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Regularized Boltzmann Operators

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Abstract—In this paper, we propose two regularization approaches for the Boltzmann collision operator. The constructed operators preserve the mass, momentum and energy; their equilibrium states are Maxwellians and they satisfy the H-theorem. In the first approach, the regularization consists in allowing microscopic collisions which do not exactly preserve energy and momentum. However, the limit of the mollified operator when the cut-off parameter tends to 0 is not the usual Boltzmann operator unless a certain condition on the distribution function is satisfied. In the second approach, the regularization relies on a smoothing of the masses of the particles and leads to a regularized operator which formally tends to the Boltzmann operator for any arbitrary distribution function, when the cut-off parameter tends to zero.

Keywords—Kinetic models, Boltzmann equation, Collisional invariants, H-theorem, Particle methods, Discrete velocity methods.

1. INTRODUCTION

In the recent past, various new numerical methods for solving the Boltzmann equation have been investigated, in particular, those based on discrete velocity models (DVMs) (see [1–4]). In such methods, the velocities lie on a fixed lattice L of $\mathbb{R}^3$. The consistency of these DVMs are closely related to the repartition of integer roots of the equation $x^2 + y^2 + z^2 = n$. So far, partial consistency results have been obtained via number theory (for example [2,5]). From the numerical and practical point of view, the main difficulty with DVMs is the small number of pairs of discrete post collisional velocities for a given pair of precollisional velocities. Indeed, the number of intersection points between the collision sphere and the lattice L of discrete velocities may be very small [6]. In such circumstances, the grid needs to be refined and the cost becomes prohibitive. To waive this difficulty, a smoothing of the collision sphere is necessary. This is the first motivation of the present work.

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The second motivation is to propose a basis for the approximation of the Boltzmann collision operator by means of the particle methods [7–9]. Monte Carlo methods allow to treat both the transport and collision operators in a fairly natural and easy way [10]. However, the Monte Carlo treatment of the collision integral generates a fairly high level of noise. It would therefore be desirable to design a particle method which would allow a flexible treatment of the transport term, together with a deterministic treatment of the collision integral in order to decrease the noise level. This goal has been achieved in linear transport theory [7–9], but has for a long time been stopped by the inability of finding a regularization of the microscopic collision process which still yields a macroscopically conservative Boltzmann operator. For short, the treatment of collisions by a deterministic particle method would essentially reduce to find a four-velocity model for velocities which are not exactly cospheric (in the center of the mass frame), but such that, after integration over all the possible four-velocity configurations, the collision operator would still be conservative (in mass, momentum and energy). This rather imprecise statement will be made clearer later on. The goal of the present paper is precisely to investigate whether it is possible to perform such regularization.

In this paper, two possible strategies to address these problems are presented. The first strategy consists in mollifying the collision sphere and in considering the collisional velocities on a spherical shell rather than on a sphere. Therefore, momentum and energy are not preserved at the level of the microscopic collision. However, they may be conserved at the macroscopic level if the scattering cross section of these unphysical collisions is carefully chosen. Indeed, in Section 2 we shall construct a mollified Boltzmann operator such that

- conservations of mass, momentum and energy holds;
- the steady state solutions are Maxwellians;
- the H-theorem holds.

These three properties are required for having a correct convergence of the distribution function towards the Maxwellian distribution at large times, which is of primary importance. We prove the following results.

- The construction of a mollified operator for which either energy or both momentum and energy conservations are relaxed at a microscopic level but such that they are satisfied at the macroscopic level is always possible (see Sections 2.1, 2.2, and 2.4). In Section 2.3, we show that the associated cross sections can be chosen in a simple form, i.e., as a piecewise constant function.
- This collision operator may be chosen in such a way that, when the regularization parameter tends to 0, it converges to the usual Boltzmann operator with a modified scattering cross section. We prove that the limit cross sections coincide with the usual one if and only if the moments of the distribution function satisfy some constraint (see Section 2.5).

A distinctive feature of this mollified collision operator is that its associated scattering cross section depends on the distribution function itself. This heavily complicates the structure of the collision operator and therefore, its implementation.

The second strategy is based on a modification of the masses of the particles during the collision and will be developed in Section 3. Once again, the microscopic collision is modified but the operator is constructed in such a way that it preserves the above three properties at the microscopic level. The main advantage of this method is to be "macroscopic" compared with the previous one in that the associated scattering cross section essentially depends on the first three moments of the distribution function instead of the microscopic details of it. Moreover, this mollified operator tends, at least formally, when the cut-off parameter tends to 0, to the usual Boltzmann operator.

We recall some classical features of the Boltzmann collision operator in the following paragraphs. We shall restrict ourselves to a monoatomic gas and consider the Boltzmann collision

operator of the form

$$Q[f](v) = \int_{\mathbb{R}^3 \times S^2_+} \sigma\left(|v - v_1|, \frac{(v - v_1, \Omega)}{|v - v_1|}\right) |v - v_1| \left(f' f'_1 - f f_1\right) d\Omega \, dv_1, \tag{1.1}$$

where σ is the differential scattering cross section and $f' = f(v')$, $f'_1 = f(v'_1)$, $f = f(v)$, $f_1 = f(v_1)$, v, and v_1 (respectively, v' and v'_1) are the particle velocities before (respectively after) the collision and are given by

$$v' = v - (v - v_1, \Omega)\,\Omega, \qquad v'_1 = v_1 + (v - v_1, \Omega)\,\Omega. \tag{1.2}$$

(x, y) denotes the dot product of the vectors x and y of $\mathbb{R}^3$ and Ω is an arbitrary angle $\Omega \in S^2$, where S^2 is the unit sphere of $\mathbb{R}^3$. These relations express the conservation of momentum and energy during a collision (the conservation of the number of particles is obviously satisfied)

$$v + v_1 = v' + v'_1, \tag{1.3}$$

$$|v|^2 + |v_1|^2 = |v'|^2 + |v'_1|^2. \tag{1.4}$$

The standard properties of the Boltzmann operator can easily be presented on the weak formulation of the Boltzmann operator. Let Ψ be a test function, we have

$$\text{P1 (Conservations):} \qquad \int_{v \in \mathbb{R}^3} Q[f](v)\Psi(v)\,dv = 0, \qquad \forall f, \tag{1.5}$$

if and only if there exists $a \in \mathbb{R}$, $b \in \mathbb{R}^3$, and $c \in \mathbb{R}$ such that $\Psi(v) = a + b.v + c|v|^2$.

$$\text{P2 (Maxwellians):} \qquad \int_{\mathbb{R}^3} Q[f](v)\Psi(v)\,dv = 0, \qquad \forall \Psi, \tag{1.6}$$

if and only if the distribution function is a Maxwellian

$$M_{\rho,u,T} = \frac{\rho}{(2\pi T)^{3/2}} \exp\left(\frac{-|v - u|^2}{2T}\right). \tag{1.7}$$

Finally, the entropy decay reads

$$\text{P3 (H-theorem):} \qquad \int_{\mathbb{R}^3} Q[f](v)\ln(f(v))\,dv \le 0, \qquad \forall f. \tag{1.8}$$

These properties hold true for sufficiently smooth and fast decaying distribution functions.

2. MOLLIFYING THE COLLISION SPHERE

Note first that the Boltzmann operator (1.1) can be equivalently written in the form

$$Q[f](v) = \int_{(\mathbb{R}^3)^4} c(v, v_1, v', v'_1)\left(f' f'_1 - f f_1\right) dv'\,dv'_1\,dv_1, \tag{2.1}$$

where the integration is now taken upon the velocities $dv'\,dv'_1\,dv_1$ and

$$c(v, v_1, v', v'_1) = \delta_0\left(v + v_1 - v' - v'_1\right)\delta_0\left(|v - v_1|^2 - |v' - v'_1|^2\right) C\left(|v - v_1|, \frac{(v - v_1, \Omega)}{|v - v_1|}\right), \tag{2.2}$$

$$C\left(|v - v_1|, \frac{(v - v_1, \Omega)}{|v - v_1|}\right) = \sigma\left(|v - v_1|, \frac{(v - v_1, \Omega)}{|v - v_1|}\right)|v - v_1|\,|v' - v'_1|, \tag{2.3}$$

where δ_0 represents the delta measure located at $x = 0$. A straightforward calculation gives (from $\Omega = ((v' - v_1') - (v - v_1))/(|(v' - v_1') - (v - v_1)|)$):

$$\left| \frac{(v - v_1, \Omega)}{|v - v_1|} \right| = \frac{1}{2} \frac{|(v' - v_1') - (v - v_1)|}{|v - v_1|}. \tag{2.4}$$

Note that the functions c and C are only defined for velocities v, v_1, v', and v_1' satisfying the conservation relations (1.3),(1.4). The conservation of momentum and energy are now taken care of by the delta measures in (2.2). Using this formulation, which can be found for instance in Cercignani [11], a natural generalization of the Boltzmann operator, consists in mollifying these measures in order to increase the number of possible post-collisional velocities.

