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Derivation of a BGK model for mixtures

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ABSTRACT

The aim of this article is to construct a BGK operator for gas mixtures starting from the true Navier–Stokes equations. That is the ones with transport coefficients given by the hydrodynamic limit of the Boltzmann equation(s). Here the same hydrodynamic limit is obtained by introducing relaxation coefficients on certain moments of the distribution functions. Next the whole model is set by using entropy minimization under moment constraints as in Brull and Schneider (2008, 2009) [23,24]. In our case the BGK operator allows to recover the exact Fick and Newton laws and satisfy the classical properties of the Boltzmann equations for inert gas mixtures.

1. Introduction

The BGK equation [1] is a seminal simplified model of the nonlinear Boltzmann equation of gas dynamics. While keeping physical and mathematical properties of the Boltzmann equation (conservation laws, H-theorem, equilibrium states, etc.) it is often used for numerical purposes. Nevertheless solutions of the BGK equation are very different from those of the Boltzmann equation far from equilibrium. In the Navier–Stokes limit things are much different and a modified version of this model – the Ellipsoidal Statistical Model [2] – allows to recover the correct transport coefficients (Prandtl number).

The Boltzmann equation can be easily extended to the case of inert gas mixtures but things are more difficult for BGK type models. For example, momentum and energy conservations stand only for the whole set of particles. Besides phenomena such as diffusion (Fick law) or thermal diffusion (Soret law) must be considered in the hydrodynamic limit. The Boltzmann equation(s) for gas mixtures has been widely studied by Japanese researchers (see for example [3–6]). Their results feature essential differences with the usual monatomic Boltzmann equation. Its theoretical aspects such as existence theorems [7–9] or study of a binary mixture close to a local equilibrium [10] confirm the specificity of multi-component gases.

Coming back to modeling there exists a great variety of BGK models which traces back to the work of Gross and Krook [11] to the most recent model by Kosuge [12]. A first idea was to mimic the monatomic simplified models in the case of multi-species [11,13–15]. In the case of Maxwellian molecules, models were designed to give the right transfers of momentum and energies far from equilibrium [14,15]. Then Garzo et al. [16] extended the previous approximations for any kind of molecular interaction. In this vein, Kosuge [12] has designed a model that is able to approximate all transfers of moments up to the order two plus the "heat transfers". But no real mathematical considerations such as nonnegativness of the distribution functions or entropy decay were addressed. This was finally done by Andries et al. [17]. This model has later been widely used in the context of reactive gas mixtures (see e.g [18] and references therein). Besides a new property was stated by Garzo et al. [16]: the indifferentiability "principle". When all molecules are of same mass and cross sections are equal then the whole set of equations must reduce to a single one when adding all distribution functions. This property is also satisfied by the model of Andries et al. [17].

Let us remark that while numerical results are quite good for some models or mathematical (and physical) properties are satisfied for others it is quite surprising that none of them has attempted to reach the right hydrodynamic limit. That is to obtain the right transport coefficients as (for example) the Ellipsoidal Statistical Model [2] does in the case of monatomic molecule. In

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general all the authors rather study the hydrodynamic limit of their model and eventually compared it with the right one [19].

Our approach goes the other way. We consider the Navier–Stokes equation with transport coefficients either computed with the hydrodynamic limit of the Boltzmann equation or given by some experiments. Then the aim of the paper is to construct a BGK model that allows to recover those coefficients – in the present case the Fick law. Our main result is in Theorem 2 where we prove that our operator enjoys that property in addition to the classical properties of the Boltzmann equations. Remark that the Fick relaxation operator is not just an abstract model since the Fick matrix coefficients can be obtained using algorithms by Ern and Giovangigli [20]. The paper is organized as follows. In Section 2 we firstly recall Boltzmann equations for gas mixtures and relevant macroscopic quantities. Secondly we introduce spaces and notations that will used in the sequel. Finally we define a class of operators (so-called properly defined) basing on the properties of the Boltzmann collision operators (Section 2.4). In Section 3 we recall in a concise and clear way the link between the thermodynamic of irreversible processes (see for example [21]) and the hydrodynamic limit of the Boltzmann equation. The computation and properties of the transport coefficients obtained from the Boltzmann equations are given in Section 3.2. Such computations easily extend to the case of properly defined operators. Section 4 is devoted to the construction of our operator. We consider linear perturbations or fluctuations around thermodynamical equilibrium. Those are classical assumptions of the thermodynamic of irreversible processes [21] and of statistical physics [22]. This is also the basis of the "theory" of relaxation coefficients introduced by two of the authors [23,24]. Our model is constructed in two step. Firstly we compute those coefficients and related moments of the distribution functions basing only on the Fick matrix (Proposition 1). Then the whole Fick relaxation model is set by using a principle of entropy minimization under moment constraints (Theorem 1). Its definition is given in 3. The simplicity of this model relies on its construction which requires only to diagonalize a modified Fick matrix. In Section 5 we prove that this operator is properly defined (Proposition 2). As a consequence the derivation of its hydrodynamic limit as well as the properties of the transport coefficients just follow the steps that were given for the Boltzmann equation itself (Section 3.2). In particular this BGK model gives at the hydrodynamic limit the exact Fick laws (Section 5.2). We finally prove in Section 5.3 a result concerning the indifferentiability property and the correct Fick law (Proposition 4).

2. The Boltzmann equation and other general kinetic equation for gas mixtures

2.1. The Boltzmann operator for inert gas mixture

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

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

where

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

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 depends on the interaction potential between species i and k. Finally $\mathbf{V} = \mathbf{w} - \mathbf{v}$ is the relative velocity. The post collisional velocities are given by

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

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

$$m_i \mathbf{v} + m_k \mathbf{w} = m_i \mathbf{v}^*_{ki} + m_k \mathbf{w}^*_{ki},$$
$$m_i \|\mathbf{v}\|^2 + m_k \|\mathbf{w}\|^2 = m_i \left\|\mathbf{v}^*_{ki}\right\|^2 + m_k \left\|\mathbf{v}^*_{ki}\right\|^2.$$

2.2. Macroscopic quantities for the mixture

We denote with $n^i, \rho^i, u^i, E^i, \mathcal{E}^i$ and T^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:

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

where k_B is the Boltzmann constant. In the same way macroscopic quantities for the mixture are defined by

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

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

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

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

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

2.3. Other considerations

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

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

This space is equipped using its natural dot product:

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

In the sequel we often use the dot product notation. This notation is valid both for list of p scalar functions and for p tensorial functions. For instance if Ψ, Φ 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 matrices. Then a notation like $\alpha\mathbf{V}, \alpha\mathbf{T}$ (where α is a scalar) means that the scalar α is distributed on each line of the list of vectors or matrix. 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 $\mathbf{S}$.

The natural set of collisional invariants $\mathbb{K}$ of $\mathbb{L}^2(\boldsymbol{M})$ is spanned 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 $\boldsymbol{\phi}^l, l \in [1, p+4]$. 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. This space will be of particular interest in the sequel. Our purpose is now to exhibit a basis of $\mathbb{C}$.

Definition 1. Let $\mathbf{C}_i$ be the vector with ith component is $\boldsymbol{v} - \boldsymbol{u}$ and others are 0line. Denote 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* $p-1$ *independent "vectors" and as a consequence the dimension of* $\mathbb{C}$ *is* $3(p-1)$.

We postpone the proof of this lemma in Appendix.

