An ES-BGK model for non polytropic gases with a general framework

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Abstract

In this paper we derive an Ellipsoidal Statistical BGK model for a polyatomic gas that is based on a general framework introduced in [10]. The distribution function of the polyatomic gas depends on its velocity and a general internal energy function, that can be discrete or continuous. We solve the minimization problem of Boltzmann entropy under suitable moments and we determine the transport coefficients (Prandtl number, first and second viscosity) in the hydrodynamic limit. At the end we obtain an ES-BGK model for a general framework covering in particular the non polytropic case.

1 Introduction

In the context of high altitude aerodynamics, it is necessary to use a kinetic description since the Knudsen number is of order 1. Since the atmosphere has a more complex structure, containing monatomic gases such as O, N and NO and polyatomic gases such as O_2 and N_2, interest has shifted to the study of kinetic models concerning mixtures of mono and polyatomic gases. A kinetic description for polyatomic gas involves a distribution function $f(t, x, v, I)$ that represents the density number of gas molecules and depends on time t, space x, velocity v and internal energy I. Polyatomic models can be split into two categories: those that assume continuous internal energy and those that consider discrete internal energy. In [9] the authors develop a microscopic model in which a certain fraction of the total energy is shared with translational and internal energy. At the mesoscopic level, tractable collisionnal models models involving energy transfers between translational and internal modes have been introduced. In [19] a kinetic model for a single polyatomic gas with continuous internal energy I presents the measure $\psi(I) = I^\alpha$ for some $\alpha \geq 0$, that is crucial to get the energy laws of polytropic gases. The generalization of the collision operator for a polyatomic gas mixture is performed in [20] together with the derivation of a polyatomic compressible Euler system. In [5] a Navier-Stokes system for any mixture of mono and polyatomic gases is derived from a Boltzmann model ([20]), providing explicit transport coefficients for Maxwell molecules. In ([17], [18]), the authors show that the linearized Boltzmann operator satisfies a Fredholm property. The

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closure problem of a Boltzmann model for a polyatomic gas is resolved in [29], using the maximum entropy principle.

In [22] a polyatomic gas has been interpreted as a mixture of monatomic gases, each of which has a discrete energy level. So, a reagent mixture of polyatomic gases is dealt with associating to each molecule the velocity of the center of mass and a discrete variable representing internal energy that can take on a set of quantized energy levels.

In order to generalize the previous models ([11]), Borsoni and al. [10] proposed a new collisional model for a single polyatomic gas, in which each molecule is defined by position, velocity and an internal state variable ζ, which varies in a measure space $(\mathcal{E}, \mathcal{A}, \omega)$ and an energy function $\epsilon(\zeta)$, which associates an energy value to each internal state. So, depending on whether the space of the internal states is assumed to be $\mathbb{N}$ or $\mathbb{R}$, the model returns the case of discrete or continuous internal energy respectively. In the case of continuous internal energy the number of degrees of freedom of internal energy does not depend on temperature, while the discrete internal energy makes this dependence. In particular, the degrees of freedom depend on the macroscopic temperature and this model encompasses non polytropic gases. This collisional model has been generalized in ([7]) to the situation of reacting gas mixtures. In ([27]), the authors developped kinetic models including translational, vibrational and rotational internal energies for reactive gas mixtures. Several scalings depending on fast and slow processes are considered and fluid systems are derived.

Another strategy for studying gases is represented by BGK models in which the Boltzmann collision operator is replaced by a relaxation term, while keeping physical and mathematical properties like conservation laws and H Theorem [8]. A BGK model for mixture of monatomic gases is defined in [1], where the interactions between particles are performed by fictitious macroscopic quantities, in order to recover conservation laws. A drawback of these BGK models is that do not provide in the hydrodynamic limit the right transport coefficients. The Ellipsoidal statistical or Gaussian model (ES-BGK) introduced by Holway ([23]) for polyatomic gases overcomes the criticality and manages to reach a Prandtl number that varies in $[\frac{2}{3}, 1[$, as proved in [2] and in [16]. Hence we aim in this paper to derive an ES-BGK model from an entropy minimization principle by using the framework developped in [10]. Entropy minimization principles as well as the idea of using different relaxation terms have been first considred by Levermore in the context of monoatomic gases ([26]). But this works leads to different models that can only reach Prandtl numbers larger than 1. In ([15], [16]) the authors proposed a derivation of the ES-BGK model in that is based on the introduction of relaxation coefficients and the resolution of an entropy minimization problem. By using the same strategy, the authors construct in ([13], [14]) a BGK model that is able to reproduce the Fick matrix. In ([32]), this operator is generalized to reacting gas mixtures by considering the operator as a sum for respectively mechnical and chemical processes. The energy variable is based on the formalism developped in ([21]). The question wheher this problem this problem admits a solution or not is subjected to the values of the relaxtion rates and the so-called realizability moments problem ([24], [26], [31]). This approach is next generalized to polyatomic gas mixtures ([12, 13]). Another investigation to do is to compare the asymptotic limit of the BGK models with the phenomenological results of Extended Thermodynamics, where the two kind of internal energy, rotational and vibrational are assumed both continuous [4, 6, 30].

In ([16], [12]) the ES-BGK is considered for a specific heat at constant volume C_v and a specific heat at constant pressure C_p constant. Such a gas is called a polytropic gas in the literature. However, as pointed out in ([25]), C_p, C_v and $\gamma = \frac{C_p}{C_v}$ should depend on temperature in order to be physically more realistic. In ([3], [25]), the authors have presented an ES-BGK model for the non polytropic case when the internal energy is a continous variable. The goal of the present paper, is to derive an ES-BGK model for the formalism developped in [10]. The method of derivation is based on the approach developped in ([15], [16]) and mentionned before.

The paper is organized as follows. In section 2 we introduce the framework and its assumptions. In section 3 we construct the Ellipsoidal Statistical model and solve the variational problem regarding the minimization of the entropy functional under suitable constraints. Then we compute the hydrodynamical limit of the model to recover proper transport coefficients and the Prandtl number. Section 4 is devoted to comparison of the present model with other models. In particular we show that we can recover some existing models. Finally, section 5 is devoted to conclusions and perspectives.

