the conservation of mass per species. Hence we must have  $\underline{\mathbf{U}} = \overline{\mathbf{U}}$  which implies (see property 1)  $\underline{\mathbf{U}} = \mathbf{U}$ .

**Property 4: Conservation laws:** Thanks to the definition of  $\mathbf{G}$  through a minimization problem with **qualified constraints** (39) the implication  $\Leftarrow$  is obvious. The converse may be obtained from the  $H$ -theorem. Assume that there holds:

$$\forall \mathbf{f} \text{ s.t. } \forall i, f_i \geq 0, \sum_{i=1}^{i=p} \int \mathcal{R}_i(\mathbf{f}) \phi_i = 0$$

where  $\phi$  is given. Then consider the particular  $\mathbf{f}$  given as  $f_i = \exp(\phi_i) \Leftrightarrow \phi_i = \ln(f_i)$ . Then from the characterization of the equilibrium states we get that:

$$\exists n^i, \mathbf{u}, T \text{ s.t. } \forall i \in [1, p], f_i = \mathcal{M}_i = \exp(\phi_i)$$

so that finally  $\phi \in \mathbb{K}$ . □

**Remark 4.** *The strategy to obtain a relaxation operator giving exact Fourier coefficient would be to generalize the ES-BGK model ([22, 12, 13, 4]) to a mixture setting.*

This is however still not enough to ensure that the Fick Relaxation operator is properly defined and we need to compute the linearized operator.

## 5.2 Linearization of Fick-Relaxation operator.

### 5.2.1 Explicit expression.

This paragraph is devoted to the computation of the linearized operator associated to the Fick-Relaxation operator defined in (42).

**Theorem 4.** *The linearized operator  $\mathcal{L}$  of the Fick-Relaxation operator around a thermodynamical equilibrium writes*

$$\mathcal{L} = \nu (\mathcal{P}_{\mathbb{K}} + R \circ \mathcal{P}_{\mathbb{C}} - \mathcal{I}),$$

where  $\mathcal{I}$  is the identity operator on  $\mathbb{L}^2(\mathbf{M})$ ,  $\mathcal{P}_{\mathbb{K}}, \mathcal{P}_{\mathbb{C}}$  respectively the orthogonal projection on  $\mathbb{K}, \mathbb{C}$  while  $R$  is the linear operator defined on  $\mathbb{C}$  by the formula:  $\forall r \in [1, p-1], R(\mathbf{w}_r) = (1 - \frac{\lambda_r}{\nu}) \mathbf{w}_r$ .

*Proof.* Let  $\mathbf{M}$  be a thermodynamical equilibrium then

$$\mathcal{L}_i(\mathbf{g}) = \frac{1}{\mathcal{M}_i} \lim_{\epsilon \rightarrow 0} \frac{\mathcal{R}_i(\mathbf{M}(1 + \epsilon \mathbf{g})) - \mathcal{R}_i(\mathbf{M})}{\epsilon} \quad \forall i \in [1, p],$$

where  $\mathbf{g}$  is any function in  $\mathbb{L}^2(\mathbf{M})$ . Remark that thanks to theorem 3  $\mathcal{R}_i(\mathbf{M}) = 0$ . Next let  $\mathbf{g}$  be fixed then there exists  $\epsilon_0$  such that for all  $\epsilon < \epsilon_0$  the problem

$$\mathbf{G} = \min\{H(h) \text{ s.t. } h \in \mathbf{K}(\mathbf{M}(1 + \epsilon \mathbf{g}))\}$$

admits a solution. Indeed the set of realizable constraints  $\mathbf{K}(\mathbf{M})$  is open [23]. Let us write this solution in the following form

$$\mathbf{G}_{i, \mathbf{M}(1 + \epsilon \mathbf{g})} = \exp \left( \sum_{l=1}^{l=p+4} \alpha_l(\epsilon, g) \phi_i^l + \sum_{r=1}^{p-1} \beta_r(\epsilon, g) w_{r,i} \right)$$

where the pseudo-Lagrange multipliers  $(\alpha_l(\epsilon, g))_l, (\beta_r(\epsilon, g))_r$  are solutions of the perturbed problem. We may compute exactly those coefficients from the form (40) given in theorem 2 and then find out that they are infinitely differentiable with respect to each variables (for  $\epsilon < \epsilon_0$ ). Thus they can be expanded in  $\epsilon$

$$\alpha_l = \alpha_l^0 + \epsilon \alpha_l^1(g) + O(\epsilon^2) \quad \forall l, \beta_r = \beta_r^0 + \epsilon \beta_r^1(g) + O(\epsilon^2) \quad \forall r.$$

The zeroth order corresponds to the Maxwellian distribution that is

$$\alpha_i^0 = \frac{-\mu_i}{k_B T} - m_i \frac{u_i^2}{2k_B T}, \quad \alpha_{p+3}^0 = \frac{\mathbf{u}_i}{k_B T}, \quad \alpha_{p+4}^0 = -\frac{1}{2k_B T}$$

$$\alpha_l^0 = 0 \quad \forall l \neq i, p+3, p+4, \quad \beta_r^0 = 0 \quad \forall r,$$

where  $\mu_i$  is defined in (17). Then  $\mathbf{G}_{i, \mathbf{M}(1 + \epsilon \mathbf{g})}$  writes

$$\mathbf{G}_{i, \mathbf{M}(1 + \epsilon \mathbf{g})} = \mathcal{M}_i \left( 1 + \epsilon \left[ \sum_{l=1}^{p+4} \alpha_l^1(g) \phi_i^l + \sum_{r=1}^{p-1} \beta_r^1(g) w_{r,i} \right] + O(\epsilon^2) \right). \quad (47)$$

