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Microreversible collisions for polyatomic gases and Boltzmann's theorem

J.-F. BOURGAT *, L. DESVILLETTES **, P. LE TALLEC *, * and B. PERTHAME *, ******

ABSTRACT. – We prove an H-Theorem for two Boltzmann models describing general polyatomic gases with the help of only one additional degree of freedom. The kinetic density is then represented by a function $f(t, x, v, \mathrm{I})$, $t \geqq 0$, $x \in \mathbb{R}^3$, $v \in \mathbb{R}^3$ and $\mathrm{I} \in \mathbb{R}^+$ where I^2 represents the internal energy of the particles. The first model is due to Borgnakke-Larsen, the second one is deduced from a monoatomic gas in higher dimension. Because of the nonlinearity of the microscopic collision process, the classical proof has to be adapted. These models are then illustrated by several numerical examples.

1. Introduction

The classical Boltzmann equation is used to describe perfect rarefied gases. In this model, the density function f satisfies

$$\partial_t f + v \cdot \nabla_x f = \mathrm{Q}(f) \tag{1}$$

where Q is the quadratic Boltzmann operator.

This model is restricted to monoatomic gases which for engineering applications is not sufficient. For pollution of satellites or re-entry problems, polyatomic gases have to be considered and Monte-Carlo simulations are usually performed using the Borgnakke & Larsen [1975] model, or variants. Our aim in this paper is to write in a general form and to prove the fundamental H-Theorem for this model, that is the inequality

$$\int \mathrm{Q}(f) \log f \leqq 0, \tag{2}$$

which guarantees that f will approach its equilibrium repartition when advancing in time.

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Moreover, we wish to introduce other models which also satisfy this inequality. The main characteristic of this type of model is to describe the polyatomic gases by means of the variables $t \geqq 0$, $x \in \mathbb{R}^3$, $v \in \mathbb{R}^3$ (the velocity of particles) and a *single* additional variable I where, for later purposes, I^2 represents the internal energy of the particles. Then, in (1), we take $f = f(t, x, v, I)$. In the fluid limit such a model should also give (*see* [Cercignani, [1988], [Vincent & Kruger, [1986]) the compressible Euler or Navier-Stokes equations with an equation of state given by $p = (\gamma - 1)\rho e$ and where the whole interval $\gamma \in (1, 5/3]$ is reachable by an appropriate choice of a parameter in the model.

In the models below, Q depends on a parameter δ (the number of additional degrees of freedom of the gas) and we will obtain the relation

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

To obtain these values, several authors have proposed a collision operator for polyatomic gases, see for instance [Berroir, 1970]; [Bird, 1976]; [McCourt *et al.*, 1990]; [Wiesen, 1991] and the references therein. Such models are physically correct but their drawback is that they require several additional degrees of freedom, which leads to an unacceptable memory storage in numerical applications. On the other hand, models with only one degree of freedom are heuristic but cheaper. D. I. Pullin [1978] and I. Kuscer [1989] have proposed such models, based on physical considerations and following the abstract formalism of E. M. Lifschitz & L. P. Pitaevskii [1981]. Here we will generalize these models making them more precise (in particular parametrizing the microscopic collision process) and show that another formalism is possible. We would also like to mention the recent interest of several authors, Esteban & Perthame [1991], Brun [1986], for inelastic collisions and simplified models with internal energy.

The main mathematical difficulty in treating models with one degree of freedom is that the collision process is then nonlinear. Thus the classical proof of the H-Theorem has to be adapted. For this purpose, we write the collision kernel in a microreversible manner (which is not the case in the original paper [B & L, 1975]) and find an adequate invariant measure.

The first section of this paper is devoted to the Borgnakke-Larsen model. In Section 2 and 3 we introduce another model, derived from a monoatomic gas in higher dimension, for which we also prove the H-Theorem. In the Appendix we relate our theory to classical Monte-Carlo schemes for solving the Boltzmann equation.

2. A model of Borgnakke-Larsen type

In this section we describe how the operator Q acts on the density $f(t, x, v, I)$ in a model proposed in [B & L, 1975]. The particles are supposed to have δ internal degrees of freedom, but δ need not be an integer. We will first show where δ enters in Q. Then we will show that, at the microscopic level the collisions are reversible and satisfy some symmetry properties. Finally we deduce the H-Theorem from some invariance property

Moreover, we wish to introduce other models which also satisfy this inequality. The main characteristic of this type of model is to describe the polyatomic gases by means of the variables $t \geqq 0$, $x \in \mathbb{R}^3$, $v \in \mathbb{R}^3$ (the velocity of particles) and a *single* additional variable I where, for later purposes, I^2 represents the internal energy of the particles. Then, in (1), we take $f = f(t, x, v, I)$. In the fluid limit such a model should also give (*see* [Cercignani, [1988], [Vincent & Kruger, [1986]) the compressible Euler or Navier-Stokes equations with an equation of state given by $p = (\gamma - 1)\rho e$ and where the whole interval $\gamma \in (1, 5/3]$ is reachable by an appropriate choice of a parameter in the model.

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of the measure defined through the cross-section in Q. This property is a consequence of the microreversibility of the collisions.

2.1. The model

We consider the following model based on a simple repartition of the kinetic and internal energy. As in the monoatomic case, the collision direction $\omega \in S^2$ is fixed and we transform the vector (v, v_*, I, I_*, r, R) with $v, v_* \in \mathbb{R}^3$, $I, I_* \geqq 0$, $r, R \in [0, 1]$ by setting

$$e^2 = \frac{1}{4}|v - v_*|^2 + I^2 + I_*^2 = \text{total energy}, \tag{4}$$

$$g = v - v_* = \text{relative velocity}, \tag{4'}$$

and by defining the post collision velocities (v', v'_*) and energies (I', I'_*) by

$$v' + v'_* = v + v_*, \tag{5}$$

$$g' = v' - v'_* = 2\,\mathrm{R}\,e\{g - 2\omega\, g.\omega\}/|g|, \tag{6}$$

$$I'^2 = r(1 - R^2)e^2, \qquad I'^2_* = (1 - r)(1 - R^2)e^2. \tag{7}$$

The factors R and r determine the quantity of energy which is exchanged between internal and kinetic energy and between the two internal energies, respectively.

We add the following definitions which, although unnecessary for the description of Q, are useful in the resulting work; r', $R' \in [0, 1]$

$$I^2 + I_*^2 = (1 - R'^2)e^2, \tag{8}$$

$$I^2 = r'(1 - R'^2)e^2, \tag{9}$$

and we have the additional relations

$$g = 2\,R'\,e\{g' - 2\omega\, g'.\omega\}/|g'|, \qquad I_*^2 = (1 - r')(1 - R'^2)e^2. \tag{10}$$

Notice that it is always possible to define R' by (8) and r' by (9) since $0 \leqq I^2 + I_*^2 \leqq e^2$. Moreover, in addition to the elementary conservation of momentum (5) we have the following conservation of energy

$$e'^2 = \frac{1}{4}|g'|^2 + I'^2 + I'^2_* = e^2. \tag{11}$$

Now, we can introduce the corresponding collision operator

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

with

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

$$\varphi_\delta(r) = [r(1 - r)]^{\delta/2 - 1}, \qquad \psi_\delta(R) = R^2 (1 - R^2)^{\delta - 1}, \tag{12}$$

(13) $B := B(e, R|g|, R|g.\omega|, I^2 r(1-R^2), I_*^2(1-r)(1-R^2), (1-R^2)(I^2+I_*^2)) > 0.$

As usual we have used the notation $f=f(v, I), f'=f(v', I'), f_*=f(v_*, I_*)$...

The arguments of the collision cross-section B will turn out to be the quantities invariant under collisions. The practical forms of φ_δ and ψ_δ given here are such that the corresponding measure is invariant in the collision process.

We keep in mind that the term $(II_*/I'I'_*)^{\delta-1}$ is introduced to give the γ-law in Euler equations according to formula (3).

Notice that the general form of the equation above is close to that of [Pullin, 1978], [Kuscer, 1989]. Only the parametrization differs.

Remarks. – 1) Variants are possible in the definition of Q, for example we could take R, $R' \in [-1, +1]$. The precise form of Q is not described in the paper [B & L, 1975] which just describes a Monte-Carlo method implementing at a discrete level.

2) Here for simplicity we have restricted the dependance of B upon certain invariant quantities. We could add $v+v^*$, $g.\omega^\perp/|g|$ *to* ω where $\omega^\perp$ denotes the space of vectors orthogonal. Also, the positivity of B is certainly too strong for the sequel but this is the usual assumption.