2 General setting

The aim of this paper is to construct a model based on the framework proposed by Borsoni and al. in [10]. A polyatomic gas is given with molecular mass $m \in \mathbb{R}^+$ and each of its molecules is defined by its velocity v and an internal state ζ that it varies in a measure space

$$(\mathcal{E}, \mathcal{A}, \omega)$$

where $\mathcal{E}$ is the space of internal states of ζ, $\mathcal{A}$ is a $\sigma-$algebra on $\mathcal{E}$ and $\omega(\mathcal{E})$ is a non negative, $\sigma-$finite measure on $(\mathcal{E}, \mathcal{A})$. We indicate with $Bor(\mathbb{R})$ the set of Borelians of $\mathbb{R}$. Let the $(\mathcal{A}, Bor(\mathbb{R}))$ measurable function

$$\epsilon : \mathcal{E} \to \mathbb{R}$$

the internal energy that associates to each internal state ζ a energy value $\epsilon(\zeta)$. We denote by the grounded internal energy function

$$\bar{\epsilon} = \epsilon - \epsilon^0$$

where

$$\epsilon^0 := inf\, ess_\omega\{\epsilon\} = sup\{R \in \mathbb{R}\, s.t.\, \omega(\epsilon < R) = 0\}$$

is the fundamental energy of configuration of the molecules.

2.1 Partition function

We define the partition function Z for the molecular internal mode of the polyatomic gas

$$Z(\beta) := \int_{\mathcal{E}} e^{-\beta\bar{\epsilon}(\zeta)} d\omega(\zeta) < \infty, \tag{1}$$

for all $\beta > 0$.
Let us now consider two particular situations.
If we consider the continuous energy space $\mathcal{E} = \mathbb{R}_+$, ([11]) the set of the Borelians of $\mathbb{R}_+$,

$\mathcal{A}$ and the measure $d\omega(I) = \psi(I)dI$, where $\psi(I) = I^\alpha$ with $\alpha > -1$ and the internal energy $\epsilon(I) = I$, the partition function takes the form

$$Z\left(\frac{1}{k_BT}\right) = \int_{\mathcal{E}} \exp\left(-\frac{I}{k_BT}\right) I^\alpha dI.$$

Instead if we consider the discrete space $\mathcal{E} = \{0, 1, \ldots, N\}$, together with $\mathcal{A} = \mathcal{P}(\mathcal{E})$ and $\epsilon(n) = \epsilon_n$ for $n = 0, \ldots, N$. In that case, the partition function (1) reads

$$Z\left(\frac{1}{k_BT}\right) = \sum_{i=0}^{N} a_i \exp\left(-\frac{\epsilon_i}{k_BT}\right), \tag{2}$$

where a_i are defined in ([21]) as the degenaracy of the i^{th} quantum energy shell.

It holds the following result, the demonstration of which is in [10]:

Proposition 2.1. *Z is $\mathcal{C}^\infty$ on $\mathbb{R}_+^*$ and its derivatives are given by*

$$(\forall\ k > 0),\ Z^{(k)}(\beta) = \int_{\mathcal{E}} (-\bar{\epsilon}(\zeta))^k e^{-\beta\bar{\epsilon}(\zeta)} d\omega(\zeta).$$

We indicate with $f(t, x, v, \zeta)$ the distribution function, such that $f(t, x, v, \zeta)dxdvd\zeta$ expresses the probability of funding a gas molecule, within the space $(x, x + dx)$ with velocity in the range $(v, v + dv)$ and internal state in $(\zeta, \zeta + d\zeta)$ at a time t. We suppose that f is non negative and

$$\forall\,(t, x)\, f(t, x, \cdot, \cdot) \in L^1(\mathbb{R}^3 \times \mathcal{E}, dv\, d\omega(\zeta)).$$

2.2 Hydrodynamic quantities

Mass density ρ, velocity u and total energy density E are defined as

$$\begin{aligned}
\rho(t, x) &:= \int_{\mathcal{E}} \int_{\mathbb{R}^3} m f(t, x, v, \zeta) dv d\omega(\zeta), \\
u(t, x) &:= \frac{1}{\rho(t, x)} \int_{\mathcal{E}} \int_{\mathbb{R}^3} m\, v f(t, x, v, \zeta) dv d\omega(\zeta), \\
E(t, x) &:= \frac{1}{\rho(t, x)} \int_{\mathcal{E}} \int_{\mathbb{R}^3} \left(\frac{m}{2}|v|^2 + \epsilon(\zeta)\right) f(t, x, v, \zeta) dv d\omega(\zeta).
\end{aligned}$$

We denote by $\delta(T)$ the number of internal degrees of freedom

$$\delta(T) := \frac{2}{k_BT}\left(\frac{\int_{\mathcal{E}} \bar{\epsilon}(\zeta) \exp\left(-\frac{\bar{\epsilon}(\zeta)}{k_BT}\right) d\omega(\zeta)}{\int_{\mathcal{E}} \exp\left(-\frac{\bar{\epsilon}(\zeta)}{k_BT}\right) d\omega(\zeta)}\right), \tag{3}$$

where k_B is the Boltzmann constant and T the temperature of the gas. We define the specific heat at constant volume

$$c_V(T) := \frac{3 + D(T)}{2} \tag{4}$$

where

$$D(T) := \frac{d(T\delta(T))}{dT}$$

for all $T > 0$. It is important to underline that here $\delta(T)$ depends on the temperature, contrary to what it turns out in [2].
The total energy density E at collision equilibrium is expressed by

$$E(u, T) = \frac{m}{2}|u|^2 + \epsilon^0 + \frac{3 + \delta(T)}{2} k_B T.$$

The choice of setting $\bar{\epsilon}$ in place of ϵ and various mathematical properties of $\delta(T)$, that make its formulation physically valid, are exposed in [10]. The specific internal energy $e(t, x) = \frac{1}{\rho(t,x)} E(t, x) - \frac{1}{2}|u|^2$ is splitted into two parts, the internal energy of translational motion $e_{tr}(t, x)$ and the energy associated with the internal structure $e_{int}(t, x)$:

