Generalization of the Grad Theory to Polyatomic Gases

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Abstract: We generalize the Grad theory to polyatomic gases with a continuous internal energy. To this end, we consider the generalized Borgnakke-Larsen model, and also a model derived of a monoatomic gas in dimension higher than three. We give an explicit fourteen moments system, computed for a diatomic gas and a Hard Sphere potential. Finally, we show how it can be reduced to standard Navier-Stokes equations.

Key-words: Grad's method, transition, Navier-Stokes, polyatomic gases.

(Résumé : tsvp)

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Généralisation de la théorie de Grad pour les Gaz polyatomiques.

Résumé :   Nous généralisons la méthode de Grad au cas des gaz polyatmiques avec énergie interne continue. Dans ce but nous utilisons le modèle de Borgnakke-Larsen et également un modèle récent, déduit d'un modèle monoatomique en dimension supérieure à trois. Nous proposons un modèle explicite aux quatorze moments, calculé pour un gaz diatomique et pour le potentiel des Sphères Dures. Finalement, nous montrons que ce système peut se réduire aux équations de Navier-Stokes.

Mots-clé :   Méthod de Grad, transition, Navier-Stokes, gaz polyatomiques.

1 Introduction

In many domain of physics, like fluid mechanics, semi-conductors or plasmas, the kinetic theory has lead to the interpretation of classical macroscopic models. For example, in fluid mechanics, Navier-Stokes equations may be derived from Boltzmann equation using the so-called Chapman-Enskog theory [3], [8], [4], valid for monoatomic dense gases with small gradients. In particular, the classical Stokes law; $\gamma = -(2/3)\mu$, appears to be valid, from the kinetic point of view, only for monoatomic gases. Furthermore, the Navier-Stokes laws and the Fourier law have a kinetic interpretation.

Different others theories have been developped to determine more general macroscopic systems of equations, valid for more general flows, especially for flows in transitional regime. We can mention here the Grad moments method [5]. More recently Levermore [6] has proposed a new theory yielding macroscopic systems of equations having good mathematical properties.

Thus, thanks to the kinetic theory we can interpret existing macroscopic systems of equations or derive new ones. The different methods we have just recalled before have been established for monoatomic gases. A natural extention consists in the interpretation or derivation of macroscopic systems of equations for more complex gases including internal energies.

We can find a first answer in the book of Chapman-Cowling [4]. The collision process is described in the context of Hamilton mechanics, which allowed to include internal energies with continuous spectrum to describe the gas. The macroscopic properties, like stress tensor and heat flux, are derived following the Chapman-Enskog arguments for a monoatomic gas. A similar approach is considered in the book of Brun [3] for internal energies with discrete spectrum. Different situations are studied depending on the relaxation time of each mode. An asymptotic expansion of the distribution function is written according to the smallest Knudsen number following Chapman-Enskog, but the solution is restricted to the zero order case. In these approaches, the kinetic modelization introduces a new variable for each internal mode, increasing difficulty at least at the microscopic level. Generally speaking, the method consists in generalizing the technique used for a monoatomic gas directly to a polyatomic gas.

In this paper, we propose a new method. The main idea follows from the introduction of a new Boltzmann polyatomic model described in Bourgat and al. [2]. This model needs only one additional variable to describe a large class of gases with continuous internal energy. Futhermore, it may be deduced from a monoatomic model written with microscopic velocities in dimension $3 + \delta$, where δ is the number of internal degrees of freedom. Then we may apply, for example, the Grad method to the monoatomic model in higher dimension and, with some appropriate assumptions on the flow, recover a consistent system of macroscopic equations for a polyatomic gas.

In section 1, we present two polyatomic models, the one mentioned above, deduced from a monoatomic model in higher dimension, and the second one which is a original mathematical formulation of the so-called Borgnakke-Larsen model. The generalization of Grad theory is detailed in section 2, yielding an explicit system of moments to describe a diatomic gas.

The corresponding calculations are developped in annex. In the following section, as an application, we derive the resulting Navier-Stokes equations for a diatomic gas. We will end this paper by some remarks.

2   Kinetic modelisation of a polyatomic gas

For a monoatomic gas, a particle is characterized by its position x and its velocity ξ at a time t. In order to describe a polyatomic gas we have to take into account the internal energy of each gas particle. To this end, supposing that each internal degree of freedom has a continuous spectrum, we introduce the variable I. This variable is nonnegative and is related to the internal energy e_{int} according to the relation $I^2 = e_{int}$. The state of the gas will be described by the distribution function $f = f(x, \xi, I, t)$. Moreover, the state equation, induced at equilibrium, is $p = (\gamma - 1) \rho \, e_{int}$, where the constant γ lies in $(1, 5/3]$, depending on the nature of the gas. The constant γ is related to the number of internal degrees of freedom by the equation

$$\gamma = \frac{\delta + 5}{\delta + 3}.$$

In this general case, the Boltzmann equation is written as follows

$$(1) \qquad \frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial x} = Q_\delta(f),$$

where Q_δ is the collision operator, quadratic with respect to f.

  We describe now two different collision modelizations, and the corresponding collision operators. The results we give here are due to J.-F. Bourgat, L. Desvillettes, P. Le Tallec and B. Perthame. For more details we refer to their paper [2].

2.1   Borgnakke-Larsen model

The model was first introduced by Borgnakke-Larsen [1] from a phenomenologycal point of view. The mathematical formulation given in [2] leads to a rigorous proof of the collision microreversibility and a H-theorem.

  To describe the collision we consider two identical molecules with velocity and internal energy (ξ, I), (ξ_*, I_*), before a collision and (ξ', I'), (ξ'_*, I'_*), after a collision. Moreover we denote by

$$(2) \qquad v_r = \xi - \xi_*, \qquad e^2 = \frac{|\xi - \xi_*|^2}{4} + I^2 + I_*^2,$$

respectively the relative velocity and the total energy of a system of two particles. After collision the total energy is conserved, and is redistributed between kinetic and internal energy.

More precisely, the post collision prime properties are deduced from the following system

$$(3) \qquad \begin{cases} \xi' + \xi'_* = \xi + \xi_*, \\[2mm] v'_r = \dfrac{2eR}{|v_r|}\,(v_r - 2v_r.\omega\,\omega), \\[2mm] I'^2 = r\,(1 - R^2)\,e^2, \qquad I'^2_* = (1 - r)(1 - R^2)\,e^2. \end{cases}$$

The parameter R, which belong to $[0, 1]$, is the fraction of total energy which becomes kinetic energy after collision and r, which belong to $[0, 1]$, is the redistribution parameter of internal energy between the colliding molecules. Finally the vector ω is a geometrical parameter belonging to the unit sphere, characterizing the collision angle in space.

According to this model, the collision operator is given by

$$(4) \qquad Q_\delta(f) = \int_\Delta \left(\frac{f' f'_*}{(I' I'_*)^{\delta-1}} - \frac{f f_*}{(I I_*)^{\delta-1}} \right) B (I I_*)^{\delta-1} d\xi_* dI_* \varphi_\delta(r) dr \psi_\delta(R) dR d\omega,$$

where the integration domain, measures and collision cross sections are given by

$$\Delta = \mathbb{R}^3 \times \mathbb{R}^+ \times [0, 1]^2 \times S^2,$$

$$\varphi_\delta(r) = [r(1 - r)]^{\delta/2 - 1}, \qquad \psi_\delta(R) = R^2(1 - R^2)^{\delta-1},$$

$$B = B(e, R|v_r|, R|v_r.\omega|, I^2 r(1 - R^2), I^2_*(1 - r)(1 - R^2), (1 - R^2)(I^2 + I^2_*)) > 0,$$

with the usual notation $f = f(\xi, I)$, $f_* = f(\xi_*, I_*)$, $f' = f(\xi', I')$ et $f'_* = f(\xi'_*, I'_*)$. All the arguments in the expression of B are collision invariants.

The Variable Hard Sphere model is obtained by setting

$$B = C|v_r|^{2\alpha}|v_r.\omega|R^{1+2\alpha},$$

and leads, by homogeneity arguments, to the following viscosity law

$$\mu = KT^{1/2 - \alpha},$$

where C and K are some constants. The Borgnakke-Larsen model satisfies the same properties as the monoatomic classical model. In particular, the following formula is verified

$$(5) \qquad \int_{\mathbb{R}^3 \times \mathbb{R}^+} Q_\delta(f)(\xi, I)\ \phi(\xi, I)\ d\xi\, dI\ =\ \frac{1}{2} \int f f_* [\phi] B d\xi_* d\xi dI_* dI \varphi_\delta(r) dr \psi_\delta(R) dR d\omega,$$

where ϕ is a function and $[\phi]$ is defined by $[\phi] = \phi + \phi_* - \phi' - \phi'_*$.