Let Ψ be a test function. We present the construction of the mollified Boltzmann operator on the following standard symmetrized weak formulation of (2.1):

$$\begin{aligned}(Q[f], \Psi) &= \int_{\mathbb{R}^3} Q[f](v)\Psi(v)\, dv, \\ &= \frac{-1}{4} \int_{(\mathbb{R}^3)^4} c(v, v_1, v', v_1') (\Psi' + \Psi_1' - \Psi - \Psi_1) (f'f_1' - ff_1)\, dv\, dv'\, dv_1'\, dv_1,\end{aligned} \tag{2.5}$$

where Ψ', Ψ_1', Ψ, and Ψ_1 again denote $\Psi(v')$, $\Psi(v_1')$, $\Psi(v)$, and $\Psi(v_1)$, respectively. Our regularization procedure consists in smoothing the delta measures δ in the Definition (2.2) of the cross section c into a positive function δ^ϵ depending on a smoothing parameter ϵ. One goal is to achieve that

$$\delta^\epsilon \left(\frac{v + v_1}{2}, \frac{v - v_1}{2}, \frac{v' + v_1'}{2}, \frac{v' - v_1'}{2} \right) \overset{\epsilon \to 0}{\longrightarrow} \delta_0 (v + v_1 - v' - v_1')\, \delta_0 \left(|v - v_1|^2 - |v' - v_1'|^2 \right), \tag{2.6}$$

while δ^ϵ being designed such that the conservation properties are not lost. We shall see that we cannot always achieve this aim. We drop the dependence upon ϵ for the moment, i.e., $\delta^\epsilon = \delta$.

The mollified Boltzmann operator $\tilde{Q}$ is written in the following symmetrized weak form:

$$\begin{aligned}\left(\tilde{Q}[f], \Psi\right) = \frac{-1}{4} \int_{(\mathbb{R}^3)^4} & \tilde{C} \left(\frac{v - v_1}{2}, \frac{v' - v_1'}{2} \right) (\Psi' + \Psi_1' - \Psi - \Psi_1) \\ & \left(f'f_1'\delta \left(\frac{v + v_1}{2}, \frac{v - v_1}{2}, \frac{v' + v_1'}{2}, \frac{v' - v_1'}{2} \right) \right. \\ & \left. - ff_1\delta \left(\frac{v' + v_1'}{2}, \frac{v' - v_1'}{2}, \frac{v + v_1}{2}, \frac{v - v_1}{2} \right) \right) dv\, dv'\, dv_1'\, dv_1,\end{aligned} \tag{2.7}$$

where $\tilde{C}$ is defined (from (2.4) and (2.3)) as

$$\tilde{C}(z, z') = C \left(\overline{|z|}, \frac{|z - z'|}{2\overline{|z|}} \right), \tag{2.8}$$

where $\overline{|z|}$ stands for some averaged value of $|z|$ and $|z'|$, like, for example

$$\overline{|z|} = \sqrt{|z|\,|z'|} \text{ or } \overline{|z|} = \frac{(|z| + |z'|)}{2}.$$

The only required properties for $\overline{|z|}$ is to coincide with $|z|$ for $z = z'$, to be smooth and symmetric (when exchanging z and z') in order to ensure the consistency of the construction. In this section, we first obtain necessary conditions on the function δ such that properties (P1), (P2), and (P3) are satisfied by $\tilde{Q}$ (Section 2.1). Then, in Section 2.2, we prove the existence of the mollified operators. When both energy and momentum conservations are smoothed we prove that the regularized operator can be chosen in a simple form (using a piecewise constant correction function S) under some conditions on the distribution function f. In Section 2.4, we show an explicit construction of the mollified operator without any conditions on the distribution function, when only the energy conservation relation is smoothed, and in Section 2.5 we study its convergence to the Boltzmann operator when the smoothing parameter tends to 0.

2.1. Construction of the Regularization Functions

2.1.1. Change of variables

We use the change of variables from the velocities v, v_1 (respectively, v' and v_1') to the velocities of the center of mass frame (denoted by w, respectively w') and relative velocity z (respectively z'). More precisely, we set

$$\begin{aligned} w &= \frac{v+v_1}{2}, & z &= \frac{v-v_1}{2}, \\ w' &= \frac{v'+v_1'}{2}, & z' &= \frac{v'-v_1'}{2}. \end{aligned} \tag{2.9}$$

We recall that conservations of momentum and energy at the binary collision level are written in these variables: $w = w'$ and $|z|^2 = |z'|^2$. The Jacobian of this transformation is$(1/2)^3$. Thus, the Boltzmann operator $\tilde{Q}$ can be written in a weak formulation

$$\begin{aligned} \left(\tilde{Q}[f], \Psi\right) = -2 \int_{(\mathbb{R}^3)^4} & \tilde{C}(z,z') \left(\Psi' + \Psi_1' - \Psi - \Psi_1\right) \left(f' f_1' \delta(w,z,w',z')\right. \\ & \left. - f f_1 \delta(w',z',w,z)\right) dz\, dz'\, dw'\, dw, \end{aligned} \tag{2.10}$$

where the functions (f or Ψ) are evaluated at the points v, v_1, v', v_1' depending on w, w', z, and z' as defined in (2.9).

2.1.2. Maxwellian steady states, i.e., (P2)

The collision operator has to vanish for Maxwellian distribution functions. This property (P2) cannot be achieved if δ is independent of the distribution function. Actually, we require a bit more indeed, that the integrand in (2.10) identically vanishes when the distribution function is a Maxwellian (as defined in (1.6)); this is the usual distinction between the global and detailed balance properties. Here the detailed balance property is written

$$M(w'+z') M(w'-z') \delta(w,z,w',z') = M(w+z) M(w-z) \delta(w',z',w,z) \tag{2.11}$$

for any Maxwellian distribution function defined by (1.7). Note that we have, for any Maxwellian $M_{\rho,u,T}$ and any vectors w and z

$$M_{\rho,u,T}(w+z) M_{\rho,u,T}(w-z) = M_{\rho,u,T/2}(w) M_{\rho,0,T/2}(z). \tag{2.12}$$

Therefore, (2.11) is achieved if and only if δ is such that

$$\delta(w,z,w',z') = M_{\rho,u,T/2}(w) M_{\rho,0,T/2}(z) S(w,z,w',z'), \tag{2.13}$$

where S is a positive symmetric function of the pairs (w,z) and (w',z')

$$S(w,z,w',z') = S(w',z',w,z), \qquad \forall (w,z,w',z') \in \left(\mathbb{R}^3\right)^4. \tag{2.14}$$

In the remainder, we shall restrict to functions S which satisfy

$$\exists \alpha \mid S(w,z,w',z') > 0, \qquad |w-w'| \le \alpha, \qquad |z-z'| \le \alpha.$$

Let us now define the Maxwellian distribution function M^f which has the same first three moments as f, i.e., $M^f = M_{\rho_f,u_f,T_f}$ such that

$$\begin{pmatrix} \rho_f \\ \rho_f u_f \\ \frac{1}{2}\rho_f \left(u_f^2 + 3T_f\right) \end{pmatrix} = \int_{\mathbb{R}^3} f(v) \begin{pmatrix} 1 \\ v \\ \frac{|v|^2}{2} \end{pmatrix} dv. \tag{2.15}$$

2.1.3. Conservations laws, i.e., (P1)

Then, we consider conservations of momentum and energy, since conservation of mass is obvious (i.e., $(\tilde{Q}, \Psi) = 0$ for $\Psi(v) = 1$). The conservation of momentum is written

$$\left(\tilde{Q}[f], v\right) = 0 \Leftrightarrow \int_{(\mathbb{R}^3)^4} \tilde{C}(z,z')(w-w')\left(f_1' f' M^f M_1^f \right.$$
$$\left. - f f_1 \left(M^f\right)' \left(M_1^f\right)'\right) S(w,z,w',z')\, dz\, dz'\, dw'\, dw,$$

and the conservation of energy

$$\left(\tilde{Q}[f], |v|^2\right) = 0 \Leftrightarrow \int_{(\mathbb{R}^3)^4} \tilde{C}(z,z')\left(|w|^2 - |w'|^2 + |z|^2 - |z'|^2\right)\left(f_1' f' M^f M_1^f \right.$$
$$\left. - f_1 f \left(M^f\right)' \left(M_1^f\right)'\right) S(w,z,w',z')\, dz\, dz'\, dw'\, dw.$$

Let us note $X = (w,z) \in (\mathbb{R}^3)^2$ (and $X' = (w',z')$). The conservation relations can then be written

$$\int_{\mathbb{R}^{12}} \tilde{S}(X,X')\begin{pmatrix} (w-w') \\ |X|^2 - |X'|^2 \end{pmatrix}\left(F(X')H(X) - F(X)H(X')\right) dX\, dX' = 0, \tag{2.16}$$

with

$$\begin{aligned} F(X) &= f(w+z)f(w-z), \\ H(X) &= M^f(w+z)M^f(w-z), \\ \tilde{S}(X,X') &= \tilde{C}(z,z')\, S(w,z,w',z'), \\ |X|^2 &= |w|^2 + |z|^2. \end{aligned} \tag{2.17}$$