2.4. The Boltzmann collision operator as model for other kinetic operators

In this section we want to define a class of operators that is based on the properties the Boltzmann collision operators. This framework is well suited to derive in a classical way the hydrodynamic limit. Moreover the corresponding Navier–Stokes equations enjoy many natural properties. So let us denote with $\mathcal{R} := (\mathcal{R}_1, \dots, \mathcal{R}_p)$ any approximation of $Q = (\mathcal{Q}_1, \dots, \mathcal{Q}_p)$. Then we will assume that $\mathcal{R}$ satisfy the following a list properties:

1. **Collisional invariants**

$$\forall \mathbf{f}, f_i \geq 0, \forall \boldsymbol{\phi}, \quad \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathcal{R}_i(\mathbf{f}) \phi_i d\mathbf{v} = 0 \Leftrightarrow \boldsymbol{\phi} \in \mathbb{K}. \tag{4}$$

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

$$\sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathcal{R}_i(\mathbf{f}) \ln(f_i)\, d\mathbf{v} \leq 0. \tag{5}$$

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

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

In such a case we denote $\mathbf{f} = \boldsymbol{M}$. Moreover $\boldsymbol{M}$ is the only set of functions such that

$$\mathcal{R}_i(\mathbf{f}) = 0, \tag{6}$$

4. **Linearized operator:** let $\mathcal{L} := (\mathcal{L}_1, \dots, \mathcal{L}_p)$ be the linearized operator of $\mathcal{R}$ then it must hold

$$Ker(\mathcal{L}) = \mathbb{K}, \tag{7}$$

$$\mathcal{L} \text{ is continuous, invertible and self adjoint negative on } \mathbb{K}^{\perp}. \tag{8}$$

Those last properties are derived from those of the linearized Boltzmann operator [25] $\mathcal{L}_B := (\mathcal{L}_{B,1}, \dots, \mathcal{L}_{B,p})$ operating on $\mathbf{g} = (g_1, \dots, g_p) \in \mathbb{L}^2(\boldsymbol{M})$ and defined by

$$\mathcal{L}_{B,i}(\mathbf{g}) = \frac{1}{\mathcal{M}_i} \left(\sum_{j=1}^{p} Q_{ji}(\mathcal{M}_j, \mathcal{M}_i g_i) + Q_{ji}(\mathcal{M}_j g_j, \mathcal{M}_i) \right). \tag{9}$$

In particular we should add to the above properties that $\mathcal{L}$ must be a Fredholm operator but we omit it for the sake of simplicity. In practice BGK operators satisfying all other properties satisfy this one as well. In the next section those seemingly abstract properties will be shown to be very physical!

Definition 2. Any kinetic operator satisfying all above properties (4)–(8) is said to be properly defined.

3. The Navier–Stokes equations for mixtures and the Boltzmann expansion

The Navier–Stokes system for a mixture of p components reads

$$\forall i \in [1,p], \quad \partial_t n^i + \nabla \cdot (n^i \mathbf{u} + \mathbf{J}_i) = 0, \tag{10}$$

$$\partial_t(\rho\, \mathbf{u}) + \nabla \cdot (\mathbb{P} + \rho\, \mathbf{u} \otimes \mathbf{u} + \mathbb{J}_{\mathbf{u}}) = 0, \tag{11}$$

$$\partial_t E + \nabla \cdot (E\mathbf{u} + \mathbb{P}[\mathbf{u}] + \mathbb{J}_{\mathbf{u}}[\mathbf{u}] + \mathbf{J}_q) = 0, \tag{12}$$

where $\mathbf{J}_i$, $\mathbb{J}_{\mathbf{u}}$ and $\mathbf{J}_{\mathbf{q}}$ 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 depend on the gradients of density, velocity and temperature. The thermodynamic of irreversible processes allows to define them properly but is not able in itself to predict transport coefficients. One of the challenge of the kinetic theory consists in approximating them. We are going to recall the two approaches for the sake of consistency though we are more concerned with the second one.

3.1. Thermodynamics of irreversible processes

The classical reference concerning the thermodynamics of irreversibility processes (TIP) for gas mixtures is the book of De Groot and Mazur [21]. In this book fluxes are expressed (in a slightly different form) as

$$\begin{aligned} \mathbf{J}_i &= \sum_{j=1}^{j=p} L_{ij} \nabla \left(\frac{-\mu_j}{T} \right) + L_{i\mathbf{q}} \nabla \left(\frac{1}{T} \right) \\ \mathbf{J}_{\mathbf{q}} &= \sum_{j=1}^{j=p} L_{\mathbf{q}j} \nabla \left(\frac{-\mu_j}{T} \right) + L_{\mathbf{qq}} \nabla \left(\frac{1}{T} \right) \\ \mathbb{J}_{\mathbf{u}} &= L_{\mathbf{uu}} \mathbb{D}(\mathbf{u}), \end{aligned} \tag{13}$$

where μ_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 given by the relation (up to some additional constant):

$$-\frac{\mu_i}{T} = k_B\left(\ln(n_i) - \frac{3}{2}\ln\left(\frac{2\pi k_B T}{m_i}\right)\right). \tag{14}$$

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

$$\mathbf{L} := \begin{bmatrix} L_{ij} & L_{i\mathbf{q}} & 0 \\ L_{\mathbf{q}i} & L_{\mathbf{qq}} & 0 \\ 0 & 0 & L_{\mathbf{uu}} \end{bmatrix} \tag{15}$$

must be symmetrical non positive.[1] Moreover global mass conservation equation reads

$$\sum_{i=1}^{i=p} m_i \mathbf{J}_i = 0 \Rightarrow \forall j \in [1,p], \qquad \sum_{i=1}^{i=p} m_i L_{ij} = 0. \tag{16}$$

As a consequence the rank of the matrix L_{ij} is at most $p-1$. Moreover using the above equation and the symmetry of the matrix $\mathbf{L}$ (15) then we can only infer that there are $p(p+1)/2+1$ unknowns to search.

Using the phenomenological point of view such fluxes are preferentially expressed as gradient of density, temperature and velocity. They read

$$\begin{aligned} \mathbf{J}_i &= \sum_{j=1}^{j=p} D_{ij}\nabla n_j + D_{iT}\nabla T, \\ \mathbf{J}_\mathbf{q} &= \sum_{j=1}^{j=p} D_{\mathbf{q}j}\nabla n_j - D_{\mathbf{qq}}\nabla T, \end{aligned} \tag{17}$$

where D_{ij} and D_{iT}, $D_{\mathbf{q}j}$ and $D_{\mathbf{qq}}$ respectively denote the Fick, Soret, Duffour and Fourier coefficients. Those coefficients may be measured from experiment while kinetic coefficients cannot be obtained directly. The drawback of this formulation is the lost of symmetry - Casimir–Onsager relations - of the phenomenological coefficients. Remark however that for mixture of ideal gases the one to one correspondence between those coefficients and the matrix $\mathbf{L}$ is straightforward. We are going to see that writing the different fluxes in term of the kinetic coefficients (13) is the most natural choice not only for the TIP but also to link them with the kinetic theory.

3.2. Link between the Boltzmann equation and the thermodynamics of irreversible processes

This subsection is devoted to the derivation of the transport coefficient from the Chapman–Enskog theory. Let us point out that this computation has already been done by Chapman and Cowling in [26] in the case of binary gas mixture. We propose here a classical and modern formulation of such a computation. Consider the rescaled equation

$$\forall i \in [1,p], \quad \partial_t f_i^\epsilon + \mathbf{v}\cdot\nabla_x f_i^\epsilon = \frac{1}{\epsilon}\sum_{k=1}^{k=p} Q_{ki}\left(f_k^\epsilon, f_i^\epsilon\right), \tag{18}$$

together with an expansion of $\mathbf{f}$ in ϵ

$$f_i^\epsilon = f_i^0 + \epsilon f_i^1 + \cdots, \quad \forall i \in [1,p].$$

As usual one compares the different orders in ϵ of the above equations and find thanks to (6) that

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

where the macroscopic parameters n^i, $\mathbf{u}$ and T depend on space and time. Then setting $f_i^1 = \mathcal{M}_i g_i$ and using the zeroth order of equations (18) the first order correction $\mathbf{g} = (g_1,\ldots,g_p)$ is solution of the following equation.