The so called H-theorem becomes for the Borgnakke-Larsen model

$$(6) \qquad \int_{\mathbb{R}^3 \times \mathbb{R}^+} Q_\delta(f)(log(f I^{1-\delta}) + 1) d\xi dI \leq 0.$$

Moreover, thanks to equation (6), $log(fI^{1-\delta})$ is a collision invariant at equilibrium, therefore a linear combination of the invariants $1, \xi, \xi^2/2 + I^2$. It follows that the equilibrium distribution function is characterized by the Maxwellian

$$(7) \qquad I^{1-\delta} f^{(0)} = \lambda_\delta \frac{\rho}{(R_g T)^{(3+\delta)/2}} e^{-(|\xi-u|^2+2I^2)/2R_g T},$$

where the parameters λ_δ and (ρ, u, T), $T > 0$, verify

$$(8) \qquad \int_{\mathbb{R}^3 \times \mathbb{R}^+} \begin{pmatrix} 1 \\ \xi_i \\ (\xi-u)_i \, (\xi-u)_j \end{pmatrix} f^{(0)} \, d\xi dI = \begin{pmatrix} \rho \\ \rho u_i \\ \rho R_g T \delta_{ij} \end{pmatrix}.$$

From a simple integration, we deduce that the total energy e_{tot} is

$$(9) \qquad \rho e_{tot} = \int_{\mathbb{R}^3 \times \mathbb{R}^+} \left(\frac{|\xi|^2}{2} + I^2 \right) f^{(0)} \, d\xi dI = \frac{\rho |u|^2}{2} + \frac{(\delta+3)}{2} \rho R_g T,$$

according to the principle of energy equipartition. For a diatomic gas, i.e. $\delta = 2$, the parameter λ_δ is

$$\lambda_2 = \frac{2}{(2\pi)^{3/2}}.$$

2.2   A model deduced of a monoatomic model in higher dimension

This model is closer to the Boltzmann equation although more complicated. It uses the collision parameters $\sigma = (a, b, \omega)$ in $[0, 2\pi]^2 \times S^2$. The prime variables are then defined by

$$(10) \qquad \begin{cases} \Lambda = \dfrac{1}{2} v_r.\omega \cos a + \sin a \, (I\alpha \cos b + I_* \alpha_* \sin b), \\ \xi' + \xi'_* = \xi + \xi_*, \end{cases}$$

$$(11) \qquad \begin{cases} v'_r = v_r - 4\Lambda \omega \cos a, \\ I'^2 = I^2 + 4\Lambda^2 \cos^2 b \, \sin^2 a - 4I\alpha\Lambda \cos b \, \sin a, \\ I_*'^2 = I_*^2 + 4\Lambda^2 \sin^2 b \, \sin^2 a - 4I_* \alpha_* \Lambda \sin b \, \sin a, \\ \alpha' = (\alpha I - 2\Lambda \cos b \, \sin a\,)/I', \\ \alpha'_* = (\alpha_* I_* - 2\Lambda \sin b \, \sin a\,)/I'_*. \end{cases}$$

The parameters α et α_*, belonging to $[0, 1]$, have a similar interpretation than the parameters r et R of the preceeding model.

The collision operator is given now by

$$(12) \qquad Q_\delta(f) = \int_\Delta \left(\frac{f' f'_*}{(I' I'_*)^{\delta-1}} - \frac{f f_*}{(I I_*)^{\delta-1}} \right) B d\xi_* (II_*)^2 dI_* d\alpha d\alpha_* d\sigma,$$

where
$$B = B(\xi + \xi_*, e, |\Lambda|, I_*^2(1 - \alpha_*^2), I^2(1 - \alpha^2), a, b, \omega) > 0,$$

$$\Delta = \mathbb{R}^3 \times \mathbb{R}^+ \times [-1, +1]^2 \times [0, 2\pi]^2 \times S^2.$$

We now recall how this model is deduced from a classical monoatomic model in dimension $3+\delta$, where δ is an interger. To this end we introduce the particle velocity variables $\underline{\xi} = (\xi, \zeta)$ in $\mathbb{R}^{3+\delta}$. In this space the collision process conserves the momentum and the total energy, ie the following equations

$$\begin{cases} \xi' + \xi_*' = \xi + \xi_*, \\ 2 \left| \dfrac{\xi' - \xi_*'}{2} \right|^2 + |\zeta'|^2 + |\zeta_*'|^2 = 2 \left| \dfrac{\xi - \xi_*}{2} \right|^2 + |\zeta|^2 + |\zeta_*|^2. \end{cases}$$

To give the complete description of the collision process we introduce the relative speed and the collision vectors

(13)
$$\begin{cases} \Xi = \left(\dfrac{\xi - \xi_*}{2}, \zeta, \zeta_* \right), \\ \Xi' = \left(\dfrac{\xi' - \xi_*'}{2}, \zeta', \zeta_*' \right), \\ \Omega = (\omega\,cosa, \eta\,sina\,cosb, \eta_*\,sina\,sinb) \quad \in S^{2+\delta}, \end{cases}$$

where η and η_* belong to the sphere $S^{\delta-1}$. The collision process is condensed into the relation
(14)
$$\Xi' = \Xi - 2\Xi.\Omega\ \Omega.$$

Then the Boltzmann equation, associated to the distribution function $g(x, \xi, \zeta, t)$ is written as
(15)
$$\frac{\partial g}{\partial t} + \xi \cdot \frac{\partial g}{\partial x} = \Gamma_\delta(g),$$

where the collision operator is

(16)
$$\Gamma_\delta(g) = \int_{\Delta'} (g'g_*' - gg_*)\, B_s d\xi_* d\zeta_* d\eta d\eta_* d\sigma,$$

under the notation

$$B_s = B_s(\xi + \xi_*, e, |\Lambda|, |\zeta|^2 - (\zeta.\eta)^2, |\zeta_*|^2 - (\zeta.\eta_*)^2, a, b, \omega),$$

$$\Delta' = \mathbb{R}^3 \times \mathbb{R}^\delta \times (S^{\delta-1})^2 \times [0, 2\pi]^2 \times S^2.$$

Now we define a distribution function f, integrating a solution g of equation (15), as follows

(17)
$$f(x, \xi, I, t) = \int_{S^{\delta-1}} 2^{\delta/2}\, I^{\delta-1}\, g(x, \xi, \sqrt{2}\, I\, \Theta, t)\, d\Theta,$$

under the notation

$$(18) \qquad \zeta = \sqrt{2}I\Theta, \quad \alpha = \frac{\zeta.\eta}{|\zeta|}, \quad \omega \in S^{\delta-1}, \quad \Lambda = \Xi.\Omega.$$

The new distribution f is solution of the Boltzmann polyatomic equation (1), with $Q_\delta(f)$ given by (12), and for a collision kernel B given by

$$(19) \qquad B = \mu_\delta(II_*)^{\delta-3}[(1 - \alpha_*^2)(1 - \alpha^2)]^{(\delta-3)/2}B_s,$$

with
$$(20) \qquad B_s = B_s(\xi + \xi_*, e, |\Lambda|, I^2(1 - \alpha^2), I_*^2(1 - \alpha_*^2)),$$

where μ_δ is a constant. The demonstration is based on some appropriate changes of variables.

Remark 2.1 *The distribution function f has the same thermodynamic properties as the Borgnakke-Larsen distribution function.*

3   Generalization of the Grad theory to a polyatomic gas

We propose below a system of macroscopic differential equations which generalizes the thirteen moments Grad system. To this end we follow the Grad theory, starting with the monoatomic equation in higher dimension (15). Then we write the distribution function g, solution of (15), as an expansion in Hermite polynomials. The coefficients of g's expansion are solutions of a first system of macroscopic differential equations. Introducing symmetry properties on the distribution g, and using the integration formula (17), we deduce an associated expansion of f and the corresponding macroscopic system of differential equations for a polyatomic gas. The right hand side of the last system is expressed as moments of the collision operator. We show that we can compute them independently of the choice of the polyatomic collision operator. Then we give an explicit formula computed for the Borgnakke-Larsen collision operator, and for a diatomic gas.

3.1   The generalized Grad expansion

Consider again the monoatomic kinetic model in dimension $(3 + \delta)$

$$(21) \qquad \frac{\partial g}{\partial t} + \underline{\xi} \cdot \frac{\partial g}{\partial \underline{x}} = \Gamma_\delta(g).$$

Here the space variable $\underline{x} = (x, y)$ and the microscopic velocities belong to $\mathbb{R}^{3+\delta}$.
    We suppose also that

- $\partial/\partial \underline{x}_4 = \partial/\partial \underline{x}_5 = ... = \partial/\partial \underline{x}_{3+\delta} = 0$,

- g is spherical by symmetric with respect to the variable ζ.

The first condition means that the transport process acts only in the physical space. Thus $x_4, ..., x_{3+\delta}$, appear as parameters of the function g. The second condition means that there is no privileged velocity direction with respect to the nonphysical velocity ζ, or equivalently that the distribution function g only depends on the norme $\sqrt{2}I$ of ζ.