3) The collision term $B\psi_\delta\varphi_\delta$ governs the kinetics of the collision process, hence the viscosity of the underlying fluid. For example, the classical Variable Hard Sphere model (VHS) associated to the viscosity law

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

will be obtained by setting

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

2.2. Microreversibility

We now set

$$T_\omega(v, v_*, I, I_*, r, R) = (v', v'_*, I', I'_*, r', R'),$$

with v', v'_*, I', I'_*, r' and R' as defined in (5)-(9).

Folllowing the classical proof of the H-Theorem (*see* [Truesdell & Muncaster, 1980]; [Cercignani, 1988]) the first step is to obtain symmetry and inversibility properties for T_ω. These properties are more difficult to obtain here due to the fact that T_ω is not a linear operator.

Proposition 1. – *For any* $\omega \in S^2$, *we have*

(i) $T_\omega \circ T_\omega = Id$,

(ii)

$$e'=e, \qquad R'|g'|=R|g|, \qquad R'g'.\omega = -Rg.\omega, \qquad I'^2 r'(1-R'^2) = I^2 r(1-R^2),$$
$$I'^2_*(1-r')(1-R'^2) = I_*^2(1-r)(1-R^2), \qquad (1-R'^2)(I'^2+I'^2_*) = (1-R^2)(I^2+I_*^2),$$
$$(1-R^2)(I^2(r-1)+rI_*^2) = -(1-R'^2)(I'^2(r'-1)+r'I'^2_*)$$

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$$(1-R^2)(I^2(r-1)+rI_*^2) = -(1-R'^2)(I'^2(r'-1)+r'I_*'^2)$$

(iii) $T_\omega(v_*, v, I_*, I, 1-r, R) = (v'_*, v', I'_*, I', 1-r', R')$,

(iv) *the collision invariants* (i.e. *the functions* φ *such that* $\varphi+\varphi_* = \varphi'+\varphi'_*$ *for all* (ω, r, R)) *are given by*

$$\varphi(v, I) = \nu + \xi.v + \mu\left(\frac{|v|^2}{2} + I^2\right), \ \mu, \nu \in \mathbb{R}, \ \xi \in \mathbb{R}^3.$$

Proof of Proposition 1. – The conservation of energy in (ii) was already derived in (11). We observe that the formulae (5), (8)-(10) defining T_ω^{-1} are identical to the formula (5)-(7) defining T_ω within the change of arguments. In other words, we have

$$w = T_\omega^{-1}(w') = T_\omega(w') = T_\omega(T_\omega(w)), \qquad \forall w = (v, v_*, I, I_*, r, R),$$

which is precisely (i). Next, we have

$$|g'| = 2Re, \qquad |g| = 2R'e$$

which gives the second conservation in (ii). The third one is deduced from the identity

$$g'.\omega = -2Reg.\omega/|g| = -\frac{R}{R'}g.\omega.$$

The three following conservations in (ii) are easily deduced combining (7)-(9) and (7)-(10). The last identity of (ii) can be obtained as follows. We multiply (9) by $(1-R^2)(r-1)$ and (10) by $(1-R^2)r$. If we add up the results, this yields

$$(1-R^2)(I^2(r-1)+rI_*^2) = e^2(1-R^2)(1-R'^2)(r-r').$$

The symmetry of this formula concludes (ii).

To check (iii) is also immediate. Finally, to prove (iv), we follow [C, 1988], [T & M, 1980]. We know that any function $\varphi(v, I)$ which is invariant under the collision operator T_ω reduces to the form given in (iv) as soon as we prove that, when (ω, R, r) varies in $S^2 \times [0, 1]^2$, then (v', v'_*, I', I'_*) takes all the possible values such that $e'=e$ and $v'+v'_* = v+v_*$. *To do so, we choose an arbitrary* (v', v'_*, I', I'_*) with $e'=e$ and $v'+v'_* = v+v_*$ and with the notation (4) set

$$\omega = \left(\frac{g}{|g|} - \frac{g'}{|g'|}\right) \Big/ \left|\frac{g}{|g|} - \frac{g'}{|g'|}\right|$$

(assuming $g/|g| \neq g'/|g'|$). Classically, this gives

$$g' = |g'|(g-2g.\omega\omega)/|g|,$$

and it remains to define R by

$$R = |g'|/2e$$

to recover (6). Since $e' = e \geqq 1/2\,|g'|$, we have R in [0, 1]. Then we fix r using (7) and R' and r' using (8) and (9). With the above choice of (w, R, r) we have

$$(v', v'_*, I', I'_*, r', R') = T_\omega(v, v_*, I, I_*, r, R).$$

This concludes the proof of (iv) and of Proposition 1.

2..3. The invariant measures

To conclude the fundamental properties of this model, it remains to find a measure which is invariant under the collision process defined above.

Proposition 2. – *For any* B *as in* (13) *and any* $\delta > 0$, *the following measure is invariant*

$$d\sigma = B\, dv\, dv_*\, I^{\delta-1}\, dI_*^{\delta-1}\, dI_*\, \varphi_\delta(r)\, dr\, \psi_\delta(R)\, dR. \tag{14}$$

In other words, $d\sigma = d\sigma'$.

Proof of Proposition 2. – By construction, $B' = B$ and, by Proposition 1 (ii), we have

$$\begin{aligned}\varphi_\delta(r)(1-R^2)^{\delta-2} I^{\delta-2} I_*^{\delta-2} &= [I^2 r(1-R^2)]^{\delta/2-1} [(1-r) I_*^2 (1-R^2)]^{\delta/2-1} \\ &= \varphi_\delta(r')(1-R'^2)^{\delta-2} I'^{\delta-2} I_*'^{\delta-2}.\end{aligned}$$

On the other hand, we have proved in Proposition 1 (ii) that

$$(1-R^2)\,|I^2(r-1) + r I_*^2| = (1-R'^2)\,|I'^2(r'-1) + r' I_*'^2|.$$

By division, Proposition 2 then reduces to the lemma

Lemma 3. – *The collision process* (4)-(10) *satisfies*

$$\begin{aligned}dA = |I^2(r-1) + r I_*^2|\, dv\, dv_*\, dI^2\, dI_*^2\, dr\, R^2 (1-R^2)^2\, dR \\ = |I'^2(r'-1) + r' I_*'^2|\, dv'\, dv_*'\, dI'^2\, dI_*'^2\, dr'\, R'^2 (1-R'^2)^2\, dR' = dA'.\end{aligned} \tag{15}$$

Proof of Lemma 3. – Standard algebraic manipulations lead to the identities

$$dv\, dv^* = \frac{1}{2} dg\, d(v + v^*)$$

$$dg = |g|^2\, d|g|\, dw = \frac{1}{2} |g|\, d|g|^2\, dw$$

with $w = g/|g|$ belonging to S^2. Since $v + v^* = v' + v'_*$, it is enough to prove that the measure

$$(1-R^2)^2\, |I^2(r-1) + r I_*^2|\, R\, |g|\, d|g|^2\, dw\, dR^2\, dI^2\, dI_*^2\, dr \tag{16}$$

is invariant. Next, if we compute the jacobian J of the map

$$(|g|^2, R^2, r, I^2, I_*^2) \to (|g|^2, R^2, e^2, (1-R^2) I^2 r, (1-R^2)(1-r) I_*^2),$$

to recover (6). Since $e' = e \geqq 1/2\,|g'|$, we have R in [0, 1]. Then we fix r using (7) and R' and r' using (8) and (9). With the above choice of (w, R, r) we have

$$(v', v'_*, \mathrm{I}', \mathrm{I}'_*, r', \mathrm{R}') = \mathrm{T}_\omega(v, v_*, \mathrm{I}, \mathrm{I}_*, r, \mathrm{R}).$$

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In other words, $d\sigma = d\sigma'$.

