Mathematical Models and Methods in Applied Sciences

CONSERVATIVE AND ENTROPY SCHEMES FOR THE BOLTZMANN COLLISION OPERATOR OF POLYATOMIC GASES

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We propose two discrete velocity models derived from the Boltzmann equation of Larsen-Borgnakke type for polyatomic gases. These two models are natural extensions of previously discussed discrete velocity models used for monoatomic gases. These two models have the same properties as the continuous one, which are conservation of mass, momentum and energy, discrete Maxwellians as equilibrium states and H-theorems.

1. Introduction

numerical methods for the Boltzmann equation of monoatomic gases, (see [5, 10, 20, 18]), are based on the kinetic theory of gases with a discrete velocity repartition [9]. These methods have been developped in the case of monoatomic gases. Only very few extensions to polyatomic gases have been made. Goldstein [11] gives the dynamics of collisions for a discrete polyatomic gas; Nanbu [17] proposes a discrete Boltzmann equation which is not related with the continuous Larsen-Borgnakke model. We present the natural extension of the discrete velocity model given in [5] to the polyatomic case. Our model is based on the Larsen-Borgnakke model [3] where the internal energy is assumed to take continuous values. Two discrete velocity models will be proposed, which both share the same properties as the continuous Larsen-Borgnakke model. The derivation of these two discrete models is a first step to obtain conservative and entropy decreasing numerical schemes for the Boltzmann equation of polyatomic gases. Space and time discretization and numerical results will be the subject of a forthcoming paper.

2. The Larsen-Borgnakke Model

A gas with δ " internal degrees of freedom", associated with a polytropic constant $\gamma = \dfrac{5+\delta}{3+\delta}$, is described by a distribution function $f(x, v, I, t)$, where $(x, v, I, t) \in \mathbb{R}^3 \times \mathbb{R}^+ \times \mathbb{R}^+$, x being the position variable of the molecule, v its velocity, I^2 its internal energy and t the time. We refer to [6] for general considerations on distribution functions and the Boltzmann equation. The number density $n(x, t)$ of parti-

cles, the momentum density $n(x,t)U(x,t)$ and the total energy density $n(x,t)E(x,t)$ are defined respectively by

$$\begin{pmatrix} n(x,t) \\ n(x,t)U(x,t) \\ n(x,t)E(x,t) \end{pmatrix} = \int_{\mathbb{R}^3\times\mathbb{R}^+} \begin{pmatrix} 1 \\ v \\ \frac{|v|^2}{2} + I^2 \end{pmatrix} f(x,v,I,t) dv I^{\delta-1} dI. \tag{2.1}$$

Following [4], the collision operator for $f(x,v,I,t)$ is defined by:

$$Q_\delta(f,f) = \int_\Delta B(f'f'_* - ff_*) dv_* I_*^{\delta-1} dI_* d\eta (r(1-r))^{\frac{\delta}{2}-1} dr R^2 (1-R^2)^{\delta-1} dR \tag{2.2}$$

with

$$g = \frac{v - v_*}{2} = \text{relative velocity,}$$
$$E^2 = |g|^2 + I^2 + I_*^2 = \text{total energy,}$$
$$(v_*, I_*, \eta, r, R) \in \Delta = \mathbb{R}^3 \times \mathbb{R}^+ \times S^{2,+} \times [0,1]^2,$$
$$B := B(E, |Rg|, |Rg.\eta|, I^2 r(1-R^2), I_*^2(1-r)(1-R^2)) > 0,$$
$$f = f(x,v,I,t),\ f_* = f(x,v_*,I_*,t),\ f' = f(x,v',I',t),\ f'_* = f(x,v'_*,I'_*,t),$$

and the collision process is defined by

$$\left\{ \begin{array}{c} v + v_* = v' + v'_* \\ g' = \dfrac{RE}{|g|}\{g - 2(g.\eta)\eta\} \\ I' = \sqrt{r(1-R^2)}E \\ I'_* = \sqrt{(1-r)(1-R^2)}E \end{array} \right. \tag{2.3}$$

S^2 is the unit sphere of $\mathbb{R}^3$. The corresponding Boltzmann equation reads:

$$\frac{\partial f}{\partial t} + v.\nabla_x f = Q_\delta(f,f). \tag{2.4}$$

The properties (see [4]) of the Boltzmann collision operator (2.2) are conservation of mass, momentum and energy, and dissipation of entropy: let $\varphi(v,I)$ be any smooth test function, we consider a weak formulation of the collision operator (2.2) which can be symmetrized as follows

$$\int_{\mathbb{R}^3\times\mathbb{R}^+} Q_\delta(f,f)\varphi dv I^{\delta-1} dI$$
$$= -\frac{1}{4}\int_{\mathbb{R}^3\times\mathbb{R}^+} Q_\delta(\varphi' + \varphi'_* - \varphi - \varphi_*) dv I^{\delta-1} dI. \tag{2.5}$$

Then the conservation of mass, momentum and energy can be written with $\varphi = 1, v, \frac{|v|^2}{2} + I^2$

$$\int_{\mathbb{R}^3\times\mathbb{R}^+} Q_\delta(f,f) \begin{pmatrix} 1 \\ v \\ \frac{|v|^2}{2} + I^2 \end{pmatrix} dv I^{\delta-1} dI = 0 \tag{2.6}$$

and the dissipation of entropy reads

$$\int_{\mathbb{R}^3\times\mathbb{R}^+} Q_\delta(f,f)\log(f)dvI^{\delta-1}dI \leq 0. \tag{2.7}$$

Any equilibrium distribution function, f satisfying $Q_\delta(f,f)=0$, is a Maxwellian

$$f(v) = C_\delta \frac{\rho}{(RT)^{(3+\delta)/2}} \quad exp(-\frac{|v-u|^2+2I^2}{2RT}), \tag{2.8}$$

where $\rho, T \in \mathbb{R}$, $\rho > 0, T > 0$, and $u \in \mathbb{R}^3$. $(\rho,\, u,\, T)$ are the density, mean velocity and temperature of the gas and C_δ is a constant of normalization.