Lemma 2. *The first order correction* $\mathbf{g}$ *satisfies the equation:*

$$\begin{aligned} \mathcal{L}_B(\mathbf{g}) = &\sum_{j=1}^{j=p} k_B^{-1}(\mathcal{I}-\mathcal{P}_\mathbb{K})(\mathbf{C}_j)\cdot\nabla\left(\frac{-\mu_j}{T}\right) \\ &+ \mathbb{A}:\mathbb{D}(\boldsymbol{u}) + \boldsymbol{B}\cdot\nabla\left(\frac{1}{T}\right) \end{aligned} \tag{19}$$

where $\mathcal{I}$ *refers to the identity operator on* $\mathbb{L}^2(\boldsymbol{M})$ *and* $\mathcal{P}_\mathbb{K}$ *is the orthogonal projection on* $\mathbb{K}$. $\mathcal{L}_B := (\mathcal{L}_{B,1},\ldots,\mathcal{L}_{B,p})$ *is the linearized Boltzmann collision operator defined in* (9)*. The list of tensors* $\mathbb{A}$, $\boldsymbol{B}$ *belong to* $\mathbb{K}^\perp$ *(up to their scalar product with a constant list of tensor) and read on their ith line:*

$$(\mathbb{A})_i = m_i\left[(\boldsymbol{v}-\boldsymbol{u})\otimes(\boldsymbol{v}-\boldsymbol{u}) - \frac{1}{3}\|\boldsymbol{v}-\boldsymbol{u}\|^2\,\mathbb{I}\right],$$

$$(\boldsymbol{B})_i = (\boldsymbol{v}-\boldsymbol{u})\left[\frac{1}{2}m_i(\boldsymbol{v}-\boldsymbol{u})^2 - \frac{5}{2}k_B T\right]$$

while $\mathbb{D}(\boldsymbol{u})$ *is the classical Reynolds tensor:*

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

The proof of this lemma is left to Appendix.

Remark 1. (19) is easily obtained generalizing an idea of Levermore ([27]). This may be as well extended to other context such as the one of polyatomic gas mixtures with chemical reactions and clarifies the computation and expressions obtained for example in the book of Giovangigli [20].

Thanks to properties (7) and (8) the Eq. (19) has one unique solution in $\mathbf{g} \in \mathbb{K}^\perp$. This leads to the Navier–Stokes systems in a setting that can be compared with the thermodynamics of irreversible processes approach. More precisely we obtain

Lemma 3.

$$L_{ij}\mathbb{I} = k_B^{-1}\left\langle \mathcal{L}_B^{-1}\left[(\mathcal{I}-\mathcal{P}_\mathbb{K})(\mathbf{C}_i)\right], (\mathcal{I}-\mathcal{P}_\mathbb{K})(\mathbf{C}_j)\right\rangle, \tag{20}$$

$$L_{i\mathbf{q}}\mathbb{I} = L_{\mathbf{q}i}\mathbb{I} = \left\langle \mathcal{L}_B^{-1}(\boldsymbol{B}), (\mathcal{I}-\mathcal{P}_\mathbb{K})(\mathbf{C}_i)\right\rangle, \tag{21}$$

$$L_{\mathbf{uu}}\mathbb{I}\otimes\mathbb{I} = \left\langle \mathcal{L}_B^{-1}(\mathbb{A}), \mathbb{A}\right\rangle, \tag{22}$$

$$L_{\mathbf{qq}}\mathbb{I} = \left\langle \mathcal{L}_B^{-1}(\boldsymbol{B}), \boldsymbol{B}\right\rangle. \tag{23}$$

This concise formalism outlines the importance on one hand of the space $\mathbb{C}$. On the other hand the symmetry and non positiveness of the linearized operator $\mathcal{L}_B^{-1}$ (8) are **necessary** conditions to obtain the Onsager–Casimir properties (15).

Remark 2. It is interesting to note that the kinetic coefficients L_{ij} are known as soon as we know the vectors $(\mathcal{I}-\mathcal{P}_\mathbb{K})(\mathbf{C}_j)$, $j \in [1,p]$ implying that Fick coefficients form a family with $p-1$ degrees of freedom.

Remark 3. Any kinetic model which is properly defined (see Definition 2) has all required properties to derive at the hydrodynamic limit the Navier–Stokes equations with transport

[1] Following precisely the TIP such a matrix must be actually symmetrical *non negative*. This difference is simply due to the definition of the entropy. We should have defined H as

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

to perfectly match the thermodynamical approach. 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.

coefficients given by (20)–(23) (replacing $\mathcal{L}_B$ with $\mathcal{L}$). All those properties are actually required except the H-theorem.

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 connections between thermodynamic forces (and associated kinetic repeal coefficients) and the kinetic theory in a simple way. We have seen that every **linear** small perturbations or fluctuations around local thermodynamic equilibrium state are moments of the perturbation $(M_1g_1,\dots,M_pg_p)$ around the local Maxwellian states. Beside transport coefficients are only connected to the properties of the linear interaction operator. Those coefficients can be interpreted as functions of relaxation rates associated to ad-hoc moments of the perturbation following the idea of two of the authors [23,24]. If one thinks of constructing BGK models that give the right hydrodynamic limit one may try to generalize the scheme of those articles. In the present work we restrict our approach to obtain the *the Fick and Newton laws*. Let us consider an operator of the form

$$\mathcal{R}(\mathbf{f}) = \nu(\mathbf{G}-\mathbf{f}). \tag{24}$$

Since diffusion coefficients depend on moments in $\mathbb{C}$ of the perturbation we may consider (unknown) vectors in $\mathbf{w}_r \in \mathbb{C}$ and set

$$\nu\sum_{j=1}^{j=p}\int_{\mathbb{R}^3}(G_j-f_j)\,\mathbf{w}_{r,j} = -\lambda_r\sum_{j=1}^{j=p}\int_{\mathbb{R}^3} f_j\mathbf{w}_{r,j}, \tag{25}$$

for a set of relaxation coefficients $(\lambda_r)_r$. The choice of a basis $(\mathbf{w}_r)_{r=1,\dots,p-1}$ $\mathbb{C}$ and relaxation coefficients $(\lambda_r)_{r=1,\dots,p-1}$ is crucial to recover the Fick law at the hydrodynamic limit. ν is eventually a free parameter that can be fitted to obtain the true viscosity coefficient. The model is designed in two steps.

1. We firstly compute the relaxation coefficients λ_r and corresponding moments $\mathbf{w}_r$ by considering the property of the Fick coefficients matrix L_{ij} (20) (property 1),
2. Secondly $\mathbf{G}$ is obtained by minimizing the entropy under the constraints (25) and the conservation laws (4) (Theorem 1).

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. We recall in this first lemma a property of (L_{ij}).

Lemma 4. *The matrix $(L_{ij})_{i,j}$ obtained in (20) has a rank $p-1$.*

We postpone the proof of this lemma to Appendix. Then we have the following result.

Lemma 5. *The symmetric non positive matrix L^*_{ij} defined by*

$$L^*_{ij} := \frac{k_BL_{ij}}{\|\mathbf{C}_i\|\,\|\mathbf{C}_j\|} = k_BL_{ij}\sqrt{\frac{m_i}{n_ik_BT}}\sqrt{\frac{m_j}{n_jk_BT}},\quad \forall i,j\in[1,p] \tag{26}$$

always diagonalizes in an orthonormal basis:

$$L^* = W^TD^*W.$$

Up to some permutation in W and D^* the corresponding eigenvalues $(d^*_r)_r$ are non null for $r=1,\dots,p-1$ while $d^*_p=0$. Moreover the vectors defined by

$$\mathbf{w}_r = \sum_{s=1}^{p} W_{rs}\frac{\mathbf{C}_s}{\|\mathbf{C}_s\|},\quad r=1,\dots,p-1 \tag{27}$$

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

$$\mathbf{w}_p = \sum_s\sqrt{\frac{\rho_s}{\rho}}\frac{\mathbf{C}_s}{\|\mathbf{C}_s\|} = \pm\sum_{s=1}^{s=p}W_{ps}\frac{\mathbf{C}_s}{\|\mathbf{C}_s\|}\in\mathbb{K}. \tag{28}$$

Proof. Since L^* is symmetric it may be diagonalized. It has exactly one vanishing eigenvalue thanks to Lemma 4. Finally we can always permute indexes so that $d^*_p=0$. Consider the vector ϖ whose components are $\sqrt{\rho_j}/\sqrt{\rho}$. Then a direct computation shows that:

$$\begin{aligned}(L^*\varpi)_i &= \sum_{j=1}^{j=p}\frac{k_BL_{ij}}{\|\mathbf{C}_i\|\,\|\mathbf{C}_j\|}\sqrt{\frac{\rho_j}{\rho}}\\ &= \frac{k_B}{\|\mathbf{C}_i\|\sqrt{\rho k_BT}}\sum_{j=1}^{j=p}L_{ij}m_j = 0\end{aligned}$$

the last equality being obtained thanks to (16). Besides, the vector ϖ is normalized for the usual vector norm. As a consequence, when diagonalizing the matrix L^* in a orthonormal basis 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 since $\|\mathbf{C}_s\| = \sqrt{n^sk_BT}/\sqrt{m_s}$ a direct computation shows that the vector $\mathbf{w}_p$ has $m_i(\mathbf{v}-\mathbf{u})/\sqrt{\rho k_BT}$ on its ith line and thus belongs to $\mathbb{K}$.

