A FICK LAW'S RECOVERING BGK MODEL FOR A MIXTURE OF MONOATOMIC AND POLYATOMIC GASES

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Abstract. Through this paper, we extend the derivation of the Fick-relaxation BGK model operated in [16], whose aim was a relaxation operator recovering the Fick Law and the shear viscosity at hydrodynamic limit, for a mixture of monoatomic gases. Here, the framework deals with a mixture of monoatomic and polyatomic gases, and we need a model including the non translational degrees of freedom and internal energies. The attractors are computed from the resolution of an entropy minimisation problem. The model is shown to satisfy a H theorem. Next, we use a Chapman-Enskog expansion in order to compute the expression for the transport coefficients; that is, the phenomenological Fick matrix as both shear and volume viscosity.

1. **Introduction.** Boltzmann equation plays a paramount role to describe simplified dilute gas dynamics, and thus has raised increasing interest in the field of kinetic theory. Indeed, the original Boltzmann operator draws its descriptive accuracy from the precise statistical microscopic transcription of gas particle collision encoded in its expression. Such a precise description enables, for instance, to recover Euler and Navier-Stokes equations at the hydrodynamic limits, with all the right transport coefficients. Such properties justifies theoretical popularity of the Boltzmann operator. As a drawback of that accuracy, the mathematical complexity of the original operator prevents effective numerical analysis and computations. In order to confront such a technical issue, alternative models have surged to conciliate simplicity and descriptive qualities. A relevant solution was to abandon cumbersome microscopic details in favor of a macroscopic overview of the gas dynamics: the BGK relaxation model, settled in 1954 in [6], has appeared as a remarkable breakthrough, thanks to a simple and intuitive relaxation operator involving the celebrated maxwellian functions.

Such convenience implies a double price to pay. The first problem deals with analysis: the simple relaxation BGK formula hides a high non linearity within the maxwellian equilibrium function which substantially complicates potential proofs for solution existences, see [39]. The second issue is of physical concern: a mere macroscopic relaxation operator misses the microscopic description needed to grasp sufficient physical accuracy, and such a model never enables to recover all the physical properties drawn from the gas dynamics, whatever complex may it be. As a

consequence, and since there are many ways to define a BGK model for gas mixture, a modelization step consists in choosing the physical properties to include in the desired BGK operator. Required fulfillments are many, and among the most fundamental : conservation laws, H-theorem - for both physical and mathematical purposes, positive maxwellian-like equilibria, positive temperatures, which are essential, but not always straightforward, properties to be recovered. Other authors require more specific phenomenons to be included, such as Andries, Aoki and Perthame, who elaborated through [2] a model observing the true microscopic exchanges relations, thus requiring additional parameters to be introduced. Such comprehensive models demand more degrees of freedom so as to absorb the extra constraints required, as was done in [2] through fictitious coefficients. Any chosen set of properties to be recovered brings with itself complications- see, for example [34], [41], [38] in which the realizability of moments is questioned. This choice even raised new subordinate models, such as the ES-BGK model, which emerged from a desire to recover the right Prandtl number at the hydrodynamic limit ([17], [18], [15]). In [43], the authors propose a polynomial model that is able to reproduce the transport coefficients. In ([45]), the ESBGK and the Shakhov model are combined in order to recover Fick, Newton and Fourier laws.

Moreover, if theory and derivation are well-known and established regarding monoatomic and monospecies gases, results in a polyatomic or polyspecies framework for the BGK model are scarcer, and would need greater investigation. Indeed, the study of atmospheric gases, which represent an important field of application for the BGK models, confronts a mixture of polyatomic gases, such as O_2 or H_2O, and monoatomic ones, He for example. That simple fact shows that avoiding polyatomic or polyspecies gases in BGK theory lacks relevance. Yet substantial models have been recently brought for more general contexts. Regarding polyatomic framework, one generally has to introduce additional non translational internal energy, as well as to choose between whether a discrete or continuous energy description. For a mere polyatomic Boltzmann model with continuous energy, see [13] for the derivation of the celebrated Borgnakke-Larsen procedure, or ([14], [24]) for an alternative polyspecies one. An adaptation to BGK model has been investigated through [8], for a mixture of monoatomic and polyatomic gases. Discrete energy models, with a finite number of energetic levels, can also be adopted, as done in [7], and then generalized in [10] to a mixture of monoatomic and polyatomic gases. In order to consider a comprehensive study of the gas behaviour, a huge litterature has been developped in the reactive case : detailed modelization, conservation and stability studies are investigated in [40] for monoatomic structures and then [29] for internal polyatomic settings. This framework entails different considerations regarding conservation laws, or the parameters of equilibrium through the mass action law or the compared relaxation times for mechanical and reactive phenomena. Consequently, various models including bimolecular reactions study could have been derived and investigated : see [30] for a generalization of [2] to slow chemical reactions, [9] for a deeper focus on the Chapman-Enskog expansion on the previous model. Also, other conservation concerns have been an equally interesting and different source of work, via [7] for a discrete polyatomic setting or [10] for a continuous one. Finally, [19] investigates the possibility of a generalization of the Fick-relaxation model of [16] for reactive mixtures.

In a polyspecies framework, other valuable quantities to be recovered are the transport coefficients, such as the phenomenological coefficients related to the Fick,

Soret, Fourier and Dufour laws, or the viscosities. Such an investigation requires to derive macroscopic equations for gases - namely, the Navier Stokes equation, from our mesoscopic considerations, near the hydrodynamic limit. The Chapman-Enskog expansion is a classical procedure to obtain these desired expression, being performed in [5] or [8] for a mixture of monoatomic and polyatomic species, and in [16] for a mixture of monoatomic species, where the linearized operator is seen to play a great role in the expression of transport coefficients.

The following work investigates a generalization of the modelization performed in [16] for a monoatomic mixture with Fick law, to a polyatomic mixture framework. More precisely, we aim to derive a BGK model for a mixture of monoatomic and polyatomic gases that is able to reproduce Fick coefficients, shear viscosity and volume viscosity.

Our investigation will proceed as follows: in a second part, general notations and remainders for the Boltzmann equation are briefly evoked. In a third part will be introduced the physical framework: in particular, we develop formulae to express the physical properties that the desired relaxation operators are required to fulfill, relying on those for the Boltzmann operator previously recalled. The fourth part establishes the desired expression for the attractor of the BGK operator, obtained from an entropy minimisation under conservation requirements as well as the supplementary constraints linked with the volume viscosity, specific to the polyatomic framework. Finally, the last part analyses the BGK operator obtained, expresses the associated physical coefficient with respect to the linearized operator , and compare their adequation with the correct coefficients in order to quantify the model relevance regarding our initial aim. In particular, we will investigate the possibility of recovering the indifferentiability principle.

2. General notations and framework.

2.1. **Kinetic framework and notations.** We consider here an ideal mixture of $N \geq 1$ ideal gases, which, for each species, can be either monoatomic or polyatomic : this distinction will be highlighted through some notations and conventions (many of them taken from [3]) and hence will not need extra indexation for the gases.

Such mixtures can be described by using Boltzmann type collision operators as in ([5]). In particular, the authors introduce collision operators for interactions beween monoatomic and polyatomic components. However, the passage for polyatomic collision operators to monoatomic collision operators is a sigular limit and cannot be proved ([4]).

Let us now introduce notations :

- The functions of interest write $g := g(x,t,v,I) := (g_i(x,t,v,I_i))_{1 \leq i \leq N}$, depending on several physical parameters: position $x \in \mathbb{R}_x^3$, time $t \in \mathbb{R}^+$, velocity $v \in \mathbb{R}_v^3$, and a N-tuple $I = (I_i)_{1 \leq i \leq N}$ where $I_i \in \mathbb{R}^+$ is a quantum number related to the internal energy of i, in the following sense: letting $\delta_i \geq 0$ be the number of non translational internal degrees of freedom of the species i (and assumed constant with respect to the temperature), $I_i^{\frac{2}{\delta_i}}$ actually corresponds with a quantum level of energy of i. As in ([15]), we use the conventions $\delta_i = 0$ and $g_i(x,t,v,0) = g_i(t,x,v)$ if and only if species i is monoatomic. That will be our only discriminant factor between monoatomic and polyatomic gases,

therefore allowing to avoid cumbersome discussions. Then, a secondary challenge will be the total generalization of both monoatomic and monospecies frameworks; such an aim motivates the general notations set above.

- Let dI_i be the associated measure with I_i. If i is monoatomic, we chose $dI_i := \delta_{\mathbf{0}}$ the usual Dirac mesure, to illustrate the fundamental level of internal energy where i always remains. If i is polyatomic, continuous level of energies invite us to chose $dI_i = d\lambda$, the usual Lebesgue mesure on $\mathbb{R}_+$. See [24] for a continuous kinetic model for polyatomic species. From now on, we will resort to the notation I_i for $I_i\chi_i$, for every real function F, so as to slightly lighten the formulae and computations.
- Given a point (x, t, v, I), $f_i(x, t, v, I_i)dxdvdI_i$ represents the density of species i at the point (x, v, I), at time t. We will note $f := (f_i)_{1\leq i\leq N}$. The natural framework is the Hilbert space $L^2(\Omega, F)$, where $\Omega = \mathbb{R}^3_v \times (\mathbb{R}^+_I)^N$ endowed with the measure $dv \otimes \bigotimes_{i=1}^N dI_i$, and $F = L^\infty_{\mathrm{loc}}(\mathbb{R}^3_x \times \mathbb{R}_t)$.

We associate the following natural dot product to this space :

$$\langle g, h\rangle := \sum_{i=1}^N \iint g_i(v, I_i)h_i(v, I_i)dvdI_i.$$

More generally, if $g := (g_1, \ldots, g_N)$ and $h = (h_1, \ldots, h_N)$ are N-tuples of p and q-tensors respectively, the dot product will be the integral of the contracted product :

$$\langle g, h\rangle := \sum_{i=1}^N \iint g_i(v, I_i) : h_i(v, I_i)dvdI_i.$$

Here, we remain that if $\mathcal{T}$ is a $p+q$-tensor and $\mathcal{V}$ is a q-tensor, then the total contracted product is a p tensor $\mathcal{T} : \mathcal{V}$ defined by :

$$\left(\mathcal{T} : \mathcal{V}\right)_{j_1\ldots j_p} := \sum_{i_1,\ldots,i_q} \mathcal{T}_{j_1\ldots j_p i_1\ldots i_q}\mathcal{V}_{i_1\ldots i_q}.$$

Moreover, real functions $F : \mathbb{R} \to \mathbb{R}$ will be implicitly extended to vectors $e \in \mathbb{R}^N$ via the notation

$$F(e) := (F(e_1), \ldots, F(e_N)),$$

so as to bring compactness and simplicity while writing.