So that

$$\mathcal{L}_i(\mathbf{g}) = \sum_{l=1}^{p+4} \alpha_l^1(g) \phi_i^l + \sum_{r=1}^{p-1} \beta_r^1(g) w_{r,i} - g. \quad (48)$$

Now remark that the set of constraints (39) depends linearly on the moments of the function  $\mathbf{M}(1 + \epsilon \mathbf{g})$  so that the perturbations at order 1 in  $\epsilon$  of the Lagrange multipliers  $\alpha_l^1(g)$ ,  $\beta_r^1(g)$  are also linear. We can compute them exactly by inserting the expression (47) in the constraints (39) with  $\mathbf{f} = \mathbf{M}(1 + \epsilon \mathbf{g})$  and considering the equalities at order one in  $\epsilon$  we get

$$\begin{aligned} \sum_{l=1}^{p+4} \langle \phi^k, \phi^l \rangle \alpha_l^1(g) &= \langle \mathbf{g}, \phi^k \rangle \quad \forall k \in [1, p+4], \\ \sum_{r=1}^{p-1} \langle \mathbf{w}_s, \mathbf{w}_r \rangle \beta_r^1(g) &= \left(1 - \frac{\lambda_r}{\nu}\right) \langle \mathbf{g}, \mathbf{w}_r \rangle \quad \forall s \in [1, p-1]. \end{aligned}$$

Here the first line corresponds exactly to the projection of  $\mathbf{g}$  on  $\mathbb{K}$  through the expression (48) of  $\mathcal{L}_i(\mathbf{g})$  while the second line amounts to project on the basis  $(\mathbf{w}_r)_r$  of  $\mathbb{C}$  and multiply each coordinates with a factor  $(1 - \frac{\lambda_r}{\nu})$ .  $\square$

### 5.2.2 Properties of the linearized operator.

In this part we easily deduce from the explicit expression of the linearized operator the following important properties.

**Proposition 1.** *The linearized operator associated to the Fick-Relaxation operator satisfies the following properties*

- i)  $\text{Ker } \mathcal{L} = \mathbb{K}$ ,
- ii)  $\mathcal{L}$  is Fredholm,
- iii)  $\mathcal{L}$  is self adjoint negative on  $\mathbb{K}^\perp$ .

Now we can finish the work by showing the last theorem.

**Theorem 5.** *The pseudo inverse  $\mathcal{L}^{-1}$  of the Fick-Relaxation operator reads as:*

$$(\forall \mathbf{g} \in \mathbb{K}^\perp), \mathcal{L}^{-1}(\mathbf{g}) = \frac{1}{\nu} \left( (R - \mathcal{I}_{\mathbb{C}})^{-1} \circ \mathcal{P}_{\mathbb{C}} + (\mathcal{P}_{\mathbb{C}} - \mathcal{I}) \right) (\mathbf{g}), \quad (49)$$

where  $\mathcal{I}_{\mathbb{C}}$  denotes the restriction on  $\mathbb{C}$  of the identity operator,  $\mathcal{P}_{\mathbb{C}}$  the projection on  $\mathbb{C}$  and  $R$  has been defined in Theorem 4.

*Proof.* For  $g \in \mathbb{K}^\perp$  it suffices to compute  $\mathcal{L}^{-1} \circ \mathcal{L}(\mathbf{g})$ .  $\square$

### 5.3 Hydrodynamical limit.

Here we want to compute the hydrodynamical limit at order 1 of the system of equations

$$\forall i \in [1, p], \partial_t f_i^\epsilon + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i^\epsilon = \frac{1}{\epsilon} \frac{(G_i^\epsilon - f_i^\epsilon)}{\nu}. \quad (50)$$

**Theorem 6.** Let  $\nu$  be defined as

$$\nu = \frac{nk_b^2 T^2}{\mu}$$

where  $\mu = \mathbf{L}_{uu}$  is the viscosity of the mixture (see equation (26)). Then the hydrodynamical limit of (50) with  $\mathbf{R}(\mathbf{f})$  defined in 28 gives at the order 1 the Navier-Stokes equations (13, 14, 15) with the fluxes given by

$$\mathbf{J}_i = \sum_{j=1}^p L_{ij} \nabla \left( \frac{-\mu_j}{T} \right), \quad \mathbf{J}_q = L_{qq}^R \nabla \left( \frac{1}{T} \right), \quad \mathbb{J}_u = \nu \mathbb{D}(\mathbf{u}). \quad (51)$$

Here  $(L_{ij})_{ij}$  is the matrix of Fick coefficients (24) computed with the (linearized) Boltzmann equation and

$$L_{qq}^R = \frac{5\mu k_b T}{2n} \sum_{i=1}^p \frac{n_i}{m_i}.$$

*Proof.* The proof is easily deduced from the fact that  $\mathcal{R}(\mathbf{f})$  is properly defined according to theorem 3 and proposition 1. Hence (see remark 1) all kinetic coefficients can be computed as soon as we know the exact form of  $\mathcal{L}^{-1}$  which is actually given in (49).