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

Finally every vector $\mathbf{w}_s$, $s\in[1,p-1]$ is a linear combination of the $\mathbf{C}_i$, $i\in[1,p]$ and orthogonal to $\mathbf{w}_p$ so that it belongs to $\mathbb{C}$. Thus this set of vectors is an orthonormal basis of $\mathbb{C}$. □

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

Proposition 1. *Assume that $\mathcal{R}(\mathbf{f})$ (see (25)) is properly defined (Definition 2). Define d^*_r and $\mathbf{w}_r (r\in[1,p])$ as in Lemma 5. Then setting*

$$\lambda_r = -d_r^{*-1},\qquad \lambda_p = 0 \tag{29}$$

the BGK model allows to recover at the hydrodynamic limit the Fick laws.

Moreover if $\mathcal{L}$-the linearized operator of $\mathcal{R}$- is such that $\mathcal{L}^{-1}(\mathbf{B})\in\mathbb{C}^\perp$, then mass fluxes read

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

Proof. In this proof we start from the conclusion and show that it is valid if and only if we take d^*_r and $\mathbf{w}_r (r\in[1,p])$ as relaxation coefficients and related moments.

Since $\mathcal{R}(\mathbf{f})$ (25) is properly defined we have thanks to (19)

$$\begin{aligned}\mathcal{L}(\mathbf{g}) &= \sum_{j=1}^{j=p}k_B^{-1}(\mathcal{I}-\mathcal{P}_{\mathbb{K}})(\mathbf{C}_j)\cdot\nabla\left(\frac{-\mu_j}{T}\right)\\ &\quad+\mathbb{A}:\mathbb{D}(\mathbf{u})+\mathbf{B}\cdot\nabla\left(\frac{1}{T}\right).\end{aligned} \tag{30}$$

We now write

$$\mathbf{J}_i = \langle\mathbf{g},\mathbf{C}_i\rangle = \sum_{j=1}^{p}L_{sj}\nabla\left(\frac{-\mu_j}{T}\right), \tag{31}$$

where the coefficients L_{ij} are defined in Eq. (20). Here the coefficients L_{iq} (21) corresponding to the operator $\mathcal{L}$ vanish since we have assumed that $\mathcal{L}^{-1}(\mathbf{B}) \in \mathbb{C}^{\perp}$. Then consider the first order expansion of relaxation equations (25)

$$\langle \mathcal{L}(\mathbf{g}), \mathbf{w}_r \rangle = -\lambda_r \langle \mathbf{g}, \mathbf{w}_r \rangle, \quad r \in [1, p]. \tag{32}$$

Using Lemma 5 and (30) the right hand sides of those equations read

$$\begin{aligned} \langle \mathbf{g}, \mathbf{w}_r \rangle &= \sum_{s=1}^{p} \frac{W_{rs}}{\|\mathbf{C}_s\|} \mathbf{J}_s \\ &= \sum_{s,j=1}^{p} \frac{W_{rs}}{\|\mathbf{C}_s\|} L_{sj} \nabla \left(\frac{-\mu_j}{T} \right), \quad r = 1, \ldots, p. \end{aligned} \tag{33}$$

Next the left hand sides can be computed thanks to (30)

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

since $\langle (\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_j), \mathbf{w}_r \rangle = \langle \mathbf{C}_j, \mathbf{w}_r \rangle$ for all $\mathbf{w}_r \in \mathbb{C}$. 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 (32) reads

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

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

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

where L_{sj}^* is defined in Eq. (26). We can also complete this set of equations with

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

thanks to (16) and the symmetry of L_{sj}^*. Multiplying both side of the above equations with W_{tj} and summing over j we obtain

$$\delta_{rt} = -\lambda_r \sum_{s,j=1}^{p} W_{rs} L_{sj}^* W_{tj}, \quad \forall r = 1, \ldots, p-1, \; t = 1, \ldots, p$$

$$0 = \sum_{s,j=1}^{p} W_{ps} L_{sj}^* W_{pj}, \quad \forall t = 1, \ldots, p$$

which amounts to diagonalize L^*. Hence since the choice of the basis $(\mathbf{w}_r)_r$ is the unique way to obtain those last equations and we have proved the proposition. □

4.3. Definition of Fick-relaxation operator

Before proving Theorem 1, we begin with some preparatory lemmas

Lemma 6. *Define $\boldsymbol{f}$ as a list of non negative and non null functions with suitable integration properties. We denote with n^i, $\boldsymbol{u}^i$, T the hydrodynamic parameters associated to the function $\boldsymbol{f}$. Let us consider the set of functions*

$$\mathbf{g} \in \boldsymbol{K}(\boldsymbol{f}) \Leftrightarrow \begin{cases} g \geq 0 \, a.e, \forall l \in [1, p+4], \\ \displaystyle\sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \phi_i^l (g_i - f_i) \, d\mathbf{v} = 0, \\ \forall r \in [1, p-1], \\ \displaystyle\sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathbf{w}_{r,i} \left(g_i - \left(1 - \frac{\lambda_r}{\nu}\right) f_i \right) d\mathbf{v} = \mathbf{0}, \end{cases} \tag{34}$$

where we have used the notations of Proposition 1. We denote respectively with $\overline{\boldsymbol{U}} = (\boldsymbol{u}^1, \ldots, \boldsymbol{u}^p)^T$, $\underline{\boldsymbol{U}} = (\boldsymbol{u}_1, \ldots, \boldsymbol{u}_p)^T$ the mean velocities of $\boldsymbol{f}$ and $\mathbf{g}$ and with $\mathbf{N}$ and Λ the diagonal matrix with diagonal terms are respectively $(\sqrt{\rho_1}, \ldots, \sqrt{\rho_p})$ and $(\lambda_1, \ldots, \lambda_p)$. Then we have

$$\underline{\boldsymbol{U}} - \boldsymbol{U} = \mathbf{N}^{-1} W^T \left(\boldsymbol{I} - \frac{1}{\nu} \Lambda \right) W \mathbf{N} \left(\overline{\boldsymbol{U}} - \boldsymbol{U} \right). \tag{35}$$

Proof. We postpone the proof of this simple calculation to Appendix. □

Remark that the conservation of energy implies

$$\begin{aligned} \sum_{i=1}^{p} \frac{1}{2} m_i \int_{\mathbb{R}^3} |v - u|^2 g_i dv &= \sum_{i=1}^{p} \frac{3}{2} n_i k_B T_i + \sum_{i=1}^{p} \frac{1}{2} \rho_i (u_i - u)^2 \\ &= \frac{3}{2} n k_B T. \end{aligned} \tag{36}$$

Here T_i stands for the temperature of g_i. This leads us to the definition of a "mean" temperature T^* for the functions $(g_i)_i$.

$$T^* = \sum_{i=1}^{p} \frac{1}{3nk_B} m_i \int_{\mathbb{R}^3} (v - u_i)^2 g_i dv.$$

Lemma 7. *Using the same notations as in Lemma 6, for any value of $\nu \geq \max_r \lambda_r / 2$ the temperature defined as*

$$T^* = T - \frac{1}{3nk_B} \left\| W^T \left(\boldsymbol{I} - \frac{1}{\nu} \Lambda \right) W \, \mathbf{N} \left(\overline{\boldsymbol{U}} - \boldsymbol{U} \right) \right\|^2 \tag{37}$$

is positive.