In this space, the macroscopic properties (density, velocity, internal energy, stress tensor and heat flux vector) are defined by the following integrals

$$(22) \qquad\qquad \rho = \int g \, d\underline{\xi},$$

$$(23) \qquad\qquad \rho u_i = \int \underline{\xi}_i \, g \, d\underline{\xi},$$

$$(24) \qquad\qquad \rho e_{int} = \int \frac{|\underline{\xi} - u|^2}{2} \, g \, d\underline{\xi},$$

$$(25) \qquad\qquad \sigma_{ij} = - \int (\underline{\xi} - u)_i \, (\underline{\xi} - u)_j \, g \, d\underline{\xi},$$

$$(26) \qquad\qquad q_i = \int (\underline{\xi} - u)_i \frac{|\underline{\xi} - u|^2}{2} \, g \, d\underline{\xi},$$

where $i, j = 1, 2, 3, 4, \cdots, 3 + \delta$. It is just a simple generalization, to dimension $3 + \delta$, of the monoatomic definitions. In addition, the pressure is defined by

$$(27) \qquad\qquad p = \frac{-1}{(3 + \delta)} \sigma_{ii}.$$

From (24) et (25) we deduce
$$(28) \qquad\qquad p = \frac{2}{3 + \delta} \rho \, e_{int}.$$

Moreover we define the temperature by

$$(29) \qquad\qquad e_{int} = \frac{(3 + \delta)}{2} R_g T.$$

It follows from (28), (29) that the state law is

$$(30) \qquad\qquad p = \rho R_g T = (\gamma - 1) \rho e_{int}.$$

Finally we define the tensor p_{ij} by

$$(31) \qquad\qquad p_{ij} = -\sigma_{ij} - p \delta_{ij}.$$

Clearly the relation $p_{ii} = 0$ is true in the space of dimension $3 + \delta$. From now on we will use the Grad notation; $S_i = 2q_i$, $p_{ij} = -\tau_{ij}$.

Remark 3.1 *Considering a diatomic gas (i.e. $\delta = 2$), it follows from the spherical symmetry of g that*

$$
\begin{aligned}
u_4 &= u_5 = 0, \\
\sigma_{i4} &= \sigma_{44}\,\delta_{i4}, \qquad \sigma_{i5} = \sigma_{55}\,\delta_{i5}, \qquad \sigma_{44} = \sigma_{55}, \\
S_4 &= S_5 = 0.
\end{aligned}
$$

Following Grad method we introduce the reduced velocity vector $\underline{v} = (v, w) \in \mathrm{IR}^{3+\delta}$, defined by

$$
v_i \;=\; \frac{\xi_i - u_i}{\sqrt{R_g T}}, \quad \text{pour } i = 1, 2, 3, \qquad w_i \;=\; \frac{\zeta_i}{\sqrt{R_g T}}, \quad \text{pour } i = 4, 5 \ldots \delta.
$$

We also introduce the first Hermite polynomials with respect to the variable $\underline{v}$

$$
\begin{aligned}
H^{(0)} &= 1, \\
H_i^{(1)} &= \underline{v}_i, \\
H_{ij}^{(2)} &= \underline{v}_i\,\underline{v}_j \,-\, \delta_{ij}, \\
H_i^{(3)} &= \underline{v}_i\,(\,|\underline{v}|^2 \,-\, (5 + \delta)\,),
\end{aligned}
$$

where $i, j = 1, 2, 3, 4, \cdots, \delta$. These polynomials are orthogonal with respect to the scalar product

$$
(p, q) \;=\; \int_{\mathrm{IR}^{3+\delta}} p(\underline{v})\, q(\underline{v})\, exp\left(-\frac{|\underline{v}|^2}{2}\right)\, d\underline{v}.
$$

The moments of the distribution g, with respect to the Hermite polynomials, are denoted by $a_i^{(m)}$ and are defined by

$$
\tag{32}
a_i^{(m)} \;=\; \frac{(R_g T)^{\left(\frac{3+\delta}{2}\right)}}{\rho} \int g\, H_i^{(m)}(\underline{v})\, d\underline{v}.
$$

By construction, these moments are related to the physical properties by the relations

$$
\tag{33}
a_{ij}^{(2)} = \frac{p_{ij}}{p}, \qquad a_i^{(3)} = \frac{S_i}{p\sqrt{R_g T}},
$$

where $S_i = 2 q_i$, for $i, j = 1, 2, 3, 4, \cdots, \delta$. Moreover, by definition of ρ and u, we have the following relations

$$
\tag{34}
a^{(0)} \;=\; 1, \qquad a_i^{(1)} \;=\; 0.
$$

Then we expand g with respect to the first Hermite polynomials $H_i^{(m)}$, as follows

$$
\tag{35}
g \;=\; g^{(0)} \left(1 \,+\, \frac{1}{2} a_{ij}^{(2)}\, H_{ij}^{(2)} \,+\, \frac{1}{2(5+\delta)}\, a_i^{(3)}\, H_i^{(3)} \right),
$$

where $g^{(0)}$ is the equilibrium Mawellian

$$
\tag{36}
g^{(0)} = \frac{\rho}{(2\pi R_g T)^{\frac{3+\delta}{2}}}\; exp\left(-\left(\frac{|v|^2 + |w|^2}{2} \right) \right).
$$

Introducing the relations (33) in (35), g can also be writen

$$(37) \quad g = g^{(0)} \left(1 + \frac{p_{ij}}{2pR_gT}(\xi - u)_i(\xi - u)_j + \frac{1}{2(5+\delta)} \frac{S_i(\xi - u)_i}{pR_gT} \left(\frac{|\xi - u)|^2}{R_gT} - (5+\delta) \right) \right).$$

Thanks to the relation (17), relating the kinetic distribution f to g, we deduce, by integration, the distribution f for a polyatomic gas. Without loss of generality, the method being the same, we can restrict ourself to a diatomic gas $\delta = 2$, i.e. $\gamma = 1.4$. In this framework, introducing the variable

$$\tau = |w| = \sqrt{\frac{1}{R_gT}} |\zeta| = \sqrt{\frac{2}{R_gT}} I,$$

we can write

$$f(x, \xi, I, t) = \int_{S^1} \sqrt{2R_gT} \, \tau \, g(\underline{x}, v, \tau\Theta, t) \, d\Theta.$$

Replacing g by (35), and introducing polar coordonates, f becomes

$$(38) \quad f = f^{(0)} \left[1 + \frac{1}{2}a_{ij}^{(2)} H_{ij}^{(2)} + \frac{(a_{44}^{(2)} + a_{55}^{(2)})}{4}(\tau^2 - 2) + \frac{1}{14} a_i^{(3)} v_i (|v|^2 + \tau^2 - 7) \right],$$

for $i, j = 1, 2, 3$, with

$$f^{(0)} = \frac{\sqrt{2}\rho\tau}{(2\pi)^{\frac{3}{2}}(R_gT)^2} exp\left(-\left(\frac{|v|^2 + \tau^2}{2} \right) \right).$$

Defining

$$H_{00}^{(2)} = \frac{1}{2}(\tau^2 - 2),$$

$$H_i^{(3)} = v_i(|v|^2 + \tau^2 - 7), i = 1, 2, 3,$$

and knowing that

$$a_{ii} = 0,$$

for $i = 1, 2, 3, 4, 5$, the expression (38) can be written

$$= f^{(0)} \left[1 + \frac{1}{2}a_{ij}^{(2)} \left(H_{ij}^{(2)} - H_{00}^{(2)}\delta_{ij} \right) + \frac{1}{14} a_i^{(3)} H_i^{(3)} \right],$$

for $i, j = 1, 2, 3$.

Finally, using dimensional variables, the expression of f becomes

$$f = f^{(0)} \left[1 + \frac{p_{ij}}{2pR_gT} \left((\xi - u)_i(\xi - u)_j - I^2\delta_{ij} \right) + \frac{1}{14} \frac{S_i(\xi - u)_i}{pR_gT} \left(\frac{|\xi - u|^2}{R_gT} + \frac{2I^2}{R_gT} - 7 \right) \right],$$

(39)

for $i, j = 1, 2, 3$. This function f is, for a diatomic gas, an approximation of the kinetic distribution solution of (1).

Remark 3.2 *The approximate expansion of f, under the form (39) has been dericed from a monoatomic kinetic model written in dimension $(3 + \delta)$. We want to point out that it can be used in any Boltzmann equation involving internal energy, and the scalar product*

$$(40) \qquad (p, q) \; = \; \int_{\mathbb{R}^3 \times \mathbb{R}_+} p(\xi, I) \, q(\xi, I) \, exp \left(-\frac{|\xi|^2 + 2I^2}{2 R_g T} \right) \, d\xi \, I \, dI.$$

3.2   The generalized Grad system

In this section, we derive an approximate system of differential equations to be satisfied by the coefficients of g's expansion (35). To this end, we replace in the Boltzmann equation the kinetic distribution g by its truncated expansion (35). In order to obtain a conservative system we multiply this last equation by the polynomials

$$(1, \underline{\xi}_i, \underline{\xi}_i \underline{\xi}_j, \underline{\xi}_i |\underline{\xi}|^2/2) = \underline{K}, \qquad \text{pour } i, j = 1, 2, 3, 4, 5,$$

then we integrate over the microscopic velocity domain $\mathbb{R}^{3+\delta}$. We obtain the generalized Grad system

$$(41) \qquad \frac{\partial}{\partial t} \int \underline{K} \, g \, d\underline{\xi} + \frac{\partial}{\partial \underline{x}_k} \int \underline{K} \, \underline{\xi}_k \, g \, d\underline{\xi} \; = \; \int \underline{K} \, \Gamma_2(g) \, d\underline{\xi},$$

whose unknown are the coefficients of the expansion (35).