Proof of Proposition 2. – By construction, B' = B and, by Proposition 1 (ii), we have

$$\varphi_\delta(r)(1-\mathrm{R}^2)^{\delta-2}\,\mathrm{I}^{\delta-2}\,\mathrm{I}_*^{\delta-2} = [\mathrm{I}^2 r(1-\mathrm{R}^2)]^{\delta/2-1}\,[(1-r)\,\mathrm{I}_*^2(1-\mathrm{R}^2)]^{\delta/2-1}$$
$$= \varphi_\delta(r')(1-\mathrm{R}'^2)^{\delta-2}\,\mathrm{I}'^{\delta-2}\,\mathrm{I}_*'^{\delta-2}.$$

On the other hand, we have proved in Proposition 1 (ii) that

$$(1-\mathrm{R}^2)\,|\mathrm{I}^2(r-1)+r\,\mathrm{I}_*^2| = (1-\mathrm{R}'^2)\,|\mathrm{I}'^2(r'-1)+r'\,\mathrm{I}_*'^2|.$$

By division, Proposition 2 then reduces to the lemma

Lemma 3. – *The collision process* (4)-(10) *satisfies*

$$d\mathrm{A} = |\mathrm{I}^2(r-1)+r\,\mathrm{I}_*^2|\, dv\, dv_*\, d\mathrm{I}^2\, d\mathrm{I}_*^2\, dr\, \mathrm{R}^2(1-\mathrm{R}^2)^2\, d\mathrm{R} \tag{15}$$
$$= |\mathrm{I}'^2(r'-1)+r'\,\mathrm{I}_*'^2|\, dv'\, dv'_*\, d\mathrm{I}'^2\, d\mathrm{I}_*'^2\, dr'\, \mathrm{R}'^2(1-\mathrm{R}'^2)^2\, d\mathrm{R}' = d\mathrm{A}'.$$

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$$dg = |g|^2\, d|g|\, dw = \frac{1}{2}|g|\, d|g|^2\, dw$$

with $w = g/|g|$ belonging to S^2. Since $v+v^* = v'+v'_*$, it is enough to prove that the measure

$$(1-\mathrm{R}^2)^2\,|\mathrm{I}^2(r-1)+r\,\mathrm{I}_*^2|\,\mathrm{R}\,|g|\,d|g|^2\, dw\, d\mathrm{R}^2\, d\mathrm{I}^2\, d\mathrm{I}_*^2\, dr \tag{16}$$

is invariant. Next, if we compute the jacobian J of the map

$$(|g|^2, \mathrm{R}^2, r, \mathrm{I}^2, \mathrm{I}_*^2) \to (|g|^2, \mathrm{R}^2, e^2, (1-\mathrm{R}^2)\mathrm{I}^2 r, (1-\mathrm{R}^2)(1-r)\mathrm{I}_*^2),$$

we get

$$\mathrm{J} = (1-\mathrm{R}^2)^2\,|\mathrm{I}^2(r-1)+r\,\mathrm{I}_*^2|.$$

This means that the measure in (16) can also be written

$$\mathrm{R}\,|g|\,d|g|^2\, dw\, d\mathrm{R}^2\, de^2\, d[(1-\mathrm{R}^2)\mathrm{I}^2 r]\, d[(1-\mathrm{R}^2)(1-r)\mathrm{I}_*^2].$$

By Proposition 1 (ii), the two last terms are clearly invariant. Also, since $e^2 = e'^2$, $|g'|^2 = 4\,\mathrm{R}^2 e^2$, and $|g|^2 = 4\,\mathrm{R}'^2 e^2$, trivially we have

$$de^2\, d|g|^2\, d\mathrm{R}^2 = de'^2\, d|g'|^2\, d\mathrm{R}'^2.$$

But $\mathrm{R}\,|g| = \mathrm{R}'\,|g'|$, $dw = dw'$ (because $w.\omega = w'.\omega$, and $w.\omega^\perp = -w.\omega^\perp$). Combined with Proposition 1 (ii), this proves that the measure (16) is invariant. Thus (15) is also invariant proving Lemma 3.

Remark. – The introduction of δ in the measure (14) is motivated by the next section and the particular form of Q_δ. The collision process itself does not see particular values of δ. In (14), the terms containing δ could be entered in B, leading to the invariant measure $\underline{\mathrm{B}}\, dv\, dv_*\, d\mathrm{I}^2\, d\mathrm{I}_*^2\, dr\, \mathrm{R}^2(1-\mathrm{R}^2)\, d\mathrm{R}$.

2.4. H-Theorem

Classically, the properties collected above are sufficient to prove invariance properties on the kernel Q_δ itself. Boltzmann's theorem follows as well as does the characterisation of the equilibrium. These results are given in the following theorem.

Theorem 4. – *Let* B *satisfy* (13), *then whenever those integrals are meaningful we have*

$$\text{(i)} \quad \int_{\mathbb{R}^3\times\mathbb{R}_+} \mathrm{Q}_\delta(f)(v, \mathrm{I})\,\varphi(v, \mathrm{I})\, dv\, d\mathrm{I} = \frac{1}{4}\int_{\mathbb{R}^3\times\mathbb{R}_+} \mathrm{Q}_\delta(f)\,[\varphi+\varphi_*-\varphi'-\varphi'_*]\, dv\, d\mathrm{I}, \tag{17}$$

$$\text{(ii)} \quad \int_{\mathbb{R}^3\times\mathbb{R}_+} \mathrm{Q}_\delta(f)\,(\log(f\,\mathrm{I}^{1-\delta})+1)\, dv\, d\mathrm{I} \leqq 0,$$

(iii) $\mathrm{Q}_\delta(f_{\mathrm{eq}}) = 0$ *if and only if*

$$f_{\mathrm{eq}} = \lambda_\delta \frac{\rho\,\mathrm{I}^{\delta-1}}{\mathrm{T}^{(3+\delta)/2}}\, e^{-(|v-u|^2+2\,\mathrm{I}^2)/2\,\mathrm{T}} \text{ for some } \rho,\ \mathrm{T}\in\mathbb{R}_+,\ u\in\mathbb{R}^3. \tag{18}$$

Before proving this result, let us give some comments.

Remarks. – 1) An equilibrium like (18) is often used to describe dense polyatomic gases (*see* [B, 1976]; [B & L, 1975]; [McC *et al.*, 1990]; [V & K, 1986]). It is also used by Deshpande [7] for numerical calculations.

2) The form (18) of the equilibrium generalizes the maxwellian. The choice of λ_δ in (18) is performed so that

$$\int_{\mathbb{R}^3\times\mathbb{R}_+} (1,\ v,\ (v-u)_i(v-u)_j)\, f_{\mathrm{eq}}\, dv\, d\mathrm{I} = (\rho,\ \rho\,u,\ \rho\,\mathrm{T}\,\delta_{ij}).$$

A simple calculation then gives

$$\int_{\mathbb{R}^3\times\mathbb{R}_+}\left(\frac{|v|^2}{2}+\mathrm{I}^2\right)f_{\mathrm{eq}}\,dv\,d\mathrm{I}=\frac{\rho|u|^2}{2}+\alpha\rho\,\mathrm{T}$$

with $\alpha=(\delta+3)/2$.

In other words, the macroscopic equations are indeed the Euler equations for a polytropic gas

$$\partial_t \mathrm{U}+\sum_{j=1}^{3}\partial_{x_j}\mathrm{F}_j(\mathrm{U})=0,$$

$$\mathrm{U}=\begin{pmatrix}\rho\\ \rho u_k\\ \mathrm{E}\end{pmatrix},\qquad \mathrm{F}_j(\mathrm{U})=\begin{pmatrix}\rho u_j\\ \rho u_j u_k+p\,\delta_{jk}\\ (\mathrm{E}+p)u_j\end{pmatrix},\qquad 1\leqq j,\,k\leqq 3,$$

with $p=\rho\,\mathrm{T}$, $\mathrm{E}=1/2\,\rho|u|^2+\alpha\rho\,\mathrm{T}$, thanks to the relation between δ and γ in (3), and $\alpha=1/(\gamma-1)$.

3) A possible application of this result is to reduce an existence proof of global solutions to the Boltzmann Eq. (1) following the recent result of Di Perna & Lions [1989]. We will not do that here, since our purpose is to settle the model rather than to perform a complete mathematical analysis. □

Proof the Theorem 4. – The proof follows the case of a monoatomic gas. Thus we indicate how the formalism goes. We have by construction

$$\int \mathrm{Q}_\delta(f)\,\varphi\,dv\,d\mathrm{I}=\int\left(\frac{f'f'_*}{(\mathrm{I}'\mathrm{I}'_*)^{\delta-1}}-\frac{ff_*}{(\mathrm{II}_*)^{\delta-1}}\right)\varphi\,d\sigma\,d\omega$$

where $d\sigma$ is the measure introduced in Proposition 2. Then the classical symmetrisation transformations used in the monoatomic case gives (i). Inequality (ii) follows by applying (i) to $\varphi=\log(f\,\mathrm{I}^{1-\delta})+1$.

Finally, at equilibrium, we must have

$$\frac{f'f'_*}{(\mathrm{I}'\mathrm{I}'_*)^{\delta-1}}=\frac{ff_*}{(\mathrm{II}_*)^{\delta-1}}.$$

Hence $\log(f\mathrm{I}^{1-\delta})$ must be a collision invariant. From Proposition 1 (iv), this implies

$$f\mathrm{I}^{1-\delta}=\exp\left(\nu+\xi.v+\mu\left(\frac{|v|^2}{2}+\mathrm{I}^2\right)\right)$$

$$=\mathrm{K}\exp[-(|v-u|^2+2\,\mathrm{I}^2)/2\,\mathrm{T}],$$

which is exactly (18). This completes our proof.