Proof. We have to find a lower bound of the right-hand side of Eq. (37). Remark now that

$$\begin{aligned} &\left\| W^T \left(\mathbf{I} - \frac{1}{\nu} \Lambda \right) W \, \mathbf{N} \left(\overline{\mathbf{U}} - \mathbf{U} \right) \right\|^2 \\ &\leq \max_r \left(1 - \frac{\lambda_r}{\nu} \right)^2 \|\mathbf{N} \left(\overline{\mathbf{U}} - \mathbf{U} \right)\|^2 \\ &\leq \left(1 - \frac{\min_r \lambda_r}{\nu} \right)^2 \|\mathbf{N} \left(\overline{\mathbf{U}} - \mathbf{U} \right)\|^2 < \sum_{i=1}^{p} \rho_i (u^i - u)^2, \end{aligned}$$

where we have used the orthogonality of the matrix W for the first inequality and the assumption on ν for the last one. Now the proof of the lemma easily follows from the equality

$$\begin{aligned} \sum_{i=1}^{p} \int_{\mathbb{R}^3} \frac{1}{2} m_i (v - u)^2 f_i dv &= \frac{3}{2} n k_B T \\ &= \frac{3}{2} \sum_{i=1}^{p} n_i k_B T^i + \sum_{i=1}^{p} \frac{1}{2} \rho_i (u^i - u)^2. \quad \square \end{aligned} \tag{38}$$

Theorem 1. *Let f and T^* be defined as above. Then for any value of $\nu \geq \max_r \lambda_r$, $K \neq \emptyset$ and there exists a unique solution $\underline{G}$ to the minimization problem*

$$\underline{G} = Argmin_{g \in K(f)} \mathcal{H}(g). \tag{39}$$

This solution reads

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

where we have used the notations of Lemmas 6 and 7.

Proof. Roughly speaking the existence (and unicity) of such a minimizer is a generalization of the complex problem of minimization of the entropy under moment constraints (see [28,29]). For example we can follow the approach of Junk [28] which consists in examining the set

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

If this set is open then the minimization problem has a unique solution as soon as $\mathbf{K}(\mathbf{f}) \neq \emptyset$. Here this set is clearly open since all exponential functions must have a negative factor (α_{p+4}) in front of monomials of order two.

Finally it is possible in this particular case to exhibit the solution itself $\underline{\mathbf{G}}$ using Lagrange multipliers. Hence $\mathbf{K}(\mathbf{f}) \neq \emptyset$. □

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

$$\mathcal{R}(f) = \nu (G - f), \tag{41}$$

where $\nu \geq \max_r \lambda_r/2$ and

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

Remark 4. The set of constraints

$$\forall r \in [1, p-1], \quad \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathbf{w}_{r,i} \left(G_i - \left(1 - \frac{\lambda_r}{\nu}\right) f_i\right) dv = \mathbf{0}$$

together with Eq. (41) is equivalent to Eq. (25). Thus if $\mathcal{R}(f)$ is properly defined it is clear that its hydrodynamic limit gives the Fick laws thanks to Proposition 1.

4.4. Practical utilization of the model

For the sake of clarity we precise in this subsection how to compute the model presented in this paper. Let us assume that the matrix of the Fick coefficients D_{ij} is measured as a function of densities $(n^i)_i$ and temperature T. In the framework of a simple explicit Euler scheme one has to compute at each time step

- the eigenelements of the matrix L^*.

$$L^*_{ij} = \frac{n_j}{k_B T} D_{ij} \sqrt{\frac{m_i m_j}{n_i n_j}}.$$

- the velocities $(\mathbf{u}_i)_i$ using the relation (35).
- the temperature T^* through formula (38).

Finally the relaxation coefficient ν must be chosen with the constraint $\nu \geq \max_r \lambda_r/2$. If the true viscosity satisfies the condition

$$\mu \leq \frac{n k_b^2 T^2}{\max_r \lambda_r}$$

then set $\nu = n k_b^2 T^2/\mu$ (see Remark 5).

5. On the Fick-relaxation operator and the transport coefficients

In this section we firstly prove that the Fick-relaxation operator is properly defined. Then we propose a mathematically well-posed derivation of the linearized operator. From those results we easily deduce the transport coefficients obtained at the hydrodynamic limit of our modified kinetic equations (Theorem 2 Section 5.2). In particular the exact Fick law is recovered. Finally Section 5.3 is devoted to a discussion about the indifferentiability property. More precisely we show that if there exists any BGK operator satisfying this property and giving the right Fick law then our model also satisfy the indifferentiability principle (Proposition 4).

5.1. $\mathcal{R}(f)$ is a properly defined operator.

Proposition 2. *The Fick-relaxation operator is a properly defined. More precisely it satisfies properties (4)–(8). Moreover the corresponding linearized operator $\mathcal{L}$ is self adjoint and negative on $\mathbb{K}^\perp$ and its kernel is $\mathbb{K}$.*

Proof. The first part of the proof is let in appendix C since it is quite usual. The explicit expression of the linearized operator allows to finish the proof. Its computation is given in the following lemma. □

Lemma 8. *The linearized operator $\mathcal{L}$ of the Fick-relaxation operator reads*

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

where $\mathcal{I}$ is the identity operator on $\mathbb{L}^2(\boldsymbol{M})$. $\mathcal{P}_{\mathbb{K}}$ and $\mathcal{P}_{\mathbb{C}}$ denote respectively the orthogonal projection on $\mathbb{K}$ and $\mathbb{C}$. Finally R is the linear operator defined on $\mathbb{C}$ by the formula:

$$\forall r \in [1, p-1], \quad R(\mathbf{w}_r) = \left(1 - \frac{\lambda_r}{\nu}\right) \mathbf{w}_r.$$

Its pseudo inverse $\mathcal{L}^{-1}$ reads:

$$\forall \mathbf{g} \in \mathbb{K}^\perp, \quad \mathcal{L}^{-1}(\mathbf{g}) = \frac{1}{\nu}\left((R - \mathcal{I}_{\mathbb{C}})^{-1} \circ \mathcal{P}_{\mathbb{C}} + (\mathcal{P}_{\mathbb{C}} - \mathcal{I})\right)(\mathbf{g}) \tag{42}$$

where $\mathcal{I}_{\mathbb{C}}$ denotes the restriction on $\mathbb{C}$ of the identity operator.

Proof. Let $\boldsymbol{M}$ be a thermodynamic equilibrium. Then $\mathcal{L}(\mathbf{g})$ is defined as usual by the formula $\mathbb{L}^2(\boldsymbol{M})$

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

for any function $\mathbf{g}$ in $\mathbb{L}^2(\boldsymbol{M})$. Remark that thanks to Proposition 2 $\mathcal{R}_i(\boldsymbol{M}) = 0$. Next for all $\mathbf{g}$ there exists $\epsilon_0(\mathbf{g})$ such that for all $\epsilon < \epsilon_0$ the problem

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

admits a solution. Indeed the set of realizable constraints $\mathbf{K}(\boldsymbol{M})$ is open [28]. Let us write this solution in the following form

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

where the pseudo-Lagrange multipliers $(\alpha_l(\epsilon, g))_l$, $(\beta_r(\epsilon, g))_r$ are solutions of the perturbated problem. We may compute exactly those coefficients from the form (40) given in Theorem 1 and find out that they are infinitely differentiable with respect to each variables for $\epsilon < \epsilon_0$. Thus they can be expanded in ϵ:

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

The zeroth order corresponds to the Maxwellian distribution thanks to property (6). That is

$$\alpha_i^0 = \frac{-\mu_i}{k_BT} - m_i\frac{\mathbf{u}^2}{2k_BT}, \qquad \alpha_{p+3}^0 = \frac{\mathbf{u}}{k_BT}, \qquad \alpha_{p+4}^0 = -\frac{1}{2k_BT}$$

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

where μ_i is defined in (14). Thus $\mathbf{G}_{i,M(1+\epsilon g)}$ can be expanded in ϵ

$$\mathbf{G}_{i,M(1+\epsilon g)} = \mathcal{M}_i\left(1+\epsilon\left[\sum_{l=1}^{p+4}\alpha_l^1(g)\phi_i^l + \sum_{r=1}^{p-1}\beta_r^1(g)\,w_{r,i}\right] + O(\epsilon^2)\right). \quad (43)$$

So that

$$\mathcal{L}_i(\mathbf{g}) = \sum_{l=1}^{p+4}\alpha_l^1(g)\phi_i^l + \sum_{r=1}^{p-1}\beta_r^1(g)\,w_{r,i} - g. \quad (44)$$