1. **Density fluxes:** We have directly

$$\mathcal{L}^{-1}(\mathbb{A}) = -\nu^{-1}\mathbb{A} \text{ and } \mathcal{L}^{-1}(\mathbf{B}) = -\nu^{-1}\mathbf{B} \in \mathbb{C}^\perp$$

so that theorem 1 applies. Hence

$$\mathbf{J}_i = \sum_{j=1}^{j=p} L_{ij} \nabla \left( \frac{-\mu_j}{T} \right) \quad \forall i \in [1, p]$$

meaning that  $L_{iq} = L_{qi} = 0$  for all  $i \in [1, p]$  ( $\mathcal{L}^{-1}$  is self-adjoint).

2. **Viscosity:** it is possible to recover the true viscosity  $\mu = L_{uu}$  defined by (26) by adjusting the relaxation rate  $\nu$  of  $\mathcal{R}(\mathbf{f})$ . Let  $L_{uu}^R$  be the viscosity of our model then

$$L_{uu}^R \mathbf{I} \otimes \mathbf{I} = \langle \mathcal{L}^{-1}(\mathbb{A}), \mathbb{A} \rangle = \frac{1}{\nu} \langle \mathbb{A}, \mathbb{A} \rangle = \frac{nk_B^2 T^2}{\nu} \mathbf{I} \otimes \mathbf{I}.$$

So obviously letting  $\nu = nk_b^2 T^2 / \mu$  we have  $L_{uu}^R = \mu$ .

3. **Fourier coefficient:** the "true" Fick and viscosity coefficients being recovered it is not possible to obtain the correct value of  $L_{qq}$  (27) with our model. Indeed

$$L_{qq}^R \mathbf{I} = \langle \mathcal{L}^{-1}(\mathbf{B}), \mathbf{B} \rangle = \frac{1}{\nu} \langle \mathbf{B}, \mathbf{B} \rangle \Leftrightarrow L_{qq}^R = \frac{5\mu k_B T}{2n} \sum_{i=1}^p \frac{n_i}{m_i} \neq L_{qq} \mathbf{I}.$$

□

Here the density fluxes are deduced from our "natural" construction (theorem 1). That is using the concept of relaxation rates associated to ad-hoc moments of the distribution functions. To recast the hydrodynamical limit in the spirit of section 3.4 we may check the following results.

**Proposition 2.** *The linearized operator  $\mathcal{L}$  satisfies*

$$\forall (i, j) \in [1, p]^2, \langle k_B^{-1} \mathcal{L}^{-1} (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_i), (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_j) \rangle = L_{ij}. \quad (52)$$

*Proof.* First let us note the one to one correspondance between the  $\mathbf{C}_i$  and the  $\mathbf{w}_k$  as:

$$\forall i \in [1, p], \mathbf{C}_i = \|\mathbf{C}_i\| \sum_{k=1}^{k=p} W_{ik}^T \mathbf{w}_k.$$

From this, it is very easy to compute  $(\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_i)$  which is simply given as:

$$(\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_i) = \|\mathbf{C}_i\| \sum_{k=1}^{k=p-1} W_{ik}^T \mathbf{w}_k.$$

Applying now the operator  $\mathcal{L}^{-1}$  is now straightforward thanks to the explicit formulation and we have

$$\mathcal{L}^{-1} (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_i) = -\|\mathbf{C}_i\| \sum_{k=1}^{k=p-1} \frac{W_{ik}^T}{\lambda_k} \mathbf{w}_k.$$

As a consequence the LHS of 3.4 reads as

$$-k_B^{-1} \|\mathbf{C}_i\| \|\mathbf{C}_j\| \sum_{k,l=1}^{k,l=p-1} \frac{1}{\lambda_k} W_{ik}^T W_{jl}^T \langle \mathbf{w}_k, \mathbf{w}_l \rangle.$$

Since the basis  $\mathbf{w}_k, k \in [1, p]$  is orthonormalized, then the sum simplifies as:

$$-k_B^{-1} \|\mathbf{C}_i\| \|\mathbf{C}_j\| \sum_{k=1}^{k=p-1} W_{ik}^T \frac{1}{\lambda_k} W_{kj} = k_B^{-1} \|\mathbf{C}_i\| \|\mathbf{C}_j\| \sum_{k=1}^{k=p} W_{ik}^T d_k^* W_{kj}$$

(this is because  $d_k^* = -1/\lambda_k, k \in [1, p-1]$ , while  $d_p^* = 0$ ). That is

$$-k_B^{-1} \|\mathbf{C}_i\| \|\mathbf{C}_j\| \sum_{k=1}^{k=p-1} W_{ik}^T \frac{1}{\lambda_k} W_{kj} = \|\mathbf{C}_i\| \|\mathbf{C}_j\| k_B^{-1} L_{ij}^* = L_{ij}$$

which ends the proof. □



## 5.4 About the indifferentiability property

Following ([1]) the indifferentiability property may be stated as follows: when in the mixture all the masses and differential cross sections are equal -which we call indifferentiable molecules- then the BGK operator for the mixture must collapse into a BGK one for a single species, that is:

$$\left[ \forall i, j \in [1, p]^2, m_i = m, \sigma_{ij} = \sigma \right] \Rightarrow \sum_{i=1}^{i=p} \mathcal{R}_i(\mathbf{f}) = \mathcal{R} \left( \sum_{i=1}^{i=p} f_i \right).$$

This "factorization" property is an algebraic one which holds when the dilute Boltzmann operator is chosen to model the particles collisions. More precisely there is:

$$\left[ \forall i, j \in [1, p]^2, m_i = m, \sigma_{ij} = \sigma \right] \Rightarrow \sum_{i=1}^{i=p} Q_i(\mathbf{f}) = Q \left( \sum_{i=1}^{i=p} f_i \right).$$

Note however that such a factorization property holds because of the bi-linearity of the dilute Boltzmann operator. But it has no particular reason to hold when the Boltzmann operator features a cubic dependancy with  $\mathbf{f}$  which happens for instance when one considers dense situations [31].