The polynomial components of the vector $\underline{K}$ can be written as a combination of the Hermite polynomials, in order to make a better use the orthogonality properties:

$$(42) \qquad 1 = H^{(0)},$$

$$(43) \qquad \underline{\xi}_i = \sqrt{R_g T} H_i^{(1)}(\underline{v}) + u_i,$$

$$(44) \qquad \underline{\xi}_i \underline{\xi}_j = R_g T H_{ij}^{(2)} + \sqrt{R_g T}(u_i H_j^{(1)} + u_j H_i^{(1)}) + R_g T \delta_{ij} + u_i u_j,$$

$$(45) \qquad \frac{\underline{\xi}_i |\underline{\xi}|^2}{2} = (R_g T)^{3/2} H_i^{(3)} + 2 R_g T u_k H_{ik}^{(2)} + u_i R_g T H_{kk}^{(2)}$$

$$+ (|u|^2 + 7 R_g T) \sqrt{R_g T} H_i^{(1)} + 2 u_i u_k \sqrt{R_g T} H_k^{(1)} + (5 R_g T + |u|^2) u_i + 2 R_g T u_k \delta_{ik},$$

for $i, j, k = 1, 2, 3, 4, 5$.

Replacing in (41) the components of $\underline{K}$ by the expressions computed above, and $\underline{\xi}_k \underline{K}$ by similar expressions, we obtain after some calculations, the following system, written with respect to the variables σ_{ij} and S_i,

$$(46) \qquad \frac{\partial U_G}{\partial t} + \frac{\partial F_k(U_G)}{\partial \underline{x}_k} \; = \; J(U_G), \qquad \text{in } \mathbb{R}^{26},$$

where

$$U_G \;=\; \begin{pmatrix} \rho \\ \rho u_i \\ \rho u_i u_j \;-\; \sigma_{ij} \\ S_i \;-\; 2u_l \sigma_{il} \;+\; 2\rho u_i e_{tot} \end{pmatrix}, \qquad i,j = 1,...,5,$$

$$F_k(U_G) \;=\; \begin{pmatrix} \bullet \rho u_k \\ \bullet \rho u_i u_k \;-\; \sigma_{ik} \\ \bullet \rho u_i u_j u_k - (u_i \sigma_{jk} + u_j \sigma_{ik} + u_k \sigma_{ij}) + \dfrac{1}{7}(\delta_{jk} S_i + \delta_{ki} S_j + \delta_{ij} S_k) \\ \bullet (S_i - 2\sigma_{il} u_l + 2\rho e_{tot} u_i) u_k - 2R_g T p \delta_{ik} - 2u_l u_i \sigma_{kl} \\ \qquad -(9R_g T + |u|^2)\sigma_{ik} + \dfrac{9}{7}u_i S_k + \dfrac{2}{7}(S_i u_k + S_l u_l \, \delta_{ki}) \end{pmatrix},$$

for $i, j = 1, ..., 5$,

$$J(U_G) \;=\; \int_{\mathbb{R}^5} \underline{K}\, \Gamma_2(g)\, d\underline{\xi}.$$

The system (46) results of a direct integration of (41) expanding K according to (42)-(45) and using the orthogonality properties of the Hermite polynomials. This calculation generalizes the one done for a monoatomic gas in dimension three [5].

Then we consider only equations of system (46) corresponding to the following moments

(47) $$K \;=\; (1, \underline{\xi}_i, \underline{\xi}_i \underline{\xi}_j, \underline{\xi}_4^2 + \underline{\xi}_5^2, \underline{\xi}_i |\underline{\xi}|^2), \quad \text{for } i, j = 1, 2, 3,$$

the others being eliminated by symmetry assumptions; and we simplify the resulting system using the fact that the following moments of g vanish

$$u_4 = u_5 = 0,$$

$$\sigma_{ij} = \sigma_{ji} = 0, \quad \text{for} \quad (i = 1, 2, 3 \quad \text{and} \quad j = 4, 5)$$
$$\text{and for} \quad (i = 4, 5 \quad \text{and} \quad j = 1, 2, 3),$$

$$S_i = 0, \quad \text{for} \quad i = 4, 5.$$

We point out that $\underline{\xi}_4^2 + \underline{\xi}_5^2$ can also be written

$$\underline{\xi}_4^2 + \underline{\xi}_5^2 \;=\; |\zeta|^2 \;=\; 2\, I^2.$$

Thanks to these assumptions, we obtain to the final 14 moments polyatomic Grad system

(48) $$\frac{\partial U_p}{\partial t} + \frac{\partial F_k(U_p)}{\partial x_k} \;=\; J(U_p), \qquad \text{in } \mathbb{R}^{14},$$

where

$$U_p \;=\; \begin{pmatrix} \rho \\ \rho u_i \\ \rho u_i u_j \;-\; \sigma_{ij} \\ 5p + \sigma_{ll} \\ S_i \;-\; 2u_l \sigma_{il} \;+\; 2\rho u_i e_{tot} \end{pmatrix}, \qquad i, j = 1, 2, 3,$$

$$F_k(U_p) = \begin{pmatrix} \bullet \rho u_k \\ \bullet \rho u_i u_k - \sigma_{ik} \\ \bullet \rho u_i u_j u_k - (u_i \sigma_{jk} + u_j \sigma_{ik} + u_k \sigma_{ij}) + \dfrac{1}{7}(\delta_{jk} S_i + \delta_{ki} S_j + \delta_{ij} S_k) \\ \bullet 5 p u_k + u_k \sigma_{ll} + \dfrac{2}{7} S_k \\ \bullet (S_i - 2\sigma_{il} u_l + 2\rho e_{tot} u_i) u_k - 2 R_g T p \delta_{ik} - 2 u_l u_i \sigma_{kl} - \\ (9RT + |u|^2)\sigma_{ik} + \dfrac{9}{7} u_i S_k + \dfrac{2}{7}(S_i u_k + S_l u_l\, \delta_{ki}) \end{pmatrix},$$

where $i, j = 1, 2, 3$.

Finally, knowing that the moments we calculate only depend on the norm of ζ, we can write

(49) $$J(U_p) = \int_{\mathbb{R}^5} \underline{K} \Gamma_2(g) d\xi d\zeta, = \int_{\mathbb{R}^3 \times \mathbb{R}_+} K\, Q_2(f) dI d\xi.$$

3.3   Extension to an arbitrary diatomic model

Formally, the system (48) can be written for an arbitrary model, not necessarily deduced from a Grad system in higher dimension. Looking apriori for a distribution function f given by (39), replacing in the Boltzmann equation in f over $\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^+ \times [0, T]$ and integrating against

$$K_{14} = \begin{pmatrix} 1 \\ \xi_i \\ \xi_i \xi_j \\ 2I^2 \\ \xi_i(|\xi|^2 + 2I^2) \end{pmatrix},$$

we get the same system (48)-(49)

(50) $$\frac{\partial}{\partial t} \int K_{14}\, f\, dI d\xi + \frac{\partial}{\partial x_k} \int K_{14}\, \xi_k\, f\, dI d\xi = \int K_{14}\, Q_2(f)\, dI d\xi.$$

Thanks to this remark, we have computed $J(U_p)$ for the Borgnakke-Larsen collision operator. For this computation we consider a diatomic gas and a Hard Sphere potential, see annex. The complete right hand side of the diatomic Grad system is then of the form

$$J = \begin{pmatrix} 0 \\ 0 \\ -(A_{kk} + 3B) \\ A_{ij} + B\,\delta_{ij} \\ -\dfrac{32\,\pi^{7/2}}{60480\, p^2 R_g T}(79\, S_i\, p_{kk} + 1520\, p\, S_i + 188\, S_k\, p_{ik}) \end{pmatrix},$$

where

$$A_{ij} = \frac{-32\pi^{7/2}}{47040\, \rho^2 (R_g T)^3}\left(784\, \rho\, (R_g T)^2\, p_{ij} + 28\, R_g T\, p_{ij}\, p_{kk} + 56\, R_g T\, p_{ik} p_{jk} + S_i S_j\right),$$

and

$$B = \frac{-32\pi^{7/2}}{47040\,\rho^2(R_g T)^3}\left(\frac{98}{9}\,\rho\,(R_g T)^2\,p_{kk} - \frac{70}{9}\,R_g T\,p_{lk}p_{lk} + \frac{175}{18}\,R_g T\,p_{kk}{}^2 - \frac{7}{36}\,S_k S_k\right).$$

Compared with the Grad thirteen moment system [5], for a monoatomic gas, the formulas differ because of a non zero trace p_{kk} of the tensor p_{ij}. In fact, as we have already mentioned, this trace does not vanish for diatomic gas, which explains why we have an additional equation in p.

4 Navier-Stokes equations for a diatomic gas

For a monoatomic gas the Navier-Stokes equations have a kinetic interpretation. The Chapman-Enskog theory is a well known procedure to derive the Navier-Stokes from the Boltzmann equation [4] [8]. This theory is quite similar in the sense that the distribution function f, solution of the Boltzmann equation, is approximated by a polynomial expansion. But Chapman-Enskog method introduces restrictive assumptions on the fluid, namely that the gas is dense and the flow has small gradients. As a result, the viscous stress tensor $\tau_{ij} = -p_{ij}$ and the heat flux vector q_i are given by the constitutive laws

$$(51)\qquad p_{ij} = -\,\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \left(\frac{2}{3}\right)\frac{\partial u_k}{\partial x_k}\,\delta_{ij}\right),$$

$$(52)\qquad q_i = -\,\kappa\,\frac{\partial T}{\partial x_i},$$

where μ is the viscosity coefficient and κ the coefficient of thermal conductivity. In this method they are functions of lower moments of the distribution function f.