Note that $\tilde{S}$ is a nonnegative symmetric function of its argument which is positive in a strip

$$\tilde{S}(X,X') \geq 0, \quad \tilde{S}(X,X') = \tilde{S}(X',X), \qquad \forall (X,X') \in \left(\mathbb{R}^6\right)^2, \tag{2.18}$$
$$\tilde{S}(X,X') > 0, \qquad \forall X, X', \quad |X - X'| < \alpha. \tag{2.19}$$

Therefore, $\tilde{S} \neq 0$ on a nonnegligible set (with respect to the Lebesgue measure $dX\, dX'$). It is easy to check that the functions F and H satisfy (from relations (2.15) and with $d = 6$)

$$\int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ X_i \\ |X|^2 \end{pmatrix} F(X)\, dX = \int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ X_i \\ |X|^2 \end{pmatrix} H(X)\, dX, \qquad \forall i = 1 \dots 3. \tag{2.20}$$

Note that the conservation relations (2.16) are symmetric with respect to the exchange of X and X'. This will be used to reduce the integration domains.

2.2. Existence of $\tilde{S}$ in the General Case

We now construct the function $\tilde{S}$ from $\mathbb{R}^{12}$ to $\mathbb{R}^+$ such that conservation of momentum and energy holds. These conservation laws can be written in the form

$$\int_{(\mathbb{R}^3)^4} G_i(X,Y)\tilde{S}(X,Y)\, dX\, dY = 0, \qquad i = 0 \dots 3, \tag{2.21}$$

where the functions G_i are defined by

$$G_0(X,Y) = \left(F(X)H(Y) - F(Y)H(X)\right)\left(|X|^2 - |Y|^2\right), \tag{2.22}$$
$$G_i(X,Y) = \left(F(X)H(Y) - F(Y)H(X)\right)(X_i - Y_i), \qquad i \in [1 \dots 3]. \tag{2.23}$$

The existence of such a function $\tilde{S}$ (or equivalently S since $\tilde{C}$ has been already chosen) in the cone of positive functions requires the following necessary and sufficient condition.

PROPOSITION 2.1. *There exists a positive and nonvanishing function $\tilde{S}$ satisfying (2.21) if and only if there exists no positive linear combination of the functions G_i.*

PROOF. The proof of the direct implication is obvious, by contradiction. We shall now prove that if the intersection of the space V generated by the functions $(G_i)_{i=1\dots4}$ and the cone C of positive functions reduces to the null function, then there exists a positive function $\tilde{S}$ satisfying (2.21), i.e., orthogonal to the functions $(G_i)_{i=1\dots4}$.

The sets C and V are considered as subsets of the Banach space $H = L^2$ and they are nonempty, convex and disjoint. Moreover, C is closed and it generates H in the sense that $C + (-C) = H$ and $C \cap (-C) = \{0\}$. If Hahn Banach theorem applies, these sets can be separated by an hyperplane, i.e., there exists a nonvanishing function $\tilde{S} \in H$ such that

$$\left\langle \tilde{S}, C \right\rangle \subset \mathbb{R}^+, \qquad \left\langle \tilde{S}, V \right\rangle = 0, \tag{2.24}$$

which gives the result. The difficulty relies on the fact that none of these sets are open. However, we still obtain the result. Let us consider $f_0 \neq 0$ in C and define $C_0 = \{f \geq f_0\}$. We show that the distance between V and C_0 is such that $\operatorname{dist}(V, C_0) = 2r > 0$: by contradiction, if $\exists\,(f_n) \in C$ and (x_n) in V such that

$$|f_n + f_0 - x_n| \to 0.$$

Then, if x_n is bounded, it converges toward $x_0 \in V$ (since V is closed) up to the extraction of a subsequence and $f_n + f_0 \to x_0$. Therefore f_n converges to $(x_0 - f_0) \in C$ (since C is closed) and hence, $x_0 = 0$. This implies that $f_0 \in (-C)$ and contradicts $f_0 \neq 0$. When x_n is not bounded, one can consider the sequence $x_n/|x_n|$ and obtain again a contradiction.

Let us now define the following mollification of V:

$$V_r \stackrel{\text{def}}{=} \{x \in H \mid \exists\, y \in V,\ x \in B(y, r)\}.$$

V_r is now an open convex set which is disjoint from C_0, since $r = \operatorname{dist}\,(V, C_0)/2$. We can now apply the Hahn Banach theorem which gives the existence of a nonvanishing function $\tilde{S} \in H$ and of a real number α such that

$$\left\langle \tilde{S}, x \right\rangle \geq \alpha, \quad \forall x \in C_0, \quad \left\langle \tilde{S}, x \right\rangle \leq \alpha, \quad \forall x \in V_r.$$

The second condition implies that $\langle \tilde{S}, x\rangle \leq \alpha$, $\forall x \in V$ and therefore (since V is a vector space) $\langle \tilde{S}, G_i\rangle = 0$, $\forall i \in [1 \dots 4]$ and $\alpha = 0$. The first condition reads $\langle \tilde{S}, th + f_0\rangle \geq 0$ forall $h \in C$ and forall $t \geq 0$. When $t \to \infty$, we obtain

$$\left\langle \tilde{S}, h \right\rangle \geq 0, \qquad \forall h \in C.$$

This implies that $\tilde{S} \in C$ and ends the proof. ∎

REMARK 2.2. The same proof holds when the functions G_i are in $L^p(\mathbb{R}^n)$ for $p < \infty$ and insures the existence of a function $f \in L^{p'}$. Since the functions G_i of interest are naturally in L^1, we have the existence of $\tilde{S} \in L^\infty$ (provided $V \cap C = \{0\}$ using the above notations).

REMARK 2.3. It can be proved that the function S can be chosen as an analytical function and everywhere strictly positive [12].

REMARK 2.4. Note that the construction of positive functions orthogonal to some subspaces of $C^2[0, T]$ is described in [13].

We now prove that the nonexistence of a positive combination of the G_i's is satisfied provided the distribution function f is not almost everywhere equal to a Maxwellian.

LEMMA 2.5. *Suppose that there exists $(\lambda_i)_{i=0,\dots,3}$ such that the function defined by*

$$G = \sum_{i=0}^{3} \lambda_i G_i$$

is positive on a nonnegligible set. Then, we have

$$F = H, \text{ a.e.}$$

PROOF. We prove this by contradiction: we suppose that $F \neq H$ on a nonnegligible set and we assume the existence of $(\lambda_i)_{i=0,\dots,3}$ such that $G(X,Y) \geq 0$ a.e., $(X,Y) \in \mathbb{R}^{2d}$ and such that $G > 0$ on a nonnegligible set of $\mathbb{R}^{2d}$.

By the definition of the function G_i we have

$$G(X,Y) = (F(X)H(Y) - H(X)F(Y))(P(X) - P(Y))$$

with $P(X) = \alpha_0|X|^2 + \sum_{i=1}^{3} \alpha_i X_i$. By integrating over Y, we obtain

$$\int_{\mathbb{R}^d} (F(X)H(Y) - H(X)F(Y))(P(X) - P(Y))\, dY > 0, \text{ a.e.}, X \in \mathbb{R}^d. \tag{2.25}$$

With the use of (2.20), we shall assume, without any loss of generality, that

$$\int_{\mathbb{R}^6} \begin{pmatrix} 1 \\ P(X) \end{pmatrix} F(X)\, dX = \int_{\mathbb{R}^6} \begin{pmatrix} 1 \\ P(X) \end{pmatrix} H(X)\, dX = \begin{pmatrix} 1 \\ \alpha \end{pmatrix}. \tag{2.26}$$

Then, (2.25) yields

$$(P(X) - \alpha)(F(X) - H(X)) > 0. \tag{2.27}$$

This gives

$$\begin{aligned}
\int_{P(X)>\alpha} P(X)(F(X) - H(X))\, dX &\geq \alpha \int_{P(X)>\alpha} (F(X) - H(X))\, dX, \\
&= -\alpha \int_{P(X)<\alpha} (F(X) - H(X))\, dX, \\
&= \alpha \int_{P(X)<\alpha} (H(X) - F(X))\, dX, \\
&\geq \int_{P(X)<\alpha} (H(X) - F(X))P(X)\, dX,
\end{aligned}$$

and one of these inequalities at least is strict by the fact that $G > 0$ on a nonnegligible set of $\mathbb{R}^{2d}$. This is in contradiction with

$$\int (H(X) - F(X))P(X)\, dX = 0,$$

and ends the proof. ∎

With Lemma 2.5, we prove the existence of a regularized operator $\tilde{Q}$ which satisfies Properties (P1)–(P3).