The above proof gives some more insight on the relation between δ and the state law. We have seen in Remark 2 that the coefficient $\alpha\mathrm{T}$ in the state law is due to the term $\mathrm{I}^{\delta-1}$ which appears in the equilibrium distribution f_{eq}. What is proved above is that this

A simple calculation then gives

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with $p=\rho\,\mathrm{T}$, $\mathrm{E}=1/2\,\rho|u|^2+\alpha\rho\,\mathrm{T}$, thanks to the relation between δ and γ in (3), and $\alpha=1/(\gamma-1)$.

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The above proof gives some more insight on the relation between δ and the state law. We have seen in Remark 2 that the coefficient $\alpha\,\mathrm{T}$ in the state law is due to the term $\mathrm{I}^{\delta-1}$ which appears in the equilibrium distribution f_{eq}. What is proved above is that this

term $\mathrm{I}^{\delta-1}$ appears only because we have added a factor $(\mathrm{II}_*/\mathrm{I}'\,\mathrm{I}'_*)^{\delta-1}$ to the source term of our collision operator.

We also observe that setting $g=f/\mathrm{I}^{\delta-1}$ we could have used the alternative formalism

$$\partial_t g+v.\nabla_x g=\int_\Delta (g'\,g'_*-gg_*)\,\mathrm{B}\,dv_*\,\mathrm{I}_*^{\delta-1}\,d\mathrm{I}_*\,\varphi_\delta(r)\,dr\,\mathrm{R}^2(1-\mathrm{R}^2)^{\delta-1}\,d\mathrm{R}. \tag{19}$$

Here, the natural measure is $dv\,\mathrm{I}^{\delta-1}\,d\mathrm{I}$ and the equilibria on g are classical maxwellians. The advantage of this formulae for f is that it is closer to the numerical method which approaches the measures $f\,dv\,d\mathrm{I}$ and which is recalled in the Appendix.

3. A model derived from a monoatomic gas in higher dimension

We now describe another possible model for polyatomic gases leading to the same equilibrium distribution. Its interest is that it is closer to the classical Boltzmann kernel. It is derived from the monoatomic case in higher dimension as will be shown in Section 3.3.

3.1. The collision process

The collisions are more complicated here than in the Borgnakke-Larsen model. The collision parameters are $\sigma=(a,\,b,\,\omega)\in[0,\,2\pi]^2\times\mathrm{S}^2$ with $d\sigma=da\,db\,d\omega$). Two particles $(v,\,\mathrm{I})$, $(v_*,\,\mathrm{I}_*)$ now collide to give the "prime" quantities defined as follows (we use the same notations as in *Sec.* 1):

$$\Lambda=\frac{1}{2}g.\omega\cos a+\sin a\,(\mathrm{I}\,\alpha\cos b+\mathrm{I}_*\,\alpha_*\sin b), \tag{20}$$

$$v'+v'_*=v+v_*,\ g'=g-4\,\Lambda\omega\cos a, \tag{21}$$

$$\mathrm{I}'^2=\mathrm{I}^2+4\,\Lambda^2\cos^2 b\sin^2 a-4\,\mathrm{I}\,\alpha\Lambda\cos b\sin a, \tag{22}$$

$$\mathrm{I}'^2_*=\mathrm{I}^2_*+4\,\Lambda^2\sin^2 b\sin^2 a-4\,\mathrm{I}_*\,\alpha_*\,\Lambda\sin b\sin a, \tag{22'}$$

$$\alpha'=(\alpha\,\mathrm{I}-2\,\Lambda\cos b\sin a)/\mathrm{I}',\ \alpha'_*=(\alpha_*\,\mathrm{I}_*-2\,\Lambda\sin b\sin a)/\mathrm{I}'_*. \tag{23}$$

Here $\alpha,\,\alpha_*\in[-1,\,+1]$ are two parameters similar to r and R in Section 2. The collision operator is defined by

$$\mathrm{Q}_\delta(f)(v,\,\mathrm{I})=\int_\Delta\left(f'\,f'_*\left(\frac{\mathrm{II}_*}{\mathrm{I}'\,\mathrm{I}'_*}\right)^{\delta-1}-ff_*\right)\mathrm{B}\,dv_*\,(\mathrm{II}_*)^{3-\delta}\,d\mathrm{I}_*\,d\alpha\,d\alpha_*\,d\sigma, \tag{24}$$

where B is given below and

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

3.2. Microreversibility and H-Theorem

As before, we set

$$\mathrm{T}_\sigma(v,\,v_*,\,\mathrm{I},\,\mathrm{I}_*,\,\alpha,\,\alpha_*)=(v',\,v'_*,\,\mathrm{I}',\,\mathrm{I}'_*,\,\alpha',\,\alpha'_*)$$

and the microreversibility of the collisions is expressed in the

PROPOSITION 5. – *For any* $\sigma=(a, b, \omega)$, *we have*

(i) $T_\sigma \circ T_\sigma = Id$

(ii) $e'=e$, $\Lambda'=-\Lambda$, $I'^2(1-\alpha'^2)=I^2(1-\alpha^2)$, $I'^2_*(1-\alpha'^2_*)=I^2_*(1-\alpha^2_*)$,

(iii) $T_{\sigma'}(v_*, v, I_*, I, \alpha_*, \alpha)=(v'_*, v', I'_*, I', \alpha'_*, \alpha')$ *for* $\sigma'=(-a, (\pi/2)-b, \omega)$.

(iv) *the collision invariants are given by the formula* (iv) *in Proposition* 1.

Proof of Proposition 5. – Let us set

$$V=\left(\frac{g}{2}, I\alpha, I_*\alpha_*\right), \qquad V'=\left(\frac{g'}{2}, I'\alpha', I'_*\alpha'_*\right) \tag{25}$$

$$\Omega=(\omega\cos a, \sin a\cos b, \sin a\sin b). \tag{26}$$

Observe that we have $\Omega.\Omega=1$. Then, the collision process is equivalently defined by

$$\Lambda=V.\Omega \tag{27}$$

$$v'+v'_*=v+v_* \tag{28}$$

$$I'^2(1-\alpha'^2)=I^2(1-\alpha^2), \qquad I'^2_*(1-\alpha'^2_*)=I^2_*(1-\alpha^2_*), \tag{29}$$

$$V'=V-2V.\Omega\Omega, \tag{30}$$

(or equivalently $V=V'-2V'.\Omega\Omega$).

These completely symmetric formulae prove (i). Moreover, from (30) we deduce $|V|^2=|V'|^2$, which added to (28) and (29) gives the conservation of energy in (ii); then $\Lambda=V.\Omega=-V'.\Omega$ concludes the proof of (ii). Finally (iii) and (iv) are tedious consequences of the formulation (25)-(30). They can also be recovered from the interpretation given in the next section.

We can now give the invariant quantities which can be arguments of B. We need that B satisfies

$$\begin{aligned} B:&=B(v+v_*, e, |\Lambda|, I^2(1-\alpha^2), I^2_*(1-\alpha^2_*), a, b, \omega) \\ &=B\left(v+v_*, e, |\Lambda|, I^2_*(1-\alpha^2_*), I^2(1-\alpha^2), -a, \frac{\pi}{2}-b, \omega\right)>0. \end{aligned} \tag{31}$$

Next the invariant measure is given by

PROPOSITION 6.

$$dv\, dv_*\, I^2_*\, dI\, dI_*\, d\alpha\, d\alpha_* = dv'\, dv'_*\, I'^2\, I'^2_*\, dI'\, dI'_*\, d\alpha'\, d\alpha'_*. \tag{32}$$

Proof of Proposition 6. – We have

$$\begin{aligned} 8\, dv\, dv_*\, I^2\, I^2_*\, dI\, dI_*\, d\alpha\, d\alpha_* &= d(v+v_*)\, dg\, dI^2\, dI^2_*\, d\alpha\, I\, d\alpha_*\, I_* \\ &= d(v+v_*)\, d((1-\alpha^2)I^2)\, d((1-\alpha^2_*)I^2_*)\, dg d(\alpha I)\, d(\alpha_* I_*) \\ &= 2\, d(v+v_*)\, d((1-\alpha^2)I^2)\, d((1-\alpha^2_*)I^2_*)\, dV. \end{aligned}$$

and the microreversibility of the collisions is expressed in the

PROPOSITION 5. – *For any* $\sigma=(a, b, \omega)$, *we have*

(i) $T_\sigma \circ T_\sigma = Id$

(ii) $e'=e$, $\Lambda'=-\Lambda$, $I'^2(1-\alpha'^2)=I^2(1-\alpha^2)$, $I'^2_*(1-\alpha'^2_*)=I^2_*(1-\alpha^2_*)$,

(iii) $T_{\sigma'}(v_*, v, I_*, I, \alpha_*, \alpha)=(v'_*, v', I'_*, I', \alpha'_*, \alpha')$ *for* $\sigma'=(-a, (\pi/2)-b, \omega)$.

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(or equivalently $V=V'-2V'.\Omega\Omega$).