In the Grad method the viscous stress and the heat flux are unknowns of the problem. This is because the Grad expansion is more general and should be valid for a larger range of flows.

Our aim in this section is to determine expressions similar to (51) and (52) for a diatomic gas. We start from the diatomic Grad system (48), that we rewrite under non conservative form,

$$(53)\qquad \frac{\partial\rho}{\partial t} + u_k\cdot\frac{\partial\rho}{\partial x_k} + \rho\frac{\partial u_k}{\partial x_k} = 0,$$

$$(54)\qquad \frac{\partial u_i}{\partial t} + u_k\cdot\frac{\partial u_i}{\partial x_k} - \frac{1}{\rho}\frac{\partial\sigma_{ik}}{\partial x_k} = 0,$$

$$(55)\qquad \frac{\partial p}{\partial t} + \frac{2}{5}p_{ik}\frac{\partial u_i}{\partial x_k} + u_k\frac{\partial p}{\partial x_k} + \frac{7}{5}p\,\frac{\partial u_k}{\partial x_k} + \frac{1}{5}\frac{\partial S_k}{\partial x_k} = 0,$$

$$\frac{\partial p_{ij}}{\partial t} + \frac{\partial u_k\, p_{ij}}{\partial x_k} + \frac{1}{7}\left(\frac{\partial S_i}{\partial x_j} + \frac{\partial S_j}{\partial x_i} - \frac{2}{5}\frac{\partial S_k}{\partial x_k}\,\delta_{ij}\right)$$

$$(56)\qquad\qquad + p_{jk}\,\frac{\partial u_i}{\partial x_k} + p_{ik}\,\frac{\partial u_j}{\partial x_k} - \frac{2}{5}\,p_{kl}\,\frac{\partial u_l}{\partial x_k}\,\delta_{ij}$$

$$+ p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{5}\frac{\partial u_k}{\partial x_k}\,\delta_{ij}\right) = J_{ij}^{(2)},$$

$$\frac{\partial S_i}{\partial t} + \frac{\partial u_k\, S_i}{\partial x_k} + \frac{9}{7}\,S_k\,\frac{\partial u_i}{\partial x_k} + \frac{2}{7}\,S_i\,\frac{\partial u_k}{\partial x_k} + \frac{2}{7}\,S_k\,\frac{\partial u_k}{\partial x_i}$$

$$(57)\qquad\qquad + \frac{2}{\rho}\,p_{il}\,\frac{\partial \sigma_{lk}}{\partial x_i} + 2R_g T\,p_{il}\,\frac{\partial p_{ik}}{\partial x_k} + 9\,p_{ik}\,\frac{\partial R_g T}{\partial x_k}$$

$$+ 7\,p\,\frac{\partial R_g T}{\partial x_i} = J_i^{(3)} - 2\,u_l\,J_{il}^{(2)},$$

for $i, j = 1, 2, 3$.

This equations are obtained by appropriate combinations of the equations of system (48). We notice that the Grad diatomic system is constituted of 14 equations with 14 unknowns ρ, u, p, p_{ij}, S_i. As already observed, compared with the monoatomic case, this new system has one additional unknown (the trace of p_{ij} does not vanish); and one more equation: the energy equation (55) is not anymore the trace of the equations in σ_{ij}, and involves a term in $I^2/2$.

We notice that the three first equations (53)-(55) of our system are the classical Navier-Stokes conservation equations, written under nonconservative form. The last equations replace the usual constitutive laws relative to p_{ij} and S_i. It follows that we just have to transform the equation into expressions similar to (51) and (52) to find again the complete Navier-Stokes equations.

To this end we suppose the flow near equilibrium in such a way that the quantities p_{ij}/p and $S_i/p\sqrt{R_g T}$ are small. Morevoer, it is natural to suppose the gradients of ρ, u, T small. Thus, neglecting the second order terms, ie. the products of two small terms, equations (56), (57) reduce to

$$(58)\quad \frac{\partial p_{ij}}{\partial t} + u_k\frac{\partial p_{ij}}{\partial x_k} + \frac{1}{7}\left(\frac{\partial S_i}{\partial x_j} + \frac{\partial S_j}{\partial x_i} - \frac{2}{5}\frac{\partial S_k}{\partial x_k}\,\delta_{ij}\right) + p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{5}\frac{\partial u_k}{\partial x_k}\,\delta_{ij}\right)$$

$$= \left(J_{ij}^{(2)}\right)_{(ordre1)} = -\frac{C p \pi^{1/2}}{30 (R_g T)^{1/2}}\left(p_{ij} + \frac{1}{72}p_{kk}\delta_{ij}\right) = -K_1\, p\left(p_{ij} + \frac{1}{72}p_{kk}\delta_{ij}\right),$$

$$(59)\qquad\qquad \frac{\partial S_i}{\partial t} + u_k\frac{\partial S_i}{\partial x_k} + 7p\frac{\partial R_g T}{\partial x_i} = \left(J_i^{(3)} - 2\,u_l\,J_{il}^{(2)}\right)_{(ordre1)}$$

$$= \frac{Cp^2}{16\pi^3(R_gT)^{1/2}}\left((R_gT)\,J(H_i^{(3)})\right)_{(ordre1)} = -K_1 p\frac{95}{63}S_i,$$

for $i,j = 1,2,3$, with

$$K_1 = \frac{C\pi^{1/2}}{30(R_gT)^{1/2}},$$

where $C = \sigma^2/m$, σ and m being respectively the diameter and the mass of a molecule. Using result of kinetic theory we can also write $\sigma^2/m = 1/\sqrt{2}\pi L\rho$, where L is the mean free path.

As for the monoatomic case, the term $1/pK_1$ has the same order of magnitude as the collision time constant. In fact, pK_1 is proportinal to c/L, where c is the sound speed and L the mean free path.

Now, if we suppose ρ, u, T constant and p_{ij}, S_i only time dependent, the solution of equations (58) and (59) are of the form

$$p_{ij}(t) = C_1 e^{-t/K_1},$$

$$S_i(t) = C_2 e^{-63t/95K_1},$$

where C_1 and C_2 are some constant.

In this case, p_{ij} and S_i tend to zero after a time comparable to the collision time constant. Thus, if we suppose the flow slowly varying, we can consider that the non homogeneous terms of (58) and (59) are not time dependent over time intervals characteristics of the mean flow which are then much larger than the collision time constant. Thus after a few collisions, a quasi-equilibrium state is reached, solved approximatively by the following spatial differential system

$$(60) \qquad u_k\frac{\partial p_{ij}}{\partial x_k} + \frac{1}{7}\left(\frac{\partial S_i}{\partial x_j} + \frac{\partial S_j}{\partial x_i} - \frac{2}{5}\frac{\partial S_k}{\partial x_k}\delta_{ij}\right) + p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{5}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right)$$

$$= -K_1\,p\left(p_{ij} + \frac{1}{72}p_{kk}\delta_{ij}\right),$$

$$(61) \qquad u_k\frac{\partial S_i}{\partial x_k} + 7\,p\frac{\partial R_gT}{\partial x_i} = -K_1\,p\frac{95}{63}\,S_i,$$

for $i,j = 1,2,3$. Finally, supposing the heat flux gradients and the viscous stress gradients to be small, the system (60), (61) reduces to the following Navier-Stokes approximations

$$(62) \qquad p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{5}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right) = -K_1\,p\left(p_{ij} + \frac{1}{72}p_{kk}\delta_{ij}\right),$$

$$(63) \qquad 7\,p\frac{\partial R_gT}{\partial x_i} = -K_1\,p\frac{95}{63}\,S_i.$$

At this level, we still have the term p_{kk} in (62). Applying the above hypothesis to the equation obtained by taking the trace of equations in p_{ij}, we write

$$(64) \qquad \frac{4}{5}\frac{\partial u_k}{\partial x_k} = -\frac{25}{24}K_1\,p_{kk}.$$

Thus, replacing p_{kk} by its expression deduced from (64), in (62), we obtain the following constitutive law

$$(65) \qquad p_{ij} = -\frac{1}{K_1}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \left(\frac{2}{5} + \frac{4}{375}\right)\frac{\partial u_k}{\partial x_k}\,\delta_{ij}\right).$$

After simplification, p_{ij} and S_i are given by

$$(66) \qquad p_{ij} = -\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \left(\frac{2}{5} + \frac{4}{375}\right)\frac{\partial u_k}{\partial x_k}\,\delta_{ij}\right),$$

$$(67) \qquad S_i = -2\,\kappa\,\frac{\partial T}{\partial x_i},$$

with

$$\mu = \frac{30\,(R_gT)^{1/2}}{C\,\pi^{1/2}} = \frac{1}{K_1}, \qquad \kappa = \frac{1323}{570}\,R_g\,\mu.$$

Introducing the viscosity coefficients λ et μ, equation (66) may also be written under the classical form

$$(68) \qquad p_{ij} = -\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \lambda\frac{\partial u_k}{\partial x_k}\,\delta_{ij},$$

with

$$(69) \qquad \lambda = -\left(\frac{2}{5} + \frac{4}{375}\right)\mu.$$

This last relation is the new Stokes relation valid for a diatomic gas. If we neglect the term $4/375$, we may write the general Stokes law as

$$\lambda = -(\gamma - 1)\mu,$$

which covers both monoatomic and diatomic gases.