In the homogeneous case, i.e. when the distribution function is independent of the space variable x,the H-theorem follows from (2.7):

$$\begin{aligned} &\frac{d}{dt}\int_{\mathbb{R}^3\times\mathbb{R}^+} f(v,I,t)\log f(v,I,t)dvI^{\delta-1}dI \\ &= \int_{\mathbb{R}^3\times\mathbb{R}^+} Q_\delta(f,f)(1+\log f)dvI^{\delta-1}dI \leq 0. \end{aligned} \tag{2.9}$$

Furthermore $H(f)$ can only be minimal if f is an equilibrium distribution (i. e. if f is a Maxwellian).

For the classical variable hard sphere (VHS) model B is simply given by:

$$B = CR^{1-2\alpha}|g|^{-2\alpha}|g.\eta| \tag{2.10}$$

with $\alpha \in [0, \frac{1}{2}]$.

At the first order in the collision dominated limit(i.e. when the Knudsen number tends to zero), the fluid limit of the Boltzmann equation (2.4) yields the Euler equations for a polytropic gas with $\gamma \in [1, \frac{5}{3}]$.

Another formulation of the Boltzmann equation for polyatomic gases is (see [7])

$$\frac{\partial f}{\partial t} + v.\nabla_x f = I^{\alpha-\delta}Q_\alpha(f,f), \tag{2.11}$$

where $\alpha \geq 1.$ and the moments are still defined by (2.1). In [7] α is taken equal to 2. This is a manner to simplify the numerical treatment of the collision operator for different values of δ.

3. Another Forms of the Collision Operator Q_δ

For our purpose the form of the collision operator (2.2) is not well adapted. We change the formulation of the collision operator to make the derivation of discrete velocity and internal energy models easier. In (2.4) we make the change of variables

$$\eta \to \omega = \frac{g}{|g|} - 2(\frac{g}{|g|}.\eta)\eta$$

with $\omega \in S^2$ for which the jacobian is $(\dfrac{|g|}{4|\eta.g|})^{-1}$. The collision process for g is now defined by

$$g' = RE\omega$$

We also make the following change of variables$(a,b) \to (R,r)$ defined by

$$R = \cos a, \quad r = \cos^2 b$$

for $(a,b) \in [0,\pi/2]^2$. The whole collision process is now defined by

$$\left\{\begin{array}{c} v' + v'_* = v + v_* \\ g' = (\cos a)E\omega \\ I' = (\sin a \cos b)E \\ I'_* = (\sin a \sin b)E \end{array}\right. \tag{3.12}$$

and the collision operator can be written

$$Q_\delta(f,f) = \int_{\mathrm{I\!R}^3\times\mathrm{I\!R}^+\times S^2\times[0,\pi/2]^2} B(f'f'_* - ff_*)d\sigma \tag{3.13}$$

and

$$d\sigma = (\cos b \sin a)^{\delta-1}(I_* \sin b \sin a)^{\delta-1} dv_* dI_* d\omega \sin a \cos^2 a da db$$

$$B := B(E, |g|.|g'|, |g.g'|, II', I_*I'_*) > 0$$

For example, in the case of the VHS model B is of the form

$$B = C|Rg|^{1-2\alpha}.$$

We introduce the following notations:

$$\Omega = \begin{pmatrix} \omega \cos a \\ \cos b \sin a \\ \sin b \sin a \end{pmatrix}, \quad V = \begin{pmatrix} g \\ I \\ I_* \end{pmatrix},$$

where $(\omega, a, b) \in S^2 \times [0,\pi/2]^2$. The superficial measure on the quarter S^4_+ of the sphere S^4 defined by $S^4_+ = \{\Omega = (\Omega_1,\Omega_2,\Omega_3,\Omega_4,\Omega_5) \in \mathrm{I\!R}^5 / |\Omega_1|^2 + |\Omega_2|^2 + |\Omega_3|^2 + |\Omega_4|^2 + |\Omega_5|^2 = 1,\ \Omega_4 > 0,\ \ \Omega_5 > 0\}$ is $d\Omega = d\omega\ db\ \sin a \cos^2 a\ da$. Then we have

$$Q_\delta(f,f) = \int_{(v_*,I_*)\in\mathrm{I\!R}^3\times\mathrm{I\!R}_+,\Omega\in S^4_+} \mathcal{B}.(f'f'_* - ff_*)dv_* dI_* d\Omega \tag{3.14}$$

with the collision process defined by

$$V' = |V|.\Omega \quad, \Omega' = \frac{V}{|V|} \tag{3.15}$$

and with:

$$f = f(x,v,I,t),\ f_* = f(x,v_*,I_*,t)$$

$$f' = f(x, \frac{v+v_*}{2} + g', I', t), \;\; f'_* = f(x, \frac{v+v_*}{2} - g', I'_*, t)$$
$$\mathcal{B} = \Omega_4^{\delta-1} I_*^{\delta-1} \Omega_5^{\delta-1} B.$$

The proof of the H-theorem with this form of the collision operator (3.14) can be easily obtained using the property (2.5). We can remark that

$$dI_* dv_* dI dv d\Omega = d(\frac{v+v_*}{2}) dV d\Omega$$

let us define the transformations

$$\begin{pmatrix} g \\ I \\ I_* \\ \Omega_1 \\ \Omega_2 \\ \Omega_3 \\ \Omega_4 \\ \Omega_5 \end{pmatrix} \rightarrow \begin{pmatrix} V' \\ \Omega' \end{pmatrix} = \begin{pmatrix} -g \\ I_* \\ I \\ \Omega_1 \\ \Omega_2 \\ \Omega_3 \\ \Omega_5 \\ \Omega_4 \end{pmatrix}$$

and

$$\begin{pmatrix} V \\ \Omega \end{pmatrix} \rightarrow \begin{pmatrix} V' \\ \Omega' \end{pmatrix} = \begin{pmatrix} |V|.\Omega \\ \frac{V}{|V|} \end{pmatrix}.$$

These transformations are both involutives and their jacobian is equal to unity. Therefore they preserve the measure $dVd\Omega$, i.e. $dVd\Omega = dV'd\Omega'$. Using the invariance of

$$B.I^{\delta-1}\Omega_4^{\delta-1} I_*^{\delta-1} \Omega_5^{\delta-1},$$

by these transformations we recover property (2.5) for the collision operator (3.14) expressed in the new variables, by exchanging (v, I) and (v_*, I_*) or (v, I, v_*, I_*) and (v', I', v'_*, I'_*) respectively. Starting from (2.2) and (2.3), we can also rewrite the collision operator in a more classical form by using the change of variables

$$\left\{ \begin{array}{c} e = I^2 \\ \omega = \frac{g}{|g|} - 2(\frac{g}{|g|}.\eta)\eta. \end{array} \right.$$