Let us now consider the following quite general form of a BGK operator for gas mixtures which we denote with  $\widetilde{\mathcal{R}}$

$$\forall i \in \{1, \dots, p\}, \widetilde{\mathcal{R}}_i(\mathbf{f}) = \tilde{\nu}_i (\widetilde{G}_i - f_i). \quad (53)$$

Here the values of the relaxation frequencies  $\tilde{\nu}_i$  may be different. We first set some quite reasonable assumptions on the above model:

1. The constraints defining the mean velocities of  $(\widetilde{G}_i)$  as functions of the mean velocities of  $(f_i)_i$  are of the form

$$\sum_{i=1}^{i=p} X_{ij} \int_{\mathbb{R}^3} \widetilde{G}_i(v - u) dv = \sum_{i=1}^{i=p} T_{ij} \int_{\mathbb{R}^3} f_j(v - u) dv$$

where the matrix  $X$  and  $T \in \mathbb{R}^p \times \mathbb{R}^p$  do not depend on  $v$ . Or in short

$$\underline{\mathbf{U}} - \mathbf{U} = X^{-1} N^{-1} T N (\overline{\mathbf{U}} - \mathbf{U}) \quad (54)$$

(here we have kept the notations of theorem 2).

2. In the indifferentiability situation the relation  $u_i = u$  holds for all  $i$ .

Let us remark that up to our knowledge the linearity of the constraints on the basis  $(\mathbf{C}_i)_i$  is the rule for all the BGK operators we have found. Those constraints are quite natural regarding to the way the true diffusion (Fick) coefficients are obtained (see (24)). Otherwise if those constraints are not linear they must be of integer degree for the sake of Galilean invariance..

The second assumption is required in most cases because the indifferenciability is obtained thanks to an "additivity" property. That is

$$\sum_i \tilde{\nu}_i (\tilde{G}_i - f_i) = \tilde{\nu} (\tilde{\mathbf{G}} - \mathbf{f})$$

when all masses and cross sections are equal. For example such assumptions are easily found when  $\tilde{G}_i$  is not a linear function of its mean velocity  $u_i$ .

We are now going to draw some conclusion about the compatibility of the indifferenciability property and the Fick law for such a model.

**Lemma 6.** *Let  $\tilde{\mathcal{R}}$  be a properly defined operator of the form (53) satisfying the conditions 1 and 2 above. Then when all molecules are the same the restriction to  $\mathbb{C}$  of the linearized BGK is proportional to minus identity.*

*Proof.* The property (11) implies that the restriction of the linearized operator on the space spanned by  $(\mathbf{C}_i)_i$  actually reduces to  $\mathbb{C}$ . Thus generalizing the calculations we have done in section 5.2.1 and using assumption 1 this restriction reads  $(\tilde{R} - \mathcal{I}_{\mathbb{C}})$  where  $\tilde{R}$  is a linear operator depending on  $\mathbf{T}$  and  $\mathcal{I}_{\mathbb{C}}$  is the restriction on  $\mathbb{C}$  of the identity operator. To be consistent with the symmetry of the linearized Boltzmann operator the operator  $\tilde{R}$  has to be symmetrical on  $\mathbb{C}$  while the operator  $\tilde{R} - \mathcal{I}_{\mathbb{C}}$  must be non positive and symmetric because of the property (12). Consequently  $\tilde{R}$  can be diagonalized in a proper orthogonal basis  $\mathbf{x}_r, r \in \{1, \dots, p-1\}$  such that

$$\forall r \in \{1, \dots, p-1\}, \tilde{R}(\mathbf{x}_r) = (1 - \alpha_r)\mathbf{x}_r, \alpha_r \geq 0.$$

And we can write (54) in the same form as((41)

$$\underline{\mathbf{U}} - \mathbf{U} = N^{-1} X^T (\mathbf{I} - A) X N (\bar{\mathbf{U}} - \mathbf{U})$$

Here the matrix  $X^T$  denotes the passage from the basis  $(\mathbf{C}_i)_i$  to the basis  $(\mathbf{x}_1, \dots, \mathbf{x}_{p-1}, \sum m_i \mathbf{C}_i)$  and the matrix  $A$  is diagonal with  $a_{rr} = \alpha_r, r \in \{1, \dots, p-1\}$  and  $a_{pp} = 0$ .

Next according to the second assumption the indifferenciability property requires  $u_i = u$  for any  $i \in \{1, \dots, p\}$  in the limit of same masses and cross sections. As a consequence the relation (54) must be valid for each values of  $u^i$  meaning that for any  $r \in \{1, \dots, p\}, \alpha_r = 1$ . Consequently  $\tilde{R} = 0$ .  $\square$

Next we prove the following alternative.