THEOREM 2.6. *There exists a positive function S such that the collision operator $\tilde{Q}$ based on the above construction satisfies properties (P1), (P2), and (P3).*

PROOF. Either $f = M^f$, a.e., and then $\tilde{Q} = 0$ or $f \neq M^f$ on a nonnegligible set, then $F \neq H$ on a nonnegligible set and there exists a function $\tilde{S}$ from Proposition 2.1. The verification of the remaining property (P3) follows from the positivity of $\tilde{S}$. Details are left to the reader. ∎

2.3. Existence of a Piecewise Constant Function S

In this section, we make an hypothesis which is a little bit restrictive but which has two main advantages: first, this assumption is easy to check numerically; second, it allows us to prove that the function S can be chosen in a very simple form, namely as a piecewise constant function. This choice is particularly convenient from the computational point of view.

First let us define the sets $\Omega_i^{\pm}, i = 0, \dots, 3$, according to the following lemma: we denote meas(A) the measure of a set A with respect to $dX\,dY$. We have the following lemmas.

LEMMA 2.7. *Assume $F(X) \neq H(X)$ on a nonnegligible set of $\mathbb{R}^d$ and define:*

$$\Omega_0^{\pm} = \left\{(X,Y) \in \mathbb{R}^{2d} \text{ s.t. } \pm G_0(X,Y) > 0\right\}, \tag{2.28}$$

$$\Omega_i^{\pm} = \left\{(X,Y) \in \mathbb{R}^{2d} \text{ s.t. } \pm G_i(X,Y) > 0\right\}. \tag{2.29}$$

Then, we have meas$(\Omega_i^{\pm}) > 0$, for all $i = 0 \dots 3$.

The proof of Lemma 2.7 follows exactly the same lines as that of Lemma 2.5 and is therefore omitted. Next, we have the following lemma.

LEMMA 2.8. *$\forall i = 0 \dots 3$, at least one of the sets Ω_i^+ or Ω_i^- defined by (2.28),(2.29) with F and H given by (2.17) is negligible (and then, both Ω_i^+ and Ω_i^- are negligible) or equivalently $F = H$ a.e. if and only if $f = M^f$, for a.e. $v \in \mathbb{R}^3$.*

PROOF. Assume one of the sets is negligible. From Lemma 2.7, we have that F is equal to H, a.e. This can be written in the form:

$$f(w+z)f(w-z) = M^f(w+z)M^f(w-z), \qquad \text{a.e. } (w,z) \in \mathbb{R}^6,$$

which implies

$$\int_{\mathbb{R}^3} f(v_1)f(v)\,dv_1 = \int_{\mathbb{R}^3} M^f(v_1)M^f(v)\,dv_1, \qquad \text{a.e. } v \in \mathbb{R}^3,$$

and yields

$$f(v) = M^f(v), \qquad \text{a.e. } v \in \mathbb{R}^3. \qquad \blacksquare$$

Now, we assume the following: any intersections of the 8 sets $\Omega_i^{\pm}$ are nonnegligible, i.e.,

$$\text{meas}\left(\cap_{j=0}^3 \Omega_j^{\alpha_j}\right) > 0, \qquad \forall (\alpha_j)_{j=0,\dots,3} \in \left(\{\pm 1\}^4\right). \tag{2.30}$$

We prove that this condition allows to construct the function S such that (2.21) holds, as a product of characteristic functions. More precisely, we set

$$S(X,X') = \prod_{i=0}^{4} \chi_i^{\pm}(X,X'), \tag{2.31}$$

where the functions $\chi_i^{\pm}$ are defined for $i = 0 \dots 3$ by

$$\chi_i^{\pm}(X,X') = \begin{cases} a_i^+, & \forall (X,X') \in \Omega_i^+, \\ a_i^-, & \text{elsewhere}, \end{cases} \tag{2.32}$$

with 8 positive real numbers $a_i^{\pm}$ to be determined. Note that $\Omega_i^- \subset (\Omega_i^+)^c$, $\forall i$, by construction. We define the following 64 constants, which depend on the distribution function f and of the choice of $\tilde{C}$

$$I_i^{\alpha} = \int_{\Omega_0^{\alpha_0} \cap \Omega_1^{\alpha_1} \cap \Omega_2^{\alpha_2} \cap \Omega_3^{\alpha_3}} \tilde{C}(z,z')\left(F(X')H(X) - F(X)H(X')\right)(X_i - X_i')\,dX\,dX', \tag{2.33}$$

$\forall i \in [0\ldots3]$ and $\forall\alpha = (\alpha_i)_{i=0\ldots3} \in \{+1,-1\}^4$ and we use the convention $X_0 = |X|^2$, for the sake of simplicity. Using (2.30), we have the following sign properties:

$$\alpha_i I_i^\alpha > 0, \tag{2.34}$$

where $\alpha = (\alpha_i)_{i=1\ldots4} \in (\{+1,-1\})^4$. With these notations and for function S of the form (2.31), the conservation of momentum (for $i = 1,2,3$) and energy (for $i = 0$) can be written as the following system of equations in the variables $a_i^\pm$ with $n = 4$:

$$\sum_{(\alpha)\in(\{+1,-1\})^n} I_i^\alpha \prod_{k=0}^{n-1} a_k^{\alpha_k} = 0, \qquad i = 0\ldots n-1. \tag{2.35}$$

We shall now prove that systems of n equations of this type for $2n$ unknowns $a_i^\pm$ have a nontrivial positive solution (with the n supplementary following constraints $a_i^- = 1$).

PROPOSITION 2.9. *Let $n \in \mathbb{N}$ and $(I_i^\alpha)_{i=0\ldots n-1,\,\alpha\in(\{+1,-1\})^n} \in (\mathbb{R})^{n2^n}$ such that (2.34) holds, be given. The system (2.35) has a nonvanishing solution $(a_i^\pm)_{i=0\ldots n-1} \in (\mathbb{R}^{+*})^{2n}$, not necessarily unique.*

PROOF. Let us fix $a_i^- = 1$ and construct sequences $((a_i)^n)_{n\in\mathbb{N}}$ which tend to a_i^+ when $n \to \infty$ as follows.

Initialize the sequences $((a_i)^n)_{n\in\mathbb{N}}$ (for $i = 1,\ldots,n$) by 1, i.e., $a_i^+ = (a_i^0)^0 = 1$. Assume a_i^m are known (in $(\mathbb{R}^+)^n$), we compute a_i^{m+1} using the i^{th} equation in (2.35) where the a_j^+ for $j \neq i$ are equal to a_j^m and $a_j^- = 1$ for all $j = 0\ldots n-1$. We have

$$a_i^{m+1} = -\frac{\sum_{(\alpha)|\alpha_i=-1} I_i^\alpha \prod_{k=0}^{n-1} a_k^{\alpha_k}}{\sum_{(\alpha)|\alpha_i=+1} I_i^\alpha \prod_{k=0,k\neq i}^{n-1} a_k^{\alpha_k}}. \tag{2.36}$$

Note that by construction we have, for all $m \in \mathbb{N}$ $a_i^{m+1} > 0$ (since $\alpha_i I_i^\alpha > 0$ for any α and the numerator contains $\prod_{k=0}^{n-1} a_k^- = 1$). We skip the term $a_i^- = 1$ in the numerator product. Then, for any of the 2^{n-1} terms (associated with a particular α^0) in the numerator sum, we have its equivalent (i.e., α with the same $\alpha_j = \alpha_j^0$, $j \neq i$) in the denominator, therefore

$$\frac{I_i^{\alpha^0} \prod_{k=0,k\neq i}^{n-1} a_k^{\alpha_k}}{\sum_{(\alpha)|\alpha_i=+1} I_i^\alpha \prod_{k=0,k\neq i}^{n-1} a_k^{\alpha_k}} \leq \frac{\max_{(\alpha),\,i=0\ldots n-1} |I_i^\alpha|}{\min_{(\alpha),\,i=0\ldots n-1} |I_i^\alpha|} \stackrel{\text{def}}{=} R. \tag{2.37}$$

Then, by adding these 2^{n-1} inequalities, we get an *a priori* upper bound for a_i^{m+1} defined by (2.36)

$$a_i^{m+1} < 2^{n-1}R. \tag{2.38}$$

Since the sum in the numerator includes a term $\prod_{k=0}^{n-1} a_k^-$ equal to unity, we also have a lower bound:

$$a_i^{m+1} > \frac{R^{-1}}{(2^{n-1}R)^{n-1}}. \tag{2.39}$$

Hence, the above constructed sequence lies in a compact set of $\mathbb{R}^n$, and thus, up to an extraction, has a limit point which gives a solution for system (2.35) which is nontrivial and positive thanks to (2.39). This ends the proof. ∎

The convergence of the whole sequence requires the uniqueness of the possible limit, which actually seems to hold, from the numerical point of view. This result may be obtained using algebra technics since (2.35) is a system of polynomial equations of degree n for the variables a_i^+ and of degree 1 with respect to each of a_i^+ separately. This remains to be proven.