- Finally, our calculations will often involve vectors indexed on the $1 \leq i \leq N$ components. To make the notations both compact and clear, we will denote :

$$\overline{v} :=^T (v_1, \ldots, v_N),$$

when no other notation fits. Among the notations that will occur most often :

$$\overline{m} :=^T (m_1, \ldots, m_N),\ \overline{I^{\frac{2}{\delta}}} :=^T (I_1^{\frac{2}{\delta_1}}, \ldots, I_N^{\frac{2}{\delta_N}}),\ \overline{\delta} =^T (\delta_1, \ldots, \delta_N),\ \overline{1} :=^T (1, \ldots, 1). \tag{1}$$

We can also note $e_i :=^T (0, \ldots, \underset{\underset{i}{\uparrow}}{1}, \ldots, 0)$, so that $\overline{v} = \sum_i v_i e_i$.

The density vector f satisfies the Boltzmann-like equation :

$$(\partial_t + v \cdot \nabla)f = S(f), \tag{2}$$

where S denotes the collision operator associated to the chosen model, and $\nabla := \nabla_x$. We will sometimes denote $D_t := (\partial_t + v \cdot \nabla)$ the transport operator.

Obviously, our framework will require deeper integrability properties, and we will assume such a framework to be set. The typical hypothesis will be to assume :

$$\sum_i \iint f_i(1 + v^2 + I_i^{\frac{2}{\delta_i}} + \ln f_i)dvdI_i < \infty.$$

2.2. **Macroscopic quantities for the mixture.** If $1 \le i \le N$, we can introduce the following macroscopic quantities associated with the gas i, i.e molecular mass m_i, respective number and volume densities n_i and ρ_i, mean velocity u_i, total, total internal, internal and translational energies E_i, $\mathcal{E}_i$, $E_{int,i}$ and $E_{tr,i}$, and finally total, internal and translational temperatures T_i, $T_{int,i}$ and $T_{tr,i}$, with the following formulae :

$$n_i := \langle f, e_i \rangle,$$

$$\rho_i := m_i n_i = \langle f, m_i e_i \rangle,$$

$$u_i := \left\langle f, \frac{1}{n_i} v e_i \right\rangle,$$

$$n_i E_{tr,i} := \left\langle f, \frac{1}{2} m_i (v - u_i)^2 e_i \right\rangle =: \frac{3}{2} n_i k T_{tr,i},$$

$$n_i E_{int,i} := \left\langle f, I_i^{\frac{2}{\delta_i}} e_i \right\rangle =: \frac{\delta_i}{2} n_i k T_{int,i},$$

$$\mathcal{E}_i := \frac{\delta_i + 3}{2} k T_i := \frac{\delta_i}{2} k T_{int,i} + \frac{3}{2} k T_{tr,i},$$

$$E_i := \left\langle f, (\frac{1}{2} m_i v^2 + I_i^{\frac{2}{\delta_i}}) e_i \right\rangle =: n_i \mathcal{E}_i + \frac{1}{2} \rho_i u_i^2.$$

Here, $k := k_B$ denotes the Boltzmann constant.

Analogous quantities for the whole gas mixture are the total number and volume densities n and ρ, the mean macroscopic velocity u, the mean degree of freedom δ, the total and internal energies E and $\mathcal{E}$, and the temperature T for the mixture, defined as :

$$n := \sum_i n_i,$$

$$\rho := \sum_i \rho_i,$$

$$u := \frac{1}{\rho} \sum_i \rho_i u_i,$$

$$\delta := \frac{1}{n} \sum_i \delta_i n_i,$$

$$nE_{tr} := \left\langle f, \frac{1}{2} \overline{m}(v - u)^2 \right\rangle = \sum_i n_i E_{tr,i} + \frac{1}{2} \sum_i \rho_i (u_i - u)^2 =: \frac{3}{2} n k T_{tr},$$

$$nE_{int} := \sum_i n_i E_{int,i} = \sum_i \frac{\delta_i}{2} n_i k T_{int,i} =: \frac{\delta}{2} n k T_{int},$$

$$n\mathcal{E} := \left\langle f, \frac{1}{2} \overline{m}(v - u)^2 + \overline{I^{\frac{2}{\delta}}} \right\rangle$$

$$= \sum_i n_i (\frac{\delta_i + 3}{2}) k T_i + \frac{1}{2} \sum_i \rho_i (u - u_i)^2 =: \frac{\delta + 3}{2} n k T,$$

$$nE := \sum_i n_i E_i = \left\langle f, \frac{1}{2}\overline{m}v^2 + \overline{I^{\frac{2}{\delta}}} \right\rangle = n\mathcal{E} + \frac{1}{2}\rho u^2.$$

3. **General properties and expressions for kinetic operators.** As one may know, BGK operators have been set to tackle the cumbersomeness issue of the Boltzmann operator, due to the complexity of its macroscopic description. To that extent, one aims to mimic its macroscopic properties. In this section, we investigate kinetic operators with well-chosen properties, inherited from the Boltzmann collision operator, whose expression and formal derivation are recalled beforehand. From the usual Chapman-Enskog expansion, we finally derive an expression for the sought transport coefficients with respect to the linearized general collision operator.

3.1. **The Boltzmann polyatomic collision operator.** The particular case of Boltzmann operator will define our criteria on $\mathcal{S}$ for physical properties, requirements of which being obviously brought by physics. We refer to [13] - for the idea of the following process, and to [14], [24], [1] and [25] for further explanations on the Boltzmann operator. The main difference of our framework with the monoatomic case consists in taking into consideration non translational energies. Considering microscopic collisions of two particles, respectively for i and j, the following conservation laws prevail for binary micro collisions :

$$\begin{cases} m_i v + m_j v_* = m_i v' + m_j v'_*, \\ \frac{1}{2}\mu_{ij}(v - v_*)^2 + I_i^{\frac{2}{\delta_i}} + I_{j*}^{\frac{2}{\delta_j}} = \frac{1}{2}\mu_{ij}(v' - v'_*)^2 + I_i'^{\frac{2}{\delta_i}} + I_{j*}'^{\frac{2}{\delta_j}} =: \mathcal{E}_{ij}, \end{cases}$$

with $\mu_{ij} := \dfrac{m_i m_j}{m_i + m_j}$ the reduced mass of the system, inherited from the associated barycentric referential.

Conservation of the system energy implies a post-collision redistribution of internal and kinetic energies, formalized by the two rates $0 \leq r, R \leq 1$, defined by:

$$\begin{cases} I_i'^{\frac{2}{\delta_i}} + I_{j*}'^{\frac{2}{\delta_j}} = (1 - R)\mathcal{E}_{ij}, \\ I_i'^{\frac{2}{\delta_i}} = r(1 - R)\mathcal{E}_{ij}. \end{cases}$$

As a consequence, considering a reflexion vector $\omega \in \mathbb{S}^2$, we obtain, thanks to computations in the mass center reference frame :

$$\begin{cases} v' = \dfrac{m_i v + m_j v_*}{m_i + m_j} + \dfrac{\sqrt{2R\mu_{ij}\mathcal{E}_{ij}}}{m_i}(u - 2(u|\omega)\omega) = v - 2\dfrac{m_j}{m_i + m_j}(v - v_*|\omega)\omega, \\ v'_* = \dfrac{m_i v + m_j v_*}{m_i + m_j} - \dfrac{\sqrt{2R\mu_{ij}\mathcal{E}_{ij}}}{m_j}(u - 2(u|\omega)\omega) = v_* + 2\dfrac{m_i}{m_i + m_j}(v - v_*|\omega)\omega, \end{cases}$$

where $(\cdot|\cdot)$ denotes the canonical scalar product in $\mathbb{R}^3$.

Further statistical considerations lead to the following definition of the polyatomic and multi-species Boltzmann operator.

Definition 3.1. The Boltzmann operator $\mathcal{B} = (\mathcal{B}_1, \ldots, \mathcal{B}_N)$ for mixtures writes as follows :

$$\mathcal{B}_i(f, f) = \sum_k \mathcal{B}_{ik}(f, f),$$

where $\mathcal{B}_{ik}$ is the operator describing collisions between the species i and k, itself defined as :

$$\mathcal{B}_{ik}(f,f) = \iiiint_{\Delta} (f_i(v'_{ik})f_k(v'_{ik*})$$

$$-f_i(v)f_k(v_*))\sigma_{ik}(v,v_*,I_i,I_{k*},r,R,\omega)(1-R)\frac{I_i^{\frac{2}{\delta_i}-1}I_{k*}^{\frac{2}{\delta_k}-1}}{|v-v_*|}dv_*dI_{i*}drdRd\omega,$$

with σ_{ik} the associated cross-section and $\Delta = \mathbb{S}^2 \times [0,1]^2 \times \mathbb{R}_+ \times \mathbb{R}^3_v$.

Theorems of existence and unicity for the Cauchy problem associated with the polyatomic Boltzmann equation, have been proved, in the case of a single polyatomic gas ([25]) and for a mixture of monoatomic and polyatomic gases ([1]).