$$e(t, x) = e_{tr}(t, x) + e_{int}(t, x), \tag{5}$$

$$e_{tr}(t, x) = \frac{1}{\rho(t, x)} \int_{\mathcal{E}} \int_{\mathbb{R}^3} \frac{m}{2}|c|^2 f(t, x, v, \zeta) dv d\omega(\zeta), \tag{6}$$

$$e_{int}(t, x) = \frac{1}{\rho(t, x)} \int_{\mathcal{E}} \int_{\mathbb{R}^3} \bar{\epsilon}(\zeta) f(t, x, v, \zeta) dv d\omega(\zeta), \tag{7}$$

where $c = v - u$ is the relative velocity. These energies are associated to the corresponding temperatures $T(t, x)$, $T_{tr}(t, x)$, $T_{int}(t, x)$

$$e(t, x) = \frac{3 + \delta(T)}{2} k_B T(t, x),$$

$$e_{tr}(t, x) = \frac{3}{2} k_B T_{tr}(t, x),$$

$$e_{int}(t, x) = \frac{\delta(T)}{2} k_B T_{int}(t, x).$$

We denote by $\Theta(t, x)$ the stress tensor s.t.

$$\rho(t, x)\Theta(t, x) := \int_{\mathcal{E}} \int_{\mathbb{R}^3} mc \otimes c f(t, x, v, \zeta) dv d\omega(\zeta).$$

We define the Boltzmann entropy as

$$\int_{\mathbb{R}^3} \int_{\mathcal{E}} \mathcal{H}(f) dv d\omega, \tag{8}$$

where $\mathcal{H}(f) = f(\ln f - 1)$.

3 Construction of the model

We propose to construct a BGK model whose relaxation term is of the form

$$R(f) = \lambda(\mathcal{G} - f).$$

More precisely, we aim to provide a BGK model that satisfies the conservation laws and main properties of the Boltzmann model and to determine the parameter λ and the Gaussian function $\mathcal{G}$ in such a way that the transport coefficients can be recovered. The strategy to obtain this model is to proceed as in ([12], [13], [15], [16]) through the mimimization of the entropy functional under moments constraints.

We will proceed in the folling way. We firstly have to choose a set of moments an thus define a set of constraints. Next, we have to compute the argmin of the entropy of the set of constraints. And the last step consists in defining relaxation parameters from the computation of the hydrodynamic limit and the comparison with the Navier-Stokes system.

3.1 Set of constraints

So, following the paper by Brull and Schneider [16], we set the variational problem:

Let f be a non negative function given, find $\mathcal{G}$ solution to the minimization problem

$$\mathcal{G} = S(\rho, u, \mathcal{T}) = \underset{g \in K_f}{\arg\min} \int_{\mathbb{R}^3} \int_{\mathcal{E}} \mathcal{H}(g) dv d\omega \tag{9}$$

where K_f is the set of functions $g \geq 0$ that satisfy the constraints

$$\int_{\mathbb{R}^3} \int_{\mathcal{E}} \left(m, mv, \frac{1}{2}mv^2 + \bar{\epsilon}(\zeta) \right) g \, dv d\omega = \int_{\mathbb{R}^3} \int_{\mathcal{E}} \left(m, mv, \frac{1}{2}mv^2 + \bar{\epsilon}(\zeta) \right) f \, dv d\omega, \tag{10}$$

$$\int_{\mathbb{R}^3} \int_{\mathcal{E}} m \left(c \otimes c - \frac{1}{3}c^2 I_d \right) \lambda(g - f) \, dv d\omega = -\lambda_1 \int_{\mathbb{R}^3} \int_{\mathcal{E}} m \left(c \otimes c - \frac{1}{3}c^2 I_d \right) f \, dv d\omega, \tag{11}$$

$$\int_{\mathbb{R}^3} \int_{\mathcal{E}} \left(\frac{1}{3}mc^2 - \frac{2}{3 + \delta(T)} \left(\frac{1}{2}mc^2 + \bar{\epsilon}(\zeta) \right) \right) \lambda(g - f) \, dv \, d\omega =$$

$$-\lambda_2 \int_{\mathbb{R}^3} \int_{\mathcal{E}} \left(\frac{1}{3}mc^2 - \frac{2}{3 + \delta(T)} \left(\frac{1}{2}mc^2 + \bar{\epsilon}(\zeta) \right) \right) f \, dv \, d\omega, \tag{12}$$

with λ_1 and λ_2 positive relaxation coefficients and I_d identical matrix in $\mathbb{R}^3$.

We observe that (10) are the conservation laws of mass, momentum and energy while (11) and (12) are suitable constraints that guarantee to find transport coefficients. Using the conservation law for the specific energy

$$\int_{\mathbb{R}^3} \int_{\mathcal{E}} \left(\frac{1}{2}mc^2 + \bar{\epsilon}(\zeta) \right) g \, dv d\omega = \int_{\mathbb{R}^3} \int_{\mathcal{E}} \left(\frac{1}{2}mc^2 + \bar{\epsilon}(\zeta) \right) f \, dv d\omega,$$

into (12), we easily get

$$\int_{\mathbb{R}^3}\int_{\mathcal{E}}\frac{1}{3}m|c|^2 g\,dvd\omega = (1-\theta)\int_{\mathbb{R}^3}\int_{\mathcal{E}}\frac{1}{3}m|c|^2 f\,dvd\omega + \theta\rho k_B T \tag{13}$$

where $\theta = \frac{\lambda_2}{\lambda}$. Using (13) and setting

$$\frac{\lambda_1}{\lambda} = 1-\nu(1-\theta), \tag{14}$$

with ν generic parameter, it is easily to turn (11) into

$$\int_{\mathbb{R}^3}\int_{\mathcal{E}} mc\otimes cg\,dvd\omega = (1-\theta)\rho\big((1-\nu)k_B T_{tr} I_d + \nu\Theta\big) + \theta\rho k_B T\, I_d = \rho\mathcal{T}, \tag{15}$$

where $\mathcal{T}$ is a tensor that can be regarded as linear combination of the stress tensor Θ and of the isotropic stress tensors $k_B T_{tr} I_d$ and $k_B T I_d$.