Now remark that the set of constraints (34) depends linearly on the moments of the function $\boldsymbol{M}(1+\epsilon\mathbf{g})$ so that the perturbations at order 1 in ϵ of the Lagrange multipliers $\alpha_l^1(g)$, $\beta_i^1(g)$ are also linear. We can compute them exactly by inserting the expression (43) in the constraints (34) with $\mathbf{f} = \boldsymbol{M}(1+\epsilon\mathbf{g})$. Hence considering the equalities at order one in ϵ we have

$$\sum_{l=1}^{p+4}\langle\boldsymbol{\phi}^k, \boldsymbol{\phi}^l\rangle\,\alpha_l^1(g) = \langle\mathbf{g}, \boldsymbol{\phi}^k\rangle \quad \forall k \in [1, p+4],$$

$$\sum_{r=1}^{p-1}\langle\mathbf{w}_s, \mathbf{w}_r\rangle\,\beta_r^1(g) = \left(1-\frac{\lambda_r}{\nu}\right)\langle\mathbf{g}, \mathbf{w}_r\rangle \quad \forall s \in [1, p-1].$$

Here the first line corresponds exactly to the projection of $\mathbf{g}$ on $\mathbb{K}$ through the expression (44) of $\mathcal{L}_i(\mathbf{g})$. The second line amounts to project on the basis $(\mathbf{w}_r)_r$ of $\mathbb{C}$ and multiply each coordinates with a factor $\left(1-\frac{\lambda_r}{\nu}\right)$.

Finally the expression (42) is readily seen to be the pseudo inverse $\mathcal{L}^{-1}$ of $\mathcal{L}$. □

5.2. Hydrodynamic limit

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

$$\forall i \in [1, p], \quad \partial_t f_i^\epsilon + \mathbf{v}\cdot\nabla_{\mathbf{x}} f_i^\epsilon = \frac{1}{\epsilon}\mathcal{R}(\mathbf{f}^\epsilon). \quad (45)$$

Theorem 2. *Define $\mathcal{R}(f)$ by the Eq. (45) and set $\nu \geq \max_r \lambda_r$ where $(\lambda_r)_r$ are defined in Lemma 5. Then the hydrodynamic limit of (45) (see definition (24)) gives at the order 1 the Navier–Stokes system of equations (10)–(12) with fluxes given by*

$$J_i = \sum_{j=1}^{p} L_{ij}\nabla\left(\frac{-\mu_j}{T}\right),$$

$$J_q = \frac{5\,k_B^3T^3}{2\,\nu}\sum_{i=1}^{p}\frac{n_i}{m_i}\nabla\left(\frac{1}{T}\right), \qquad \mathbb{J}_u = \frac{n\,k_B^2T^2}{\nu}\,\mathbb{D}(\mathbf{u}). \quad (46)$$

Here $(L_{ij})_{ij}$ is the matrix of Fick coefficients (20) computed with the linearized Boltzmann operator.

Proof. The proof is easily deduced from the fact that $\mathcal{R}(\mathbf{f})$ is properly defined according to Proposition 2 (see Remark 3). Hence all kinetic coefficients can be computed since we know the exact form of $\mathcal{L}^{-1}$ (42).

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

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

   so that Proposition 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:** A direct computation gives

   $$L_{\mathbf{uu}}^{\mathcal{R}}\mathbf{I}\otimes\mathbf{I} = \langle\mathcal{L}^{-1}(\mathbb{A}), \mathbb{A}\rangle = \frac{1}{\nu}\langle\mathbb{A}, \mathbb{A}\rangle = \frac{n\,k_B^2T^2}{\nu}\mathbf{I}\otimes\mathbf{I}.$$
3. **Fourier coefficient:**

   $$L_{\mathbf{qq}}^{\mathcal{R}}\mathbf{I} = \langle\mathcal{L}^{-1}(\mathbf{B}), \mathbf{B}\rangle = \frac{1}{\nu}\langle\mathbf{B}, \mathbf{B}\rangle$$

   $$\Leftrightarrow L_{\mathbf{qq}}^{R} = \frac{5\,k_B^3T^3}{2\,\nu}\sum_{i=1}^{p}\frac{n_i}{m_i} \neq L_{\mathbf{qq}}\mathbf{I}. \quad \square$$

Remark 5. Let $\mu = \mathbf{L}_{uu}$ be the true viscosity of the mixture (see Eq. (22)). Then if the condition

$$\mu \leq \frac{nk_b^2T^2}{\max_r \lambda_r}$$

is satisfied one can recover the true viscosity by setting $\nu = nk_b^2T^2/\mu$.

Here the density fluxes are deduced from our "natural" construction (Proposition 1). That is using the concept of relaxation rates associated to ad-hoc moments of the distribution functions. To recast the hydrodynamic limit in the spirit of Section 3.2 we may check the following results.

Proposition 3. *The linearized operator $\mathcal{L}$ satisfies*

$$\forall (i,j) \in [1, p]^2,$$
$$\langle k_B^{-1}\mathcal{L}^{-1}(\mathcal{I}-\mathcal{P}_{\mathbb{K}})(\mathbf{C}_i), (\mathcal{I}-\mathcal{P}_{\mathbb{K}})(\mathbf{C}_j)\rangle = L_{ij}. \quad (47)$$

Proof. First let us note that:

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

It is then very easy to compute $(\mathcal{I}-\mathcal{P}_{\mathbb{K}})(\mathbf{C}_i)$ which reads:

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

Applying now the operator $\mathcal{L}^{-1}$ 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 left hand side of (47) reads:

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

Since the basis $(\boldsymbol{w}_k)$ is orthonormal this sum simplifies in the above equation:

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

$$= k_B^{-1}\|\mathbf{C}_i\|\,\|\mathbf{C}_j\|\sum_{k=1}^{k=p}W_{ik}^Td_k^*W_{kj}$$

(recall that $d_k^* = -1/\lambda_k$, $k \in [1, p-1]$ and $d_p^* = 0$). 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. □

5.3. About the indifferentiability property

Following the articles by Garzo et al. [16] and Andries et al. [17] the indifferentiability property may be stated as follows. When all particle masses and differential cross sections are equal in the mixture – which define the so-called indifferentiable molecules – the BGK operator for the mixture must reduce to a single one for the sum of all distribution functions:

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

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 dependency with $\mathbf{f}$ which happens for instance when one considers dense situations (see for example [30]).

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

$$\forall i \in \{1,\dots,p\},\quad \widetilde{\mathcal{R}}_i(\mathbf{f}) = \tilde{\nu}_i(\widetilde{G}_i - f_i). \tag{48}$$

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 "linear" in the following sense. There exist X and $T \in \mathbb{R}^p \times \mathbb{R}^p$ which do not depend on v such that
$$\sum_{i=1}^{i=p} X_{ij}\int_{\mathbb{R}^3}\widetilde{G}_i(v-u)\,dv = \sum_{i=1}^{i=p} T_{ij}\int_{\mathbb{R}^3} f_i(v-u)\,dv.$$
Or in short
$$\underline{\mathbf{U}} - \mathbf{U} = X^{-1}N^{-1}T\,N\,(\overline{\mathbf{U}} - \mathbf{U}) \tag{49}$$
(here we have kept the notations of Lemma 6 and Theorem 1).
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. This is for example the case of [17]. Those constraints are quite natural regarding to the way the true diffusion (Fick) coefficients are obtained (see (20)). 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 indifferentiability is obtained thanks to an "additivity" property. That is

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

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

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

Lemma 9. *Let $\widetilde{\mathcal{R}}$ be a properly defined operator of the form (48) satisfying the above assumptions. Then when all molecules are indifferentiable the restriction to $\mathbb{C}$ of the linearized BGK operator is proportional to minus identity.*

Proof. The property (7) implies that the restriction of the linearized operator on the space spanned by $(\mathbf{C}_i)_i$ actually reduces to the space $\mathbb{C}$. Thus generalizing the calculations we have done in Section 5.1 and using Assumption 1 this restriction reads $(\widetilde{R} - \mathcal{I}_{\mathbb{C}})$ where $\widetilde{R}$ is a linear operator depending on T (see Assumption 1). Here $\mathcal{I}_{\mathbb{C}}$ is as usual the restriction on $\mathbb{C}$ of the identity operator. To be consistent with the symmetry of the linearized Boltzmann operator the operator $\widetilde{R}$ has to be symmetric on $\mathbb{C}$ while the operator $\widetilde{R} - \mathcal{I}_{\mathbb{C}}$ must be non positive and symmetric because of the property (8). Consequently $\widetilde{R}$ can be diagonalized in a proper orthogonal basis $\mathbf{x}_r$, $r \in \{1,\dots,p-1\}$ such that

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

And we can write (49) in the same form as (35)

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

Here the matrix X^T denotes the passage from the basis $(\mathbf{C}_i)_i$ to the new 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 $a_{pp} = 0$.