3.2. **Conservation laws and equilibria.** The Boltzmann operator $\mathcal{S} = \mathcal{B}$ expresses physical relevance since it satisfies conservations of mass, total quantity of movement and energy, which can be expressed as the following:

Property 1. (Conservation laws) $\mathcal{S} = \mathcal{B}$ verifies :

$$\forall 1 \leq j \leq N+4, \langle \mathcal{S}(f), \phi_j \rangle = 0, \tag{3}$$

where the associated collisional invariants $(\phi_i)_i$, with $1 \leq i \leq N+4$, are :

$$\begin{cases} \phi_1 = \begin{pmatrix} 1 \\ \vdots \\ 0 \end{pmatrix}, \dots, \phi_N = \begin{pmatrix} 0 \\ \vdots \\ 1 \end{pmatrix}, \\ \phi_{N+k} = \begin{pmatrix} m_1 v_k \\ \vdots \\ m_N v_k \end{pmatrix}, \ k \in \{1; 3\}, \\ \phi_{N+4} = \begin{pmatrix} \frac{1}{2}m_1 v^2 + I_1^{\frac{2}{\delta_1}} \\ \vdots \\ \frac{1}{2}m_N v^2 + I_N^{\frac{2}{\delta_N}} \end{pmatrix}. \end{cases} \tag{4}$$

The space spanned by the collisional invariants $(\phi_i)_i$, $1 \leq i \leq N+4$ will be denoted by $\mathbb{K}$ and $P_{\mathbb{K}}$ will represent the orthogonal projection on $\mathbb{K}$.

Definition 3.2. The Boltzmann entropy $\mathcal{H}(f)$ is defined by the following formula:

$$\mathcal{H}(f) := \langle f, \log f - \bar{1} \rangle = \sum_i \iint f_i(\log f_i - 1)dvdI_i. \tag{5}$$

This definition is consistent with the natural additivity of entropy.

As has been proved, the entropy enables to quantify distance of the gas from equilibrium. In particular is proved its Lagrangian decrease in the Boltzmann operator case :

Property 2. (H-Theorem: Entropy dissipation) The entropy associated with $\mathcal{S} = \mathcal{B}$ is dissipative, in the following sense :

$$\partial_t \mathcal{H}(f) + \nabla \cdot \Phi[\mathcal{H}](f) = \langle \mathcal{S}(f), (\log f) \rangle \leq 0, \tag{6}$$

where :

$$\Phi[\mathcal{H}](f) := \sum_i \iint v f_i (\log f_i - 1) dv dI_i,$$

is the entropy flux, for $f := (f_i)_{1 \le i \le N}$.

Such a behaviour invites to investigate entropy minima, and the Lagrange Multiplier method performed to minimize $\mathcal{H}$, under the physical constraint set (3) associated with the macroscopic parameters evoked above, lead to the well known maxwellian forms of equilibrium :

Definition 3.3. The maxwellian equilibrium distribution corresponding with a macroscopic triplet (ρ, u, T) is $\mathcal{M} := (\mathcal{M}_1, \dots, \mathcal{M}_N)$ where :

$$\mathcal{M}_i = n_i \left(\frac{m_i}{2\pi kT}\right)^{\frac{3}{2}} \left(\frac{1}{kT}\right)^{\frac{\delta_i}{2}} \Lambda_i^{-1} \exp\left(-\frac{m_i(v-u)^2}{2kT} - \frac{I_i^{\frac{2}{\delta_i}}}{kT}\right), \ 1 \le i \le N, \qquad (7)$$

$$\Lambda_i = \int \exp\left(-I_i^{\frac{2}{\delta_i}}\right) dI_i = \frac{\delta_i}{2} \Gamma\left(\frac{\delta_i}{2}\right), \qquad (8)$$

where Γ denotes the usual gamma function. Also, we will note $\mathcal{M}(f)$ (or $\mathcal{M}$ when the context is not misleading) the maxwellian corresponding with the macroscopic parameters of f.

From this expression, we can introduce the natural dot product for the weighted space $L^2(\Omega, F, \mathcal{M})$, i.e :

$$\forall h, g \in L^2(\Omega, F, \mathcal{M}), \langle h, g \rangle_{\mathcal{M}} := \sum_i \iint h_i g_i \mathcal{M}_i dv dI_i. \qquad (9)$$

This definition can also be extended to tensors, as evoked above. The assiociated Hilbert norm will be denoted by $\| \ \|_{\mathcal{M}}$. This product will be used often, as collisional invariants ; that will sometimes require to take profits out of the underlying geometrical structure, by Schmidt-orthogonalizing the basis of $\mathbb{K}$.

These calculations are performed so as to express the orthogonal projection on $\mathbb{K}$, $P_{\mathbb{K}}$ that has been defined in property 1. It leads to the orthogonalized family :

$$\psi_i = \phi_i, \ \|\psi_i\|_{\mathcal{M}}^2 = n_i, 1 \le i \le N,$$

$$\psi_{N+k,j} = m_j(v_k - u_k), 1 \le k \le 3, \ \|\psi_{N+k}\|_{\mathcal{M}}^2 = \rho kT, 1 \le j \le N,$$

$$\psi_{N+4,j} = \frac{1}{2} m_j(v-u)^2 + I_j^{\frac{2}{\delta_j}} - \left(\frac{\delta_j + 3}{2}\right) kT, \ \|\psi_{N+4}\|_{\mathcal{M}}^2 = \frac{\delta+3}{2} n(kT)^2, 1 \le j \le N.$$

Definition 3.4. If $1 \le j \le N$, let us define the tensor C_j by the following :

$$\begin{cases} (C_j)_j := v - u, \\ (C_j)_{j \neq i} := 0. \end{cases} \qquad (10)$$

Definition 3.5. If $1 \le j \le N$, we denote $\Phi_j := (\mathbb{I}_d - P_{\mathbb{K}})(C_j)$, $\alpha := \frac{2}{3kT}(\mathbb{I}_d - P_{\mathbb{K}})(\overline{I^{\frac{2}{\delta}}})$ as well as the generated spaces :

$$\begin{cases} \mathbb{C} := Vect\{\Phi_j, 1 \le j \le N\}, \\ \tilde{\mathbb{C}} := \mathbb{C} \bigoplus \mathbb{R}\alpha. \end{cases}$$

We shall later proceed in a further investigation of such spaces. Easy calculations bring :

$$\begin{cases} (\Phi_j)_i = (\chi_{ij} - \dfrac{m_i n_j}{\rho})(v - u), \\[3mm] \dfrac{3}{2}kT\alpha_i = -\dfrac{\delta}{2(\delta + 3)}m_i(v - u)^2 + \dfrac{3}{\delta + 3}I_i^{\frac{2}{\delta_i}} + \dfrac{3}{2}(\dfrac{\delta - \delta_i}{\delta + 3})kT, \end{cases} \quad (11)$$

where $\mathbb{I}_d$ is the identity operator and χ_{ij} is the characteristic function associated with the pair $\{i, j\}$, i.e :

$$\chi_{ij} = \begin{cases} 1 \text{ if } i = j, \\[2mm] 0 \text{ else.} \end{cases}$$

Introducing the following reduced velocities:

$$V^j := \sum_i V_i^j e_i, \ j \in \mathbb{N}, \qquad V_i := \sqrt{\dfrac{m_i}{kT}}(v - u),$$

we can write :

$$\alpha_i = -\dfrac{\delta}{3(\delta + 3)}V_i^2 + \dfrac{2}{\delta + 3}\dfrac{I_i^{\frac{2}{\delta_i}}}{kT} + (\dfrac{\delta - \delta_i}{\delta + 3}).$$

We can now link maxwellians with equilibrium :

Property 3. (Equilibrium) For $\mathcal{S} = \mathcal{B}$, $\langle \mathcal{S}(f) \log f \rangle = 0$ if and only if $f = \mathcal{M}$ - where $\mathcal{M}$ is the maxwellian vector introduced at Definition 3.3, i.e f is at thermodynamic equilibrium.

The last remarkable inner property of $\mathcal{B}$ is related to this linearized operator, which, as we shall see, plays a great role for recovering Navier Stokes equations :

Definition 3.6. The linearized operator $\mathcal{L}[\mathcal{S}]$ associated with $\mathcal{S}$ is defined by the following directional derivative of the collisional operator near equilibrium :

$$\mathcal{L}[\mathcal{S}](g) := \mathcal{M}^{-1}\dfrac{\mathrm{d}}{\mathrm{d}\epsilon}\Big(\mathcal{S}(\mathcal{M}(\bar{1} + \epsilon g))\Big)\Big|_{\epsilon = 0},$$

with $\mathcal{M}g := (\mathcal{M}_1 g_1, \ldots, \mathcal{M}_N g_N)$.

This definition is quite formal for the sake of generality but has an obviously simpler expression in the Boltzmann case thanks to its bilinear operator.

Property 4. With $\mathcal{S} = \mathcal{B}$, $\mathcal{L}[\mathcal{S}]$ induces a continuous, self-adjoint and definite negative operator on $\mathbb{K}^\perp$.

As we shall see, such properties enable an operator to recover a Navier-Stokes-like system of equations near equilibrium, and justifies to prove Fredholm alternatives when studying collision operator, as has been performed in [20] in the diatomic case and in [21] in the general case for monospecies Boltzmann operator.

Definition 3.7. A collision operator $\mathcal{S}$ satisfying properties 1, 2, 3, 4 will be said properly defined.

3.3. **Thermodynamics of irreversible processes.** This part is devoted to the description of the fluxes appearing in the compressible Navier-Stokes system. They can be expressed in function of different variables.

The fluxes associated to the gases can expressed as ([16], [23]):

$$
\begin{aligned}
\text{Mass fluxes } &: J_i = \sum_{j=1}^{N} L_{ij} \nabla(-\frac{\mu_j}{kT}) + L_{iq} \nabla(-\frac{1}{kT}), \\
\text{Heat fluxes } &: J_q = \sum_{j=1}^{N} L_{qj} \nabla(-\frac{\mu_j}{kT}) + L_{qq} \nabla(-\frac{1}{kT}), \\
\text{Velocity flux } &: J_u = -\eta \Sigma(u) - \eta_V (\nabla \cdot u)\mathbb{I}_3,
\end{aligned}
\tag{12}
$$

where $\mathbb{I}_3$ is the identity matrix in $\mathbb{R}^3$, $(L_{ij})_{1 \le i,j \le N}$ is the Onsager matrix, μ_j is the chemical potential of the species j. These quantities are defined by :

$$
\mu_j = -kT \ln \left(\frac{n_j \Lambda_j^{-1}}{\left(\frac{2\pi kT}{m_j}\right)^{\frac{3}{2}}} \right),
\tag{13}
$$

and :

$$
\Sigma := \frac{\nabla u + (\nabla u)^T}{2} - (\frac{1}{3}\nabla \cdot u)\mathbb{I}_3,
$$

is the Reynolds tensor, η is the shear viscosity and η_V the volume viscosity.