Now E is given by $|g|^2 + e + e_*$, the collision process is defined by

$$\left\{ \begin{array}{c} v + v_* = v' + v'_* \\ g' = R\sqrt{E}\omega \\ e' = r(1-R^2)E \\ e'_* = (1-r)(1-R^2)E \end{array} \right. \tag{3.16}$$

and the collision operator can be written

$$Q_\delta(f,f) = \int_{\mathbb{R}^3 \times \mathbb{R}^+ \times S^2 \times [0,1]^2} B(f'f'_* - ff_*) d\sigma \tag{3.17}$$

with

$$d\sigma = dv_* e_*^{\frac{\delta}{2}-1} de_* d\omega R^2(1-R^2)^{\delta-1} dR [r(1-r)]^{\frac{\delta}{2}-1} dr,$$
$$B := B(E, |g|.|g'|, |g.g'|, ee', e_* e'_*) > 0.$$

4. Discrete Velocity and Energy Models

We start from (3.14) and (3.17) to derive discrete Boltzmann equations. We obtain two models which differ by the dicretization of the internal energy e. In the first one we discretize uniformly $\sqrt{e}$ while in the second model the discretization is uniform in e. With these two models, it is straightforward to derive a discrete version of the equation (2.11).

4.1. A first discrete velocity and energy model

We consider the space homogeneous problem

$$\begin{cases} \dfrac{df}{dt} = Q_\delta(f,f) \\ f_{|t=0} = f_0(v,I) \end{cases} \tag{4.18}$$

where $Q_\delta(f,f)$ is given by (3.14).

4.1.1. *Discretization*

We take a regular discretization of $\mathbb{R}^3 \times \mathbb{R}_+$:

let us introduce $\Delta v > 0$, $\{e_1, e_2, e_3, e_4\}$ the canonical base of $\mathbb{Z}^4$, $z_i = (v_i, I_i) = (i + \frac{1}{2}e_4)\Delta v$, $i = (i_1, i_2, i_3, i_4) \in L = \mathbb{Z}^3 \times \mathbb{N}$, and an approximation $f_i(t)$ of $(\Delta v)^4 f(z_i, t)$. We introduce a particle approximation of the problem (4.18). Given any test function $\varphi(v, I)$ we have

$$\int_{\mathbb{R}^3\times\mathbb{R}_+} \frac{df}{dt}\varphi(v,I) I^{\delta-1} dv dI$$
$$= \frac{1}{4}\int_{\mathbb{R}^3\times\mathbb{R}_+} Q_\delta(\varphi(v,I) + \varphi(v_*, I_*) - \varphi(v'_*, I'_*) - \varphi(v', I')) I^{\delta-1} dv dI \tag{4.19}$$

and

$$\frac{1}{4}\int_{\mathbb{R}^3\times\mathbb{R}_+} Q_\delta(\varphi + \varphi_* - \varphi' - \varphi'_*) I^{\delta-1} dv dI$$
$$= \int_{\mathbb{R}^3\times\mathbb{R}_+\times\mathbb{R}^3\times\mathbb{R}_+\times S^4_+} \mathcal{C}(\varphi + \varphi_* - \varphi' - \varphi'_*)(f'f'_* - ff_*) d\Omega dv_* dI_* dv dI \tag{4.20}$$

where we have set for simplicity

$$\varphi = \varphi(v,I),\ \ \varphi_* = \varphi(v_*, I_*),$$
$$\varphi' = \varphi(\frac{v+v_*}{2} + g', I'),\ \ \varphi'_* = \varphi(\frac{v+v_*}{2} - g', I'_*),$$

$$\mathcal{C} = \frac{1}{4}\mathcal{B}I^{\delta-1} = \frac{1}{4}I^{\delta-1}\Omega_4^{\delta-1}I_*^{\delta-1}\Omega_5^{\delta-1}B := \mathcal{C}(e, |g|.|g'|, |g.g'|, II', I_*I'_*).$$

We obtain an approximation of the two terms of the equality (4.19) by using quadrature formulaes for the integrals with respect to $(v_*, I_*), (v, I)$, the quadrature points of which are the lattice points of $\Delta v.L$. First, we get an approximation of the left hand side, of the form

$$\int_{\mathbb{R}^3\times\mathbb{R}_+} \frac{df}{dt}\varphi(v, I)I^{\delta-1}dvdI \simeq (\Delta v)^4 \sum_{i\in L} \frac{df_i}{dt}\varphi(z_i)I_i^{\delta-1} \tag{4.21}$$

For the right hand side we make some transformations . We set

$$U = \frac{v + v_*}{2}$$

we have

$$dvdv_*dIdI_* = 8dUdV$$

and, therefore,

$$\begin{aligned}&\int_{\mathbb{R}^3\times\mathbb{R}_+\times\mathbb{R}^3\times\mathbb{R}_+\times S_+^4} \mathcal{C}(\varphi + \varphi_* - \varphi' - \varphi'_*)(f'f'_* - ff_*)dv_*dI_*dvdId\Omega \\ &\quad = 8\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}_+^2\times S_+^4} \mathcal{C}.(\varphi + \varphi_* - \varphi' - \varphi'_*)(f'f'_* - ff_*)dUdVd\Omega.\end{aligned} \tag{4.22}$$

We discretize first in the variable U. Since $z_i \in \Delta vL$ then for U the quadrature points U_m are the elements of $\frac{\Delta v}{2}\mathbb{Z}^3$. We obtain a quadrature formula for the collision operator of the form

$$\begin{aligned}&\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}_+^2\times S_+^4} \mathcal{C}(\varphi + \varphi_* - \varphi' - \varphi'_*)(f'f'_* - ff_*)d\Omega dUdV \\ &\simeq \Delta v^3 \sum_{m\in\mathbb{Z}^3} \int_{\mathbb{R}^3\times\mathbb{R}_+^2\times S_+^4} \mathcal{C}(\varphi(U_m + g, I) + \varphi(U_m - g, I_*) \\ &\qquad -\varphi(U_m + g', I') - \varphi(U_m - g', I'_*)) \\ &(f(U_m + g', I')f(U_m - g', I'_*) - f(U_m + g, I)f(U_m - g, I_*))dVd\Omega.\end{aligned} \tag{4.23}$$