3.2 Minimization problem

This section is devoted to the resolution of the minimization problem (9). As we consider a general mesure for the internal energy variable, the entropy minimization problem cannot be solved like in ([16])

Theorem 3.1. *For symmetric positive definite tensor* Θ, $-\frac{1}{2}\le\nu<1$ *and* $0<\theta<1$ *we have*

(i) the tensor $\mathcal{T}$ *defined in* (15) *is symmetric positive definite and the set* K_f *is not empty;*

(ii) the unique solution of the minimization problem (9) *is the Gaussian function*

$$\mathcal{G}(v,\bar\epsilon) = \frac{\rho}{m\sqrt{det(2\pi\mathcal{T})}}\exp\Big(-\frac{1}{2}\big\langle (v-u)\mathcal{T}^{-1},(v-u)\big\rangle - \frac{\bar\epsilon(\zeta)}{k_B T_{rel}}\Big) Z\left(\frac{1}{k_B T_{rel}}\right)^{-1} \tag{16}$$

where $T_{rel} = \theta T + (1-\theta)T_{int}$.

Proof. (i) We prove the definite positivity of the matrix $\mathcal{A} = \rho\big((1-\nu)k_B T_{tr} I_d + \nu\Theta\big)$ In fact this implies that the matrix $\mathcal{T}$ is positive definite as a convex combination of positive definite matrices since $0\le\theta<1$. If we consider a basis of eigenvectors of Θ, the tensor $\mathcal{A}$ is diagonal

$$\mathcal{A}_i = \frac{1-\nu}{3}(\theta_1+\theta_2+\theta_3) + \nu\theta_i, \quad i = 1, 2\,\text{or}\,3.$$

Since $-\frac{1}{2}\le\nu<1$ the matrix $\mathcal{A}$ is positive definite. The definite positivity of the matrix $\mathcal{T}$ guarantees that the set K_f is not empty (see for more details [16]).

(ii) Here we proceed as in [2]. Since the functional $\mathcal{H}$ is strictly convex, we can infer that for all $g \geq 0$, with $g \neq \mathcal{G}$, with $\mathcal{G}$, given by 16, the following relation holds

$$\mathcal{H}(g) > \mathcal{H}(\mathcal{G}) + \mathcal{H}'(\mathcal{G})(g - \mathcal{G}).$$

Invoking the Lagrange multiplier

$$\alpha = \left(\ln \frac{\rho}{m\sqrt{det(2\pi k_B \mathcal{T})}} Z^{-1}\left(\frac{1}{k_B T_{rel}}\right) - \frac{1}{2} u\mathcal{T}^{-1}u, \mathcal{T}^{-1}u, -\frac{1}{2}\mathcal{T}^{-1}, -\frac{1}{k_B T_{rel}} \right),$$

we can express

$$\mathcal{H}'(\mathcal{G}) = \ln \mathcal{G} = \alpha.m(v), \tag{17}$$

where

$$m(v) = (1, v, v \otimes v, \bar{\epsilon}(\zeta))^T.$$

So, we deduce from (17) and from the fact that $g \in K_f$, with $g \neq \mathcal{G}$, that

$$\int_{\mathbb{R}^3} \int_{\mathcal{E}} \mathcal{H}(\mathcal{G}) dv d\omega < \int_{\mathbb{R}^3} \int_{\mathcal{E}} \mathcal{H}(g) dv d\omega.$$

□

3.3 H Theorem

Now we prove that the ES-BGK model satisfies the H theorem.

Theorem 3.2. *Let $\mathcal{G}^{\nu,\theta}$ the Gaussian function, provided by* (16), $\forall \nu \in [-\frac{1}{2}, 1]$ *and* $\theta \in [0,1]$. *Hence, the entropy dissipation satisfies*

$$\mathcal{D}(f) = \int_{\mathbb{R}^3} \int_{\mathcal{E}} (\mathcal{G}^{\nu,\theta} - f) \ln f dv\, d\omega \leq 0,$$
$$\mathcal{D}(f) = 0 \quad \textit{iff} \quad f = \mathcal{M}_f$$

$\forall \nu \in \left[-\frac{1}{2}, 1\right)$ *and* $\theta \in (0,1)$, *where*

$$\mathcal{M}_f = \frac{\rho}{m} \exp\left(-\frac{m(v-u)^2}{2k_B T} - \frac{\bar{\epsilon}(\zeta)}{k_B T} \right) \left(\frac{2\pi k_B T}{m} \right)^{-\frac{3}{2}} Z\left(\frac{1}{k_B T}\right)^{-1} \tag{18}$$

is the Maxwellian corresponding to the equilibrium states of the collision operator [10].

Proof. We follow the proof developed by Andries et al [2]. Thanks to the convexity of the entropy function, we can derive the inequality

$$\int_{\mathbb{R}^3} \int_{\mathcal{E}} (\mathcal{G}^{\nu,\theta} - f) \ln f dv d\omega \leq \int_{\mathbb{R}^3} \int_{\mathcal{E}} \mathcal{G}^{\nu,\theta} \ln \mathcal{G}^{\nu,\theta} dv\, d\omega - \int_{\mathbb{R}^3} \int_{\mathcal{E}} f \ln f dv d\omega.$$