When all molecules are indifferentiable and under Assumption 2 $u_i = u$ for any $i \in \{1,\dots,p\}$. As a consequence the relation (49) must be valid for each values of u^i meaning that for any $r \in \{1,\dots,p\}$, $\alpha_r = 1$. Consequently $\widetilde{R} = 0$. □

Remark 6. The above lemma is valid without any assumption on the entropy decay meaning that it is also valid for BGK operator where functions (G_i) are not positive everywhere (see for example [16]). Moreover the conclusion of the lemma implies that all frequencies $\tilde{\nu}_i$ reduces to a single one $\tilde{\nu}$.

Next we prove the following alternative.

Proposition 4. *Two situations are possible.*

- *Either there exists at least one properly defined BGK operator of the form (48) satisfying the above assumptions,the indifferentiability property and giving the Fick law at the hydrodynamic limit. In that case the Fick relaxation operator $\mathcal{R}$ (Definition 3) satisfies the indifferentiability as well. Moreover when all molecules are indifferentiable $\tilde{\nu}_i = \nu$, $\forall i$.*
- *Or there are no properly defined BGK operator satisfying the indifferentiability property and Fick law together Assumptions 1 and 2.*

Proof. Consider a properly defined BGK operator satisfying Assumptions 1 and 2. Its associated Fick coefficients $L_{ij}^{\widetilde{\mathcal{R}}}$ are given by (20) replacing $\mathcal{L}_B$ with $\mathcal{L}_{\widetilde{\mathcal{R}}}$ (see Remark 3). Thus according to Lemma 9 and the above remark when all molecules are indifferentiable

$$L_{ij}^{\widetilde{\mathcal{R}}}\mathbb{I} = -\frac{1}{k_B\tilde{\nu}}\left\langle(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_i),(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\mathbf{C}_j)\right\rangle,\quad \tilde{\nu} > 0. \tag{50}$$

If the model satisfies the Fick law as well we have $(L_{ij}^{\widetilde{\mathcal{R}}})_{i,j} = (L_{ij})_{i,j}$ where the second matrix is defined either by (20) or by

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

where we have used (42) and (47). The comparison between this equation and (50) imposes firstly that $R = 0$. Coming back to Eq. (35) 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 indifferentiability property. But according to Lemma 9, in the situation of indifferentiability L_{ij} is given by a formula analogous to (50) leading to $\tilde{\nu} = \nu$.

The last assertion is self evident. □

When all molecules are indifferentiable we do not know exactly if the kinetic coefficients obtained by the linearized Boltzmann operator can match those obtained by a BGK operator satisfying the indifferentiability property. But in reality we do not care because the correctness of the linearized BGK operator is much more important. If the two requirements contradict we prefer to sacrify indifferentiability.

In concrete situations masses and cross sections are always different. Therefore the indifferentiability principle is only a continuity principle. That is why we prefer to conserve the correctness of the hydrodynamic 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 [23,24] as a new way to understand the ellipsoidal 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 Newton 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, Newton and Fourier coefficients could be possible by generalizing for gas mixture the approach described in [23]. More difficult however seems the possibility to get at the same time the correct (so called "cross") kinetic coefficients $(L_{i\mathbf{q}})_i$ (15), (21). In our model (as it is also the model of [17]) such cross kinetic coefficients are zero and give incorrect 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 [20] and the experimental work of Kestin et al. [31] will be of precious help when actually computing the Fick relaxation operator.

Acknowledgments

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Appendix

A.1. Proof of Lemma 1

Proof. A direct computation shows that the lth 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:

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

To know if this linear system on the α_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 independent or not), one has to discuss the determinant of the k by k matrix M defined as:

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

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

$$(\forall j \in \{1; k\}), \quad \sum_{i=1}^{p} x_i = \frac{\rho}{\rho_j} x_j. \tag{51}$$

Therefore it comes that

$$(\forall j \in \{1; k\}), \quad \frac{\rho}{\rho_j} x_j = \frac{\rho}{\rho_1} x_1. \tag{52}$$

Now assume by contradiction that $x \neq 0$. In that case for example $x_1 \neq 0$. According to (52), for any $i \in \{1,k\}, x_i \neq 0$. So (51) implies that $\sum_{i=1}^{k} x_i \neq 0$. From (52) 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 $x \in KerN$. So N is non invertible. □

A.2. Proof of Lemma 2

Proof. Here we follow the path of Levermore [27]. The first problem consists in computing $(\partial_t + \mathbf{v}\cdot\nabla_\mathbf{x})[\mathcal{M}_i]$ for $i \in [1,p]$. Now let write $\mathcal{M}_i$ as:

$\forall i \in [1,p]$,

$$\mathcal{M}_i = \exp\left(\left(\frac{-\mu_i}{k_BT} - m_i\frac{\mathbf{u}^2}{2k_BT}\right) + \frac{\mathbf{u}}{k_BT}\cdot m_i\mathbf{v} - \frac{m_i\mathbf{v}^2}{2k_BT}\right).$$

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

$\forall i \in [1,p]$,

$$(\partial_t + \mathbf{v}\cdot\nabla_\mathbf{x})(\mathcal{M}_i) = \sum_{k=1}^{k=p+4} [(\partial_t + \mathbf{v}\cdot\nabla_\mathbf{x})\alpha_k]\,\boldsymbol{\phi}_i^k\mathcal{M}_i, \tag{53}$$

where

$$\forall k \in [1,p],\quad \alpha_k = \left(\frac{-\mu_k}{T} - \frac{m_k\mathbf{u}^2}{2k_BT}\right)$$

$$\alpha_{p+1} = \frac{u_x}{k_BT},\qquad \alpha_{p+2} = \frac{u_y}{k_BT},\qquad \alpha_{p+3} = \frac{u_z}{k_BT},$$

$$\alpha_{p+4} = -\frac{1}{2k_BT}.$$

The zeroth order of (45) gives after integration the Euler equations

$$\forall l \in [1,p+4],\quad \sum_{i=1}^{i=p}\int_{\mathbb{R}^3} ((\partial_t + \mathbf{v}\cdot\nabla_\mathbf{x})(\mathcal{M}_i)\,\phi_i^l)\,d\mathbf{v} = 0. \tag{54}$$

Using (53) we they can be rewritten as

$$\forall l \in [1,p+4],\quad \sum_{k=1}^{k=p+4} \langle(\partial_t + \mathbf{v}\cdot\nabla_\mathbf{x})(\alpha_k)\,\phi^k, \phi^l\rangle = 0. \tag{55}$$

The orthogonal projection $\mathcal{P}_\mathbb{K}(b)$ on $\mathbb{K}$ of any vector $b \in \mathbb{L}^2(\mathbf{w}(\mathbf{v})\,d\mathbf{v})$ reads

$$\mathcal{P}_\mathbb{K}(b) = \sum_{k=1}^{k=p+4}\left[\sum_{l=1}^{l=p+4} (S^{-1})_{kl}\langle b, \phi^l\rangle\right]\phi^k, \tag{56}$$

where S denote the symmetrical matrix such that $S_{lk} = \langle\phi^l, \phi^k\rangle$. Let us consider now

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

The Eq. (55) 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 $\mathbb{K}$ (56) 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

$$\sum_{k=1}^{k=p+4} (\partial_t + \mathbf{v}\cdot\nabla_\mathbf{x})(\alpha_k)\,\boldsymbol{\phi}^k = (\mathcal{I} - \mathcal{P}_\mathbb{K})\left(\sum_{k=1}^{k=p+4} [\mathbf{v}\cdot\nabla_\mathbf{x}](\alpha_k)\,\phi^k\right). \tag{57}$$