We now discretize in the variable V. For a fixed U_m we can write $U_m = \Delta v(\frac{\varepsilon}{2} + p)$ where $p \in \mathbb{Z}^3$ and $\varepsilon = (\varepsilon_1, \varepsilon_1, \varepsilon_1) \in \{0, 1\}^3$. Since the points (v, I) lie in L, the quadrature points for V are then necessarily in $\Delta v\big((\frac{\varepsilon}{2} + \mathbb{Z}^3) \times (\mathbb{N} + \frac{1}{2})^2\big)$. Using the same type of quadrature formula as for U, we have the approximation

$$\begin{aligned}&\sum_{m\in\mathbb{Z}^3} \int_{\mathbb{R}^3\times\mathbb{R}_+^2\times S_+^4} \mathcal{C}(\varphi(U_m + g, I) + \varphi(U_m - g, I_*) - \varphi(U_m + g', I') \\ &\quad -\varphi(U_m - g', I'_*))(f(U_m + g', I')f(U_m - g', I'_*) - f(U_m + g, I)\end{aligned}$$

$$f(U_m - g, I_*))dV d\Omega \simeq \Delta v^8 \sum_{i,j \in L\times L} \int_{S^4_+} \mathcal{C}(V = V_{ij})$$
$$(\varphi(z_i) + \varphi(z_j) - \varphi(U_{ij} + g'_{ij}, I'_{ij}) - \varphi(U_{ij} - g'_{ij}, I'_{*ij}))$$
$$(f(U_{ij} + g'_{ij}, I'_{ij}) f(U_{ij} - g'_{ij}, I'_{*ij}) - f(z_i) f(z_j)) d\Omega, \qquad (4.24)$$

where we have set

$$V_{ij} = \begin{pmatrix} \dfrac{z_{i_1} - z_{j_1}}{2} \\ \dfrac{z_{i_2} - z_{j_2}}{2} \\ \dfrac{z_{i_3} - z_{j_3}}{2} \\ z_{i_4} \\ z_{j_4} \end{pmatrix} = \begin{pmatrix} g_{ij} \\ I_i \\ I_j \end{pmatrix},$$

$$U_{ij} = \begin{pmatrix} \dfrac{z_{i_1} + z_{j_1}}{2} \\ \dfrac{z_{i_2} + z_{j_2}}{2} \\ \dfrac{z_{i_3} + z_{j_3}}{2} \end{pmatrix},$$

and $V^{'}_{ij} = (g^{'}_{ij}, I^{'}_{ij}, I^{'}_{*ij})$ is the image of V_{ij} by the transformation (3.15). Formula (3.15) shows that, when Ω varies in S^4_+, $V^{'}_{ij}$ varies on the sphere of radius $|V_{ij}|$ and centered at the point U_{ij}. As we have seen we can write $U_m = \Delta v(\dfrac{\varepsilon_{ij}}{2} + p_{ij})$. So we define

$$\begin{aligned} S_{ij} &= \{(k,l) \in L^2 \text{ and such that } U_{ij} = U_{kl} \text{ and } |V_{ij}| = |V_{kl}|\} \\ &= \{(z_k, z_l) = \Big((U_{ij} + g_{kl}, (V_{kl})_4), (U_{ij} - g_{kl}, (V_{kl})_5)\Big) \text{ with} \\ &\quad V_{kl} \in \Delta v(\frac{\varepsilon_{ij}}{2} + \mathbb{Z}^3) \times (\mathbb{N} + \frac{1}{2})^2 \text{ such that } |V_{ij}| = |V_{kl}|\}. \end{aligned} \qquad (4.25)$$

For $(k,l) \in S_{ij}$, we can define a unique $\Omega^{kl}_{ij} \in S^4_+$, such that the first of formula (3.15) holds for $(v, I) = z_i, (v_*, I_*) = z_j, (v', I') = z_k, (v'_*, I'_*) = z_l$. The sets S_{ij} are not empty. For the integral with respect to Ω which appears at the right hand side of (4.24), we use a quadrature formula using the Ω^{kl}_{ij} as quadrature points. We make the assumption that the points Ω^{kl}_{ij} are well distributed over S^4_+. By definition of $\mathcal{C}$ we have

$$\int_{S^4_+} \mathcal{C}(V = V_{ij}).(\varphi(z_i) + \varphi(z_j) - \varphi(U_{ij} + g'_{ij}, I'_{ij}) - \varphi(U_{ij} - g'_{ij}, I'_{*ij}))$$
$$(f(U_{ij} + g'_{ij}, I'_{ij}) f(U_{ij} - g'_{ij}, I'_{*ij}) - f(z_i) f(z_j)) d\Omega$$
$$= \frac{I_i^{\delta-1} I_j^{\delta-1}}{4} \int_{S^4_+} B(V = V_{ij}).(\varphi(z_i) + \varphi(z_j) - \varphi(U_{ij} + g'_{ij}, I'_{ij}) - \varphi(U_{ij} - g'_{ij}, I'_{*ij}))$$
$$(f(U_{ij} + g'_{ij}, I'_{ij}) f(U_{ij} - g'_{ij}, I'_{*ij}) - f(z_i) f(z_j)) \Omega_4^{\delta-1} \Omega_5^{\delta-1} d\Omega.$$