The problem of minimizing of the entropy functional in the case $\nu = 1$ and $\theta = 0$ provides

$$\int_{\mathbb{R}^3} \int_{\mathcal{E}} \mathcal{G}^{1,0} \ln \mathcal{G}^{1,0} dv d\omega \leq \int_{\mathbb{R}^3} \int_{\mathcal{E}} \mathcal{H}(f) dv d\omega,$$

because the functions that belong to the set K_f when $\nu = 1$ and $\theta = 0$ satisfy the same constrains of the function f. So, we have that

$$\int_{\mathbb{R}^3}\int_{\mathcal{E}}(\mathcal{G}^{\nu,\theta} - f)\ln f dv d\omega \leq \int_{\mathbb{R}^3}\int_{\mathcal{E}}\mathcal{G}^{\nu,\theta}\ln\mathcal{G}^{\nu,\theta} dv d\omega - \int_{\mathbb{R}^3}\int_{\mathcal{E}}\mathcal{G}^{1,0}\ln\mathcal{G}^{1,0} dv d\omega.$$

It is derived from computations that

$$\int_{\mathbb{R}^3}\int_{\mathcal{E}}\mathcal{G}^{\nu,\theta}\ln\mathcal{G}^{\nu,\theta} dv d\omega = \ln\left[\frac{\rho}{m\sqrt{det(2\pi k_B\mathcal{T})}}Z^{-1}\left(\frac{1}{k_B T_{rel}}\right)\right] - \frac{\rho}{2}(1+\delta(T)).$$

So, we recover

$$\int_{\mathbb{R}^3}\int_{\mathcal{E}}(\mathcal{G}^{\nu,\theta} - f)\ln f dv d\omega \leq \rho\ln\sqrt{\frac{det\Theta}{det\mathcal{T}}}\frac{Z^{-1}\left(\frac{1}{k_B T_{rel}}\right)}{Z^{-1}\left(\frac{1}{k_B T_{int}}\right)}. \tag{19}$$

Using analitical arguments on general convex combinations of matrix, as in [2], it is proved that $det\mathcal{T} \geq det\Theta$ and hence the entropy dissipation is non positive. Finally, when $\mathcal{D}(f) = 0$, it has

$$f = \mathcal{G}^{\nu,\theta} = \mathcal{G}^{1,0},$$

from which we derive

$$det\mathcal{T} = det\Theta = \left(\frac{k_B}{m}T\right)^3.$$

This directly proves that $f = \mathcal{M}_f$. □

3.4 Definition of λ_1, λ_2 and λ

This section is devoted to the derivation of the hydrodynamic limit of the equation

$$\partial_t f(t,x,v,\zeta) + v\cdot\nabla_x f(t,x,v,\zeta) = \frac{\lambda}{\tau}(\mathcal{G} - f), \tag{20}$$

where τ is the Knudsen number. The aim is to determine the relaxation coefficients λ_1, λ_2 and λ in order to obtain the right transport coefficients.

In the Chapman-Enskog expansion we let $\tau \to 0$ and we expand f and G w.r.t τ around the Maxwellian function defined in (18).

So, we obtain

$$f = \mathcal{M}_f + \tau f^{(1)} + \mathcal{O}(\tau^2),$$
$$\mathcal{G} = \mathcal{M}_f + \tau G^{(1)} + \mathcal{O}(\tau^2).$$

Since f and $\mathcal{G}$ have the same moments the orthogonality relation holds

$$\int_{\mathbb{R}^3}\int_{\mathcal{E}}\left(m, mv, \frac{1}{2}mv^2 + \bar{\epsilon}(\zeta)\right)f^{(1)}\, dv d\omega = \int_{\mathbb{R}^3}\int_{\mathcal{E}}\left(m, mv, \frac{1}{2}mv^2 + \bar{\epsilon}(\zeta)\right)G^{(1)}\, dv d\omega = 0. \tag{21}$$

By considering the scaled Boltzmann equation (20) at order 0 we get

$$\left(\frac{\partial}{\partial t} + v \cdot \nabla\right) \mathcal{M}_f = \lambda(G^{(1)} - f^1).$$

If we multiply the previous equation with the collision invariants and integrate it over v and ϵ, we derive as in [10] the compressible Euler system, that we can recast in the following form,

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -\rho \nabla \cdot u - \nabla \rho \cdot u, && (22) \\ \frac{\partial u}{\partial t} &= -u \cdot \nabla u - \frac{k_B}{\rho m} \nabla \rho T - \frac{k_B}{m} \nabla T, && (23) \\ \frac{\partial T}{\partial t} &= -\nabla T \cdot u - \frac{T \nabla \cdot u}{c_V(T)}. && (24) \end{aligned}$$

Next, by using (22, 23, 24) in order to eliminate temporal derivatives, we get

$$\begin{aligned} \frac{(\partial_t + v \cdot \nabla_x)\mathcal{M}_f}{\mathcal{M}_f} &= \frac{m}{k_B}\left(V \otimes V - \frac{1}{3}V^2 Id\right) : \nabla u \\ &+ \left(\frac{1}{3}\frac{m}{k_B}V^2 - 1 - \frac{mV^2}{2k_B c_V(T)} - \frac{\bar{\epsilon}}{k_B T c_V(T)} + \frac{3}{2c_V(T)} + \frac{\delta(T)}{2c_V(T)}\right) \nabla \cdot u \\ &+ \left(-\frac{5}{2} - \frac{\delta(T)}{2} + \frac{mV^2}{2k_B} + \frac{\bar{\epsilon}}{k_B T}\right) V \cdot \frac{\nabla T}{\sqrt{T}} \end{aligned} \qquad (25)$$

where we adopted the substitution $V = \frac{v-u}{\sqrt{T}}$. We point out the particularities of the previous formula. The term involving the divergence of velocity, $\nabla \cdot u$ characterizes non polytropic gases by the presence of $c_V(T)$ that depends non linearly on temperature, while the last term involving the gradient of temperature ∇T has a form that depends on the monatomic or polyatomic nature of gas. We proceed to determine the dissipative terms in the system of Navier Stokes equations by considering Chapman expansion at first order. We write down the compressible Navier Stokes equations, neglecting terms of order ϵ^2 in (20), then we multiply it by the collision invariants and integrate it on v and ϵ. So we obtain the following form,