**Proposition 3.** *Two situations are possible.*

- *Either there is a properly defined BGK operator of the form (53) satisfying conditions 1 and 2 above, the indifferenciability property and giving the Fick law at the hydrodynamical limit. In that case the Fick Relaxation operator  $\mathcal{R}$  (definition 3) satisfies the indifferenciability as well. Moreover when all masses and cross sections the operator must obey a law in the indifferenciability case that is  $\tilde{\nu}_i = \tilde{\nu} = \nu \forall i$ .*

- Or there are no well defined BGK operator satisfying the conditions 1) and 2) and in the same time indifferenciability and Fick law.

*Proof.* Consider a properly defined BGK operator defined (53) satisfying Fick law and the indifferenciability condition. Its associated Fick coefficients  $L_{ij}^{\tilde{\mathcal{R}}}$  are given by (24) replacing  $\mathcal{L}_B$  with  $\mathcal{L}_{\tilde{\mathcal{R}}}$  (see remark 1). Thus according to lemma 6 when all masses and all differential cross sections are equal

$$L_{ij}^{\tilde{\mathcal{R}}}\mathbb{I} = -\frac{1}{k_B\tilde{\nu}} \langle (\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_i), (\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_j) \rangle, \quad \tilde{\nu} > 0. \quad (55)$$

If the model satisfies the Fick law as well we have  $(L_{ij}^{\tilde{\mathcal{R}}})_{i,j} = (L_{ij})_{i,j}$  where the second matrix is defined either by (24) or by

$$L_{ij}\mathbb{I} = -\frac{1}{k_B\nu} \left\langle (R - \mathcal{I}_C)^{-1} (\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_i), (\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_j) \right\rangle,$$

where we have used (49) and (52). The comparison between this equation and (55) imposes firstly that  $R = 0$ . Coming back to equation (41) this means that  $\underline{\mathbf{U}} = \mathbf{U}$  whatever are the values of  $\overline{\mathbf{U}}$ . Hence using the definition of  $G_i$  (40) the Fick-Relaxation model satisfies the indifferenciability property. But according to lemma 6, in the situation of indifferenciability,  $L_{ij}$  is given by a formula analogous to (55) leading to  $\tilde{\nu} = \nu$ .

The last assertion is self evident. □

In a situation of same masses and same differential cross sections, we do not know exactly if the kinetic coefficients obtained by the linearized Boltzmann operator can match those obtained by a BGK satisfying the indifferenciability property. But in reality we do not care because the correctness of the linearized BGK operator is much more important, it seems, that the indifferenciability property and if they contradict, we prefer to sacrifice indifferenciability.

In concrete situations masses and cross sections are always different. Therefore the indifferenciability principle is only a continuity principle. That is why we prefer to conserve the correctness of the hydrodynamical coefficients which are more physically pertinent.

## 6 Conclusion and perspectives.

In this paper we have introduced a new relaxation operator for gas mixtures. Our construction features two ideas. The first one is that we have constructed it within the framework of moments relaxations that were introduced in [12, 13] as a new way to understand the ellispodal model for monospecies systems. Here we have also taken into account the relaxation on velocities species which is necessary to obtain mass diffusion, thus shedding in light the space of vectors of moments of order one orthogonal to the space of collisional invariants. The second characteristic of this work is that we have focused the construction

of this relaxation operator so that its associated linear mass and momentum transports coefficients exactly match those obtained by the Chapman-Enskog expansion applied to the Boltzmann operator. While it is classical to have such concerns to recover the right Newtown viscosity and Fourier coefficient when constructing BGK models in the case of a single specie, it is not the usual track which is followed when considering gas mixtures as we pointed it in introduction. Interestingly our relaxation operator also enjoy important properties of the Boltzmann collision terms (H theorem for instance) which are not always satisfied when pure linear models are at stake. Besides we have pointed out the remarkable link existing between the eigenvalues of Fick coefficient matrix and the rate of relaxation for the vanishing moments associated to functions of degree one in velocity. Up to our knowledge such a perspective has never been expressed so clearly. Finally a key aspect of the Fick Relaxation Operator we have defined lies in the very simplicity of its computation which only requires the diagonalization of the Fick matrix! It seems to us that this could be an important thing for future users if any. Unfortunately when writing these lines, we are not still able to propose a Relaxation operator that could be able to match in the linear regime all the transport coefficients. It seems to us that obtaining simultaneously the *correct* Fick, Newtown and Fourier coefficients could be possible by generalizing for gas mixture the approach described in [12]. More difficult however seems the possibility to get at the same time the correct (so called "cross") kinetic coefficients  $(L_{i\mathbf{q}})_i$  (18),(25). In our model (as it is also the model of [1]) such cross kinetic coefficients are zero and give uncorrect Soret and Dufour coefficients (except for Maxwellian molecules). This might be a problem for situations featuring non negligible thermodiffusion for instance. Finally the approach we have described in this paper requires the knowledge of the kinetic coefficients. Unfortunately such a knowledge is not obvious at all but combining both the numerical algorithm to compute them given in [15] and the experimental work of Kestin [24] will be of precious help when actually computing the Fick Relaxation Operator.