We can remark that

$$\int_{S_+^4} \Omega_4^{\delta-1}\Omega_5^{\delta-1} d\Omega = C_\delta \tag{4.26}$$

where C_δ is a constant just depending of δ. The use of the above mentionned quadrature formule yields

$$\begin{aligned}
&\int_{S_+^4} B(V = V_{ij})(\varphi(z_i) + \varphi(z_j) - \varphi(U_{ij} + g'_{ij}, I'_{ij}) - \varphi(U_{ij} - g'_{ij}, I'_{*ij}) \\
&\qquad (f(U_{ij} + g'_{ij}, I'_{ij}) f(U_{ij} - g'_{ij}, I'_{*ij}) - f(z_i)f(z_j))\Omega_4^{\delta-1}\Omega_5^{\delta-1} d\Omega \\
&\qquad \simeq \sum_{(k,l)\in S_{ij}} \frac{\mathcal{M}(S_+^4)}{\mathrm{Card}(S_{ij})} B(V = V_{ij}, V' = V_{kl}) (\frac{I_k I_l}{|V_{ij}|})^{\delta-1} \\
&\qquad (\varphi(z_i) + \varphi(z_j) - \varphi(z_k) - \varphi(z_l))(f(z_k)f(z_l) - f(z_i)f(z_j))
\end{aligned} \tag{4.27}$$

and

$$\int_{S_+^4} \Omega_4^{\delta-1}\Omega_5^{\delta-1} d\Omega \simeq \sum_{(k,l)\in S_{ij}} \frac{\mathcal{M}(S_+^4)}{\mathrm{Card}(S_{ij})} (\frac{I_k I_l}{|V_{ij}|})^{\delta-1}. \tag{4.28}$$

It is thus legitimate to identify the right hand side of equation (4.28) with C_δ according to (4.26), and to insert the resulting identity into (4.27). This yields:

$$\begin{aligned}
&\int_{S_+^4} \mathcal{C}(V = V_{ij}).(\varphi(z_i) + \varphi(z_j) - \varphi(U_{ij} + g'_{ij}, I'_{ij}) - \varphi(U_{ij} - g'_{ij}, I'_{*ij})) \\
&\qquad (f(U_{ij} + g'_{ij}, I'_{ij}) f(U_{ij} - g'_{ij}, I'_{*ij}) - f(z_i)f(z_j)) d\Omega \\
&\qquad \simeq \frac{I_i^{\delta-1} I_j^{\delta-1}}{4} \sum_{(k,l)\in S_{ij}} p_{kl} B_{ij}^{kl} (\varphi(z_i) + \varphi(z_j) \\
&\qquad -\varphi(z_k) - \varphi(z_l))(f(z_k)f(z_l) - f(z_i)f(z_j))
\end{aligned} \tag{4.29}$$

with

$$B_{ij}^{kl} = C_\delta B(V = V_{ij}, V' = V_{kl})$$

and

$$p_{kl} = \frac{I_k^{\delta-1} I_l^{\delta-1}}{\sum_{(k,l)\in S_{ij}} I_k^{\delta-1} I_l^{\delta-1}}.$$

For the VHS model in which

$$B = C\left(\frac{|g||g'|}{|V|}\right)^{1-2\alpha} = \left(|g|\sqrt{\Omega_1^2 + \Omega_2^2 + \Omega_3^2}\right)^{1-2\alpha}$$

we can make another approximation for the integral with respect to Ω which appears in the left hand side of (4.29) which gives a better approximation of the collision frequencies. By noticing that in this case

$$\int_{S_+^4} (\frac{|g'|}{|V|})^{1-2\alpha} \Omega_4^{\delta-1}\Omega_5^{\delta-1} d\Omega = D_{\delta,\alpha} \tag{4.30}$$

where $D_{\delta,\alpha}$ is a constant just depending on α and δ, we can also make the following approximations of (4.30)

$$D_{\delta,\alpha} \simeq \sum_{(k,l)\in S_{ij}} \frac{\mathcal{M}(S^4_+)}{\mathrm{Card}(S_{ij})} \left(\frac{|g_{kl}|}{|V_{ij}|}\right)^{1-2\alpha} \left(\frac{I_k I_l}{|V_{ij}|}\right)^{\delta-1}. \tag{4.31}$$

We obtain the same type of approximation (4.29) with

$$B^{kl}_{ij} = D_{\delta,\alpha}|g_{ij}|^{1-2\alpha}$$

and

$$p_{kl} = \frac{|g_{kl}|^{1-2\alpha} I_k^{\delta-1} I_l^{\delta-1}}{\displaystyle\sum_{(k,l)\in S_{ij}} |g_{kl}|^{1-2\alpha} I_k^{\delta-1} I_l^{\delta-1}}$$

This approximation for the VHS model forces the discrete model to give us the good collision frequency between z_i and z_j.

No error estimates for the quadrature formula (4.29) is available up to now. One problem is that the number of quadrature points Ω^{kl}_{ij} on S^4_+ is a non monotone function of $|V_{ij}|$. Another one is that very few things can be said about the location of the points Ω^{kl}_{ij} on S^4_+. The only known result about the well distribution of these points is for the class of spheres which have their centers lying exactly on the velocity lattice(see for example [2]). The problem is then equivalent to find the distribution over the unit sphere of all the decompositions of an integer number into a sum of n square of integer numbers. In this case and by eliminating some values of n it can be proved that the set of the decompositions is well distributed over the unit sphere (see [8, 15]). When the center is not in the velocity lattice, the problem is now equivalent to the well distribution of special subsets of the decompositions of an integer number into a sum of n square of integer numbers, for which no results seems to be known. For the discrete monoatomic model ([5, 10]), this result allows, by eliminating the sphere that have not their centers of the velocity lattice, to prove the consistency of the discrete model with the continuous one (see[2]).

We shall estimate the number of the points Ω^{kl}_{ij} by adapting a very classical theorem of number theory, about the number of decompositions of an integer number into a sum of squares of integers numbers (see [13]). This estimate will show that the discrete sphere are non empty and that the number of points Ω^{kl}_{ij} "tends" to infinity with the diameter. We give the result in the general case. We suppose that the dimension of space is $d \geq 1$. We set $\varepsilon = (\varepsilon_1, ..., \varepsilon_d) \in \{0,1\}^d$. For $i \in \mathbb{Z}^d$, we have $|i - \frac{\varepsilon}{2}|^2 \in \mathbb{N} + |\frac{\varepsilon}{2}|^2$ where, for $i \in \mathbb{Z}^d$, $|i|^2 = \sum_{p=1}^{d} i_p^2$. Let

$$r_{\varepsilon,d}(n) = \mathrm{Card}\Big(\big\{i \in \mathbb{Z}^d \;/\; \Big|i - \frac{\varepsilon}{2}\Big|^2 = n + \Big|\frac{\varepsilon}{2}\Big|^2\big\}\Big), \quad for\ n \in \mathbb{N}$$

the number of points of $\mathbb{Z}^d$ on the sphere having the center $\frac{\varepsilon}{2}$ and the radius