$$\begin{aligned} &\partial_t \int_{\mathbb{R}^3} \int_{\mathcal{E}} m\mathcal{M}_f \, dv d\omega + \nabla \cdot \int_{\mathbb{R}^3} \int_{\mathcal{E}} mv\mathcal{M}_f \, dv d\omega = 0 \\ &\partial_t \int_{\mathbb{R}^3} \int_{\mathcal{E}} mv\mathcal{M}_f \, dv d\omega + \nabla \cdot \int_{\mathbb{R}^3} \int_{\mathcal{E}} mv \otimes v\mathcal{M}_f \, dv d\omega \\ &\qquad = -\tau \nabla \cdot \int_{\mathbb{R}^3} \int_{\mathcal{E}} mv \otimes v f^1 \, dv d\omega \\ &\partial_t \int_{\mathbb{R}^3} \int_{\mathcal{E}} \left(\frac{1}{2}mv^2 + \bar{\epsilon}(\zeta)\right) \mathcal{M}_f \, dv d\omega + \nabla \cdot \int_{\mathbb{R}^3} \int_{\mathcal{E}} \left(\frac{1}{2}mv^2 + \bar{\epsilon}(\zeta)\right) v\mathcal{M}_f \, dv d\omega \\ &\qquad = -\tau \nabla \cdot \int_{\mathbb{R}^3} \int_{\mathcal{E}} \left(\frac{1}{2}mv^2 + \bar{\epsilon}(\zeta)\right) v f^1 \, dv d\omega. \end{aligned}$$

After some intermediate computations, we are able to derive Navier Stokes equations,

$$\begin{aligned} \partial_t\rho + \nabla\cdot(\rho u) = 0 \\ \partial_t(\rho u) + \nabla\cdot(\rho u\otimes u) + \nabla P = \tau\nabla\cdot P\big[(\nabla u + \nabla u^T) - 2\Lambda(T)\nabla\cdot u\, I_d\big] \\ \partial_t\left(\frac{1}{2}\rho|u|^2 + \frac{\rho}{m}e\right) + \nabla\cdot\left(\frac{1}{2}\rho|u|^2u + \frac{\rho}{m}eu + Pu\right) = \\ \tau\nabla\cdot P\big[(\nabla u + \nabla u^T) - 2\Lambda(T)\nabla\cdot u\, I_d\big]\cdot u + \tau\nabla\cdot\frac{5+D(T)}{2}P\frac{k_B}{m}\nabla T \end{aligned}$$

with

$$P = \rho\frac{k_B}{m}T, \quad \Lambda(T) = \frac{1}{2c_V(T)}, \quad D(T) = \frac{d(T\delta(T))}{dT}.$$

We recognize stress tensor and heat flux

$$\Pi = P\big[(\nabla u + \nabla u^T) - 2\Lambda(T)\nabla\cdot u\, I_d\big] \tag{26}$$

$$q = -\frac{5+D(T)}{2}P\frac{k_B}{m}\nabla T, \tag{27}$$

that will be used in the identification of transport coefficients λ_1, λ_2 and λ, taking into account their generic formulations

$$\Pi = \mu(\nabla u + \nabla u^T) - \alpha\mu\nabla\cdot u\, I_d, \tag{28}$$

$$q = -\kappa\nabla T, \tag{29}$$

where μ is the first viscosity, $\mu\alpha$ the second viscosity and κ the heat conductivity. We firstly compute

$$\int_{\mathbb{R}^3}\int_{\mathcal{E}} v\otimes v(\partial_t + v\partial_x)\mathcal{M}_f\, dvd\omega = \Pi \tag{30}$$

in order to compare it with the conditions (11)-(12) to find the transport coefficients λ_1 and λ_2.

So, Chapman-Enskog expansion of (12) at first order, together with (21), provides

$$\int_{\mathbb{R}^3}\int_{\mathcal{E}}|c|^2 f^{(1)}dvd\omega = -\frac{1}{\lambda_2}\int_{\mathbb{R}^3}\int_{\mathcal{E}} v\otimes v(\partial_t + v\partial_x)\mathcal{M}_f dvd\omega \tag{31}$$

and comparison with (30) gives

$$\int_{\mathbb{R}^3}\int_{\mathcal{E}}|c|^2 f^{(1)}dvd\omega = \frac{P}{\lambda_2}\Lambda(T)\nabla\cdot u.$$

Finally, from comparison with the trace of the stress tensor (28), we find

$$\lambda_2(T) = \frac{2P\Lambda(T)}{(2-3\alpha)\mu}.$$

Similarly the Chapman-Enskog expansion of the relation (11) at first order, taking into account (30), provides

$$\int_{\mathbb{R}^3}\int_{\mathcal{E}} c\otimes c f^{(1)}dvd\omega = \frac{P}{\lambda_1}(\nabla u + \nabla u^T)$$

and comparing this relation with the part without trace of the stress tensor (28), one has

$$\lambda_1 = \frac{P}{\mu}. \tag{32}$$

Since the polynomials in (25) are orthogonal to $\mathcal{P}$, we get

$$\int_{\mathbb{R}^3}\int_{\mathcal{E}}\Big(-\frac{5}{2}-\frac{\delta(T)}{2}+\frac{mV^2}{2k_B}+\frac{\bar{\epsilon}}{k_BT}\Big)V(G^{(1)}-f^{(1)})dVd\omega = \frac{1}{\lambda}[\Pi\cdot u - q]$$

and from comparison with (29), we find the last coefficient

$$\lambda(T) = \frac{(5+D(T))Pk_B}{2m\kappa}.$$

We are now able to define the relaxation type term of the Ellipsoidal Statistical BGK model

$$R(f) = \lambda(\mathcal{G}-f),$$

in which $\mathcal{G}$ is the Gaussian function, derived by Theorem 3.1 and λ, using relation (14) and (32), is given by

$$\lambda = \frac{P}{\mu(1-\nu+\theta\nu)}.$$

Finally, we provide the expression of Prandtl number

$$Pr = \frac{\lambda}{\lambda_1} = \frac{5+D(T)}{2}\frac{k_B\mu}{m\kappa}. \tag{33}$$

4 Comparison with other models

In this section we show how we can recover some existing models from the present formalism. More precisely, by assigning parameters to space $(\mathcal{E}, \mathcal{A}, \omega)$ and energy ϵ, the model allows to study various cases, such as monatomic gas, polyatomic gas with discrete energy and polyatomic gas with continuous energy.