We apply Proposition 2.9 with I_i^α given by (2.33) and $n = 4$. Then, we can also satisfy a normalization constraint of the form

$$\sum_{(\alpha)\in(\{+1,-1\})^4} \left(\int_{\cap_{i=0}^{3} \Omega_i^{\alpha_i}} \tilde{C}(X,X') F(X) H(X')\, dX\, dX' \right) \prod_{k=0}^{3} a_k^{\alpha_k} = N_{\text{coll}} > 0, \tag{2.40}$$

where the right-hand side is the given number of collisions for the exact Boltzmann operator defined by

$$N_{\text{coll}} \overset{\text{def}}{=} \int_{(\mathbb{R}^3)} \tilde{C}(z,z)(f(w+z)f(w-z))\, dz\, dw = \int_{\mathbb{R}^3\times\mathbb{R}^3\times S_2} C f f_1\, dv\, dv_1\, d\Omega > 0. \tag{2.41}$$

Therefore, it suffices to consider an arbitrary solution given by Proposition 2.9 and to multiply the pair (a_1^+, a_1^-) by a constant in order to satisfy the normalization requirement (2.40).

Note that the coefficients I_i^α are defined from the distribution function as integrals over $\Omega_j^\pm$ (also defined from the distribution function). Thus, the assumption (2.30) on the intersections of $\Omega_i^\pm$ naturally depends on the details of the distribution function and has to be checked. Efficient algorithms to achieve this computation practically still need to be designed.

2.4. Description of the Energy Mollified Operator

In this section, we prove that a generalized Boltzmann operator can be constructed in the particular case in which only the microscopic energy conservation is relaxed. More precisely, it consists in assuming that $\delta(w,z,w',z')$ in (2.10) is of the form

$$\delta(w,z,w',z') = \delta_z\left(|z|^2, |z'|^2\right) \delta_0(w-w'), \tag{2.42}$$

where δ_0 is the delta function. Then, the conservation of momentum is automatically verified. The detailed balanced property (2.11) can be simplified using $(w = w')$ and leads to

$$\exp\left(\frac{-|z|^2}{T_f}\right) \delta_z(z,z') = \exp\left(\frac{-|z'|^2}{T_f}\right) \delta_z(z',z), \tag{2.43}$$

where T_f is the temperature of f defined by (2.15). This condition (2.43) reads

$$\delta_z(z,z') = \exp\left(\frac{|z|^2 - |z'|^2}{2T_f}\right) S(z,z'), \tag{2.44}$$

with $S(z,z')$ symmetric and positive. The conservation of energy can be written in the following form:

$$\int_{(\mathbb{R}^3)^3} \tilde{C}(z,z')\left(|z'|^2 - |z|^2\right)\left(f(w+z)f(w-z)\exp\left(\frac{|z|^2-|z'|^2}{2T_f}\right) \right.$$
$$\left. - f(w+z') f(w-z') \exp\left(\frac{|z'|^2 - |z|^2}{2T_f}\right)\right) S(z,z')\, dz\, dz'\, dw = 0, \tag{2.45}$$

and, after integration with respect to the variable w,

$$\int_{(\mathbb{R}^3)^2} \tilde{C}(z,z')\left(|z|^2 - |z'|^2\right)\left(\alpha_f(z)\exp\left(\frac{-|z'|^2}{T_f}\right) - \alpha_f(z')\exp\left(\frac{-|z|^2}{T_f}\right)\right)$$
$$\exp\left(\frac{\left(|z'|^2 + |z|^2\right)}{2T_f}\right) S(z,z')\, dz\, dz' = 0. \tag{2.46}$$

with

$$\alpha_f(z) = \int_{\mathbb{R}^3} f(w+z)f(w-z)\,dw. \tag{2.47}$$

A corollary of Lemma 2.8 proves that the function inside the integral in (2.46)

$$G(z,z') = \left(|z|^2 - |z'|^2\right)\left(\alpha_f(z)\exp\left(\frac{|z|^2 - |z'|^2}{2T_f}\right) - \alpha_f(z')\exp\left(\frac{|z'|^2 - |z|^2}{2T_f}\right)\right),$$

is strictly positive (respectively negative) on a nonnegligible set denoted by Ω^+ (respectively Ω^-) if and only if f is not almost everywhere equal to the Maxwellian M^f. Then, a positive function S such that the energy conservation holds can be found. It can be chosen constant on the set $\Omega^\pm$ in the spirit of the Section 2.3 without any supplementary hypothesis on the distribution function in this case. Then we have Theorem 2.10.

THEOREM 2.10. *There exists a positive function S such that the operator $\tilde{Q}$ of the form (2.7) with $\tilde{C}$ given by (2.8), δ given by (2.42) and δ_z by (2.44) verifies Properties (P1)–(P3).*

2.5. Convergence When $\varepsilon \to 0$

In this section, we intend to see if we can make the regularization depend on a (small) smoothing parameter ε such that (2.6) holds when $\varepsilon \to 0$. We restrict to the energy regularization investigated in the previous section. We now consider scattering cross sections of the form

$$S_\varepsilon(z,z') = S_\varepsilon\left(|z|^2, |z'|^2\right) = \xi_\varepsilon\left(|z|^2 - |z'|^2\right).\chi_\varepsilon\left(|z|^2, |z'|^2\right), \tag{2.48}$$

with ξ an even and positive function such that $\xi_\varepsilon(t) = 1/\varepsilon\,\xi(t/\varepsilon)$ and $\int \xi(t)\,dt = 1$. We shall now prove Proposition 2.11.

PROPOSITION 2.11. *A necessary condition for the energy operator $\tilde{Q}^\varepsilon$ with S^ε given by (2.48) to be such that*

$$\lim_{\varepsilon\to 0} \tilde{Q}^\varepsilon = Q(f,f), \qquad \text{in } \mathcal{D}$$

(for smooth distribution function f) is that

$$\int_0^\infty s\,c\left(\frac{s}{2}, \frac{s}{2}\right)\mu_f(s)\,ds = 0, \tag{2.49}$$

where $\mu_f(s)$ a particular moment of f defined below. In the case where $\tilde{c}$ is a constant (Variable Hard Sphere models), condition (2.49) is written

$$\int_{w,z} C(|z|)\left(|z| - \frac{T_f}{|z|}\right) f(w+z)f(w-z)\,dw\,dz = 0. \tag{2.50}$$

PROOF. The conservation of energy can be written (after angular integration of the variables z and z')

$$\begin{aligned} 0 = \int_0^\infty \int_0^\infty \bar{c}\left(|z|^2, |z'|^2\right)\left(|z|^2 - |z'|^2\right)\Bigg(&\bar{\alpha_f}\left(|z|^2\right)\exp\left(\frac{|z'|^2 - |z|^2}{2T_f}\right) \\ &-\bar{\alpha_f}\left(|z'|^2\right)\exp\left(\frac{|z|^2 - |z'|^2}{2T_f}\right)\Bigg) S_\varepsilon\left(|z'|^2, |z|^2\right)|z|^2\,d|z|\,|z'|^2\,d|z'|, \end{aligned} \tag{2.51}$$

where we assume that the scattering cross section verifies the simplifying assumption

$$\tilde{C}\left(|z|\beta, |z'|\beta'\right) = \bar{c}\left(|z|^2, |z'|^2\right).\tilde{c}(\beta, \beta'), \tag{2.52}$$

with $z = |z|\beta$, $\beta \in S^2$, $z' = |z'|\beta'$, $\beta' \in S^2$ are the expressions of z and z' in spherical coordinates and where $\bar{\alpha_f}$ is defined by

$$\bar{\alpha_f}\left(|z|^2\right) = \int_{\beta\in S^2}\int_{\beta'\in S^2}\int_{w\in\mathbb{R}^3} \bar{c}(\beta,\beta')\, f(w+|z|\beta) f(w-|z|\beta)\, d\beta\, d\beta'\, dw. \tag{2.53}$$

We use the following change of variable $u = |z|^2$, $u' = |z'|^2$ in (2.51):

$$0 = \int_0^\infty \int_0^\infty \bar{c}(u,u')\,(u-u')\left(\bar{\alpha_f}(u)\exp\left(\frac{u'-u}{2T_f}\right) - \bar{\alpha_f}(u')\exp\left(\frac{u-u'}{2T_f}\right)\right)$$
$$\xi_\varepsilon(u-u')\,\chi_\varepsilon(u,u')\,\sqrt{u}\,du\sqrt{u'}\,du'. \tag{2.54}$$