$(n + \left|\frac{\varepsilon}{2}\right|^2)^{\frac{1}{2}}$. We write $\mathcal{M}(E)$ for the Lebesgue measure of a mesurable subset E of $\mathbb{R}^n$. We have the

Lemma 4.1 *For* $d \geq 2$,

$$\sum_{k=0}^{n} r_{\varepsilon,d}(k) = \mathcal{M}(S^{d-1})n^{\frac{d}{2}} \; + O(n^{\frac{d-1}{2}})$$

and $r_{\varepsilon,d}(n) = O(n^{\frac{d-2}{2}+\delta})$ *for all* $\delta > 0$*, or equivalently,* $r_{\varepsilon,d}(n) = o(n^{\frac{d-2}{2}+\delta})$ *for all* $\delta > 0$.

Proof. By setting $E_n = \left\{ i \in \mathbb{Z}^d \; / \; \left|i - \frac{\varepsilon}{2}\right|^2 \leq n + \left|\frac{\varepsilon}{2}\right|^2 \right\}$, we have

$$\sum_{k=0}^{n} r_{\varepsilon,d}(k) = \mathrm{Card}(E_n).$$

At each point i we associate the cube C_i having $i + \alpha$ for vertices with $\alpha = (\alpha_1, .., \alpha_d) \in \{0, \; 1\}^d$. We have $\mathcal{M}(C_i) = 1$ and therefore,

$$\mathrm{Card}(E_n) = \sum_{i \in E_n} \mathcal{M}(C_i) = \mathcal{M}(\bigcup_{i \in E_n} C_i).$$

It is clear that

$$\bigcup_{i \in E_n} C_i \subset B\Big(\frac{\varepsilon}{2}, \; \sqrt{n + \left|\frac{\varepsilon}{2}\right|^2} + \sqrt{d}\Big).$$

For $x \in B\Big(\frac{\varepsilon}{2}, \sqrt{n + \left|\frac{\varepsilon}{2}\right|^2} - \sqrt{d}\Big)$ we have

$$\sqrt{n + \left|\frac{\varepsilon}{2}\right|^2} - \sqrt{d} \geq \left|x - \frac{\varepsilon}{2}\right| = \left|[x] + \{x\} - \frac{\varepsilon}{2}\right| > \left|[x] - \frac{\varepsilon}{2}\right| - |\{x\}|$$

where $[x]$ is the integer part of x and $\{x\} = x - [x]$. Hence, $[x] \in E_n$ and in consequense we have then

$$B\Big(\frac{\varepsilon}{2}, \; \sqrt{n + \left|\frac{\varepsilon}{2}\right|^2} - \sqrt{d}\Big) \subset \bigcup_{i \in E_n} C_i$$

and consequently

$$\mathcal{M}(S^{d-1})\Big(\sqrt{n + \left|\frac{\varepsilon}{2}\right|^2} - \sqrt{d}\Big)^d \leq \sum_{k=0}^{n} r_{\varepsilon,d}(k) \leq \mathcal{M}(S^{d-1})\Big(\sqrt{n + \left|\frac{\varepsilon}{2}\right|^2} + \sqrt{d}\Big)^d.$$

Since

$$\mathcal{M}(S^{d-1})\Big(\sqrt{n + \left|\frac{\varepsilon}{2}\right|^2} \pm \sqrt{d}\Big)^d$$

is clearly $\mathcal{M}(S^{d-1})n^{\frac{d}{2}} \; + O(n^{\frac{d-1}{2}})$ we have proved the first part of the lemma. The second assertion is in fact a consequence of the following lemma (see [13]):

Lemma 4.2 *If we call $s(n)$ the number of decompositions of n in a sum of two squares of integer numbers then $s(n) = O(n^{\delta})$ for all $\delta > 0$ or, equivalently, $s(n) = o(n^{\delta})$ for all $\delta > 0$.*

We prove the second assertion by recursion on the dimension of the space. The lemma yields the result for $d = 2$. We shall prove that the result holds for $d > 2$. Assume that the result holds for one $d \geq 2$. Let i such that $\displaystyle\sum_{p=1}^{d+1} i_p^2 = n$. We have then $i_{d+1}^2 \leq n$ which give $|i_{d+1}| \leq [\sqrt{n}\,]$ and now

$$r_{0,d+1}(n) \leq \sum_{i_{d+1}=0}^{[\sqrt{n}\,]} r_{0,d}(n - i_{d+1}^2)$$

Using the assumption for d, we have

$$r_{0,d+1}(n) = O\Big(\sum_{i_{d+1}=0}^{[\sqrt{n}\,]} (n - i_{d+1}^2)^{\delta + \frac{d-2}{2}}\Big)$$

For simplicity we set $\alpha = \delta + \dfrac{d-2}{2}$. By the precedent equality, we obtain

$$r_{0,d+1}(n) = O\bigg(([\sqrt{n}\,]+1)^{2\alpha+1}.\frac{1}{[\sqrt{n}\,]+1}\sum_{i_{d+1}=0}^{[\sqrt{n}\,]}\Big(\frac{n}{([\sqrt{n}\,]+1)^2} - (\frac{i_{d+1}}{[\sqrt{n}\,]+1})^2\Big)^{\alpha}\bigg).$$

The function $x \ \rightarrow \ (x-a)^{\alpha}$ is increasing in x for all $\alpha > 0$ and then

$$r_{0,d+1}(n) = O\bigg(([\sqrt{n}\,]+1)^{2\alpha+1}.\frac{1}{[\sqrt{n}\,]+1}\sum_{i_{d+1}=0}^{[\sqrt{n}\,]}\Big(1 - (\frac{i_{d+1}}{[\sqrt{n}\,]+1})^2\Big)^{\alpha}\bigg)$$