4.1 Monatomic case

The behavior of monatomic gases is described by a distribution function $f(t, x, v)$ that depends only on time, space and velocity of the gas. Therefore we set $\mathcal{E} = \{0\}, \mathcal{A} = \mathcal{P}(\mathcal{E})$ and $\omega(\{0\}) = 1$ and we recover the following expression for the Gaussian function that solves the minimization problem (9),

$$\mathcal{G}[\rho, u, \mathcal{T}](v) = \frac{\rho}{m\sqrt{det(2\pi\mathcal{T})}}\exp\Big(-\frac{1}{2}\big\langle(v-u)\mathcal{T}^{-1}, (v-u)\big\rangle\Big).$$

We notice that the Gaussian for the monatomic gases we have determined coincides with that obtained by Andries et al. in [2]. In the case of monatomic gases only elastic collision occur, so the conservation law of momentum and the conservation law of energy hold. We observe that the number of internal degrees of freedom $\delta = 0$, according to the fact that a monatomic gas can only translate in the three directions of space and we determine the heat capacity at constant volume $c_V = \frac{3}{2}$. Moreover if we set $\theta = 0$ and $\nu = -\frac{1}{2}$, we recover the correct value of Prandtl number for monatomic gas, $Pr = \frac{2}{3}$.

4.2 Polyatomic case with continuous internal energy

In a polyatomic gas the macroscopic internal energy is given by two contributions: the translational energy due to the fact that the molecule translates in the three directions of space and the energy associated with other degrees of freedom, which are rotation and vibration. Monatomic gases have only internal energy translation, which is linked to the trace of stress tensor. In the case of polyatomic gases, it is only the translational component of internal energy that is related to the stress tensor trace. To take into account the additional degrees of freedom of a polyatomic gas, expressed by $\delta(T)$, the state of a polyatomic gas at the microscopic level is defined not only by its velocity but also by a function, the microscopic internal energy I, that can be continuous or discrete. In the model of polyatomic gases with continuous internal energy, it is necessary to introduce a weight function $\psi(I)$ built ad hoc, in order to obtain the caloric law of energy at the equilibrium,

$$e = c_V \frac{k_B}{m} T, \tag{34}$$

where e and T are the internal energy density and the temperature. So the space in which the distribution function $f(t, x, v, I)$ is defined is of the type $L^1(\psi(I) d\omega dv)$. We determine the caloric law of energy for polyatomic gas as it is developed in [28]. First of all, by computing the internal macroscopic energy at the kinetic level, we obtain

$$\rho e = \frac{3}{2} n k_B T - n \frac{Z'(\frac{1}{k_B T})}{Z\left(\frac{1}{k_B T}\right)} \tag{35}$$

where

$$Z\left(\frac{1}{k_B T}\right) = \int_{\mathbb{R}_+} e^{-\frac{1}{k_B T} I} \psi(I) dI \tag{36}$$

is determined from the partition function (1) by setting $\mathcal{E} = \mathbb{R}_+, \epsilon = I$ and $d\mu = \psi(I) dI$. We observe also that the term

$$\frac{Z'(\frac{1}{k_B T})}{Z(\frac{1}{k_B T})} = \delta(T) k_B \frac{T}{2} \tag{37}$$

is related to the internal degrees of freedom according to (3). It is easy to recover the following formula if we define the notation $\tau = \frac{1}{k_B T}$,

$$\frac{Z'\left(\frac{1}{k_B T}\right)}{Z\left(\frac{1}{k_B T}\right)} = -\frac{\frac{dZ(\tau)}{d\tau}}{Z(\tau)} = -\frac{d}{d\tau} \log Z(\tau).$$

Since we aim that the two equations (34) and (35) are equivalent, we deduce that

$$-\frac{d}{d\tau} \log Z(\tau) = \lambda \frac{1}{\tau}$$

with λ a generic constant. The previous relation is a ODE that yields the solution $Z(\tau) = \tau^{-\lambda}$. Observing from (36) that $Z(\tau)$ is the Laplace transform of $\psi(I)$, we can conclude that

$$\psi(I) = \mathcal{L}^{-1}(\tau^{-\lambda}) = \frac{I^{\lambda-1}}{\Gamma(\lambda)}$$

with $\Gamma(\lambda)$ the Gamma function. We here refer to the simpler formula, defined by Desvillettes and al. in [20],

$$\psi(I) = I^{\alpha} \tag{38}$$

with $\alpha > -1$.

Following Prop. 6.1 in the work [10] with the formula of the weight function (38) we compute that the number of internal degrees of freedom δ is constant and yields

$$\delta = 2(\alpha + 1) \tag{39}$$

and accordingly

$$c_V = \frac{5}{2} + \alpha.$$

So the caloric equation for internal energy (35) together with (39) and (37) assumes the formula (34) as we wanted. We recover in that case the situation of a polytropic gas. Summing up, for a polyatomic gas with continuous internal energy we set $\mathcal{E} = \mathbb{R}_+$, $\mathcal{A}$ the set of the Borelians of $\mathbb{R}_+$, $d\mu(I) = \psi(I)dI$, where $\psi(I) = I^{\alpha}$ with $\alpha > -1$ and $\epsilon(I) = I$. We obtain that the Gaussian (16) takes the form

$$\mathcal{G}[\rho, u, T, \mathcal{T}](v, I) = \frac{\rho}{m\sqrt{det(2\pi\mathcal{T})}} \exp\left(-\frac{1}{2}\langle (v-u)\mathcal{T}^{-1}, (v-u)\rangle - \frac{I}{K_B T}\right) Z\left(\frac{1}{k_B T}\right)^{-1}.$$

In this case we recover the Ellipsoidal Statistical Model that has been developed in [2, 16]. This model recovers values of Prandtl number less than 1. In fact if we consider a diatomic gas, the formula of the Prandtl number (33) returns the experimental value of $\frac{5}{7}$ setting $\theta = \frac{1}{5}$ and $\nu = -\frac{1}{2}$.