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## 7 Appendix

### 7.1 Proof of Lemma 1.

*Proof.* A direct computation shows that the  $l$ -th component of  $(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_i)$  is

$$[(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_i)]_l = \left( \delta_{il} - \frac{n^i m_l}{\rho} \right) (\mathbf{v} - \mathbf{u}).$$

Now assume that for  $k \in [1, p]$  there holds

$$\sum_{i=1}^{i=k} \alpha_i (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_i) = \mathbf{0}$$

then, working on the  $k$  first line of this equation we get that:

$$(\forall l \in [1, k]) \sum_{i=1}^{i=k} \left( \delta_{il} - \frac{n^i m_l}{\rho} \right) \alpha_i = 0.$$

To know if this linear system on the  $\alpha_i$  has the unique trivial solution or not (and then to know if the family  $(\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_i), i \in [1, k]$  is independant or not), one has to discuss the determinant of the  $k$  by  $k$  matrix  $M$  defined as:

$$(\forall i, l \in [1, k]^2) M_{il} = \left( \delta_{il} - \frac{n^i m_l}{\rho} \right).$$

Elementary algebraic calculations show that the determinant of such a matrix may be computed as

$$\det M = \left( \prod_{i=1}^{i=k} \frac{\rho^i}{\rho} \right) \det N,$$

with

$$N = \begin{bmatrix} \frac{\rho}{\rho^1} & 0 & \cdots & 0 \\ 0 & \frac{\rho}{\rho^2} & 0 & \vdots \\ \vdots & \cdots & \ddots & \cdots \\ 0 & \cdots & 0 & \frac{\rho}{\rho^k} \end{bmatrix} - \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & \ddots & \cdots & 1 \\ \vdots & \cdots & \cdots & \vdots \\ 1 & \cdots & \cdots & \ddots \end{bmatrix}.$$

Consider first the case where  $k < p$ . Let  $x \in Ker(N)$ . Hence by definition of  $N$ , it holds that

$$(\forall j \in \{1; k\}), \sum_{i=1}^p x_i = \frac{\rho}{\rho_j} x_j. \quad (56)$$

Therefore it comes that

$$(\forall j \in \{1; k\}), \frac{\rho}{\rho_j} x_j = \frac{\rho}{\rho_1} x_1. \quad (57)$$

Now assume by contradiction that  $x \neq 0$ . In that case for example  $x_1 \neq 0$ . According to (57), for any  $i \in \{1, k\}, x_i \neq 0$ . So (56) implies that  $\sum_{i=1}^k x_i \neq 0$ . From (57) it holds that  $x_j = \frac{\rho_j}{\rho_1} x_1$ . Hence

$$\sum_{j=1}^p x_j = \sum_{j=1}^k \frac{\rho_j}{\rho_1} x_1 = \frac{\rho}{\rho_1} x_1$$

and it follows that

$$\sum_{j=1}^k \rho_j = \rho.$$

Therefore for any  $j \in \{k+1; n\}$ ,  $\rho_j = 0$  and we get a contradiction. Then it follows that  $N$  is invertible.

Next consider the case where  $k = p$ . Let  $x = (\rho_1, \dots, \rho_p) \neq 0$ . In that case

$$\rho_i \frac{\rho}{\rho_i} = \sum_{j=1}^k \rho_j.$$

Then  $x \neq 0$  and  $x \in \text{Ker} N$ . So  $N$  is non invertible.  $\square$

## 7.2 Proof of Lemma 2.

*Proof.* The first problem consists in computing the left-hand side of (22), namely any of the  $(\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}}) [\mathcal{M}_i]$  for  $i \in [1, p]$ . Now introduce the following decomposition of  $\mathcal{M}_i$  given as:

$$\forall i \in [1, p], \mathcal{M}_i = \exp \left( \left( \frac{-\mu_i}{k_B T} - m_i \frac{\mathbf{u}^2}{2k_B T} \right) + \frac{\mathbf{u}}{k_B T} \cdot m_i \mathbf{v} - \frac{m_i \mathbf{v}^2}{2k_B T} \right).$$

Then, introducing the natural basis of  $\mathbb{K}$ ,  $\phi^k$ ,  $k \in [1, p+4]$  there holds:

$$\forall i \in [1, p], (\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}}) (\mathcal{M}_i) = \sum_{k=1}^{k=p+4} [(\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}}) \alpha_k] \phi_i^k \mathcal{M}_i \quad (58)$$

where

$$\begin{aligned} \forall k \in [1, p], \alpha_k &= \left( \frac{-\mu_k}{T} - \frac{m_k \mathbf{u}^2}{2k_B T} \right) \\ \alpha_{p+1} &= \frac{u_x}{k_B T}, \quad \alpha_{p+2} = \frac{u_y}{k_B T}, \quad \alpha_{p+3} = \frac{u_z}{k_B T} \\ \alpha_{p+4} &= -\frac{1}{2k_B T} \end{aligned}$$

But since  $\mathbf{w} := (\mathcal{M}_1, \dots, \mathcal{M}_p)$  satisfies the Euler equations, then we know

$$\forall l \in [1, p+4], \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} ((\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}}) (\mathcal{M}_i) \phi_i^l) d\mathbf{v} = 0. \quad (59)$$

By introducing now the left-hand side expression (58) we obtain that

$$\forall l \in [1, p+4], \sum_{k=1}^{k=p+4} \langle (\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}}) (\alpha_k) \phi^k, \phi^l \rangle = 0. \quad (60)$$