These completely symmetric formulae prove (i). Moreover, from (30) we deduce $|V|^2=|V'|^2$, which added to (28) and (29) gives the conservation of energy in (ii); then $\Lambda=V.\Omega=-V'.\Omega$ concludes the proof of (ii). Finally (iii) and (iv) are tedious consequences of the formulation (25)-(30). They can also be recovered from the interpretation given in the next section.

We can now give the invariant quantities which can be arguments of B. We need that B satisfies

$$\begin{aligned} B:&=B(v+v_*, e, |\Lambda|, I^2(1-\alpha^2), I^2_*(1-\alpha^2_*), a, b, \omega) \\ &=B\left(v+v_*, e, |\Lambda|, I^2_*(1-\alpha^2_*), I^2(1-\alpha^2), -a, \frac{\pi}{2}-b, \omega\right)>0. \end{aligned} \tag{31}$$

Next the invariant measure is given by

PROPOSITION 6.

$$dv\, dv_*\, I^2_*\, dI\, dI_*\, d\alpha\, d\alpha_* = dv'\, dv'_*\, I'^2\, I'^2_*\, dI'\, dI'_*\, d\alpha'\, d\alpha'_*. \tag{32}$$

Proof of Proposition 6. – We have

$$\begin{aligned} 8\, dv\, dv_*\, I^2\, I^2_*\, dI\, dI_*\, d\alpha\, d\alpha_* &= d(v+v_*)\, dg\, dI^2\, dI^2_*\, d\alpha\, I\, d\alpha_*\, I_* \\ &= d(v+v_*)\, d((1-\alpha^2)\, I^2)\, d((1-\alpha^2_*)\, I^2_*)\, dg d(\alpha I)\, d(\alpha_* I_*) \\ &= 2\, d(v+v_*)\, d((1-\alpha^2)\, I^2)\, d((1-\alpha^2_*)\, I^2_*)\, dV. \end{aligned}$$

From the invariance property (ii) of the formulation (26)-(30), we immediately deduce the announced result.

These properties, used at the microscopic level, directly yield the results of the H-Theorem 4 exactly as in Section 2. Therefore, these results do hold for this new model but we do not state, neither prove, them again. We prefer to go directly to our motivations for this model.

3.3. A MONOATOMIC GAS IN HIGHER DIMENSION

We now explain the origin of our model. It comes about when considering a classical Boltzmann equation in dimension $3+\delta$ where δ is an integer. We therefore introduce the variable $(v, w)\in\mathbb{R}^{3+\delta}$. In this space, the collision process

$$(v, w, v_*, w_*)\to(v', w', v'_*, w'_*)$$

has to satisfy the conservation of momentum and energy *i.e.*

$$v+v_*=v'+v'_*, \quad \frac{|v-v_*|^2}{4}+|w|^2+|w_*|^2=\frac{|v'-v'_*|^2}{4}+|w'|^2+|w'_*|^2. \tag{33}$$

Such a collision is obtained by considering a symmetry in $\mathbb{R}^{3+2\delta}$, associated to the unit vector $\underline{\Omega}$ which here is parametrized by

$$\underline{\Omega}=(\omega\cos a, \eta\sin a\cos b, \eta_*\sin a\sin b) \tag{34}$$

Above $a, b\in[0, 2\pi]$, and $\omega\in\mathbb{R}^3$, η, $\eta_*\in\mathbb{R}^\delta$ are unit vectors. Then we set

$$\underline{v}=\left(\frac{v-v_*}{2}, w, w_*\right), \qquad \underline{v}'=\left(\frac{v'-v'_*}{2}, w', w'_*\right), \tag{35}$$

and (v', v'_*, w', w'_*) is defined by

$$\underline{v}'=\underline{v}-2\underline{v}.\underline{\Omega}\underline{\Omega}=T_{\underline{\Omega}}(\underline{v}). \tag{36}$$

The corresponding Boltzmann equation associated with the function $g(x, v, w, t)$ is then

$$\partial_t g+v.\nabla_x g=\Gamma_\delta(g), \tag{37}$$

with a collision operator given by

$$\Gamma_\delta(g)=\int_{\mathbb{R}^3\times\mathbb{R}^\delta\times[0, 2\pi]^2\times S^2\times(S^{\delta-1})^2}\{g'g'_*-gg_*)\,\mathscr{B}\, dv_*\, dw_*\, d\eta\, d\eta_*\, d\sigma. \tag{38}$$

and

$$\mathscr{B}=\mathscr{B}(v+v_*, e, |\Lambda|, |w|^2-(w-\eta)^2, |w_*|^2-(w_*.\eta_*)^2, a, b, \omega).$$

This new model is related to our previous model in the following way. The parameters a, b, ω the total energy are the same and Λ can be defined either by (27) or by

$$I=|w|, \qquad \alpha=w.\eta/|w|, \qquad \Lambda=\underline{v}.\underline{\Omega}. \tag{39}$$

More precisely we have

THEOREM 7. — *If* $g(x, v, w, t)$ *satisfies* (36)-(38), *then*

$$f(x, v, \mathrm{I}, t) = \int_{\mathrm{S}^{\delta-1}} \mathrm{I}^{\delta-1} g(x, v, \mathrm{I}\theta, t)\, d\theta$$

satisfies the Boltzmann Eq. (1), *with a collision kernel given by* (20)-(24) *where, for some constant* μ_δ, B *is given by*

$$\begin{cases} \mathrm{B} = \mu_\delta (\mathrm{II}_*)^{\delta-3} [(1-\alpha_*^2)(1-\alpha^2)]^{(\delta-3)/2} \mathscr{B} \\ \mathscr{B} = \mathscr{B}(v+v_*, \mathrm{E}, |\Lambda|, \mathrm{I}^2(1-\alpha^2), \mathrm{I}_*^2(1-\alpha_*^2)). \end{cases} \tag{40}$$

Proof of Theorem 7. — Let $w = \mathrm{I}\theta$ with $\theta \in \mathrm{S}^{\delta-1}$, then integrating (38) with respect to $\mathrm{I}^{\delta-1}\, d\theta$, the collision term becomes

$$\int_{\mathrm{S}^{\delta-1}} \Gamma_\delta(g)\, \mathrm{I}^{\delta-1}\, d\theta = \int_\Sigma \{g' g'_* - g g_*\} \mathscr{B}\, d\theta\, d\eta\, d\theta_*\, d\eta_*\, (\mathrm{II}_*)^{\delta-1}\, d\mathrm{I}_*\, dv_*\, d\sigma \tag{41}$$

where we have used $dw_* = \mathrm{I}_*^{\delta-1}\, d\mathrm{I}_*\, d\theta$ and set

$$\Sigma = (\mathrm{S}^{\delta-1})^4 \times \mathbb{R}_+ \times \mathbb{R}^3 \times [0, 2\pi]^2 \times \mathrm{S}^2.$$

But, with θ, θ_* fixed, η and η_* only appear in $\mathscr{B}$ through $\alpha = \eta \cdot \theta$ and $\alpha_* = \eta_* \cdot \theta_*$. For the scattering term we can therefore replace $d\eta\, d\eta_*$ by

$$\mu_\delta (1-\alpha^2)^{(\delta-3)/2} (1-\alpha_*^2)^{(\delta-3)/2}\, d\alpha\, d\alpha_*$$

for some constant μ_δ. Indeed $(1-\alpha^2)^{(\delta-3)/2}$ is the density measure of the first component α of an element of the sphere $\mathrm{S}^{\delta-1}$ and μ_δ is a normalization constant coming from the other components of η which do not appear in the integral (41). The scattering term in (41) then becomes

$$\begin{aligned} \Gamma_s = -\mu_\delta \int \left(\int_{\mathrm{S}^{\delta-1}} g\, \mathrm{I}^{\delta-1}\, d\theta \right) \left(\int_{\mathrm{S}^{\delta-1}} g_*\, \mathrm{I}_*^{\delta-1}\, d\theta_* \right) \mathscr{B} \\ [(1-\alpha^2)(1-\alpha_*^2)]^{(\delta-3)/2}\, d\alpha\, d\alpha_*\, d\mathrm{I}_*\, dv_*\, d\sigma \\ = -\int f f_*\, \mathrm{B}\, (\mathrm{II}_*)^{3-\delta}\, d\alpha\, d\alpha_*\, d\mathrm{I}_*\, dv_*\, d\sigma, \end{aligned}$$

thanks to the relation (40). This is exactly the scattering term of (24). The source term can be treated in a similar way; indeed using the measure invariance $d\underline{v} = d\underline{v}'$ and the