To end this section, we also give the associated Navier-Stokes approximation of the particles distribution. It is obtained by replacing p_{ij} and S_i by (66) and (67) in (39), yielding

$$(70) \qquad f = f^{(0)}\left[1 - \frac{2\mu}{pR_gT}\left((\xi_i - u_i)(\xi_j - u_j) - \left(\frac{2}{5} + \frac{4}{375}\right)|\xi - u|^2\delta_{ij}\right.\right.$$

$$\left.\left. + \left(1 - \left(\frac{3}{5} + \frac{2}{375}\right)\right)I^2\delta_{ij}\right)\frac{\partial u_i}{\partial x_j} - \frac{\kappa}{7}\frac{(\xi - u)_i}{pR_gT}\left(\frac{|\xi - u|^2}{R_gT} + \frac{2I^2}{R_gT} - 7\right)\frac{\partial T}{\partial x_i}\right],$$

for $i, j = 1, 2, 3$.

Compared with the monoatomic expansion, new terms appear taking into account internal energy. But the mathematical structure of the expansion of f is unchanged.

5 Conclusion

In this paper we have reviewed recent mathematical formulations of the Boltzmann equation for polyatomic gases, and in particular a model deduced from a monoatomic model in higher dimension. Thanks to this last model, we can generalize the Grad theory, and deduce a system of macroscopic 14 moments equations for a polyatomic gas. Finally, we give an explicit formulation of this system, from which we derive, at the limit of small Knudsen numbers and small gradients, the corresponding Navier-Stokes equations. This kinetic interpretation of the Navier-Stokes equations leads to a new Stokes law for the viscosity coefficient.

As for the monoatomic case, the fourteen moment system does not have nice mathematical properties. In particular this system is not hyperbolic. Nevertheless, we can use it to analyse the validity, from a kinetic point of view, of a numerical solution of the Navier-Stokes equations, as showed in [7].

The idea we have used, which consists in extending the classical monoatomic Grad method to the monoatomic model in higher dimension, may be applied to any classical or modern asymptotic theory. In particular, it seems possible to extend it to the recent Levermore theory.

Moreover, it would be interesting to try to obtain a mathematical formulation of the Boltzmann collision operator, in the same spirit, including discrete rotation or vibrational energies, with the aim of studying then the asymptotic transition between kinetic and hydrodynamic models, for such generalized collision models.

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Annexe 1: Computation of the right hand side of the Grad system. The case of a diatomic gas

In this section we compute $J(U_p)$ for the collision Borgnakke-Larsen model with hard sphere potential, in the case of a diatomic gas. The tedious part of the computation will be done by MAPLE.

Consider again the expression (49) of $J(U_p)$. Thanks to the formula (5), we can write

$$(71) \qquad\qquad J(U_p) \; = \; \frac{1}{2} \int_\Delta \, [K] \, \frac{ff_*}{II_*} \, d\sigma,$$

where

$$d\sigma \; = \; II_* R^2 (1 - R^2) B d\xi d\xi_* \, dI dI_* \, dr dR d\omega,$$

$$\Delta \; = \; (\mathbb{R}^3)^2 \times (\mathbb{R}_+)^2 \times [0,1]^2 \times S^2.$$

We will restrict ourselves to the hard sphere collision model

$$B \; = \; C \, R \, |v_r . \omega|,$$

where C is a constant. This model leads to a macroscopic viscosity law of the form $C_o T^{1/2}$, where C_o is a constant.

Moreover we denote the components of $J(U_p)$ by

$$J(U_p) \; = \; (\, J^{(0)}, J_i^{(1)}, J_{ij}^{(2)}, J_{00}^{(2)}, J_i^{(3)} \,) \; = \; (\, J_i^{(m)} \,) \; = \; \frac{1}{2} \int [K_i^{(m)}] \frac{ff_*}{II_*} \, d\sigma,$$

with

$$K_i^{(m)} = (\, K^{(0)}, K_i^{(1)}, K_{ij}^{(2)}, K_{00}^{(2)}, K_i^{(3)} \,),$$

for $i, j = 1, 2, 3$.

It is clear that $J^{(0)}$ and $J_i^{(1)}$ vanish because $K^{(0)}$ and $K_i^{(1)}$ are collision invariants. Moreover, $|\xi|^2 + 2I^2$ being a collision invariant, we may write

$$J_{ii}^{(2)} + J_{00}^{(2)} = 0.$$

We compute now the other components of $J_i^{(m)}$.

First of all, we transforme integral (71) introducing reduced variables and the function

$$(72) \qquad\qquad h \; = \; \frac{(2\pi)^{3/2} \, (R_g T)^{5/2}}{2\rho I} \, f.$$

With this notation, the collision term writes

$$(73) \qquad J_i^{(m)} \quad = \quad \frac{C\rho p}{16\pi^3 (R_g T)^{1/2}} \int h h_* \, [K_i^{(m)}](v, \tau, v_*, \tau_*) R^3 (1 - R^2) \, |V.\omega| \tau \tau_*$$

$$dv dv_* d\tau d\tau_* dr dR d\omega,$$

where $V = v_r/\sqrt{R_g T}$, $v_r = v - v_*$.

We introduce the notation

(74)
$$J(H_i^{(m)}) = \int h h_* [H_i^{(m)}](v, \tau, v_*, \tau_*) R^3 (1 - R^2) |V.\omega| \tau \tau_*$$

$$dv dv_* d\tau d\tau_* dr dR d\omega.$$

Taking into account the formulas (44) et (45), and knowing that $\Sigma_{k=1}^5 H_{kk}^{(2)}$ is a collision invariant, we deduce that

(75)
$$J_{ij}^{(2)} = \frac{C p^2}{16\pi^3 \sqrt{R_g T}} J(H_{ij}^{(2)}),$$

(76)
$$J_i^{(3)} = \frac{C p^2}{16\pi^3 \sqrt{R_g T}} \left[R_g T J(H_i^{(3)}) + 2 u_k J(H_{ik}^{(2)}) \right].$$

Thus we have to compute the quantities $J(H_i^{(m)})$. Recall that, according to (39), h is given by

$$h(v, \tau) = P(v, \tau) \exp\left(-\left(\frac{|v|^2 + \tau^2}{2}\right)\right),$$

where

$$P(v, \tau) = \left[1 + \frac{p_{ij}}{2p}\left(H_{ij}^{(2)} - H_{00}^{(2)}\delta_{ij}\right) + \frac{1}{14}\frac{S_i}{p\sqrt{R_g T}} H_i^{(3)}\right].$$

We introduce now the auxilarily velocities variable. (V, V_*), defined by

(77)
$$\begin{cases} V = v - v_* \\ V_* = v + v_* \end{cases} \leftrightarrow \begin{cases} v = \dfrac{V_* + V}{2} \\ v_* = \dfrac{V_* - V}{2}. \end{cases}$$

Doing this change of variables in $J(H_i^{(m)})$, we obtain

$$J(H_i^{(m)}) = \int \exp\left(-\left(\frac{|v|^2 + \tau^2}{2}\right)\right) \exp\left(-\left(\frac{|v_*|^2 + \tau_*^2}{2}\right)\right) P(v, \tau) P(v_*, \tau_*)$$

$$|V.\omega| [H_i^{(m)}](v, \tau, v_*, \tau_*) R^3 (1 - R^2) \tau \tau_* dv dv_* d\tau d\tau_* dr dR d\omega,$$

$$= \frac{1}{64} \int \exp\left(-\left(\frac{|V|^2 + |V_*|^2}{4}\right)\right) \exp\left(-\left(\frac{\tau^2 + \tau_*^2}{2}\right)\right) P(\frac{V_* + V}{2}, \tau) P(\frac{V_* - V}{2}, \tau_*)$$

$$|V.\omega| [H_i^{(m)}](\frac{V_* + V}{2}, \tau, \frac{V_* - V}{2}, \tau_*) R^3 (1 - R^2) \tau \tau_* dV dV_* d\tau d\tau_* dr dR d\omega,$$

$$= \frac{1}{64} \int exp\left(-(\frac{|V|^2 + |V_*|^2}{4})\right) exp\left(-(\frac{\tau^2 + \tau_*^2}{2})\right) I_i^{(m)} P(\frac{V_* + V}{2}, \tau) P(\frac{V_* - V}{2}, \tau_*)$$

$$R^3 (1 - R^2) \tau \tau_* dV dV_* d\tau d\tau_* dr dR,$$

where

$$I_i^{(m)} = \int_S |V.\omega| [H_i^{(m)}] d\omega.$$

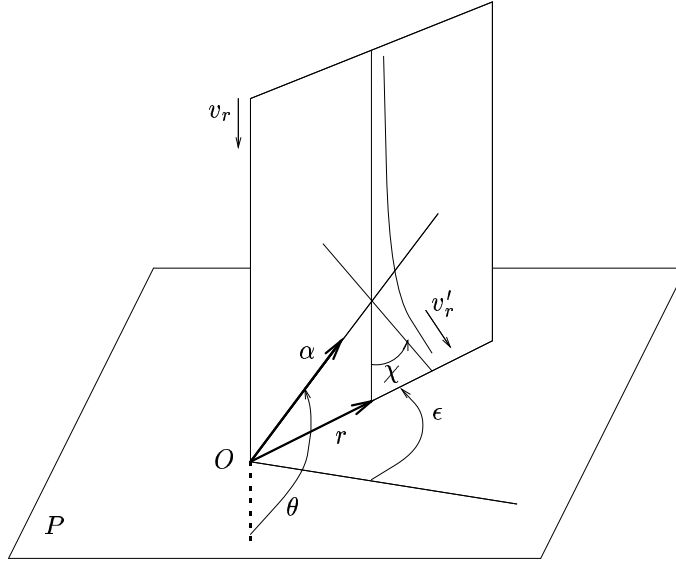In the coordinate system of figure (1), $I_i^{(m)}$ reduces to