We set $s = u + u'$ and $t = u' - u$ and define

$$\bar{G_0}(s,t) = \sqrt{s^2-t^2}\; t\; \bar{c}\left(\frac{s-t}{2},\frac{s+t}{2}\right)\left(\bar{\alpha_f}\left(\frac{s-t}{2}\right)\exp\left(\frac{t}{2T_f}\right) - \bar{\alpha_f}\left(\frac{s+t}{2}\right)\exp\left(\frac{-t}{2T_f}\right)\right), \tag{2.55}$$

for all $(s,t) \in \{s>0, |t|\le s\} \stackrel{\text{def}}{=} \Delta$. The energy conservation now reads

$$\int_\Delta \bar{G_0}(s,t)\xi_\varepsilon(t)\chi_\varepsilon\left(\frac{s-t}{2},\frac{s+t}{2}\right) ds\,dt = 0. \tag{2.56}$$

When $\varepsilon \to 0$, the function ξ_ε tends to a delta measure, and, by a classical result about smoothing kernels, the above constructed collision operator converges to the usual Boltzmann one, at least formally, provided first that

$$\bar{c}\left(\frac{s}{2},\frac{s}{2}\right) = c(s), \tag{2.57}$$

where $c(s)$ is the physical scattering cross section defined at (2.2) and second, that

$$\lim_{t\to 0}\chi_\varepsilon\left(\frac{s-t}{2},\frac{s+t}{2}\right) = 1, \qquad \forall s>0, \tag{2.58}$$

uniformly for $\varepsilon > 0$. We now investigate under what condition it is possible to find a family of functions χ_ε satisfying (2.58) which guarantee that the energy conservation (2.56) is satisfied. Let us suppose that (2.56) holds. Then, when $t \to 0$, we have, assuming enough regularity on the distribution function,

$$\lim_{t\to 0}\bar{G_0}(s,t) = \frac{1}{2}\, s\, t^2\, \bar{c}\left(\frac{s}{2},\frac{s}{2}\right)\mu_f(s), \tag{2.59}$$

with

$$\mu_f(s) = \bar{\alpha_f}'\left(\frac{s}{2}\right) + \frac{\bar{\alpha_f}(s/2)}{T_f}. \tag{2.60}$$

Therefore, at the leading order when $\varepsilon \to 0$, (2.56) leads to

$$\int_0^\infty s\bar{c}\left(\frac{s}{2},\frac{s}{2}\right)\mu_f(s)\int_{-s}^{s}\xi_\varepsilon(t)\chi_\varepsilon\left(\frac{s-t}{2},\frac{s+t}{2}\right)t^2\,dt\,ds = 0. \tag{2.61}$$

But, by (2.58), we can write

$$\chi_\varepsilon\left(\frac{s-t}{2},\frac{s+t}{2}\right) = 1 + \eta_\varepsilon(s,t), \tag{2.62}$$

with for all s,

$$\lim_{t\to 0}\eta_\varepsilon(s,t) = 0, \tag{2.63}$$

uniformly when $\varepsilon \to 0$. Inserting (2.62) in (2.61), we get

$$\int_0^\infty s\bar{c}\left(\frac{s}{2},\frac{s}{2}\right)\mu_f(s)\left(\int_{-s}^{s} t^2\xi_\varepsilon(t)\,dt\right)\left(1+\int_{-s}^{s}\eta_\varepsilon(s,t)\,d\nu_\varepsilon(t)\right)ds = 0, \tag{2.64}$$

with

$$d\nu_{\varepsilon,s}(t) = \frac{t^2\xi_\varepsilon(t)\,dt}{\int_{-s}^{s} t^2\xi_\varepsilon(t)\,dt}. \tag{2.65}$$

It is easy to see that

$$d\nu_{\varepsilon,s}(t) \to \delta(t), \text{ as } \varepsilon \to 0, \qquad \forall s > 0, \tag{2.66}$$

vaguely. Therefore, with (2.63), we have

$$\int_{-s}^{s} \eta_\varepsilon(s,t)\,d\nu_{\varepsilon,s}(t) \to 0, \text{ as } \varepsilon \to 0. \tag{2.67}$$

$\forall s > 0$, which by means of the Lebesgue theorem, implies

$$\int_0^\infty s\bar{c}\left(\frac{s}{2},\frac{s}{2}\right)\mu_f(s)\,ds = 0. \tag{2.68}$$

It is easily seen that, by the same argument as in Lemma 2.8, $\mu_f(s)$ is not of constant sign. Therefore, a function $\bar{c}$ such that (2.68) is satisfied can always be found. However, here, we require (2.57), i.e., $c = \bar{c}$ where c is the physical scattering cross section defined by (2.2). Therefore, (2.68) is no more a constraint on $\bar{c}$, but rather a constraint on f. And, obviously, this constraint is in general not satisfied. ∎

REMARK 2.12. *Note that $\mu_f = 0$ if and only if $f = M^f$ (at least when $\tilde{C}$ is constant which is the case with Variable Hard Sphere (VHS) models). The constructed collision operator for the energy relaxation case is thus a good approximation of the Boltzmann operator for distribution functions close to equilibrium.*

3. MOLLIFYING THE MASSES DURING THE COLLISION

The second regularization approach is based on the introduction of artificial masses belonging to a certain interval around the physical mass. The scattering cross section for collisions of particle with unphysical masses is designed to provide Properties (P1)–(P3). The main advantage of this method is that this generalized scattering cross section only depends on the first three moments of the distribution function (the number density, the mean velocity and the temperature). This is very interesting from the practical point of view since, for example in the homogeneous case, these corrections are computed once for all at the beginning. The principle of the mass regularization, is to act as if the particles do not have the same masses before and after the collision. For a similar approach devoted to multispecies flows, the reader can also refer to [14].

3.1. Description of the Collision Process

In this section, we describe the collision process. Let $\vec{v}$ and $\vec{v_1}$ be two incident velocities (in $\mathbb{R}^3$) corresponding to two particles of masses m and m_1. We consider post collisional velocities $\vec{v'}$ and $\vec{v_1'}$ associated with particles of masses m' and m_1' such that conservation of momentum and energy hold for this particular collision (see (1.3) and (1.4), for comparison)

$$m\vec{v} + m_1\vec{v_1} = m'\vec{v'} + m_1'\vec{v_1'}, \tag{3.1}$$

$$m|\vec{v}|^2 + m_1|\vec{v_1}|^2 = m'|\vec{v'}|^2 + m_1'|\vec{v_1'}|^2. \tag{3.2}$$

The case $m = m'$ and $m_1 = m_1'$ may be physically interpreted as a collision between particles of different species (and different masses: $A + B \to A' + B'$), whereas the general case could be interpreted as a collision with chemical reactions ($A+B \to C+D$), with a conservation of the total mass. However, in this paper, we shall distinguish the physical masses of the particles (which are the same) and the artificial masses (which serve us to generalize the collision operator). Although there is no physical justification, this procedure allows to build a collision operator satisfying Properties (P1)–(P3) defined in Section 1. We denote

$$x = \frac{m}{m+m_1}, \qquad 1-x = \frac{m_1}{m+m_1}, \tag{3.3}$$

$$y = \frac{m'}{m'+m_1'}, \qquad 1-y = \frac{m_1'}{m'+m_1'}, \tag{3.4}$$

with $(x,y) \in]0,1[^2$. The conservation relations (3.1) and (3.2) can be written

$$x\vec{v} + (1-x)\vec{v_1} = y\vec{v'} + (1-y)\vec{v_1'}, \tag{3.5}$$

$$x|\vec{v}|^2 + (1-x)|\vec{v_1}|^2 = y\left|\vec{v'}\right|^2 + (1-y)\left|\vec{v_1'}\right|^2. \tag{3.6}$$

We search now to parametrize the velocities $(\vec{v'}, \vec{v_1'})$ for a fixed pair $(\vec{v}, \vec{v_1})$ and fixed parameters x and y. We define the velocities of the pre- and post-colisional center of mass frames

$$\vec{V}(x) = x\vec{v} + (1-x)\vec{v_1}, \tag{3.7}$$

$$\vec{V'}(y) = y\vec{v'} + (1-y)\vec{v_1'}. \tag{3.8}$$

To ensure momentum conservation it is enough to take (remember that $\vec{V'}(y) = \vec{V}(x)$)

$$\vec{v'} = \vec{V}(x) + (1-y)r\vec{\omega}, \tag{3.9}$$

$$\vec{v_1'} = \vec{V}(x) - yr\vec{\omega}, \tag{3.10}$$

with $\vec{\omega} \in S^2$ and $r > 0$, S^2 being the unit sphere of $\mathbb{R}^3$ and r to be determined later on. We now impose the conservation of energy (3.6). We calculate the two quantities $|\vec{v'}|^2$ and $|\vec{v_1'}|^2$, with (3.9) and (3.10)

$$\left|\vec{v'}\right|^2 = \left|\vec{V}(y)\right|^2 + 2r(1-y)\left(\vec{\omega}, \vec{V}(y)\right) + (1-y)^2 r^2, \tag{3.11}$$

$$\left|\vec{v_1'}\right|^2 = \left|\vec{V}(y)\right|^2 + 2ry\left(\vec{\omega}, \vec{V}(y)\right) + y^2 r^2, \tag{3.12}$$

with $(.,.)$ the scalar product of two vectors of $\mathbb{R}^3$. We deduce that

$$y\left|\vec{v'}\right|^2 + (1-y)\left|\vec{v_1'}\right|^2 = \left|\vec{V}(y)\right|^2 + y(1-y)r^2. \tag{3.13}$$

We shall compute the quantity r using the conservation of energy, in terms of $\vec{v_1}$, x, and y

$$\left|\vec{V}(x)\right|^2 + y(1-y)r^2 = \left|\vec{V}(x)\right|^2 + x(1-x)\left|\vec{v} - \vec{v_1}\right|^2. \tag{3.14}$$

This equation has a unique solution $r > 0$ given by

$$r \stackrel{\text{def}}{=} \left(\frac{x(1-x)}{y(1-y)}\right)^{1/2} \left|\vec{v} - \vec{v_1}\right|. \tag{3.15}$$

3.2. Microreversibility and Invariant Measures

We define the transformation $\mathcal{T}$ as follows (the exponent $\top$ denotes the transpose of a vector).