But

$$\frac{1}{[\sqrt{n}\,]+1}\sum_{i_{d+1}=0}^{[\sqrt{n}\,]}\Big(1 - (\frac{i_{d+1}}{[\sqrt{n}\,]+1})^2\Big)^{\alpha} = O\Big(\int_0^1 (1-y^2)^{\alpha} dy\Big)$$

and

$$([\sqrt{n}\,]+1)^{2\alpha+1} = O\big(n^{\frac{1}{2}+\alpha}\big)$$

Then we get the desired estimate for $r_{0,d+1}(n)$:

$$r_{0,d+1}(n) = O\big(n^{\frac{1}{2}+\alpha}\big) = O\big(n^{\frac{d+1-2}{2}+\delta}\big)$$

In the case of $\varepsilon \neq 0$ we can go back to the case $\varepsilon = 0$ by noting that if i is such that

$$\Big|i - \frac{\varepsilon}{2}\Big|^2 = n + \Big|\frac{\varepsilon}{2}\Big|^2$$

or, equivalently

$$|2i - \varepsilon|^2 = 4n + |\varepsilon|^2$$

this implies

$$2i - \varepsilon \in \left\{ j \ / \ |j|^2 = 4n + |\varepsilon|^2 \right\}$$

and we have then the following inequality

$$r_{\varepsilon,d}(n) \le r_{0,d}(4n + |\varepsilon|^2).$$

Using the result for $r_{0,d}(n)$ and the fact that $|\varepsilon|^2 \le d$ we have

$$r_{\varepsilon,d}(n) = O\left\{ (4n + |\varepsilon|^2)^{\frac{d-2}{2} + \delta} \right\} = O\left\{ n^{\frac{d-2}{2} + \delta} \right\}$$

This ends the proof. $\square$

This result shows that in the sense of the Cesaro mean value, $\mathrm{Card}(S_{ij})$, which is $\frac{1}{4} r_{\varepsilon,5}(|V|^2)$ with $\varepsilon = (\eta_1, \eta_2, \eta_3, 1, 1)$ and $(i - j) \equiv \eta (\mathrm{mod}\ 2)$, behaves like $|V|^3$. A similar weak result can be easily obtained for the well distribution of the points of S_{ij} on the corresponding continuous quarter of sphere. Given a function g defined and continuous on the unit sphere S^4 we define G on $\mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}_+$ by:

$$G(x) = g\left(\frac{x}{|x|}\right).$$

A classical result on the well distribution of the points of a regular lattice $\Delta v \mathbb{Z}^n$ which lye in a regular domain of $\mathbb{R}^n$, states that

$$\lim_{\Delta v \to 0} \frac{\sum_{i\Delta v \in D \cap \Delta v \mathbb{Z}^n} \phi(x)}{\sum_{i \Delta v \in D} 1} = \int_D \phi(x) dx$$

for all smooth test functions ϕ. This gives us by setting $N = \dfrac{1}{\Delta v}$, $x_i = (i + \dfrac{\varepsilon}{2})\Delta v$ with i in $\mathbb{Z}^n$ and by taking $n = 5$, the following identity:

$$\lim_{N \to \infty} \frac{\int_{B(\frac{\varepsilon}{2}\Delta v, 1) \cap \mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}_+} dx}{\sum_{j=1}^{N} \frac{1}{4} r_{\varepsilon,5}(j)} \sum_{j=1}^{N} \sum_{i \in \mathcal{I}_j} G(x_i)$$
$$= \int_{B(\frac{\varepsilon}{2}\Delta v, 1) \cap \mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}_+} G(x) dx.$$

with

$$\mathcal{I}_j = \{ i \text{ such that } x_i \in \mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}_+ \text{ and } |x_i - \frac{\varepsilon}{2}\Delta v|^2 = j \Delta v^2 \}.$$

But

$$\int_{B(\frac{\varepsilon}{2}\Delta v, 1) \cap \mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}_+} G(x) dx = \frac{1}{5} \int_{S^4_+} g(\omega) d\omega$$

so in the sense of the Cesaro mean value, the points of $\left\{|x_i - \frac{\varepsilon}{2}\Delta v|^2 = j\Delta v^2\right\}$ are well distributed that is

$$\lim_{j\to\infty} \frac{r_{\varepsilon,5}(j)}{4} \int_{S^4_+} d\omega \sum_{|x_i - \frac{\varepsilon}{2}\Delta v|^2 = j\Delta v^2} G(x_i) = \int_{S^4_+} g(\omega) d\omega$$

These two results tends to show that the approximation (4.29) is "reasonably accurate".

The overall approximation of the right hand side of (4.19) is now of the form

$$\begin{aligned} \frac{1}{4}\int_{\mathbb{R}^3\times\mathbb{R}_+} & Q_\delta(\varphi(v,I) + \varphi(v_*,I_*) - \varphi(v_*^{'},I_*^{'}) - \varphi(v^{'},I^{'}))I^{\delta-1} dvdI \\ & \simeq \frac{1}{4} \sum_{i,j\in L\times L} \sum_{k,l\in S_{i,j}} (\varphi(z_i) + \varphi(z_j) \\ & -\varphi(z_k) - \varphi(z_l)(f_k f_l - f_i f_j) p_{kl} B_{ij}^{kl} I_i^{\delta-1} I_j^{\delta-1}. \end{aligned} \tag{4.32}$$

By setting $\bar{f} = f_i, i \in L$, and noticing that

$$p_{kl} B_{ij}^{kl} I_i^{\delta-1} I_j^{\delta-1} = p_{kl} B_{ji}^{kl} I_i^{\delta-1} I_j^{\delta-1} = p_{lk} B_{ij}^{lk} I_i^{\delta-1} I_j^{\delta-1} = p_{ij} B_{kl}^{ij} I_k^{\delta-1} I^{\delta-1}$$

we obtain the following approximation of the continuous homogeneous problem

$$\frac{df_i}{dt} = \bar{Q}_\delta(\bar{f},\bar{f})_i \tag{4.33}$$

with

$$\bar{Q}_\delta(\bar{f},\bar{f})_i = \sum_{j\in L} \sum_{(k,l)\in S_{ij}} (A_{kl}^{ij} f_k f_l - A_{ij}^{kl} f_i f_j) \tag{4.34}$$

or

$$\bar{Q}_\delta(\bar{f},\bar{f})_i = \sum_{(j,k,l)\in (L)^3} (A_{k,l}^{i,j} f_k f_l - A_{ij}^{kl} f_i f_j), \tag{4.35}$$

where we have extended the definition of A_{ij}^{kl} and for further purposes, we also introduce the tensor $\mathcal{A}_{ij}^{kl}$ by:

$$A_{ij}^{kl} = \frac{\mathcal{A}_{ij}^{kl}}{I_i^{\delta-1}} = \begin{cases} I_j^{\delta-1} p_{kl} B_{ij}^{kl} & \text{if} \quad (k,l) \in S_{ij} \\ 0 \quad \text{otherwise.} \end{cases} \tag{4.36}$$