Figure 1:

$$(78) \qquad I_i^{(m)} = -\int_{\frac{\pi}{2}}^{\pi} \int_0^{2\pi} |V| \cos\theta \sin\theta [H_i^{(m)}] d\varepsilon d\theta,$$

knowing that in this coordinate system $V = (|V|, 0, 0)$ and $\omega = (\cos\theta, \sin\theta \cos\varepsilon, \sin\theta \sin\varepsilon)$.

In the expression of $[H_i^{(m)}]$, given by

$$(79) \qquad [H_i^{(m)}] = H_i^{(m)}(v', \tau') + H_i^{(m)}(v'_*, \tau'_*) - H_i^{(m)}(v, \tau) - H_i^{(m)}(v_*, \tau_*),$$

we calculate the prime's variables with respect to variables without prime. From expressions (2) et (3), we deduce

$$(80) \quad \begin{cases} v' = \dfrac{V_*}{2} + \dfrac{R\,E}{|V|}\,(V - 2\,|V|cos\theta\,\omega) \\[4mm] v'_* = \dfrac{V_*}{2} - \dfrac{R\,E}{|V|}\,(V - 2\,|V|cos\theta\,\omega), \end{cases}$$

$$(81) \quad \begin{cases} \tau'^2 = 2\,r\,(1 - R^2)E^2, \\[4mm] \tau_*'^{\,2} = 2\,(1 - r)(1 - R^2)E^2, \end{cases}$$

$$E^2 = \frac{|V|^2}{4} + \frac{\tau^2}{2} + \frac{\tau_*^2}{2}.$$

To compute $[H_i^{(m)}]$, we introduce the following notations

$$\delta = (\delta_{ij})_{ij}, \quad x^2 = (x_i x_j)_{ij}, \quad x \otimes y = (x_i y_j + x_j y_i)_{ij},$$

$$H^{(2)} = (H_{ij}^{(2)})_{ij}, \quad H^{(3)} = (H_i^{(3)})_i, \quad I^{(2)} = (I_{ij}^{(2)})_{ij},$$

$$I^{(3)} = (I_i^{(3)})_i, \quad M \underline{\otimes} x = (M_{ij} x_j)_i,$$

where x is a vector, M is a matrix and $i, j = 1, 2, 3$.

According to these notations, we compute $[H^{(2)}]$, whose expression is given by

$$(82) \quad [H^{(2)}] = v'^2 + v_*'^2 - v^2 - v_*^2.$$

Computing v'^2 and $v_*'^2$ from (80) and $v^2 + v_*^2$ from (77), we obtain

$$(83) \quad v'^2 = \frac{V_*^2}{4} + \frac{RE}{2|V|}\,(V - 2|V|\cos\theta\,\omega).V_* + \frac{(RE)^2}{|V|^2}(V - 2|V|\cos\theta\,\omega)^2,$$

$$(84) \quad v_*'^2 = \frac{V_*^2}{4} - \frac{RE}{2|V|}\,(V - 2|V|\cos\theta\,\omega).V_* + \frac{(RE)^2}{|V|^2}(V - 2|V|\cos\theta\,\omega)^2,$$

$$(85) \quad v^2 + v_*^2 = \frac{V^2 + V_*^2}{2}.$$

Replacing (83),(84) and (85) in (82), $[H^{(2)}]$ is written, after simplifications,

$$(86) \quad [H^{(2)}] = 2\,\frac{(RE)^2}{|V|^2}\,(V - 2\,|V|\,cos\theta\,\omega)^2 - \frac{V^2}{2},$$

$$= \left[2\,\frac{(RE)^2}{|V|^2} - \frac{1}{2}\right]\,V^2 + 2\,\frac{(RE)^2}{|V|^2}\,(4\,|V|^2\,cos^2\theta\,\omega^2 - 2|V|cos\theta\,V \otimes \omega).$$

Knowing now the expression of $[H^{(2)}]$, we can compute $I^{(2)}$. Replacing $[H^{(2)}]$ by (86) in (78), we write

$$
\begin{aligned}
I^{(2)} \quad = \quad & - \left[2\frac{(RE)^2}{|V|^2} - \frac{1}{2} \right] V^2 \int_{\frac{\pi}{2}}^{\pi} |V| cos\theta \, sin\theta \int_0^{2\pi} d\varepsilon \, d\theta \\
\\
& - \quad 8\frac{(RE)^2}{|V|} \int_{\frac{\pi}{2}}^{\pi} cos^3\theta \, sin\theta \int_0^{2\pi} |V|^2 \omega^2 d\varepsilon \, d\theta \\
\\
& + \quad 4\frac{(RE)^2}{|V|} \int_{\frac{\pi}{2}}^{\pi} cos^2\theta \, sin\theta \int_0^{2\pi} |V| V \otimes \omega d\varepsilon \, d\theta.
\end{aligned}
$$

(87)

To determine this integral, at first we integrate with respect to the variable ε and then with respect to the variable θ. Thus integrating with respect to ε, we can write

$$
\begin{aligned}
\int_0^{2\pi} |V| V \otimes \omega \, d\varepsilon \quad &= |V| V \otimes \int_0^{2\pi} \omega \, d\varepsilon \\
\\
&= |V| V \otimes \begin{pmatrix} 2\pi \, cos\theta \\ 0 \\ 0 \end{pmatrix} = 4\pi \, cos\theta \, V^2,
\end{aligned}
$$

(88)

$$
\int_0^{2\pi} |V|^2 \, \omega^2 \, d\varepsilon =
$$

(89)

$$
= \int_0^{2\pi} |V|^2 \begin{pmatrix} cos^2\theta & cos\theta \, sin\theta \, cos\varepsilon & cos\theta \, sin\theta \, sin\varepsilon \\ \\ cos\theta \, sin\theta \, cos\varepsilon & sin^2\theta \, cos^2\varepsilon & sin^2\theta \, sin\varepsilon cos(\varepsilon) \\ \\ cos\theta \, sin\theta \, sin\varepsilon & sin^2\theta \, sin\varepsilon \, cos\varepsilon & sin^2\theta \, cos^2\varepsilon \end{pmatrix} d\varepsilon
$$

$$
= \pi |V|^2 \, sin^2\theta \, \delta + \pi (2cos^2\theta - sin^2\theta) \, V^2,
$$

and the expression (87) becomes

$$
I^{(2)} = -2\pi \left[2 \frac{(RE)^2}{|V|^2} - \frac{1}{2} \right] V^2 |V| \int_0^{2\pi} cos\theta \, sin\theta \, d\theta
$$

$$
-8\pi (RE)^2 |V| \delta \int_0^{2\pi} cos^3\theta \, sin^3\theta d\theta
$$

(90)

$$
-8\pi \frac{(RE)^2}{|V|} V^2 \int_0^{2\pi} (2cos^5\theta \, sin\theta - cos^3\theta \, sin^3\theta) d\theta
$$

$$
+16\pi \frac{(RE)^2}{|V|} V^2 \int_0^{2\pi} cos^3\theta \, sin\theta \, d\theta.
$$

The values of the integrals with respect to θ are

$$
(91) \qquad \int_{\frac{\pi}{2}}^{\pi} sin\theta \, cos\theta \, d\theta = -\frac{1}{2}, \qquad \int_{\frac{\pi}{2}}^{\pi} sin^3\theta \, cos\theta \, d\theta = -\frac{1}{12},
$$

$$
(92) \qquad \int_{\frac{\pi}{2}}^{\pi} sin(\theta) \, cos(\theta)^5 \, d\theta = -\frac{8}{15}, \qquad \int_{\frac{\pi}{2}}^{\pi} sin(\theta) \, cos(\theta)^3 \, d\theta = -\frac{1}{4}.
$$

Finally, replacing the preceeding integrals in (90), $I^{(2)}$ is written, after simplification

$$
(93) \qquad I^{(2)} = -\pi \left(-\frac{2}{3}(RE)^2 |V| \delta + \frac{|V|}{2} V^2 \right).
$$