Another formulation of the fluxes is more relevant for real applications since they are expressed in function of phenomenological coefficients ([42])

$$
J_i = -\sum_{j=1}^{N} \rho_i D_{ij} \frac{\nabla p_j}{p} - \rho_i \theta_i \frac{\nabla T}{T},
\tag{14}
$$

$$
J_q = -\hat{\lambda}\nabla T - p \sum_{i=1}^{N} \theta_i \frac{\nabla p_i}{p} + \sum_{i=1}^{N} h_i J_i,
\tag{15}
$$

where (D_{ij}) is the Fick matrix, θ_i are the thermal coefficients and $\hat{\lambda}$ is the thermal conductivity.

Therefore, the Fick matrix is directly connected to the Onsager matrix L_{ij} by the relation

$$
D_{ij} = -n\frac{kL_{ij}}{n_i n_j}.
$$

These coefficients can be measured experimentally. The link between these two formulations has been shown by Kurochkin, Makarenko, and Tirskii ([37]). $(D_{ij})_{ij}$ is called the Fick Matrix for the system, and contains the so-called Fick coefficients we aim to recover with our BGK oper ator. Casimir-Onsager relations imply that the associated Onsager matrix associated with the Boltzmann operator $\left(\frac{L_{ij}[\mathcal{B}]}{\|C_i\|_{\mathcal{M}} \|C_j\|_{\mathcal{M}}}\right)_{ij}$, is symmetric non positive. This result can be found in [16]. We will later point out that this condition has as direct consequence the assumption of symmetry and non positiveness of $\mathcal{L}$ itself.

Since η_V only appears within polyatomic frameworks, we expect it to be a function $\eta_V = \eta_V(\bar{\delta})$, with $\eta_V(\bar{0}) = 0$.

In particular, these fluxes play a crucial role in the gas dynamics, drawn by the isotropic Navier Stokes equations fulfilled by the mixture:

$$\begin{cases} \partial_t \rho_i + \nabla \cdot (\rho_i u + J_i) = 0, \\\\ \partial_t(\rho u) + \nabla \cdot (\rho u \otimes u + p\mathbb{I}_3 + J_u) = 0, \\\\ \partial_t(\rho E) + \nabla \cdot ((\rho E + p)u) + \nabla \cdot (J_q + J_u \cdot u) = 0. \end{cases} \tag{16}$$

3.4. **General expression of the transport coefficients.** As Boltzmann equation leads to the Euler equations at hydrodynamic limit as well as to Navier-Stokes system at first approximation, it is of particular interest to seek an operator able to deliver correct fluxes ; equivalently, correct phenomenological coefficients are to be recovered. It may be useful to recall that the limit and the first approximation are taken with respect to $\epsilon := Kn$, which is the Knudsen number associated with the mixture.

It is well known that BGK models do not fail at providing Euler equations at hydrodynamic limit. To obtain the inherent Navier Stokes system, we perform a Chapman Enskog expansion. Starting from the kinetic equation (2) with a compressible scaling

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} S(f)$$

where ε is proportional to the Knudsen number, f around its local maxwellian, for any properly defined collision operator :

$$f = \mathcal{M}(f)(1 + \epsilon g + O(\epsilon^2)), \tag{17}$$

where $\mathcal{M}(f)$ and f and share the same conserved moments

$$\langle f, \phi_j \rangle = \langle \mathcal{M}(f), \phi_j \rangle, \quad j \in \{1; N+4\}$$

where $(\phi_j)_{1,N+4}$ has been defined in (4). In relation (17), g corresponds to the first order correction.

Lemma 1. *Let $\mathcal{S}$ be any properly defined operator. The first order correction g satisfies the equation:*

$$\mathcal{L}[\mathcal{S}](g) = \sum_{j=1}^{N} \Phi_j \cdot \nabla(-\frac{\mu_j}{kT}) + kT \mathbb{A}(V) : \Sigma(u) + \tilde{B}(v, I) \cdot \nabla(-\frac{1}{kT}) - \alpha(V, I) \nabla \cdot u, \tag{18}$$

where we have defined the following quantities :

$$\begin{cases} \mathbb{A}(V) := V \otimes V - \frac{1}{3} V^2 \mathbb{I}_3, \\\\ V^j := \sum_i V_i^j e_i, \ j \in \mathbb{N}, \qquad V_i := \sqrt{\frac{m_i}{kT}}(v - u), \\\\ \tilde{B}(v, I) := (v - u)\Big(\frac{1}{2} kT V^2 + \overline{I^{\frac{2}{\delta}}} - \frac{n\overline{m}}{\rho}(\frac{\delta + 5}{2}) kT\Big), \end{cases} \tag{19}$$

where Φ_j refers to Definition 3.5 and equation (11), and the overlined quantities have been previously defined through relations (1).

Remark 1. Actually, α corresponds with $-\frac{1}{3}\phi^\kappa$, where ϕ^κ is part of the Chapman-Enskog first-order decomposition derived from [27].

Remark 2. The last two terms in the expression (18) above are inherited from the polyatomic framework; computing $\delta = 0$ and $\delta_i = 0$ from (2) will bring us back to the monoatomic framework. See [27] or [42] for such a derivation within a discrete framework.

Proof. Let us write the Chapman-Enskog expansion (17), at first at 0 order:

$$\partial_t \mathcal{M} + v \cdot \nabla \mathcal{M} = \mathcal{M} \mathcal{L}(g) + O(\epsilon). \tag{20}$$

For each component i, by using the expressions of (7), (8) and thanks to (13), a direct computation gives

$$\log \mathcal{M}_i = -\frac{\mu_i}{kT} - \frac{(v-u)^2 + I_i^{\frac{2}{\delta_i}}}{2kT} = \sum_j \alpha_j \phi_{j,i}, \tag{21}$$

$$\text{with:} \quad \begin{cases} \alpha_j = -\dfrac{\mu_j}{kT} - \dfrac{m_j u^2}{2kT}, \\[2mm] \alpha_{N+j} = \dfrac{u_{x_j}}{kT}, 1 \le j \le 3, . \\[2mm] \alpha_{N+4} = -\dfrac{1}{kT} \end{cases}$$

Hence the relation (21) gives $\ln \mathcal{M} \in \mathbb{K}$ and $P_{\mathbb{K}}(\ln \mathcal{M}) = \ln \mathcal{M}$. So dividing (20) by $\mathcal{M}$, applying the conservation projection $P_{\mathbb{K}}$ and using that $\mathcal{L}(g) \in \mathbb{K}^{\perp}$ leads to :

$$\frac{\partial_t \mathcal{M}}{\mathcal{M}} = -P_{\mathbb{K}}(v \cdot \frac{\nabla \mathcal{M}}{\mathcal{M}}) + O(\epsilon). \tag{22}$$

Next, using (22) after dividing once more by $\mathcal{M}$ in (20):

$$\mathcal{L}(g) = (\mathbb{I}_d - P_{\mathbb{K}})(v \cdot \frac{\nabla \mathcal{M}}{\mathcal{M}}) = (\mathbb{I}_d - P_{\mathbb{K}})((v-u) \cdot \nabla \log \mathcal{M})$$

where $\mathbb{I}_d$ is the identity operator.

We are only left with mere computations.

- If $1 \le j \le N, (v-u) \cdot \nabla \alpha_j = (v-u) \cdot \nabla(-\frac{\mu_j}{kT}) + \frac{m_j}{2} u^2 (v-u) \cdot \nabla(-\frac{1}{kT}) - \frac{m_j}{kT}(v-u) \cdot (\nabla u)^T \cdot u$,
- If $1 \le j \le 3, (v-u) \cdot \nabla \alpha_{N+j} = -u_{x_j}(v-u) \cdot \nabla(-\frac{1}{kT}) + \frac{(v-u)}{kT} \cdot \nabla u_{x_j}$,
- $(v-u) \cdot \nabla \alpha_{N+4} = (v-u) \cdot \nabla(-\frac{1}{kT})$.

Finally, we obtain the following expression, for the i-th line :

$$\sum_j (v-u) \cdot \nabla \alpha_j \phi_{j,i} = (v-u) \cdot \nabla(-\frac{\mu_i}{kT})\chi_{ij} + (m_i \frac{(v-u)^2}{2} + I_i^{\frac{2}{\delta_i}})(v-u) \cdot \nabla(-\frac{1}{kT})$$

$$+ (\frac{m_i(v-u) \otimes (v-u)}{kT}) : (\frac{\nabla u + (\nabla u)^T}{2}).$$

Now let us finally compute the orthogonal projection of this sum, component by component.

- To begin with, we simply apply the projection to our first term, which provides $\sum_{j=1}^N \Phi_j \cdot \nabla(-\frac{\mu_j}{kT})$.
- Then, the projection applied to the second term leads to $m_i(v-u)(\frac{1}{2}(v-u)^2 - \frac{5}{2}\frac{n}{\rho}kT)$, plus an additional term which is $(I_i^{\frac{2}{\delta_i}} - \frac{1}{2}\frac{n}{\rho}\delta kT m_i)(v-u)$, correlated which our polyatomic framework.

- Finally, the last term is, at i-th line,

$$\frac{m_i}{kT}(v-u)\otimes(v-u) - [\frac{(\frac{\delta-\delta_i}{2})kT + \frac{1}{2}m_i(v-u)^2 + I_i^{\frac{2}{\delta_i}}}{\frac{\delta+3}{2}kT}]\mathbb{I}_3.$$

Note that this term is indeed a generalization of the monoatomic case (assuming that the term $I_i^{\frac{2}{\delta_i}}$ goes formally to 0 when we revert back to this case) : with this hypothesis, we get the traceless tensor $V_i \otimes V_i - \frac{1}{3}V_i^2\mathbb{I}_3$.