DEFINITION 3.1. To a given $(\vec{v}, \vec{v_1}) \in (\mathbb{R}^3)^2$, $\vec{\omega} \in S^2$, $(x, y) \in]0,1[^2$, the transformation $\mathcal{T}$ associates $(\vec{v'}, \vec{v'_1}) \in (\mathbb{R}^3)^2$, $\vec{\omega'} \in S^2$, $(x', y') \in]0,1[^2$ such that

$$\mathcal{T}(\vec{v}, \vec{v_1}, x, y, \omega)^\top \stackrel{\text{def}}{=} \left(\vec{v'}, \vec{v'_1}, y, x, \frac{\vec{v} - \vec{v_1}}{|\vec{v} - \vec{v_1}|}\right)^\top, \tag{3.16}$$

where $(\vec{v'}, \vec{v'_1})$ are defined by (3.9),(3.10). This transformation describes the collision process.

We also define the space of collisional parameters by

$$\mathcal{E} = \left\{(\vec{v}, \vec{v_1}, x, y, \vec{\omega})^\top \in \left(\mathbb{R}^3\right)^2 \times]0,1[^2 \times S^2\right\}. \tag{3.17}$$

This transformation can be decomposed in the center of mass frame according to $\mathcal{T} = \Phi^{-1} \circ \mathcal{C} \circ \Phi$ with $\mathcal{C}$ the collision process in the center of mass frame and Φ being defined by Definition 3.2.

DEFINITION 3.2. $\forall (\vec{v}, \vec{v_1}, x, y, \vec{\omega})^\top \in \mathcal{E}$, we define

$$\Phi(\vec{v}, \vec{v_1}, x, y, \vec{\omega})^\top \stackrel{\text{def}}{=} \left(\vec{V(x)} = x\vec{v} + (1-x)\vec{v_1}, \vec{g} = \vec{v} - \vec{v_1}, x, y, \vec{\omega}\right)^\top. \tag{3.18}$$

Its Jacobian determinant verifies:

$$\det(\partial\mathcal{T}) = \det\left(\partial\Phi^{-1}\right) \circ \det(\partial\mathcal{C}) \circ \det(\partial\Phi).$$

We calculate the Jacobian of the transformation Φ:

$$|\det(\partial\Phi)| = 1.$$

The Jacobian of $\mathcal{T}$ can be written

$$|\det(\partial\mathcal{T}(\mathcal{V}))| = \sqrt{\frac{|g|^2}{g_y^2 + g_z^2}} \sin(\theta), \tag{3.19}$$

with $\vec{g} = (g_x, g_y, g_z)$ and with the classical parametrization of $\vec{\omega}$

$$\vec{\omega} = (\cos(\theta), \sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi)). \tag{3.20}$$

Parameterizing $\vec{\omega'} = (v - v_1/|v - v_1|)$ by

$$\vec{\omega'} = \left(\cos(\theta'), \sin(\theta')\cos(\phi'), \sin(\theta')\sin(\phi')\right), \tag{3.21}$$

and remarking that

$$\sqrt{\frac{g_y^2 + g_z^2}{|g|^2}} = \sin(\theta'),$$

we can put the Jacobian of $\mathcal{T}$ in the form

$$\det(\partial\mathcal{T}(\mathcal{U})) = \frac{J(\mathcal{U})}{J(\mathcal{U}')},$$

with $\mathcal{U} = (v, v_1, x, y, \omega)$, $\mathcal{U}' = \mathcal{T}(\mathcal{U})$ and

$$J(\mathcal{U}) = (x(1-x))^{3/2} \sin(\theta).$$

Now we set, for simplicity

$$p(x) = 32\left(x - x^2\right)^{3/2}. \tag{3.22}$$

Note that the factor 32 is chosen such that $p(1/2) = 1$ since it will allow to recover the standard Boltzmann operator in a following section. We deduce Proposition 3.3.

PROPOSITION 3.3. *The following measure*

$$p(x)\sin(\theta)\,dx\,dy\,d\vec{v_1}\,d\vec{v}\,d\vec{\omega}, \tag{3.23}$$

is invariant under the transformation $\mathcal{T}$.

REMARK 3.4. Let $\mathcal{T}$ be an involutive differentiable application of $\mathcal{E}$. Then, the measure $\sqrt{|\det(\partial\mathcal{T}(X))|}\,dX$ is invariant under the the transformation $\mathcal{T}$. Indeed, by the use of the property $\mathcal{T} = \mathcal{T}^{-1}$, we deduce

$$\partial\mathcal{T}(X) = \left(\partial\mathcal{T}^{-1}(\mathcal{T}(X))\right)^{-1}. \tag{3.24}$$

By taking the determinant of each member and by putting $X' = \mathcal{T}(X)$

$$\det(\partial\mathcal{T}(X)) = \frac{1}{\det(\partial\mathcal{T}(X'))}, \tag{3.25}$$

then we have

$$dX' = d(\mathcal{T}(X)) = \det(\partial\mathcal{T}(X))\,dX = \sqrt{\frac{|\det(\partial\mathcal{T}(X))|}{|\det(\partial\mathcal{T}(X'))|}}\,dX. \tag{3.26}$$

Invariants quantities by the transformation $\mathcal{T}$ can be easily built: let h be defined on $\mathcal{E}$ and taking values in $\mathbb{R}^d$ and g be a real function. For example, we can consider the quantities of the form

$$g(\langle h(X), h(\mathcal{T}(X))\rangle),$$

where $\langle x, y\rangle$ stands for the inner product in $\mathbb{R}^d$.

3.3. Definition of the Mass Regularized Operator

We consider a sub interval $\mathcal{I}$ of $]0,1[$ having the form $\mathcal{I} =]\eta, 1-\eta[$, with $1/2 > \eta > 0$ and '*cut off*' functions of the form

$$h_\varepsilon\left(x - \frac{1}{2}\right) = \frac{1}{\varepsilon}\xi\left(\frac{x - 1/2}{\varepsilon}\right), \tag{3.27}$$

with $\xi(z)$ an even, positive and sufficiently smooth function verifying

$$\int_{z\in\mathcal{I}} \xi\left(z - \frac{1}{2}\right)dz = 1.$$

We consider also the function χ defined by

$$\chi(a,b,c,d,x,y) = \begin{cases} 1, & \text{if } (x\ln(a) + (1-x)\ln(b) - y\ln(c) - (1-y)\ln(d))(cd - ab) \le 0, \\ 0, & \text{elsewhere.} \end{cases} \tag{3.28}$$

DEFINITION 3.5. *For all $\varepsilon > 0$ and for any given distribution function f, we define*

$$\begin{aligned} \mathcal{C}_\varepsilon(f,f) = \int_{\mathbb{R}^3}\int_{S^2}\int_{(x,y)\in\mathcal{I}^2} & q\left(\frac{|\vec{v} - \vec{v_1}| + \left|\vec{v'} - \vec{v_1'}\right|}{2}, \vec{\omega}\right) \\ & \chi\left(\frac{f}{M}, \frac{f_1}{M_1}, \frac{f'}{M'}, \frac{f_1'}{M_1'}, x, y\right) \\ & \left(\frac{M_1 M f' f_1' - M_1' M' f f_1}{\sqrt{M_1 M M_1' M'}}\right) \\ & h_\varepsilon\left(x - \frac{1}{2}\right) h_\varepsilon\left(y - \frac{1}{2}\right) d\vec{v_1}\, d\vec{\omega} 2xp(x)\,dx\,dy, \end{aligned}$$

where $(\vec{v'}, \vec{v_1'}, \vec{\omega'}, x', y') = \mathcal{T}(\vec{v}, \vec{v_1}, \vec{\omega}, x, y)$ ($\mathcal{T}$ being defined in Definition 3.1), $q(u,\vec{\omega}) = u\sigma(u,\omega)$, and σ is the differential scattering and $M = M^f$ is the Maxwellian with the same first five moments as f.