To compute $I^{(3)}$, we follow the same steps as to compute $I^{(2)}$. After some calculation, $[H_i^{(3)}]$ is given by

$$
[H_i^{(3)}] = v' \left(|v'|^2 + \tau'^2 - 7 \right) + v'_* \left(|v'_*|^2 + {\tau'_*}^2 - 7 \right)
$$

(94)

$$
- v \left(|v|^2 + \tau^2 - 7 \right) - v_* \left(|v_*|^2 + \tau_*^2 - 7 \right).
$$

To achieve this computation we introduce the following notations

$$
(95) \qquad v' = \frac{V_*}{2} + \beta T, \qquad v'_* = \frac{V_*}{2} - \beta T,
$$

where

$$
\beta = \frac{RE}{|V|}, \qquad T = V - 2(V.\omega) \, \omega.
$$

Replacing (95) in (94), we can write

$$[H_i^{(3)}] = \frac{V_*}{2}\left[\frac{|V_*|^2}{2} + 2\beta^2|T|^2 + 2(1-R^2)E^2 - 14\right]$$

(96)
$$+ \beta T\left[2\beta V_*.T + 2(1-R^2)(2r-1)E^2\right]$$

$$- v\left(|v|^2 + \tau^2 - 7\right) - v_*\left(|v_*|^2 + \tau_*^2 - 7\right).$$

Moreover, knowing that

$$v\left(|v|^2 + \tau^2 - 7\right) + v_*\left(|v_*|^2 + \tau_*^2 - 7\right) =$$

(97)
$$= \frac{1}{4}\left[(|V_*|^2 + |V|^2)V_* + 2(V_*.V)V\right]$$

$$+ \frac{(V_* + V)}{2}\tau^2 + \frac{(V_* - V)}{2}\tau_*^2 - 7V_*,$$

and after simplification, (96) is writen

$$[H_i^{(3)}] = 2\beta^2(V_*.T)T + 2\beta(1-R^2)(2r-1)E^2T$$

(98)
$$- \frac{V}{2}(V_*.V) - \frac{V}{2}(-\tau^2 + \tau_*^2).$$

Remplacing $T = V - 2(V.\omega)\omega$ in (98), $[H_i^{(3)}]$ is finally written

(99)
$$\begin{cases} [H_i^{(3)}] = 2\beta^2(V.V_*)V + 2\beta E^2(2r-1)(1-R^2)V - \frac{(V.V_*)}{2}V \\[2mm] \quad - \frac{1}{2}(\tau^2 - \tau_*^2)V - 4\beta^2(V.\omega)(V_*.\omega)V - 4\beta^2(V_*.V)(V.\omega)\omega \\[2mm] \quad - 4\beta E^2(2r-1)(1-R^2)(V.\omega)\omega \\[2mm] \quad + 8\beta^2(V.\omega)^2(V_*.\omega)\omega. \end{cases}$$

To compute $I^{(3)}$, we integrate with respect to ε the different terms of (99) which depend on ε. Thus we have

$$\int_0^{2\pi}(V.\omega)\,\omega\,d\varepsilon = \int_0^{2\pi}\begin{pmatrix}|V|cos^2\theta \\ sin\theta\,cos\varepsilon \\ sin\theta\,sin\varepsilon\end{pmatrix}d\varepsilon = 2\pi\,cos^2\theta\,V,$$

$$\int_0^{2\pi}(V.\omega)\,(V_*.\omega)\,d\varepsilon = \int_0^{2\pi}|V|cos\theta\,V_*.\begin{pmatrix}cos\theta \\ sin\theta\,cos\varepsilon \\ sin\theta\,sin\varepsilon\end{pmatrix}d\varepsilon = 2\pi\,cos^2\theta\,(V_*.V),$$

$$\int_0^{2\pi} (V.\omega)^2 \, (V_*.\omega)\omega \, d\varepsilon,$$

$$= |V|^2 cos^2\theta \int_0^{2\pi} V_*. \begin{pmatrix} cos\theta \\ sin\theta \, cos\varepsilon \\ sin\theta \, sin\varepsilon \end{pmatrix} \begin{pmatrix} cos\theta \\ sin\theta \, cos\varepsilon \\ sin\theta \, sin\varepsilon \end{pmatrix} d\varepsilon,$$

$$= |V|^2 cos^2\theta \int_0^{2\pi}$$

$$\begin{pmatrix} V_{*1} cos^2\theta + V_{*2} sin\theta \, cos^2\theta \, cos\varepsilon + V_{*3} sin\theta \, cos^2\theta \, sin\varepsilon \\ V_{*1} sin\theta \, cos^2\theta \, sin\varepsilon + V_{*2} sin^2\theta \, cos^2\varepsilon + V_{*3} sin^2\theta \, sin\varepsilon \, cos\varepsilon \\ V_{*1} sin\theta \, cos^2\theta \, sin\varepsilon + V_{*2} sin^2\theta \, cos\varepsilon \, sin\varepsilon + V_{*3} sin^2\theta \, sin^2\varepsilon \end{pmatrix} d\varepsilon,$$

$$= \pi |V|^2 cos^2\theta \begin{pmatrix} 2V_{*1} cos^2\theta \\ V_{*2} sin^2\theta \\ V_{*3} sin^2\theta \end{pmatrix},$$

$$= \pi |V|^2 cos^2\theta \begin{pmatrix} 2cos^2\theta & 0 & 0 \\ 0 & sin^2\theta & 0 \\ 0 & 0 & sin^2\theta \end{pmatrix} \underline{\otimes} V_*,$$

$$= \pi cos^2\theta \left[sin^2\theta \, |V|^2 \, \delta \underline{\otimes} V_* + (2cos^2\theta - sin^2\theta) \, V^2 \underline{\otimes} V_* \right].$$

Replacing the preceeding integrals in

(100) $$I^{(3)} = \int_{\frac{\pi}{2}}^{\pi} \int_0^{\pi} |V| cos\theta \, sin\theta [H^{(3)}] d\varepsilon \, d\theta,$$

the expression of $I^{(3)}$ can still be writen

$$I^{(3)} = -2\pi \left[\quad 2\beta^2(V.V_*)\,V \; + \; 2\beta E^2(2r-1)(1-R^2)V - \right.$$

$$\left. \frac{(V.V_*)}{2}V - \frac{1}{2}(\tau^2 - \tau_*^2)\,V \right] \int_{\frac{\pi}{2}}^{\pi} sin\theta\, cos\theta\, d\theta$$

$$+16\pi\beta^2|V|(V_*.V)V \int_{\frac{\pi}{2}}^{\pi} sin\theta\, cos^3\theta\, d\theta$$

(101)

$$-8\pi\beta E^2(2r-1)(1-R^2)|V|V \int_{\frac{\pi}{2}}^{\pi} sin\theta\, cos^3\theta\, d\theta$$

$$-8\pi\beta^2|V|^3\delta\underline{\otimes}V_* \int_{\frac{\pi}{2}}^{\pi} sin\theta\, cos^3\theta\, d\theta$$

$$-8\pi\beta^2|V|V^2\underline{\otimes}V_* \int_{\frac{\pi}{2}}^{\pi} (2cos^5\theta\, sin\theta \,-\, cos^3\theta\, sin^3\theta)d\theta.$$

Using the relations (91) - (92), the final expression of $I^{(3)}$ is

$$I^{(3)} \quad = \quad -\frac{\pi}{2}\left[(V.V_*) \,+\, \tau^2 \,-\, \tau_*^2 \,+\, 2\beta^2\,(V.V_*)\right]|V|\,V$$

$$+ \quad \frac{2}{3}\pi\beta^2\,|V|\,\left[|V|^2\,\delta \,+\, 3\,V^2\right].V_*.$$

This end our part of the computations. Now it is the turn to MAPLE. Before giving the final results we want to point out that the computation of $H_i^{(m)}$ is not trivial with MAPLE because of the special coordinate system (1), connected to a particle. We compute now the integrals with respect to the variables $r, R, \tau, \tau_*, V, V_*$ with MAPLE.

All computations being done, introducing

$$A_{ij} \;=\; \frac{-32\pi^{7/2}}{47040\,\rho^2(R_gT)^3}\left(784\,\rho\,(R_gT)^2\,p_{ij} \,+\, 28\,R_gT\,p_{ij}\,p_{kk} \,+\, 56\,R_gT\,p_{ik}p_{jk} \,+\, S_iS_j\right),$$

and

$$B \;=\; \frac{-32\pi^{7/2}}{47040\,\rho^2(R_gT)^3}\left(\frac{98}{9}\,\rho\,(R_gT)^2\,p_{kk} \,-\, \frac{70}{9}\,R_gT\,p_{lk}p_{lk} \,+\, \frac{175}{18}\,R_gT\,{p_{kk}}^2 \,-\, \frac{7}{36}\,S_kS_k\right),$$

we can write, for the second order term,

(102) $$J(H_{ij}^{(2)}) \;=\; A_{ij} \,+\, B\,\delta_{ij}.$$

Moreover, for the third order term, we have

$$(103) \qquad J(H_i^{(3)}) = -\frac{32\,\pi^{7/2}}{60480\,p^2 R_g T}\left(79\,S_i\,p_{kk} + 1520\,p\,S_i + 188\,S_k\,p_{ik}\right).$$