The desired expression follows easily. □

Lemma 2. *The following useful alternative formula for $\mathcal{L}[\mathcal{S}]$ is true :*

$$\mathcal{L}[\mathcal{S}](g) = \sum_{j=1}^{N}\Phi_j\cdot\frac{\nabla p_j}{p_j} + kT\mathbb{A}(V):\Sigma(u) + B'(v,I)\cdot\nabla(-\frac{1}{kT}) - \alpha(V,I)\nabla\cdot u, \quad (23)$$

with the new quantity:

$$B'(v,I) = (v-u)(\frac{1}{2}\overline{m}(v-u)^2 + \overline{I^{\frac{2}{\delta}}} - \frac{\delta+5}{2}kT\overline{1}) \in \tilde{\mathbb{C}}^\perp. \quad (24)$$

Also, that expression brings, following the way of the previous lemma, the following alternative formula for the masses and heat fluxes introduced in (12):

$$J_i = \sum_{j=1}^{N}kL_{ij}[\mathcal{S}]\frac{\nabla p_j}{p_j} + \theta_i[\mathcal{S}]T\nabla(-\frac{1}{kT}),$$

$$\theta_i[\mathcal{S}] = \frac{L_{iq}[\mathcal{S}]}{T} + \sum_{j=1}^{N}(\frac{\delta_j+5}{2})kTL_{ij}[\mathcal{S}], \quad (25)$$

$$J_q = k\sum_{i=1}^{N}L_{iq}[\mathcal{S}]\frac{\nabla p_i}{p_i} + \beta[\mathcal{S}]\nabla(-\frac{1}{kT}),$$

$$\beta[\mathcal{S}] = L_{qq}[\mathcal{S}] + \sum_{j=1}^{N}(\frac{\delta_j+5}{2})kTL_{jq}[\mathcal{S}].$$

For a similar expression in a discrete framework we refer to [27].

Proof. Let us simply remark that the formula (13) brings :

$$\nabla(-\frac{\mu_i}{kT}) = \frac{\nabla p_i}{p_i} - \frac{\delta_i+5}{2}\frac{\nabla T}{T} = \frac{\nabla p_i}{p_i} + \left(\frac{\delta_i+5}{2}\right)kT\nabla\left(-\frac{1}{kT}\right).$$

Now inserting this expression into (18) :

$$\mathcal{L}[\mathcal{S}](f) = \sum_{j=1}^{N}\Phi_j\cdot\frac{\nabla p_i}{p_i} + kT\mathbb{A}(V):\Sigma(v) + \left\{\tilde{B}(v,I) + P_{\mathbb{K}^\perp}\mathcal{V}\right\}\cdot\nabla\left(-\frac{1}{kT}\right) - \alpha(V,I)\nabla\cdot u,$$

with

$$\mathcal{V} = \left(\sum_i\left(\frac{\delta_i+5}{2}\right)kTC_i\right).$$

But the lth component of $P_{\mathbb{K}}(\mathcal{V})$ writes:

$$\left[P_{\mathbb{K}}(\mathcal{V})\right]^{(l)} = \left[\sum_{i=1}^{3}\frac{\langle\mathcal{V},\psi_{N+i}\rangle}{\|\psi_{N+i}\|_{\mathcal{M}}^2}\psi_{N+i}\right]^{(l)} = \frac{\frac{\delta+5}{2}nkT}{\rho kT}\overline{m}kT(v_l - u_{x_l}), \quad (26)$$

where u_{x_l} is the lth component of u. (26) is exactly the opposite of the last term in the definition (24) of $\tilde{B}(v, I)$. Consequently, the term newly associated with the vector $\nabla\left(-\frac{1}{kT}\right)$ is:

$$B'(v,I) = (v-u)\left(\frac{1}{2}kTV^2 + \overline{I^{\frac{2}{\delta}}}\right) - P_{\mathbb{K}^\perp}\left(\sum_i \left(\frac{\delta_i + 5}{2}\right)kTC_i - P_{\mathbb{K}}\left(\sum_i \left(\frac{\delta_i + 5}{2}\right)kTC_i\right)\right),$$

i.e :

$$B'(v, I) = (v - u)\left(\frac{1}{2}kTV^2 + \overline{I^{\frac{2}{\delta}}}\right) - \sum_i \left(\frac{\delta_i + 5}{2}\right)kTC_i$$

and the result follows by applying the definition (10) for the C_i family. $\qquad\square$

As one is aware of the link between linearized operator and approximation around the equilibrium, the previous formula provides, more particularly, the expression of the desired phenomenological coefficients, as stated by the following lemma.

Lemma 3. *Let $\mathcal{S}$ be a properly defined operator. Then, if f satisfies (2), the associated gas mixture verifies the Navier Stokes system (16) at order 1 in ϵ, where ϵ denotes the Knudsen number for the mixture, and with the following transport coefficients, as defined in (12) :*

$$\forall i, j, L_{ij}[\mathcal{S}] = \frac{1}{3}\left\langle \Phi_i, \mathcal{L}[\mathcal{S}]^{-1}\Phi_j \right\rangle_{\mathcal{M}}, \tag{27}$$

$$\forall i, L_{iq}[\mathcal{S}] = \frac{1}{3}\left\langle \Phi_i, \mathcal{L}[\mathcal{S}]^{-1}(\tilde{B}) \right\rangle_{\mathcal{M}}, \tag{28}$$

$$\eta[\mathcal{S}] = -\frac{1}{10}k^2T^2\left\langle \mathbb{A}, \mathcal{L}[\mathcal{S}]^{-1}(\mathbb{A}) \right\rangle_{\mathcal{M}}, \tag{29}$$

$$\eta_V[\mathcal{S}] = -kT\left\langle \alpha, \mathcal{L}[\mathcal{S}]^{-1}(\alpha) \right\rangle_{\mathcal{M}}, \tag{30}$$

$$\forall j, L_{qj}[\mathcal{S}] = \frac{1}{3}\left\langle \tilde{B}, \mathcal{L}[\mathcal{S}]^{-1}\Phi_j \right\rangle_{\mathcal{M}}, \tag{31}$$

$$L_{qq}[\mathcal{S}] = \frac{1}{3}\left\langle \tilde{B}, \mathcal{L}[\mathcal{S}]^{-1}(\tilde{B}) \right\rangle_{\mathcal{M}}. \tag{32}$$

Proof. Taking anew the Chapman-Enskog expansion at order 1 brings :

$$D_t\mathcal{M} + \epsilon D_t(\mathcal{M}g) = S(f) + O(\epsilon^2). \tag{33}$$

Applying the unweighted dot product against ϕ_i, for every $1 \leq i \leq N+4$, we obtain the following $N + 4$ conservation equations :

$$\forall 1 \leq i \leq N + 4, \langle D_t\mathcal{M}, \phi_i\rangle_{\mathcal{M}} + \epsilon\langle D_t(\mathcal{M}g), \phi_i\rangle_{\mathcal{M}} = O(\epsilon^2).$$

Here we seek to develop the Navier-Stokes remainder part to obtain an expression of the fluxes depending on the linearized operator. Note that the first consideration is to find a new expression of the fluxes depending on the linearized Boltzmann operator. From this, we then deduce a correct expression for any "well-enough defined" collision operator.

Let us finally remark that, since $g \in \mathbb{K}^\perp$, our term of interest simplifies into:

$$\langle D_t(\mathcal{M}g), \phi_i\rangle_{\mathcal{M}} = \nabla \cdot \langle (v - u)\phi_i, g\rangle_{\mathcal{M}}. \tag{34}$$

Let us compute the right-hand side dot product of (34), for $1 \leq i \leq N + 4$.

- $\underline{1 \leq i \leq N}$: $(v - u)\phi_i = C_i$, so that, identifying first orders,

$$J_i = \langle C_i, g \rangle_{\mathcal{M}} = \langle \Phi_i, g \rangle_{\mathcal{M}}.$$

Relying on the phenomenological expression of the mass fluxes, and assuming mutual functional independance of the family $\{\nabla(-\frac{\mu_1}{kT}), \ldots, \nabla(-\frac{\mu_N}{kT}), \nabla(-\frac{1}{kT})\}$, we finally obtain (27) and (28).

- $\underline{N + j, 1 \leq j \leq 3}$: Due to $g \in \mathbb{K}^{\perp}$, we can consider ψ_{N+j} instead of ϕ_{N+j}, and given the equality :

$$(v - u)\phi^{N+j} = kT(\mathbb{A}(V) + \frac{1}{3}V^2\mathbb{I}_3)e_j,$$

we obtain the following expression :

$$J_u = kT \left\langle \mathbb{A}(V) + \frac{1}{3}V^2\mathbb{I}_3, g \right\rangle_{\mathcal{M}}. \tag{35}$$

Note here that the dot product implying $\frac{1}{3}V^2$ does not vanish if the mixture is not strictly monoatomic, because of a more complex invariant basis. In particular, $\psi_{N+4,i}$ contains the supplementary term $I_i^{\frac{2}{\delta_i}}$, causing $\frac{1}{3}V^2 \notin \mathbb{K}$ within the polyatomic framework, causing the volume viscosity to appear. Indeed, one notice that:

$$P_{\mathbb{K}}(\frac{1}{3}V^2) = \frac{1}{3}V^2 + \alpha,$$

causing $\alpha = -P_{\mathbb{K}^{\perp}}(\frac{1}{3}V^2)$, which truly contributes as soon as the δ_i do. Since $g \in \mathbb{K}^{\perp}$, (35) becomes :

$$J_u = kT \langle \mathbb{A} - \alpha\mathbb{I}_3, g \rangle_{\mathcal{M}}.$$

Then, (18) brings the following equalities :

$$\begin{cases} -\eta\sigma(u) = k^2T^2 \left\langle \mathbb{A} - \alpha\mathbb{I}_3, \mathcal{L}[\mathcal{S}]^{-1}(\mathbb{A} : \Sigma(u)) \right\rangle_{\mathcal{M}}, \\ \eta_V = kT \left\langle \mathbb{A} - \alpha\mathbb{I}_3, \mathcal{L}[\mathcal{S}]^{-1}\alpha \right\rangle_{\mathcal{M}}. \end{cases}$$

Now, applying the matrix trace to the first equation provides :

$$\left\langle \alpha, \mathcal{L}[\mathcal{S}]^{-1}(\mathbb{A} : \Sigma(u)) \right\rangle_{\mathcal{M}} = 0.$$

So :

$$-\eta\sigma(u) = k^2T^2 \left\langle \mathbb{A}, \mathcal{L}[\mathcal{S}]^{-1}(\mathbb{A} : \Sigma(u)) \right\rangle_{\mathcal{M}}.$$

Then, symmetry of the involved tensors brings (29). Similarly, applying matrix trace to the second equation of our system, provides (30).