We formally have Proposition 3.6.

PROPOSITION 3.6. *The limit when $\varepsilon \to 0$ of $\mathcal{C}_\varepsilon(f,f)$ given by Definition 3.5 is the usual Boltzmann operator*

$$\lim_{\varepsilon\to 0} \mathcal{C}_\varepsilon(f,f) = \int_{\mathbb{R}^3}\int_{S^2} (f'f_1' - ff_1)\, q\left(|\vec{v}-\vec{v_1}|,\vec{\omega}\right) d\vec{v_1}\, d\vec{\omega}, \qquad \text{in } \mathcal{D}. \tag{3.29}$$

PROOF. In the limit $\varepsilon \to 0$, we have, in the distributional sense

$$\lim_{\varepsilon\to 0} h_\varepsilon\left(x-\frac{1}{2}\right) = \delta_{1/2}, \tag{3.30}$$

where $\delta_{1/2}$ is the delta measure located at $x = 1/2$ and, for $x = y = 1/2$ we have $p(1/2) = 1$ and $\chi(a,b,c,d,1/2,1/2) \equiv 1$: indeed, $\forall (a,b,c,d) \in \mathbb{R}_+^4$, we verify

$$\lim_{x\to 1/2,\, y\to 1/2} \chi(a,b,c,d,x,y) = 1. \tag{3.31}$$

This is obvious in the case $ab = cd$ and, in the converse case, $ab \neq cd$ and for (x,y) close enough of $(1/2,1/2)$, we have $\chi = 1$ by monotony of the logarithm

$$(a-b)(\ln(b)-\ln(a)) \le 0, \qquad \forall a,b \ge 0.$$

Finally, for any Maxwellian, any 4-tuple of velocities $(\vec{v},\vec{v'},\vec{v_1},\vec{v_1'})$ satisfying the conservation of momentum and energy (3.1),(3.2) and for $x = y = 1/2$, we have

$$M_1 M = M' M_1'.$$

This ends the proof. ∎

3.4. Properties of the Operator $\mathcal{C}_\varepsilon$

We now check Properties (P1)–(P3) for $\mathcal{C}_\varepsilon(f,f)$ given by Definition 3.5. For that purpose, we introduce the weak formulation of this operator and we symmetrize it as follows: by Definition 3.5, momentum and energy conservation relation (3.3),(3.4) and Proposition 3.3 on invariant measures, we have, for all test functions ϕ

$$\begin{aligned}\int_{\mathbb{R}^3} \mathcal{C}_\varepsilon(f,f)\phi(\vec{v})\, d\vec{v} = \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{S^2}\int_{(x,y)\in\mathcal{I}^2} & q\left(\frac{|\vec{v}-\vec{v_1}|+|\vec{v}-\vec{v_1}|}{2},\vec{\omega}\right)\\ & \chi\left(\frac{f}{M},\frac{f_1}{M_1},\frac{f'}{M'},\frac{f_1'}{M_1'},x,y\right)\\ & \left(\frac{M_1 M f' f_1' - M_1' M' f f_1}{\sqrt{M_1 M M_1' M'}}\right)(x\phi + (1-x)\phi_1 - y\phi' - (1-y)\phi_1')\\ & h_\varepsilon\left(x-\frac{1}{2}\right) h_\varepsilon\left(y-\frac{1}{2}\right) d\vec{v_1}\, d\vec{\omega}\, d\vec{v} p(x)\, dx\, dy.\end{aligned}$$

3.4.1. Conservation laws, i.e., (P1)

PROPOSITION 3.7. *Conservations of mass, momentum and energy hold true*

$$\int_{\vec{v}\in\mathbb{R}^3} \begin{pmatrix} 1 \\ \vec{v} \\ |\vec{v}|^2 \end{pmatrix} \mathcal{C}_\varepsilon(f,f)\, d\vec{v} = \vec{0}. \tag{3.32}$$

PROOF. By taking successively $\phi = 1$, $\vec{v}$ and $|\vec{v}|^2$ in the above weak formulation, we can easily verify from (3.5) and (3.6) that (3.32) holds. This ends the proof. ∎

We note that the term

$$\chi\left(\frac{f}{M},\frac{f_1}{M_1},\frac{f'}{M'},\frac{f_1'}{M_1'},x,y\right),$$

in the definition of the collision operator, does not play any role for the establishment of the conservation laws.

3.4.2. Entropy Dissipation, i.e., (P3)

PROPOSITION 3.8. *We have the following inequality*

$$\int_{\mathbb{R}^3} \mathcal{C}_\varepsilon(f,f)\ln(f)\,d\vec{v} \le 0. \tag{3.33}$$

PROOF. Using the weak formulation of $\mathcal{C}_\varepsilon(f,f)$ and replacing ϕ by $\ln(f)$ in it, we obtain

$$\begin{aligned}\int_{\mathbb{R}^3} \mathcal{C}_\varepsilon(f,f)\ln(f)\,d\vec{v} =& \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{S^2}\int_{(x,y)\in\mathcal{I}^2} q\left(\frac{|\vec{v}-\vec{v_1}|+|\vec{v}-\vec{v_1}|}{2},\vec{\omega}\right)\\ &\chi\left(\frac{f}{M},\frac{f_1}{M_1},\frac{f'}{M'},\frac{f_1'}{M_1'},x,y\right)\\ &\left(\frac{M_1Mf'f_1'-M_1'M'ff_1}{\sqrt{M_1MM_1'M'}}\right)\\ &(x\ln(f)+(1-x)\ln(f_1)-y\ln(f')-(1-y)\ln(f_1'))\\ &h_\varepsilon\left(x-\frac{1}{2}\right)h_\varepsilon\left(y-\frac{1}{2}\right)\,d\vec{v_1}\,d\vec{v}\,d\vec{\omega}p(x)\,dx\,dy.\end{aligned} \tag{3.34}$$

By the use of the conservations of mass, momentum and energy, we have that $\ln(M)$ is an invariant for the collision operator, for any Maxwellian M. Therefore, (3.34) can be written as

$$\begin{aligned}\int_{\mathbb{R}^3} \mathcal{C}_\varepsilon(f,f)\ln(f)\,d\vec{v} =& \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{S^2}\int_{(x,y)\in\mathcal{I}^2} q\left(\frac{|\vec{v}-\vec{v_1}|+|\vec{v}-\vec{v_1}|}{2},\vec{\omega}\right)\\ &\chi\left(\frac{f}{M},\frac{f_1}{M_1},\frac{f'}{M'},\frac{f_1'}{M_1'},x,y\right)\\ &\left(\frac{f'f_1'}{M'M_1'}-\frac{ff_1}{MM_1}\right)\sqrt{M_1MM_1'M'}\\ &\left(x\ln\left(\frac{f}{M}\right)+(1-x)\ln\left(\frac{f_1}{M_1}\right)-y\ln\left(\frac{f'}{M'}\right)-(1-y)\ln\left(\frac{f_1'}{M_1'}\right)\right)\\ &h_\varepsilon\left(x-\frac{1}{2}\right)h_\varepsilon\left(y-\frac{1}{2}\right)\,d\vec{v_1}\,d\vec{v}\,d\vec{\omega}p(x)\,dx\,dy.\end{aligned}$$

Definition (3.28) of $\chi(f/M, f_1/M_1, f'/M', f_1'/M_1', x, y)$ ensures artificially the positivity of the above expression and ends the proof. ∎

3.4.3. Maxwellian steady states, i.e., (P2)

By construction, we easily verify Proposition 3.9.

PROPOSITION 3.9.

$$f(\vec{v}) = M_{\rho,u,T}(\vec{v}) \Rightarrow \mathcal{C}_\varepsilon(f,f) = 0. \tag{3.35}$$

The converse implication is not clear, because the term χ can vanish for some velocities even if the distribution function is not identically a Maxwellian. The only equilibrium states of an operator of the form

$$Q_{\alpha,\varepsilon}(f,f) = (1-\alpha)\mathcal{C}_\varepsilon(f,f) + \alpha Q(f,f), \tag{3.36}$$

with $\alpha \in]0,1[$, $\mathcal{C}_\varepsilon(f,f)$ given by Definition 3.5 and $Q(f,f)$ the standard Boltzmann operator given by (3.29) are the Maxwellians. Indeed, since the only steady states of $Q(f,f)$ are the Maxwellians, we have proved that $Q_{\alpha,\varepsilon}$ satisfies Properties (P1)–(P3). The modification of $\mathcal{C}_\varepsilon$ into $Q_{\alpha,\varepsilon}$ is not unnatural from the numerical point of view. It can be seen as a splitting of the collision operator between the regularized operator which allows much more collisions and the standard operator which eliminates spurious steady states.

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