More precisely we have

THEOREM 7. – *If* $g(x, v, w, t)$ *satisfies* (36)-(38), *then*

$$f(x, v, \mathrm{I}, t) = \int_{\mathrm{S}^{\delta-1}} \mathrm{I}^{\delta-1} g(x, v, \mathrm{I}\theta, t)\, d\theta$$

satisfies the Boltzmann Eq. (1), *with a collision kernel given by* (20)-(24) *where, for some constant* μ_δ, B *is given by*

$$\text{(40)} \qquad \begin{cases} \mathrm{B} = \mu_\delta (\mathrm{II}_*)^{\delta-3} [(1-\alpha_*^2)(1-\alpha^2)]^{(\delta-3)/2}\, \mathscr{B} \\ \mathscr{B} = \mathscr{B}(v+v_*, \mathrm{E}, |\Lambda|, \mathrm{I}^2(1-\alpha^2), \mathrm{I}_*^2(1-\alpha_*^2). \end{cases}$$

Proof of Theorem 7. – Let $w = \mathrm{I}\theta$ with $\theta \in \mathrm{S}^{\delta-1}$, then integrating (38) with respect to $\mathrm{I}^{\delta-1}\, d\theta$, the collision term becomes

$$\text{(41)} \qquad \int_{\mathrm{S}^{\delta-1}} \Gamma_\delta(g)\, \mathrm{I}^{\delta-1}\, d\theta = \int_\Sigma \{ g' g'_* - g g_* \}\, \mathscr{B}\, d\theta\, d\eta\, d\theta_*\, d\eta_*\, (\mathrm{II}_*)^{\delta-1}\, d\mathrm{I}_*\, dv_*\, d\sigma$$

where we have used $dw_* = \mathrm{I}_*^{\delta-1}\, d\mathrm{I}_*\, d\theta$ and set

$$\Sigma = (\mathrm{S}^{\delta-1})^4 \times \mathbb{R}_+ \times \mathbb{R}^3 \times [0, 2\pi]^2 \times \mathrm{S}^2.$$

But, with θ, θ_* fixed, η and η_* only appear in $\mathscr{B}$ through $\alpha = \eta \cdot \theta$ and $\alpha_* = \eta_* \cdot \theta_*$. For the scattering term we can therefore replace $d\eta\, d\eta_*$ by

$$\mu_\delta (1-\alpha^2)^{(\delta-3)/2} (1-\alpha_*^2)^{(\delta-3)/2}\, d\alpha\, d\alpha_*$$

for some constant μ_δ. Indeed $(1-\alpha^2)^{(\delta-3)/2}$ is the density measure of the first component α of an element of the sphere $\mathrm{S}^{\delta-1}$ and μ_δ is a normalization constant coming from the other components of η which do not appear in the integral (41). The scattering term in (41) then becomes

$$\Gamma_s = -\mu_\delta \int \left(\int_{\mathrm{S}^{\delta-1}} g\, \mathrm{I}^{\delta-1}\, d\theta \right) \left(\int_{\mathrm{S}^{\delta-1}} g_*\, \mathrm{I}_*^{\delta-1}\, d\theta_* \right) \mathscr{B}$$
$$[(1-\alpha^2)(1-\alpha_*^2)]^{(\delta-3)/2}\, d\alpha\, d\alpha_*\, d\mathrm{I}_*\, dv_*\, d\sigma$$
$$= -\int f f_*\, \mathrm{B}\, (\mathrm{II}_*)^{3-\delta}\, d\alpha\, d\alpha_*\, d\mathrm{I}_*\, dv_*\, d\sigma,$$

thanks to the relation (40). This is exactly the scattering term of (24). The source term can be treated in a similar way; indeed using the measure invariance $d\underline{v} = d\underline{v}'$ and the

change of variable $(v, v_*, w, w_*) \to (v', v'_*, w', w'_*)$, for any function $\varphi(|w|, v)$ we have

$$\text{(42)} \qquad \int \Gamma_\delta \varphi\, dv\, dw = \int g' g'_* \varphi(\mathrm{I}, v)\, \mathscr{B}\, dv\, dv_*\, dw\, dw_*\, d\eta\, d\eta_*\, d\sigma$$
$$= \int g' g'_* \varphi(\mathrm{I}, v)\, \mathscr{B}'\, dv'\, dv'_*\, dw'\, dw'_*\, d\eta\, d\eta_*\, d\sigma$$
$$= \int g g_* \varphi(\mathrm{I}', v')\, \mathscr{B}\, dv\, dv_*\, dw\, dw_*\, d\eta\, d\eta_*\, d\sigma.$$

Next, the same changes of variables as before yield that (42) is also

$$\int \Gamma_\delta \varphi\, dv\, dw = \int f f_* \varphi(\mathrm{I}', v')\, \mathscr{B}\, dv\, dv_*\, (\mathrm{II}_*)^{3-\delta}\, d\mathrm{I}\, d\mathrm{I}_*\, d\alpha\, d\alpha_*\, d\sigma.$$

Now, with (39), the pair (I', v') defined by the collision process (35) is identical to the pair (I', v') obtained by the collision process (20)-(23). Applying Proposition 6, we can then write

$$\int \Gamma_\delta \varphi\, dv\, dw = \int f f_* \varphi(\mathrm{I}', v')\, (\mathrm{II}_*)^{1-\delta}\, \mathrm{B}'\, dv'\, dv'_*\, (\mathrm{I}'\, \mathrm{I}'_*)^2\, d\mathrm{I}'\, d\mathrm{I}'_*\, d\alpha'\, d\alpha'_*\, d\sigma.$$

Changing variables, this can be rewritten as

$$\int \Gamma_\delta \varphi\, dv\, dw = \int f' f'_* \varphi(\mathrm{I}, v)\, (\mathrm{I}'\, \mathrm{I}'_*)^{1-\delta}\, \mathrm{B}\, dv\, dv_*\, (\mathrm{II}_*)^2\, d\alpha\, d\alpha_*\, d\sigma.$$

Since this equality holds for any function φ, it implies that

$$\int_\Sigma g' g'_*\, \mathscr{B}\, d\theta\, d\eta\, d\theta_*\, d\eta_*\, (\mathrm{II}_*)^{\delta-1}\, d\mathrm{I}_*\, dv_*\, d\sigma$$
$$= \int f' f'_* (\mathrm{I}'\, \mathrm{I}'_*)^{1-\delta}\, \mathrm{B}\, dv_*\, (\mathrm{II}_*)^{3-\delta+\delta-1}\, d\mathrm{I}_*\, d\alpha\, d\alpha_*\, d\sigma.$$

This means that we have also recovered the source temr of (24). Since the transport equation on g, once integrated by $\mathrm{I}^{\delta-1}\, d\theta$, gives the transport equation on f, we obtain Theorem 7.

APPENDIX

Relation with a discretization through a particle method

In this appendix, we show the relation between the collision operator Q_δ we have introduced in Section 1, and its numerical discretization in the spirit of [B & L, 1975]. We have choosen to present the method of Babovski [1986] because it is closer to the Boltzmann equation, but the main conclusions would be true for the Monte-Carlo

methods (*see* B, 1976]; [I & R, 1988]). The random choice for r, R has to incorporate the law $\varphi_\delta(r)\psi_\delta(\mathrm{R})\,\mathrm{B}$.

In order to present the random particle method of [B, 1986], let us introduce the notation

$$\langle f, g\rangle = \int_{\mathbb{R}^3\times\mathbb{R}_+} f(v, \mathrm{I})\, g(v, \mathrm{I})\, dv\, d\mathrm{I}, \tag{43}$$

and assume that $\varphi_\delta(r)\psi_\delta(\mathrm{R})\,dr\,d\mathrm{R}\,d\omega$ is normalized so as to be a probability measure on $[0, 1]^2\times S^2$. After a splitting between transport and collisions, we are led to solve the homogeneous equation below which is written in a weak form. For any g continuous solve

$$\frac{d}{dt}\langle f(t), g\rangle = \langle Q_\delta(f), g\rangle = \frac{1}{2}\int ff_*(g'+g'_*)\,\mathrm{B}\,dm - \frac{1}{2}\int ff_*(g+g_*)\,\mathrm{B}\,dm. \tag{44}$$

Here we have used the notation

$$dm = dv\,dv_*\,d\mathrm{I}\,d\mathrm{I}_*\,\varphi_\delta\psi_\delta\,dr\,d\mathrm{R}\,d\omega.$$

This formulation is obtained using Theorem 4(i) and Proposition 2. It still makes sense when f is a sum of delta masses

$$f = \frac{\rho}{2\mathrm{N}}\sum_{i=1}^{2\mathrm{N}} \delta(v-v_i)\,\delta(\mathrm{I}-\mathrm{I}_i). \tag{45}$$

For such f, the scattering term is then simply

$$\frac{\rho^2}{8\mathrm{N}^2}\sum_{i,j}[g(v_i, \mathrm{I}_i)+g(v_j, \mathrm{I}_j)]\,\mathrm{W}_{ij} \tag{46}$$

with weight W_{ij} given by

$$\mathrm{W}_{ij} = \int \mathrm{B}(v=v_i,\ v_*=v_j,\ \mathrm{I}=\mathrm{I}_i,\ \mathrm{I}_*=\mathrm{I}_j,\ r,\ \mathrm{R},\ \omega)\,\varphi_\delta\psi_\delta\,dr\,d\mathrm{R}\,d\omega. \tag{47}$$

Similarly, the source term in (44) is

$$\frac{\rho^2}{8\mathrm{N}^2}\sum_{i,j}\int \mathrm{B}(\ldots)[g(v'_i, \mathrm{I}'_i)+g(v'_j, \mathrm{I}'_j)]\,\varphi_\delta\psi_\delta\,dr\,d\mathrm{R}\,d\omega, \tag{48}$$

where... means the same argument as before and v'_i, v'_j, I'_i, I'_j is the result of the collision of (v_i, I_i) with (v_j, I_j) according to (4)-(7).