- $\underline{i = N + 4}$: Computations provides us with the following expression :

$$(v - u)\phi_{N+4} = B(v) + \frac{5}{2}\frac{n}{\rho}\overline{m}kT + kT(\mathbb{A} + \frac{1}{3}V^2\mathbb{I}_3) \cdot u + \frac{1}{2}\overline{m}u^2(v - u) + \overline{I^{\frac{2}{\delta}}}(v - u)$$

$$= B(v) + kT(\mathbb{A} + \frac{1}{3}V^2\mathbb{I}_3) \cdot u + \overline{I^{\frac{2}{\delta}}}(v - u) + e,$$

with $e \in \mathbb{K}$. As a consequence,

$$J_q = \left\langle (v - u)\phi^{N+4}, g \right\rangle_{\mathcal{M}} - J_u[u] = \langle B(v), g \rangle_{\mathcal{M}} + \left\langle \overline{I^{\frac{2}{\delta}}}(v - u), g \right\rangle_{\mathcal{M}}.$$

It finally results in the previous formulae (31) and (34).

$\square$

Remark 3. Let us remark that only the mutual independency of the macroscopic functions brought

$$\begin{cases} \beta = \frac{1}{3} \left\langle B' + \overline{(\frac{\delta + 5}{2})kT(v - u)}, \mathcal{L}[\mathcal{S}]^{-1}(B') \right\rangle_{\mathcal{M}}, \\ L_{jq} = \frac{1}{3} \left\langle B' + \overline{(\frac{\delta + 5}{2})kT(v - u)}, \mathcal{L}[\mathcal{S}]^{-1}(\Phi_j) \right\rangle_{\mathcal{M}}, \end{cases}$$

without assuming anything on the $\mathcal{L}[\mathcal{S}]^{-1}$-stability of the orthogonal sum $\mathbb{C} \overset{\perp}{\oplus} \mathbb{C}^\perp = \mathbb{K}^\perp$. This stability is established for $\mathcal{S} := \mathcal{B}$. It will be proved for Fick-relaxation operators as well.

Remark 4. Lemma 1 also provides the following expression :

$$\theta_i T = \frac{1}{3} \left\langle \Phi_i, \mathcal{L}[\mathcal{S}]^{-1}(B') \right\rangle_{\mathcal{M}}, \tag{36}$$

where θ_i has been defined in (14, 15).

Lemma 4. *Alternative expressions are given for the coefficients :*

$$\beta = \frac{1}{3} \left\langle B' + (\frac{\delta + 5}{2})kT(v - u)\overline{1}, \mathcal{L}[\mathcal{S}]^{-1}(B') \right\rangle_{\mathcal{M}},$$

$$L_{jq} = \frac{1}{3} \left\langle B' + (\frac{\delta + 5}{2})kT(v - u)\overline{1}, \mathcal{L}[\mathcal{S}]^{-1}(\Phi_j) \right\rangle_{\mathcal{M}}. \tag{37}$$

Proof. Following the steps of the previous proof leads to the expression :

$$J_q = \left\langle B' + \overline{(\frac{\delta + 5}{2})kT(v - u)}, g \right\rangle_{\mathcal{M}}.$$

Now, replacing g by its alternative expression brought by (24), and identifying with the alternative expression of J_q above, brings the result. $\qquad\square$

4. **Definition of a Fick-relaxation operator.** Here, we seek to define a BGK model for which the Fick law holds, thus having the following expression :

$$\mathcal{R}(f) = \nu(f)(G(f) - f), \tag{38}$$

where the collision frequency $\nu(f)$ depends on f through its macroscopic fields and G is a function to be suitably chosen. This operator must, on the one hand, be properly defined, i.e satisfy the properties (conservation laws, entropy dissipation, correct equilibrium states, and well-defined linearized operator) introduced above. But those constraints are not fully satisfactory, as we have highlighted the necessity to recover (all or parts of) the Navier Stokes equation near equilibria. Lagrange multipliers method shows that, in absence of other constraints, the BGK model is fully determined by the formula (3), leaving only one insufficient degree of freedom to our operator. The constraints (3) garantee that the BGK model will satisfy the right conservation laws. Supplementary constraints on non conserved moments introduced on $\mathcal{R}$ will partially solve this problem. They rely the moments of the relaxation operator and the moments of the distribution function f and are re-stated as linear relations between the moments of f and those of G. The following problem is to define G once its moments are known. This part is overcome by minimizing the natural entropy under moment constraints. In a last step, performing a Chapmann-Enskog expansion starting from (38) up to Navier-Stokes, we compute

transport coefficients. The goal is therefore to recover the Fick matrix (from (27)), the shear viscosity and the the volume viscosity (from 30) associated to the Boltzmann operator considered here as the reference. We could also consider transport coefficients measured from experiments as the reference.

This section is therefore devoted to expressing convenient conditions to obtain a Fick-relaxation operator. As done in [16], the space $\tilde{\mathbb{C}}$ is of particular interest for those constraints.

Hypothesis 1. We assume $w_r \in \mathbb{C}, 1 \leq r \leq N-1$ to be well-chosen elements of $\mathbb{C}$, as well as the following constraints to be verified :

$$\begin{cases} \langle \mathcal{R}(f), w_r \rangle &= -\lambda_r \langle f, w_r \rangle \\ \\ \langle \mathcal{R}(f), \alpha \rangle &= -\lambda \langle f, \alpha \rangle \end{cases} \tag{39}$$

4.1. **Properties of** $\mathbb{C}$. Let us first recall two lemmas from [16] describing the supplementary constraints space $\mathbb{C}$ as well as its link with the Boltzmann operator. The proofs of these lemmas remain unchanged.

Lemma 5. *The matrix* $(L_{ij}[\mathcal{B}])_{1 \leq i,j \leq N}$ *is of rank* $N-1$, *where* $L_{ij}[\mathcal{B}]$ *is defined through* (27), *with* $\mathcal{S} = \mathcal{B}$ *being the multispecies polyatomic Boltzmann operator.*

Lemma 6. *Let us introduce, if* $1 \leq i, j \leq N$, $L_{ij}^*[\mathcal{B}] := k \dfrac{L_{ij}[\mathcal{B}]}{\|C_i\|_{\mathcal{M}} \|C_j\|_{\mathcal{M}}}$. *Then* $L^*[\mathcal{B}]$ *is symmetric, non-positive. Noting* $W[\mathcal{B}]$ *a matrix such that:*

$$W[\mathcal{B}]^T L^*[\mathcal{B}] W[\mathcal{B}] := Diag(d_1, \ldots, d_N), \tag{40}$$

with $d_1, \ldots, d_{N-1} < 0$ *and* $d_N = 0$, *then, the family* $\left(w_r[\mathcal{B}] := \displaystyle\sum_{s=1}^{N-1} W_{rs}[\mathcal{B}] \dfrac{C_s}{\|C_s\|_{\mathcal{M}}} \right)_{r < N}$ *provides an orthonormal basis of* $\mathbb{C}$ *for our weighted product, while*

$$w_N[\mathcal{B}] := \sum_{s=1}^{N} W_{Ns}[\mathcal{B}] \frac{C_s}{\|C_s\|_{\mathcal{M}}} \in \mathbb{K},$$

with :

$$W_{Ns}[\mathcal{B}] := \pm \sqrt{\frac{\rho_s}{\rho}}.$$

Finally, $\sigma(L^*[\mathcal{B}]) - \{0\} = \sigma(\mathcal{L}^{-1}[\mathcal{B}]_{|\mathbb{C}})$, *with:*

$$\begin{cases} w_r[\mathcal{B}] \in Ker(\mathcal{L}^{-1}[\mathcal{B}] - d_r), W_r[\mathcal{B}] \in Ker(L^*[\mathcal{B}] - d_r), \ r < N, \\ \\ w_N[\mathcal{B}] \in Ker(\mathcal{L}[\mathcal{B}]), W_N \in Ker(L^*[\mathcal{B}]). \end{cases}$$

Under the following conditions, BGK-type collisional operators can provide the correct Fick law near the hydrodynamical limit.

Property 5. Let us assume that $\mathcal{R}$ is a properly defined BGK operator, defined from (38). Then, taking $\lambda_r := -d_r^{-1}$ for $r < N$, $\lambda_N := 0$, and $w_r := w_r(\mathcal{B})$, then $\mathcal{R}$ allows to recover the correct Fick law at hydrodynamic limit if and only if

$$\mathcal{L}^{-1}[\mathcal{R}](B') \in \mathbb{C}^\perp. \tag{41}$$

Proof. Let us assume that $\mathcal{R}$ is properly defined and fulfills the phenomenologic Fick law from (12) at the hydrodynamic limit, that is, since this is the case for the Boltzmann operator :

$$\forall i, j, L_{ij}[\mathcal{R}] = L_{ij}[\mathcal{B}].$$

The order one for the Chapman-Enskog expansion as in (17) for our relaxation condition (39) leads to the following spectral requirements on $\mathcal{L}[\mathcal{R}]$:

$$\langle \mathcal{L}[\mathcal{R}](g), w_r \rangle_{\mathcal{M}} = -\lambda_r \langle g, w_r \rangle_{\mathcal{M}}, r < N, \tag{42}$$

where $\{w_r, r < N\}$ is a basis for $\mathbb{C}$ and $\lambda_r < 0, r < N$. Let us recall that $\{\mathbf{\Phi}_i, i < N\}$ is a generating family for $\mathbb{C}$. Hence we can write:

$$w_r = \sum_{s=1}^{N} W_{rs} \frac{(\mathbb{I}_d - P_{\mathbb{K}})(C_s)}{\|C_s\|_{\mathcal{M}}}, \tag{43}$$

since $w_r \in \mathbb{C}$. Let us also remark that the additional condition :

$$\langle \mathcal{L}[\mathcal{R}](g), w_N \rangle_{\mathcal{M}} = -\lambda_N \langle g, w_N \rangle_{\mathcal{M}}, \tag{44}$$

is trivial because $w_N \in \mathbb{K}$ and $\lambda_N = 0$. Firstly, the right-hand term of (42)-(44) gives :

$$\langle g, w_r \rangle_{\mathcal{M}} = \sum_{s=1}^{N} \frac{\langle g, C_s \rangle_{\mathcal{M}}}{\|C_s\|_{\mathcal{M}}} W_{rs} = \sum_{s=1}^{N} \frac{W_{rs}}{\|C_s\|_{\mathcal{M}}} J_s[\mathcal{R}]. \tag{45}$$