If we denote by  $S$  the symmetrical matrix such that  $S_{lk} = \langle \phi^l, \phi^k \rangle$  then for any vector  $b \in \mathbb{L}^2(\mathbf{w}(\mathbf{v}) d\mathbf{v})$  we have clearly

$$\mathcal{P}_{\mathbb{K}}(b) = \sum_{k=1}^{k=p+4} \left[ \sum_{l=1}^{l=p+4} (S^{-1})_{kl} \langle b, \phi^l \rangle \right] \phi^k \quad (61)$$

the orthogonal projection of  $b$  on  $\mathbb{K}$ . Let us consider now

$$b_1 := \sum_{k=1}^{k=p+4} [\partial_t \alpha_k] \phi^k, \quad b_2 := \sum_{k=1}^{k=p+4} [(\mathbf{v} \cdot \nabla_{\mathbf{x}}) \alpha_k] \phi^k.$$

The equation (60) gives that  $\forall l \in [1, p+4], \langle b_1, \phi^l \rangle = -\langle b_2, \phi^l \rangle$ . So using the explicit expression of the orthogonal projection on  $\mathbb{K}$  (61) we have necessary that:  $\mathcal{P}_{\mathbb{K}}(b_1) = -\mathcal{P}_{\mathbb{K}}(b_2)$ . Now remark that the vector  $b_1$  belongs to  $\mathbb{K}$  (this is because  $\partial_t \alpha_k$  does not depends on  $\mathbf{v}$ ) so that  $b_1 = \mathcal{P}_{\mathbb{K}}(b_1) = -\mathcal{P}_{\mathbb{K}}(b_2)$ . Finally we get that  $b_1 + b_2 = b_2 - \mathcal{P}_{\mathbb{K}}(b_2)$ , that is

$$\sum_{k=1}^{k=p+4} (\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}}) (\alpha_k) \phi^k = (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) \left( \sum_{k=1}^{k=p+4} [\mathbf{v} \cdot \nabla_{\mathbf{x}}] (\alpha_k) \phi^k \right). \quad (62)$$

Using this equality with the relation (58) enables us to see the equation (22) as:

$$\mathcal{L}(\mathbf{g}) = (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) \left( \sum_{k=1}^{k=p+4} [\mathbf{v} \cdot \nabla_{\mathbf{x}}] (\alpha_k) \phi^k \right). \quad (63)$$

Now we need to establish the detailed expression of the right-hand side of (63). Since  $\alpha_k$  does not depend on the variable  $\mathbf{v}$ , then  $\sum_{k=1}^{k=p+4} [(\mathbf{u} \cdot \nabla_{\mathbf{x}}) \alpha_k] \phi^k \in \mathbb{K}$ . By consequence, in the argument of  $(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\cdot)$  the  $(\mathbf{v} \cdot \nabla_{\mathbf{x}}) (\alpha_k)$  can be replaced by  $[(\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}}] (\alpha_k)$ . Finally, a direct computation of the latter shows that for any  $k \in [1, p]$

$$(\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} (\alpha_k) = (\mathbf{v} - \mathbf{u}) \cdot \left[ \nabla_{\mathbf{x}} \left( \frac{-\mu_k}{k_B T} \right) - m_k \frac{[\nabla_{\mathbf{x}} \mathbf{u}]^T [\mathbf{u}]}{k_B T} + m_k \mathbf{u}^2 \frac{\nabla_{\mathbf{x}} T}{2k_B T^2} \right] \quad (64)$$

as well as

$$\begin{aligned} (\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} (\alpha_{p+1}) &= \frac{(\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} u_x}{k_B T} - \frac{u_x (\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} T}{k_B T^2} \\ (\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} (\alpha_{p+2}) &= \frac{(\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} u_y}{k_B T} - \frac{u_y (\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} T}{k_B T^2} \\ (\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} (\alpha_{p+3}) &= \frac{(\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} u_z}{k_B T} - \frac{u_z (\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} T}{k_B T^2} \end{aligned}$$

and finally

$$(\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} (\alpha_{p+4}) = (\mathbf{v} - \mathbf{u}) \cdot \frac{\nabla_{\mathbf{x}} T}{2k_B T^2}.$$

Now multiplying the former terms by the functions  $\phi^k$ , summing over  $k$  and gathering the terms in  $\nabla_{\mathbf{x}} \left( \frac{1}{T} \right)$ , those in  $[\nabla_{\mathbf{x}} \mathbf{u}]^T$  and the others we get that the  $i^{\text{th}}$  line of  $\sum_{k=1}^{p+4} (\mathbf{v} - \mathbf{u}) \cdot \nabla_{\mathbf{x}} (\alpha_k) \phi^k$  is given as the sum of the following terms:

$$\begin{aligned} \nabla_{\mathbf{x}} \left( \frac{-\mu_i}{k_B T} \right) \cdot (\mathbf{v} - \mathbf{u}), \quad & [\nabla_{\mathbf{x}} \mathbf{u}]^T : \frac{m_i (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u})}{k_B T}, \\ & \frac{m_i (\mathbf{v} - \mathbf{u})^2 (\mathbf{v} - \mathbf{u})}{2k_B} \cdot \nabla_{\mathbf{x}} \left( \frac{1}{T} \right). \end{aligned}$$

Thanks to the symmetry of  $(\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u})$  we have

$$[\nabla_{\mathbf{x}} \mathbf{u}]^T : \frac{m_i (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u})}{k_B T} = \left( [\nabla_{\mathbf{x}} \mathbf{u}]^T + \nabla_{\mathbf{x}} \mathbf{u} \right) : \frac{m_i (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u})}{2k_B T}.$$