The random particle method of [B, 1986] consists of three steps:

(1) Replace the double sum in (46) or (48) by a random choice of N pairs of particles (thus covering the set of 2 N particles, which explains the reed to deal with even numbers

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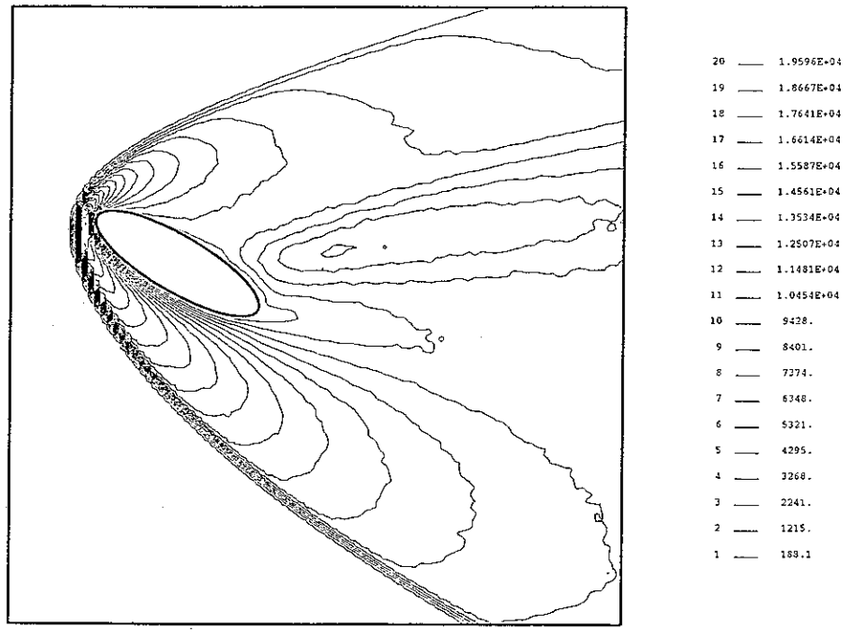

Fig. 1. – Temperature contours. Monoatomic.

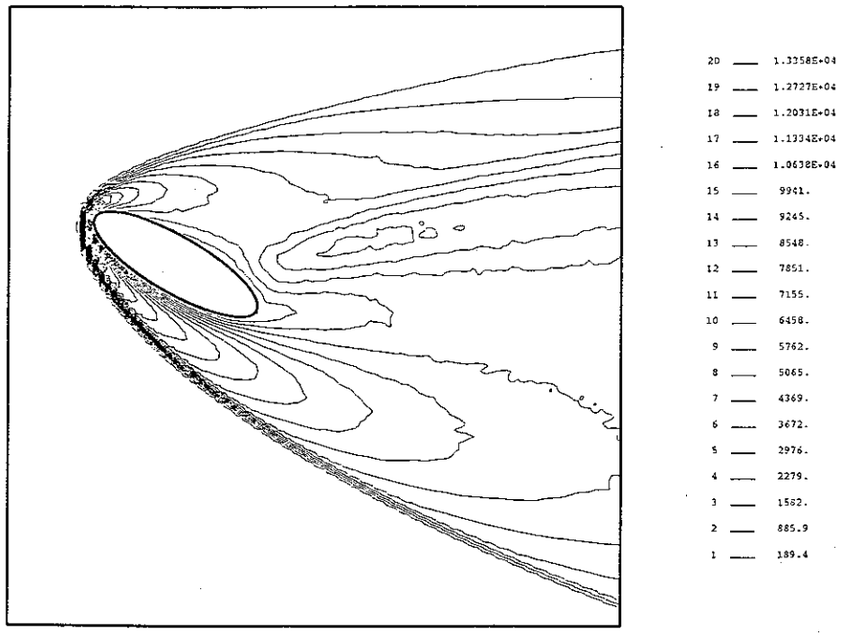

Fig. 2. – Temperature contours. Diatomic BL model.

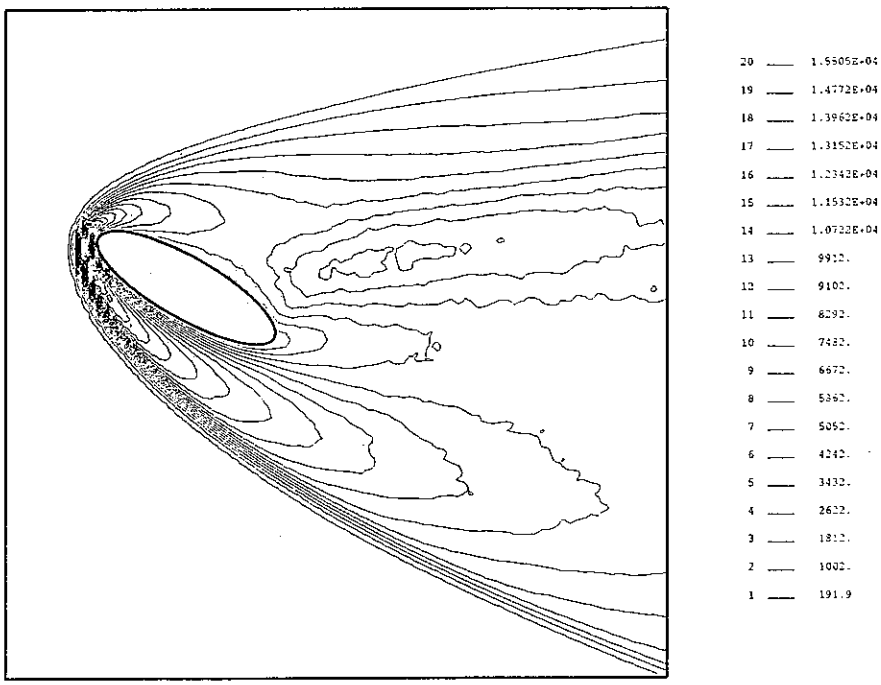

Fig. 3. – Temperature contours. Diatomic MGHD model.