By hypothesis, the Fick law is recovered at the hydrodynamic limit, i.e, by (25):

$$J_i[\mathcal{R}] = \sum_{j=1}^{N} k L_{ij}[\mathcal{B}] \frac{\nabla p_j}{p_j} + \theta_i T \nabla(-\frac{1}{kT}). \tag{46}$$

Therefore according to (46), (45) becomes :

$$\langle g, w_r \rangle_{\mathcal{M}} = \sum_j (\sum_s \frac{W_{rs}}{\|C_s\|_{\mathcal{M}}} L_{sj}[\mathcal{B}]) \frac{\nabla p_j}{p_j} + (\sum_{s=1}^{N} \frac{\theta_s}{\|C_s\|_{\mathcal{M}}} W_{rs} T) \nabla(-\frac{1}{kT}). \tag{47}$$

Secondly, the left-hand term of the expansion (42)-(44) expresses :

$$\langle \mathcal{L}[\mathcal{R}](g), w_r \rangle_{\mathcal{M}} = \sum_{j=1}^{N} (\sum_{s=1}^{N} \langle C_j, C_s \rangle_{\mathcal{M}} \frac{W_{rs}}{\|C_s\|_{\mathcal{M}}}) \frac{\nabla p_j}{p_j}. \tag{48}$$

Injecting (47)-(48) into (42)-(44) leads, by algebraic identification, to the following conditions :

$$\begin{cases} \lambda_r \|C_j\|_{\mathcal{M}} W_{rj} = \sum_{s=1}^{N} \frac{W_{rs}}{\|C_s\|_{\mathcal{M}}} L_{sj}[\mathcal{B}], \\ \\ \sum_{s=1}^{N} W_{rs} \frac{\theta_s}{\|C_s\|_{\mathcal{M}}} = 0. \end{cases}$$

The first condition writes :

$$\lambda_r W_{rj} = \sum_{s=1}^{N} W_{rs} L_{sj}^*[\mathcal{B}], \forall r \geq N \Leftrightarrow W L^* W^T = Diag(\lambda_1, \dots, \lambda_N).$$

The second condition writes according to relation (36):

$$\langle w_r, \mathcal{L}^{-1}[\mathcal{R}](B') \rangle_{\mathcal{M}} = 0, r < N,$$

which is exactly asking $\mathcal{L}^{-1}[\mathcal{R}](B') \in \mathbb{C}^{\perp}$. $\square$

Let us finally notice that developing the λ constraint of (39) at order one for Chapman-Enskog expansion, brings that the right λ eigenvalue for the Boltzmann operator is :

$$\lambda[\mathcal{B}] = kT \frac{\|\alpha\|_{\mathcal{M}}^2}{\eta_V[\mathcal{B}]}. \tag{49}$$

As a consequence, we will, from now on, take this value for λ in order to recover the correct volume viscosity. Hence the following straightforward condition :

Lemma 7. *If $\mathcal{R}$ satisfies $\lambda[\mathcal{R}] = \lambda[\mathcal{B}]$, then $\eta_V[\mathcal{R}] = \eta_V[\mathcal{B}]$ is the correct volume viscosity for the gas mixture.*

Remark 5. Finally, let us also notice that this last condition becomes, a priori, singular at monoatomic limit.

4.2. **Definition of a Fick-relaxation operator.** The previous sections lead to the derivation a BGK-type operator satisfying the Fick Law with correct Onsager coefficients, as well as the obvious physical conservation laws and, in the strict polyatomic case, the correct volume viscosity. The next aim deals with the obtention of our so-called properly defined operator. In particular, we aim to obtain entropy dissipation and the right behaviour at equilibrium.

Lemma 8. *Let $f \geq 0$ such that:*

$$\sum_i \iint f_i (1 + v^2 + I_i^{\frac{2}{\delta_i}} + \ln f_i) dv dI_i < \infty.$$

We introduce the following set of constraints:

$$K(f) := \left\{ g \geq 0, g \in L^1(v, \mathcal{H}), \left\{ \begin{array}{c} \forall 1 \leq l \leq N+4, \langle f, \phi_l \rangle = \langle g, \phi_l \rangle \\ \forall r < N, \langle g, w_r(\mathcal{B}) \rangle = (1 - \dfrac{\lambda_r(\mathcal{B})}{\nu}) \langle f, w_r[\mathcal{B}] \rangle \\ \langle g, \alpha \rangle = (1 - \dfrac{\lambda}{\nu}) \langle f, \alpha \rangle \end{array} \right. \right\}. \tag{Cons}$$

Let $g \in K(f)$, and let us note ρ_i, n_i, m_i, δ_i the common macroscopic quantities for g and f, whereas u^i, T^i (resp. u_i, T_i) are the proper quantities for g (resp f). Then, the velocity tensor $\overline{U} := (u^1, \ldots, u^N)^T$ of g can be expressed only with parameters from f, via the following formula :

$$\overline{U} - U = N^{-1} W^T[\mathcal{B}] (I - \frac{\Lambda}{\nu}) W[\mathcal{B}] N(\underline{U} - U), \tag{50}$$

where $U := (u, \ldots, u)^T$, $N := Diag(\sqrt{\rho_1}, \ldots, \sqrt{\rho_N})$, $\Lambda := Diag(\lambda_1[\mathcal{B}], \ldots, \lambda_N[\mathcal{B}])$, and $\underline{U} := (u_1, \ldots, u_N)^T$ is the velocity tensor associated with f.

Proof. The demonstration for that formula is similar to the proof in the monoatomic case, see [16]. $\square$

On the one hand, conservation laws (3) imply :

$$\tfrac{\delta+3}{2} nkT = \mathcal{E} = \sum_i \iint (\tfrac{1}{2} m_i (v-u)^2 + I_i^{\frac{2}{\delta_i}}) f_i dv dI_i = \sum_i \iint (\tfrac{1}{2} m_i (v-u)^2 + I_i^{\frac{2}{\delta_i}}) g_i dv dI_i. \tag{51}$$

On the other hand, fictitious temperature for g can be defined by :

$$T^* := \sum_i \frac{n_i}{n} T^i = \frac{2}{(\delta+3)nk} \sum_i \iint (\frac{1}{2} m_i (v-u^i)^2 + I_i^{\frac{2}{\delta_i}}) g_i dv dI_i.$$

From these two statements, we can deduce :

Lemma 9. *The mean temperature of g can be defined exclusively via parameters of f, with the following formula :*

$$T^* = T - \frac{1}{(\delta + 3)nk} \left\| W^T(\mathcal{B})(I - \frac{\Lambda(\mathcal{B})}{\nu})WN(\overline{U} - U) \right\|^2, \tag{52}$$

where $\| \|$ is the Euclidean norm. Moreover, $T^* \geq 0$ if we chose $\nu \geq \dfrac{\max_r \lambda_r(\mathcal{B})}{2}$.

Proof. Let us first notice that (51), combined with the original expression of T^*, give the following relation between T and T^*:

$$T - T^* = \frac{1}{(\delta + 3)nk} \sum_i \rho_i (u_i - u)^2. \tag{53}$$

Evaluating the norm of (50) leads, thanks to the symmetry of $W^T(I - \dfrac{\Lambda(\mathcal{B})}{\nu})W$:

$$T^* \geq T - \frac{1}{(\delta + 3)nk} \max \sigma (I - \frac{\Lambda(\mathcal{B})}{\nu})^2 \|\overline{U} - U\|^2$$

$$= T - (1 - \frac{\min \lambda_r}{\nu})^2 \frac{1}{(\delta + 3)nk} \sum_i \rho_i (u_i - u)^2$$

$$\geq \sum_i \frac{\delta_i + 3}{2} n_i k T_i \geq 0,$$

with the correct choice of ν. $\qquad\square$

Lemma 10. *The last constraint of (Cons) expresses :*

$$T^*_{int} = T^*_{tr} + (1 - \frac{\lambda}{\nu})\{T_{int} - T_{tr}\},$$

with :

$$\begin{cases} \frac{3}{2}nkT^*_{tr} := \left\langle g, \frac{1}{2}\overline{m}(v - u)^2 \right\rangle_{\mathcal{M}} \\ \frac{\delta}{2}nkT^*_{int} := \left\langle g, \overline{I^{\frac{2}{\delta}}} \right\rangle_{\mathcal{M}} \end{cases},$$

the respective translational and non translational temperatures for g. For $\nu \geq \dfrac{\lambda}{1 + \min\{\frac{\delta}{3}, \frac{3}{\delta}\}}$, we have $T^*_{int}, T^*_{tr} \geq 0$.