4.3 Polyatomic case with discrete internal energy

Groppi and Spiga in [22] provided a model for a polyatomic gas with discrete internal energy in order to focus on the vibrational motions of molecules. The internal energy varies in a set of discrete values $\epsilon_0, \epsilon_1, \ldots, \epsilon_N$, with $N \in \mathbb{N}$. So the microscopic state of a molecule is described by $(v, n) \in \mathbb{R}^3 \times [0, N]$ and to each internal state n a value of microscopic internal energy $\epsilon_n \in \mathbb{R}^3$ is associated.

Setting $\mathcal{E} = \{0, 1, \ldots, N\}$, $\mathcal{A} = \mathcal{P}(\mathcal{E})$ and $\epsilon(n) = \epsilon_n$ for $n = 0, \ldots, N$, we obtain that the partition function Z defined in (1) takes the form (2). The number of internal degrees of freedom writes from (3) as

$$\delta(T) = \frac{2}{k_B T} \frac{\sum_{n=0}^{N} (\epsilon_n - \epsilon^0) \exp\left(-\frac{(\epsilon_n - \epsilon^0)}{k_B T}\right)}{\sum_{n=0}^{N} \exp\left(-\frac{(\epsilon_n - \epsilon^0)}{k_B T}\right)}$$

while the heat capacity at constant volume from (27) is

$$c_V = \frac{3}{2} - \frac{\delta(T)^2}{4} + \frac{2}{k_B^2 T^2} \frac{\sum_{n=0}^{N} (\epsilon_n - \epsilon^0)^2 \exp\left(-\frac{(\epsilon_n - \epsilon^0)}{k_B T}\right)}{\left[\sum_{n=0}^{N} \exp\left(-\frac{(\epsilon_n - \epsilon^0)}{k_B T}\right)\right]^2}.$$

4.4 Polyatomic case with discrete and continuous parts of internal energy

Let us consider a model in which the microscopic internal energy takes into account both contributions: the rotational part represented by a continuous variable and the vibrational part expressed by a discrete variable. We assume that the measure space is

$$(\mathcal{E}, \mathcal{A}, d\omega) = (\mathbb{R}_+ \times [0, N], Bor(\mathbb{R}_+) \otimes \mathcal{P}([0, N]), \psi(I)dI \times 1),$$

where 1 represents the counting measure. So the Gaussian function (16) takes the form

$$\mathcal{G}[\rho, u, T, \mathcal{T}](v, I, i) = \frac{\rho}{m\sqrt{det(2\pi\mathcal{T})}} \exp\left(-\frac{1}{2}\langle(v-u)\mathcal{T}^{-1}, (v-u)\rangle - \frac{\epsilon_i - \epsilon^0}{k_B T} - \frac{I}{k_B T}\right)$$

$$Z_c\left(\frac{1}{k_B T}\right)^{-1} Z_d\left(\frac{1}{k_B T}\right)^{-1}$$

where

$$Z_c\left(\frac{1}{k_B T}\right) = \int_{\mathbb{R}^+} e^{-\frac{I}{k_B T}} I^\alpha dI, \qquad Z_d\left(\frac{1}{k_B T}\right) = \sum_{n=0}^{N} e^{-\frac{\epsilon_n - \epsilon^0}{k_B T}}.$$

Regarding the number of degrees of freedom and the heat capacity, there are two contributions due to the two rotational and vibrational effects, as follows

$$\delta(T) = \delta_c(T) + \delta_d(T) = 2(\alpha+1) + \frac{2}{k_B T} \frac{\sum_{n=0}^{N}(\epsilon_n - \epsilon^0)\exp\left(-\frac{(\epsilon_n - \epsilon^0)}{k_B T}\right)}{\sum_{n=0}^{N}\exp\left(-\frac{(\epsilon_n - \epsilon^0)}{k_B T}\right)},$$

$$c_V = c_V^c + c_V^d = \frac{5}{2} + \alpha + \frac{3}{2} - \frac{\delta_d(T)^2}{4} + \frac{2}{k_B^2 T^2} \frac{\sum_{n=0}^{N}(\epsilon_n - \epsilon^0)^2\exp\left(-\frac{(\epsilon_n - \epsilon^0)}{k_B T}\right)}{\left[\sum_{n=0}^{N}\exp\left(-\frac{(\epsilon_n - \epsilon^0)}{k_B T}\right)\right]^2}.$$

In that case, δ_c does not depend on temperature. The advantage of this model is that it allows to investigate separately the rotational internal energy and on the vibrational internal energy.

5 Conclusion and perspectives

We have constructed an Ellipsoidal Statistical Model for mono and polyatomic gases, in which each molecule is characterized by an internal state ζ that varies in a generic measure space ($\mathcal{E}$, $\mathcal{A}$, ω) and the non translational degrees of freedom are outlined by an energy function that depends on the internal state variable $\epsilon(\zeta)$. We proved the minimization problem of the entropy functional under moment constraints and we recovered the Maxwellian equilibria. The model is consistent with conservation laws and it verifies H Theorem. We determined the coefficients of transport (first viscosity, second viscosity and thermal conductivity) and we derived the analytical expression of the Prandtl number that provides consistent values for mono and polyatomic gases. We have also studied the number of internal degrees of freedom and derived the fluid-dynamic Navier-Stokes equations. The peculiarity of this model is that recovers usual models, i.e. the monatomic gas, the continuous internal description and the discrete one for polyatomic gas, fitting appropriately the measure space of internal states and the internal energy function.

The next step in the research is to construct a BGK-model for mixture of polyatomic gases within the framework of [10]. In particular, a generalization of the papers ([13], [12]) in the non polytropic case based on the present framework is postponed to future papers.

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