Using this equality with the relation (53) enables us to write the Eq. (19) at order 0 in the form

$$\mathcal{L}(\mathbf{g}) = (\mathcal{I} - \mathcal{P}_\mathbb{K})\left(\sum_{k=1}^{k=p+4} [\mathbf{v}\cdot\nabla_\mathbf{x}](\alpha_k)\,\phi^k\right). \tag{58}$$

Now we need to establish the detailed expression of the right-hand side of (58). Since α_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 $k \in [1,p]$

$$(\mathbf{v}-\mathbf{u})\cdot\nabla_\mathbf{x}(\alpha_k) = (\mathbf{v}-\mathbf{u})\cdot\left[\nabla_\mathbf{x}\left(\frac{-\mu_k}{k_BT}\right) - m_k\frac{[\nabla_\mathbf{x}\mathbf{u}]^T[\mathbf{u}]}{k_BT} + m_k\mathbf{u}^2\frac{\nabla_\mathbf{x}T}{2k_BT^2}\right] \tag{59}$$

as well as

$$(\mathbf{v}-\mathbf{u})\cdot\nabla_\mathbf{x}(\alpha_{p+1}) = \frac{(\mathbf{v}-\mathbf{u})\cdot\nabla_\mathbf{x}u_x}{k_BT} - \frac{u_x(\mathbf{v}-\mathbf{u})\cdot\nabla_\mathbf{x}T}{k_BT^2}$$

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

$$(\mathbf{v}-\mathbf{u})\cdot\nabla_\mathbf{x}(\alpha_{p+3}) = \frac{(\mathbf{v}-\mathbf{u})\cdot\nabla_\mathbf{x}u_z}{k_BT} - \frac{u_z(\mathbf{v}-\mathbf{u})\cdot\nabla_\mathbf{x}T}{k_BT^2}$$

and finally

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

Now multiplying the former terms by the functions ϕ^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 ith line of $\sum_{k=1}^{p+4}(\mathbf{v}-\mathbf{u})\cdot\nabla_\mathbf{x}(\alpha_k)\,\boldsymbol{\phi}^k$ is given as the sum of the following terms:

$$\nabla_\mathbf{x}\left(\frac{-\mu_i}{k_BT}\right)\cdot(\mathbf{v}-\mathbf{u}),\qquad [\nabla_\mathbf{x}\mathbf{u}]^T : \frac{m_i(\mathbf{v}-\mathbf{u})\otimes(\mathbf{v}-\mathbf{u})}{k_BT},$$

$$\frac{m_i(\mathbf{v}-\mathbf{u})^2(\mathbf{v}-\mathbf{u})}{2k_B}\cdot\nabla_\mathbf{x}\left(\frac{1}{T}\right).$$

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

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

The proof is easily completed by computing the orthogonal projection on $\mathbb{K}$ of the vectors having respectively

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

$$\frac{m_i\,(\mathbf{v}-\mathbf{u})^2\,(\mathbf{v}-\mathbf{u})}{2k_B}\cdot\nabla_{\mathbf{x}}\left(\frac{1}{T}\right)$$

on their ith line. □

A.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:

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

where $\mathcal{C}_i$ is the contribution on the ith line of the collision operator (Boltzmann or BGK one). Multiplying such an equation by ϕ_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:

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

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

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

To have the diffusion term associated to the density n_l, we must considerate the list of function $(\mathbf{v}-\mathbf{u})\,\boldsymbol{\phi}^l = \mathbf{C}_l$, $l \in [1, p]$ 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 $(\mathcal{I}-\mathcal{P}_{\mathbb{K}})\,\mathbf{C}_l$ is 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 $\mathbb{J}_{\mathbf{u}} = \langle \mathbb{A}, \mathbf{g}\rangle$. 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 $\langle \mathbf{B}, \mathbf{g}\rangle$. □

A.4. Proof of Lemma 4

Proof. Note by $L_{:,j}$ the jth 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:

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

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 β_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 readily 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. □

A.5. Proof of Lemma 6

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 $(\mathbf{w}_r)_{r=1,\ldots,p-1}$ and secondly those expressing conservation of momentum (moments $\boldsymbol{\phi}^{i=p+1,p+2,p+3}$). 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 $\mathbf{w}_p$ (28). Then the whole set of constraints on the moments $(\mathbf{w}_r)_r$ reads

$$\sum_{j=1}^{p}W_{rj}\frac{1}{\|\mathbf{C}_j\|}\int g_j\,(\mathbf{v}-\mathbf{u})dv = \left(1-\frac{\lambda_r}{\nu}\right)\sum_{j=1}^{p}W_{rj}\frac{1}{\|\mathbf{C}_j\|}\int f_j\,(\mathbf{v}-\mathbf{u})dv$$

$$\Longleftrightarrow \sum_{j=1}^{p}W_{rj}\frac{n^j}{\|\mathbf{C}_j\|}\,(\mathbf{u}_j-\mathbf{u}) = \left(1-\frac{\lambda_r}{\nu}\right)\sum_{j=1}^{p}W_{rj}\frac{n^j}{\|\mathbf{C}_j\|}\,(\mathbf{u}^j-\mathbf{u}),\quad r = 1,\ldots,p$$

$$\Longleftrightarrow \sum_{j=1}^{p}W_{rj}\sqrt{\rho_j}\,(\mathbf{u}_j-\mathbf{u}) = \left(1-\frac{\lambda_r}{\nu}\right)\sum_{j=1}^{p}W_{rj}\sqrt{\rho_j}\,(\mathbf{u}^j-\mathbf{u}),\quad r = 1,\ldots,p.$$

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 (35). □

A.6. Proof of Proposition 2

Property 3: Equilibrium states

$\mathcal{R}(\mathbf{f}) = 0$ if only if $\mathbf{f} = \underline{\mathbf{G}}$. But then $T^\star = T^i$ and $\mathbf{u}_i = \mathbf{u}^i$ so $\|\underline{\mathbf{U}}-\mathbf{U}\| = \|\overline{\mathbf{U}}-\mathbf{U}\|$. But from (35) such an equality norm can only occur if $\underline{\mathbf{U}} = \mathbf{U} = \overline{\mathbf{U}}$ (this is because $\lambda_r > 0$, $r \in [1, p-1]$) which ends the proof since all the function f_i are now Maxwellians at the same temperature and velocity.

Property 2: H theorem

The convexity of the function $x \to x\ln x - x$ implies

$$\sum_{i=1}^{i=p}\int_{\mathbb{R}^3}(G_i - f_i)\ln f_i\,dv \leq \mathbf{H}\left(\underline{\mathbf{G}}\right) - \mathbf{H}\,(\mathbf{f})\,. \tag{60}$$

On one side we have

$$\mathbf{H}(\underline{\mathbf{G}}) = \sum_i n^i\left(\ln n^i - \frac{3}{2}\ln\left(\frac{2\pi k_BT^\star}{m_i}\right)\right) - n.$$

On the other side let us consider the classical problem of finding the entropy minimizer of functions having the same moments as f_i

for a given i. This function reads

$$\Gamma_i = \frac{n^i}{\left(2\pi k_b T^i/m_i\right)^{3/2}} \exp\left(-\frac{m_i\left(\mathbf{v}-\mathbf{u}^i\right)^2}{2k_b T^i}\right)$$

and it is easily seen that

$$\mathbf{H}(\mathbf{f}) \geq \sum_{i=1}^{p} \int \Gamma_i \ln(\Gamma_i) - \Gamma_i$$

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

Moreover using (36) and (37), it comes that $-nT^\star \leq -\sum_i n^i T^i$. So the function $x \to \ln x$ being concave and non decreasing, it holds that

$$\mathbf{H}(\underline{\mathbf{G}}) - \mathbf{H}(\mathbf{f}) \leq -\frac{3}{2} n \ln T^\star + \frac{3}{2}\sum_i n^i \ln T^i \leq 0.$$

Property 1: *Conservation laws*

Thanks to the definition of **G** through a minimization problem with **qualified constraints** (34) the implication $\Leftarrow$ is obvious. The converse may be obtained from the H-theorem. Assume that there holds:

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

where ϕ 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:

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

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

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