Proof. The equality :

$$\begin{pmatrix} 1 & -1 \\ \frac{\delta}{2} & \frac{3}{2} \end{pmatrix} \begin{pmatrix} T^*_{int} \\ T^*_{tr} \end{pmatrix} = \begin{pmatrix} (1 - \frac{\lambda}{\nu})(T_{int} - T_{tr}) \\ (\frac{\delta + 3}{2})T \end{pmatrix}$$

leads to :

$$\begin{cases} T^*_{int} = T + \frac{3}{\delta + 3}(1 - \frac{\lambda}{\nu})(T_{int} - T_{tr}), \\ T^*_{tr} = T - \frac{\delta}{\delta + 3}(1 - \frac{\lambda}{\nu})(T_{int} - T_{tr}). \end{cases} \tag{54}$$

Now, let us denote $\beta := 1 - \frac{\lambda}{\nu} \leq 1$. The first equation of (54) becomes :

$$T^*_{int} = (\frac{\delta}{\delta + 3} + \frac{3}{\delta + 3}\beta)T_{int} + \frac{3}{\delta + 3}(1 - \beta)T_{tr}.$$

We easily find the desired sufficient condition, requiring the first right-hand side coefficient to be positive, and performing similar computations from the expression of T^*_{tr}. $\qquad\square$

Remark 6. This supplementary constraint fits with the distinction between translational and non-translational internal temperatures, which introduces a new degree of freedom. Thanks to the relation :

$$\frac{\delta+3}{2}nkT = \frac{\delta}{2}nkT_{int} + \frac{3}{2}nkT_{tr},$$

we can obtain the following expression for fictitious temperature :

$$\frac{\delta+3}{2}nkT^* = \frac{\delta+3}{2}nkT_{tr}^* + \frac{\delta}{2}(1 - \frac{\lambda}{\nu})(T_{int} - T_{tr})$$

Theorem 4.1. *If* $\nu \geq \max \lambda_r(\mathcal{B})/2$, *then* $K(f) \neq \emptyset$ *and there exists a unique solution to the minimization problem* $\underline{G} = Argmin_{K(f)}\mathcal{H}$, *its coordinates read :*

$$G_i = n_i \left(\frac{m_i}{2\pi kT_{tr}^*}\right)^{\frac{3}{2}} \left(\frac{1}{kT_{int}^*}\right)^{\frac{\delta_i}{2}} \Lambda_i^{-1} \exp\left(-\frac{m_i(v-ui)^2}{2kT_{tr}^*} - \frac{I_i^{\frac{2}{\delta_i}}}{kT_{int}^*}\right),$$

where $(u^i)_{1\leq i \leq N}$ *has been defined in* (50) *and with the notations of Lemmas* 8, 9, 10.

Proof. We rely on [34], or [31] to argue that this minimization problem always has a unique solution, as soon as:

$$\Omega_0 := \{(A_l)_{1\leq l \leq N+4}, (B_r)_{1\leq r \leq N-1}, C; \textstyle\sum_i \exp(A \cdot \phi_i + B \cdot w_{.,i} + C\alpha) \in L^1(\mathbb{R}^3 \times \mathbb{R}_+)\} \subset \mathbb{R}^{2N+3},$$

is open, where $\phi_i, w_{.,i}$ and α refer to the constraint vectors defined respectively in Property 1, Lemma 6 and Equation (19). Indeed, Ω_0 is open (for the usual norm topology). □

5. **On the Fick-relaxation operator and the transport coefficients.** Now that we have explicited all the parameters necessary to describe our Fick-relaxation operator with the desired constraints - i.e the frequency ν and the attractor G, it remains to compute the associated parameters. In particular, we are now able to give an expression of the linearized operator $\mathcal{L}[\mathcal{R}]$, and therefore to all the phenomenological coefficients. This process will finally enable us to verify the physical compatibility of our model. In particular, the correct Onsager matrix and the two viscosities are to be recovered - under conditions.

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

Property 6. With the hypotheses of Theorem 4.1, $\mathcal{R}$ is properly defined, and the associated linearized operator satisfies :

$$\mathcal{L}[\mathcal{R}] = \nu(R \circ P_{\tilde{\mathbb{C}}} - P_{\mathbb{K}^\perp}),$$

with R the linear operator on $\tilde{\mathbb{C}}$ such that $Rw_r = (1 - \frac{\lambda_r(\mathcal{B})}{\nu})w_r$, for $r < N$, and $R\alpha = (1 - \frac{\lambda}{\nu})\alpha$, while

$$\mathcal{L}^{-1}[\mathcal{R}] = \frac{1}{\nu}((R - Id)^{-1} \circ P_{\tilde{\mathbb{C}}} - P_{\tilde{\mathbb{C}}^\perp}). \tag{55}$$

Remark 7. Let us notice that once again, this formula still holds in the monospecies case, since $\tilde{\mathbb{C}} = \{0\}$ within this particular framework. Likewise, we recover the monoatomic case when $\alpha = 0$.

We can also remark once again (this is also clear from the above properties of $\mathcal{L}[\mathcal{R}]$ that the orthogonal sum $\tilde{\mathbb{C}} \oplus \tilde{\mathbb{C}}^\perp = \mathbb{K}^\perp$ is stable by $\mathcal{L}$. Therefore we cannot make simple hypothesis such as $\mathcal{L}^{-1}[\tilde{B}] \in \tilde{\mathbb{C}}^\perp$ within the pure polyatomic framework.

Finally, we shall see that this writing of $\mathcal{L}^{-1}$ lacks convenience, since the expression of $w_r[\mathcal{B}]$ is not known.

Proof. To prove that $\mathcal{R}(f)$ is properly defined, the only part differing from [16] is the proof of the H-theorem from Property 2.

The convexity of $F : x \mapsto x \ln x - x$ enables us to obtain the following inequality on the entropy variation:

$$\nu \iint \sum_i (G_i - f_i) \ln f_i dv dI \leq \mathcal{H}(\underline{G}) - \mathcal{H}(f). \tag{56}$$

Now easy computations bring, from (2) :

$$\mathcal{H}(\underline{G}) = \sum_i n_i (\ln n_i + \frac{3}{2} \ln(\frac{m_i}{2\pi k T^*}) - \frac{\delta_i + 3}{2} \ln k T^* - \frac{\delta_i + 3}{2} - 1 - \ln \Lambda_i).$$

$f \notin K(f)$ implies that $\mathcal{H}(f)$ cannot be directly compared with $\mathcal{H}(\underline{G})$ ($\lambda_r \not\equiv 0$); however, classic entropy minimization in the monospecies case leads to $\mathcal{H}(f) \geq \mathcal{H}(\Gamma)$, with :

$$\Gamma_i := n_i \Lambda_i^{-1} (\frac{m_i}{2\pi k T^i})^{\frac{3}{2}} (\frac{1}{k T^i})^{\frac{\delta_i}{2}} \exp(-\frac{m_i(v - u^i)^2}{2k T^i} - \frac{I^{\frac{2}{\delta_i}}}{k T^i}).$$

Therefore, (56) becomes :

$$\nu \iint \sum_i (G_i - f_i) \ln f_i dv dI \leq n \frac{\bar{\bar{\delta}} + 3}{2} \ln \frac{\sum_i n_i \frac{\delta_i + 3}{2} k T^i}{\frac{\bar{\bar{\delta}} + 3}{2} n k T^*} \leq 0$$

thanks to the concavity of ln and definition of T^*. $\qquad \square$

5.2. **Hydrodynamic limit.** Thanks to our previous computations combined with the expression (52) for the inverse linearized operator, we are able to recover the sought coefficients.

Property 7. The transport coefficients computed from our Fick relaxation operator defined in (37) can be expressed by the following formulae :

$$L_{ij} = L_{ij}[\mathcal{B}],$$

$$L_{iq} = -kT \sum_j (\frac{\delta_j + 5}{2}) L_{ij},$$

$$L_{qq} = k^2 T^2 \sum_{i,j=1}^N (\frac{\delta_i + 5}{2})(\frac{\delta_j + 5}{2}) L_{ij}$$

$$+ \frac{5}{2\nu} k^2 T^3 (\sum_{i=1}^N \frac{n_i}{m_i}) + \frac{1}{4\nu} \delta^2 (\sum_{i=1}^N \frac{n_i}{m_i})$$

$$+ \frac{13 - \delta}{6\nu} (\sum_{i=1}^N \frac{n_i}{m_i} \delta_i) + \frac{1}{4\nu} (\sum_{i=1}^N \frac{n_i}{m_i} \delta_i^2),$$

$$\eta = \frac{n k^2 T^2}{\nu},$$

$$\eta_V = \frac{2\delta n k T}{3\lambda(\delta + 3)}.$$

Moreover, if $\eta[\mathcal{B}] \leq \dfrac{2nk^2T^2}{\max_r \lambda_r[\mathcal{B}]}$, then taking $\nu := \dfrac{nk^2T^2}{\eta[\mathcal{B}]}$, the model enjoys the true shear viscosity. Finally, if $\eta[\mathcal{B}] \leq \dfrac{3}{2}(1+\dfrac{3}{\delta})(1+a)kT\eta_V[\mathcal{B}]$, with $a := \min\{\frac{\delta}{3}, \frac{3}{\delta}\}$, the model enjoys the true volume viscosity.

Proof. • If (41) is fulfilled, then the correct Fick coefficients are recovered,
  • $\mathcal{L}^{-1}(B') \in \mathbb{C}^{\perp}$, so $\theta_i = 0$, thanks to the formula (36). As a consequence, (25) brings :

$$L_{iq} = -kT \sum_{j=1}^{N} (\frac{\delta_j + 5}{2})L_{ij}.$$

  • That equality, coupled with the expression of β, provides :

$$L_{qq} = k^2T^2 \sum_{i,j=1}^{N} (\frac{\delta_i + 5}{2})(\frac{\delta_j + 5}{2})L_{ij} - \frac{1}{3\nu}\left\langle B' + \frac{\delta + 5}{2}T(v - u)\overline{1}, \mathcal{L}^{-1}(B')\right\rangle_{\mathcal{M}}.$$

Finally, further computations lead to the desired result.

$\square$

Obviously, although L and both viscosities were shown to be recovered at hydrodynamic limit, nothing tends to prove - and cumbersome results rather tend to disprove, that the other phenomenological coefficients are correct.

6. **Conclusions and perspectives.** Throughout this paper, has been investigated a generalization to a mixture of both monoatomic and polyatomic gases, of the Fick relaxation operator initiated in [16]. Two purposes were involved: on the one hand, the sought operator was expected, within a polyatomic modelization inherited from [13], to recover the correct Fick matrix, the shear viscosity and the volume viscosity at the vicinity of hydrodynamic limit. This investigation has been shaped as an inverse problem involving the desired coefficients. To that extent, a Chapman-Enskog expansion at order 1 enabled a useful expression of our relaxation model's own coefficients with respect to its inversed linearized operator. These expressions have then been used to provide equivalent constraints on our system, themselves finally taking part of an entropy minimization, to solve the inverse problem while fulfilling the H Theorem.

On the other hand, all these calculations have been performed in order to construct a model which would strictly contains its monoatomic counterpart; the aim was here to be able to revert back to a mixture of monoatomic gases from this model, through a simple affectation of value.

Finally, this model can be made more realistic. For example, one is aware of the fact that, within a context of sufficient variations of temperature, $\delta = \delta(T)$. We mention a recent paper ([12]) in that direction where a new collision operator intergrating varying δ has been constructed.

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