Finally, by computing the orthogonal projection on  $\mathbb{K}$  of the vectors having respectively

$$\left( [\nabla_{\mathbf{x}} \mathbf{u}]^T + \nabla_{\mathbf{x}} \mathbf{u} \right) : \frac{m_i (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u})}{2k_B T}, \quad \frac{m_i (\mathbf{v} - \mathbf{u})^2 (\mathbf{v} - \mathbf{u})}{2k_B} \cdot \nabla_{\mathbf{x}} \left( \frac{1}{T} \right)$$

on their  $i^{\text{th}}$  line, we get exactly the expression 22.  $\square$

### 7.3 Proof of Lemma 3

*Proof.* The equation which is satisfied by the perturbation (list of) function  $\mathbf{g}$  reads for any  $i \in [1, p]$  as:

$$(\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}}) (\mathcal{M}_i (1 + \epsilon g_i)) = \frac{1}{\epsilon} \mathcal{C}_i (\mathcal{M}_1 (1 + \epsilon g_1), \dots, \mathcal{M}_p (1 + \epsilon g_p)),$$

where  $\mathcal{C}_i$  is the contribution on the  $i^{\text{th}}$  line of the collision operator (Boltzmann or BGK one). Multiplying such an equation by  $\phi_i^l$ , integrating over  $\mathbb{R}^3$ , summing on  $i$  and taking into account that the perturbation  $\mathbf{g}$  is in  $\mathbb{K}^\perp$  gives us:

$$\forall l \in [1, p+4], \partial_t \langle \phi^l, \mathbf{M} \rangle + \nabla_{\mathbf{x}} \langle \mathbf{v} \otimes \phi^l, \mathbf{M} \rangle + \epsilon \nabla_{\mathbf{x}} \langle \mathbf{v} \otimes \phi^l, \mathbf{g} \rangle = \mathbf{0}$$

which is exactly the Euler equation which are perturbed by the flux terms  $\langle \mathbf{v} \otimes \phi^l, \mathbf{g} \rangle$  that need to be clarified.

First let us remark that  $\langle \mathbf{u} \otimes \phi^l, \mathbf{g} \rangle = \mathbf{0}$  so we can replace  $\mathbf{v}$  by  $\mathbf{v} - \mathbf{u}$  when computing  $\langle \mathbf{v} \otimes \phi^l, \mathbf{g} \rangle$ .

To have the diffusion term associated to the density  $n_l$ , we must considerate the list of function  $(\mathbf{v} - \mathbf{u}) \phi^l = \mathbf{C}_l$ ,  $l \in [1, p]$  and we get directly the following expression  $\mathbf{J}_l = \langle \mathbf{C}_l, \mathbf{g} \rangle = \langle (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) \mathbf{C}_l, \mathbf{g} \rangle$ : the fact that we can replace  $\mathbf{C}_l$  by  $(\mathcal{I} - \mathcal{P}_{\mathbb{K}}) \mathbf{C}_l$  in the bracket is due to the fact that  $\mathbf{g} \in \mathbb{K}^\perp$ .

Following the same idea, the diffusion of momentum is obtained when  $\phi_i^l = m_i \mathbf{v}$ . Since  $\mathbf{g} \in \mathbb{K}^\perp$  this may be replaced by  $m_i (\mathbf{v} - \mathbf{u})$  so finally we get that  $\mathbb{J}_{\mathbf{u}} = \langle \mathbf{A}, \mathbf{g} \rangle$ . To get heat diffusion, we need to consider  $\phi_i^l = \frac{1}{2} m_i \mathbf{v}^2$ . This gives us an energy diffusive flux given as  $\langle \mathbf{B}, \mathbf{g} \rangle$ .  $\square$

## 7.4 Proof of Lemma 4.

*Proof.* Note by  $L_{:,j}$  the  $j^{\text{th}}$  column of the matrix  $L_{ij}, (i, j) \in [1, k]^2$  and assume that  $\sum_{j=1}^{j=k} \alpha_j L_{:,j} = 0$ . Then there is

$$\sum_{i=1}^{i=k} \sum_{j=1}^{j=k} \alpha_i \alpha_j L_{ij} = 0$$

when the matrix  $L_{ij}$  comes from a Chapman-Enskog expansion this means:

$$\sum_{i=1}^{i=k} \sum_{j=1}^{j=k} \alpha_i \alpha_j \langle \mathcal{L}^{-1} (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_i), (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_j) \rangle = 0.$$

As the operator  $\mathcal{L}^{-1}$  is negative on  $\mathbb{K}^{\perp}$  this implies

$$\sum_{i=1}^{i=k} \alpha_i (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_i) = 0$$

Now using the lemma 1, for any  $k < p$ , this implies that  $\forall i \in [1, k], \alpha_i = 0$ . For  $k = p$ , one can find from lemma (1) a set of real  $\beta_i, i \in [1, p]$  which are not all zero such that:

$$\sum_{j=1}^{j=p} \beta_j (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_j) = \mathbf{0}$$

then using the expression of the  $L_{ij}$  from the Chapman-Enskog expansion one sees redily that

$$\sum_{j=1}^{j=p} \beta_j L_{:,j} = 0$$

meaning that the matrix  $L_{ij}, (i, j) \in [1, p]^2$  has not a full rank. □