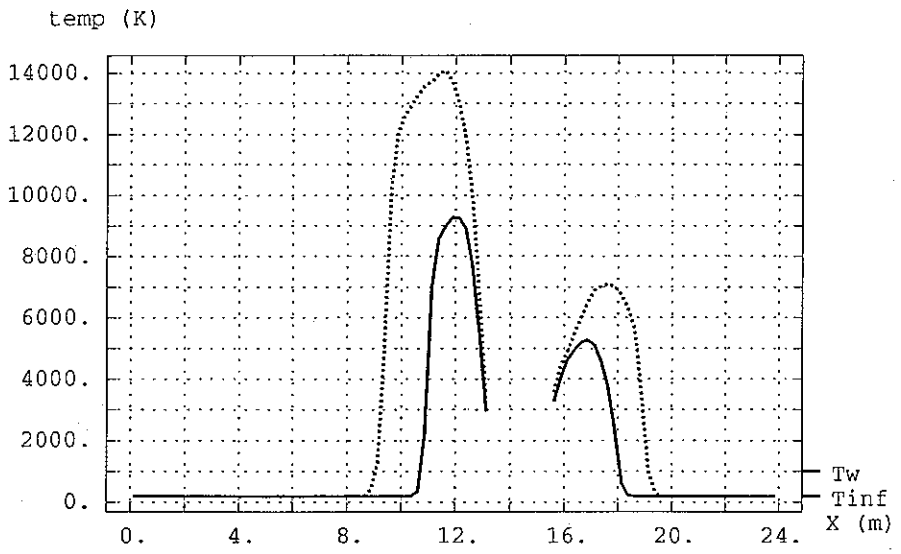

Fig. 4. – Vertical section of the temperature.
——— diatomic BL
····· monoatomic

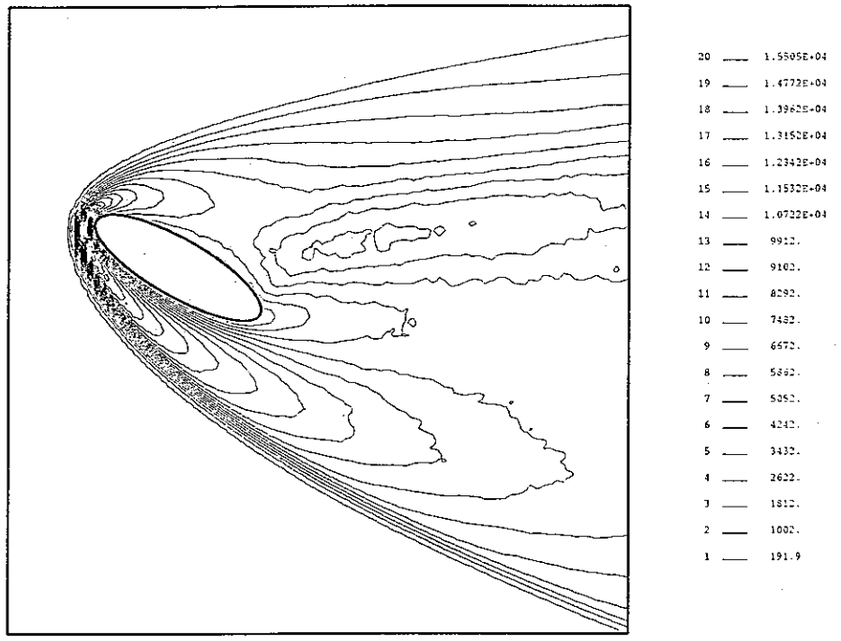

Fig. 3. – Temperature contours. Diatomic MGHD model.

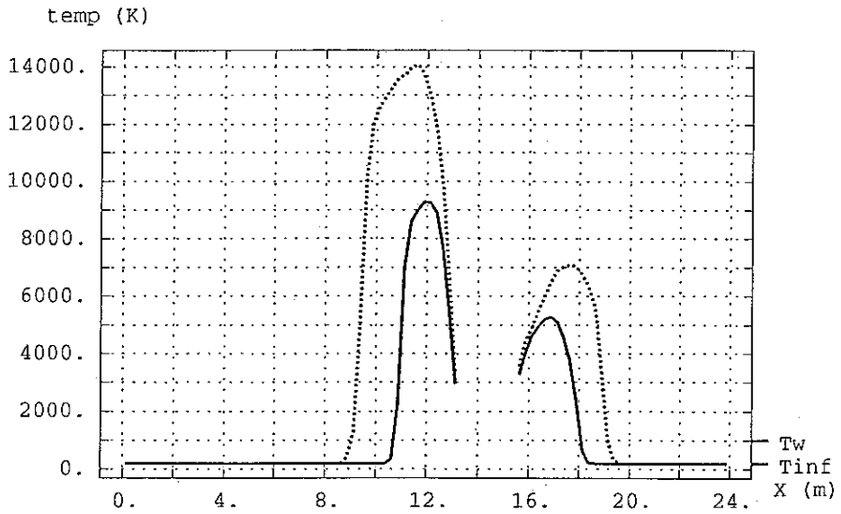

Fig. 4. – Vertical section of the temperature.
——— diatomic BL
····· monoatomic

of particles), say

$$\sigma=\{(v_1, \mathrm{I}_1)\,(v_{*1}, \mathrm{I}_{*1})\}, \{(v_2, \mathrm{I}_2), (v_{*2}, \mathrm{I}_{*2})\}, \ldots \{(v_\mathrm{N}, \mathrm{I}_\mathrm{N}), (v_{*\mathrm{N}}, \mathrm{I}_{*\mathrm{N}})\}.$$

This can be seen as the integration of a discrete measure through a random choice of the variable. Indeed, for any quantity $q(v, \mathrm{I}, w, \mathrm{J})$ such that $q(v, v, \mathrm{I}, \mathrm{I})=0$, one has

$$\frac{1}{(2\mathrm{N})^2}\sum_{i,j=1}^{2\mathrm{N}} q(v_i, v_j, \mathrm{I}_i, \mathrm{I}_j)=\frac{1}{|\Omega|}\sum_{\underline{\sigma}\in\Omega}\left[\frac{2\mathrm{N}-1}{2\mathrm{N}^2}\sum_{i=1}^{\mathrm{N}} q(v_i, v_{*i}, \mathrm{I}_i, \mathrm{I}_{*i})\right],$$

$$\simeq\frac{2\mathrm{N}-1}{2\mathrm{N}^2}\sum_{i=1}^{\mathrm{N}} q(v_i, v_{*i}, \mathrm{I}_i, \mathrm{I}_{*i})$$

where Ω denotes the set of all possible N-pairs $\underline{\sigma}$.

(2) Discretize in time with a forward Euler rule; then, if step 1 has been performed, (44) becomes

$$\langle f^{n+1}, \varphi\rangle=\langle f^n, \varphi\rangle+\rho^2\,\Delta t\,[\text{source-scattering}]$$

$$=\frac{\rho}{2\mathrm{N}}\sum_{i=1}^{\mathrm{N}}\Big\{[\varphi(v_i, \mathrm{I}_i)+\varphi(v_{*i}, \mathrm{I}_{*i})](1-\underline{\rho}\,\Delta t\,\mathrm{W}_i)$$

$$+\underline{\rho}\,\Delta t\int[\varphi(v_i', \mathrm{I}_i')+\varphi(v_{*i}', \mathrm{I}_{*i}')]\,\mathrm{B}_i\,\varphi_\delta\,\psi_\delta\,dr\,d\mathrm{R}\,d\omega\Big\} \tag{49}$$

where $\underline{\rho}=2\mathrm{N}-1/2\mathrm{N}\,\rho$ and B_i, W_i stands for the quantities in (46), (48) replacing $(v, \mathrm{I})_i$, $(v, \mathrm{I})_j$ by $(v, \mathrm{I})_i$, $(v_*, \mathrm{I}_*)_i$.

(3) The remaining integrals are computed using a Monte-Carlo method. We perform a random choice of r, R, ω according to the law $\varphi_\delta\,\psi_\delta\,dr\,d\mathrm{R}\,d\omega$, and a number $s\in(0, 1)$ is chosen (uniformly). Then, if $s\leqq\underline{\rho}\,\Delta t\,\mathrm{B}_i$, the collision is processed and the particles $(v, \mathrm{I})_i$, $(v_*, \mathrm{I}_*)_i$ are replaced by the particles $(v', \mathrm{I}')_i$, $(v_*', \mathrm{I}_*')_i$ corresponding to collisions with the parameters r, R, ω. In the other case the initial particles are kept. Under the condition on Δt

$$\underline{\rho}\,\Delta t\,\mathrm{B}_i\leqq 1, \tag{50}$$

this method amounts to writing

$$\underline{\rho}\,\Delta t\,\mathrm{B}_i\,\varphi_\delta\,\psi_\delta\,dr\,d\mathrm{R}\,d\omega=\int\mathbf{1}_{0\leqq s\leqq\underline{\rho}\,\mathrm{B}_i\,\Delta t}\,ds\,\varphi_\delta\,\psi_\delta\,dr\,d\mathrm{R}\,d\omega,$$

$$1-\underline{\rho}\,\Delta t\,\mathrm{W}_i=\iint\mathbf{1}_{\underline{\rho}\,\mathrm{B}_i\,\Delta t\leqq s\leqq 1}\,ds\,\varphi_\delta\,\psi_\delta\,dr\,d\mathrm{R}\,d\omega,$$

and replacing these two integrals by a random choice of s, r, R, ω. Then, depending on s compared to $\underline{\rho}\,\mathrm{B}_i\,\Delta t$, one of them is 0 the other is 1. In the right-hand side of (49), only one of the two terms is kept (collision or not) which enforces perfect conservation.

After this step, (49) gives a simple sum of N terms $\varphi_i+\varphi_{*i}$ or $\varphi_i'+\varphi_{*i}'$. This identifies f^{n+1} to a new repartition of the same form (45) with 2N new particles.

We have used this method to perform some calculations for the models described before in the diatomic case $\delta = 2$. The Borgnakke-Larsen model (BL) of Section 1, in the hard sphere case *i.e.* $B = R|g.\omega|$, is presented in Figure 2 and compared with a monoatomic gas in Figure 4. The Monoatomic Gas in Higher Dimension (MGHD) model is presented in Figure 3. The test problem is a global flow around a two dimensional ellipse at Mach 20 with a Knudsen number equal to 0.014. A partial accomodation equal to 0.8 is taken on the body. These calculations where run using 300,000 particles.

The BL and MGHD models give similar results compared to the monoatomic case (*Fig.* 1). The differences between BL and MGHD results certainly come from the collisional laws which are rather different.

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