We consider now a bounded velocity domain. The issue is to replace the Boltzmann equation in the whole velocity space domain, by a bounded space one, for which the algebraic properties displayed in section 3.1 still hold. We proceed as in [18, 19]. Let $\mathcal{D}_{v,I}$ be a bounded domain of $\mathbb{R}^3 \times \mathbb{R}_+$, and let $\chi((v,I),(v_*,I_*),(v',I'),(v'_*,I'_*))$ be the following characteristic function

$$\chi(a,b,c,d) = \begin{cases} 1 \quad \text{if} \quad (a,b,c,d) \in \mathcal{D}_{v,I}^4 \\ 0 \quad \text{otherwise.} \end{cases} \tag{4.37}$$

Now, let us consider the Boltzmann operator

$$Q_\delta(f,f)(v) = \int_{\mathcal{D}_{v,I}} \int_{S^4_+} \chi\big((v,I),(v_*,I_*),(v',I'),(v'_*,I'_*)\big)\mathcal{B} \\ (f'f'_* - ff_*)dv_* I_*^{\delta-1} dI_* d\Omega. \tag{4.38}$$

For $v \in \mathcal{D}_{v,I}$, it is easy to show that properties (2.6) to (2.9) still hold, with the only difference that the coefficient of $\frac{|v|^2}{2} + I^2$ in (2.8) is no more necessarily positive. Indeed, its positivity for the full space case follows from integrability requirements on the Maxwellian, which can no more be used because of the boundedness of the domain. The particle approximation of problem (4.18) is now restricted to approximations f_i of $(\Delta v)^4 f(z_i)$ for $z_i \in \Delta v L \cap \mathcal{D}_{v,I}$. Let E be the set of indices, which is included in L, for which $z_i \in \mathcal{D}_{v,I}$. The discrete homogeneous problem for $i \in E$ is now written

$$\frac{df_i(t)}{dt} = \bar{Q}_\delta(\bar{f},\bar{f})_i = \sum_{j\in E} \sum_{(k,l)\in \tilde{S}_{ij}} (A^{i,j}_{k,l} f_k f_l - A^{kl}_{ij} f_i f_j)$$

with

$$\tilde{S}_{ij} = \{(k,l) \in S_{ij} \quad \text{such that} \quad k,l \in E\} \tag{4.39}$$

where

$$A^{kl}_{ij} = \frac{\mathcal{A}^{kl}_{ij}}{I_i^{\delta-1}} = \begin{cases} I_j^{\delta-1} \tilde{p}_{kl} B^{kl}_{ij} \quad \text{if} \quad z_i, z_j \in \mathcal{D}_{v,I} \quad \text{and} \quad (k,l) \in \tilde{S}_{ij} \\ 0 \quad \text{otherwise.} \end{cases} \tag{4.40}$$

with

$$\tilde{p}_{kl} = \frac{I_k^{\delta-1} I_l^{\delta-1}}{\sum_{(k,l)\in\tilde{S}_{ij}} I_k^{\delta-1} I_l^{\delta-1}}.$$

For example, in the VHS model case, we can take

$$\tilde{p}_{kl} = \frac{|g_{kl}|^{1-2\alpha} I_k^{\delta-1} I_l^{\delta-1}}{\sum_{(k,l)\in\tilde{S}_{ij}} |g_{kl}|^{1-2\alpha} I_k^{\delta-1} I_l^{\delta-1}}.$$

4.1.2. *Properties of the discrete collision operator*

It is easy to check that the tensor $\mathcal{A}^{kl}_{ij}$ is non negative and satisfies the following symmetry properties

$$\mathcal{A}^{kl}_{ij} = \mathcal{A}^{kl}_{ji} = \mathcal{A}^{lk}_{ij} \tag{4.41}$$

and also the microreversibility property

$$\mathcal{A}^{kl}_{ij} = \mathcal{A}^{ij}_{kl} \tag{4.42}$$

Therefore, see (4.32), we have the discrete analogue of identity (2.5): let $\bar\varphi = (\varphi_i)_{i\in E}$ be a test sequence, then

$$\sum_{i\in E} \bar Q_\delta(\bar f,\bar f)_i \varphi_i I_i^{\delta-1} = \frac{1}{4}\sum_{(i,j,k,l)\in(E)^4} \mathcal{A}_{ij}^{kl}(f_k f_l - f_i f_j)(\varphi_i+\varphi_j-\varphi_k-\varphi_l) \quad (4.43)$$

Using the definition of tensor $\mathcal{A}_{ij}^{kl}$ and equality (4.43) it is easy to show that the discrete analogue of conservation of mass, momentum and energy

$$\sum_{i\in E} \bar Q_\delta(\bar f,\bar f)_i I_i^{\delta-1}\begin{pmatrix} 1 \\ v_i \\ \frac{|v_i|^2}{2}+I_i^2\end{pmatrix} = 0, \quad (4.44)$$

holds. Also using (4.43) and the classical inequality $(y-x)(\log x - \log y) \le 0$ for any $x, y > 0$, a discrete H-theorem holds that yields dissipation of entropy $H(t) = \sum_{i\in E} f_i(t)\log f_i(t) I_i^{\delta-1}$

$$\begin{aligned}\frac{dH(t)}{dt} &= \sum_{i\in E}\bar Q_\delta(\bar f,\bar f)_i I_i^{\delta-1}\log(f_i) \\ &= \frac{1}{4}\sum_{(i,j,k,l)\in(E)^4}\mathcal{A}_{ij}^{kl}(f_k f_l - f_i f_j)(\log(f_i)+\log(f_j)-\log(f_k)-\log(f_l)) \\ &= \frac{1}{4}\sum_{(i,j,k,l)\in(E)^4}\mathcal{A}_{ij}^{kl}(f_k f_l - f_i f_j)(\log(f_i f_j)-\log(f_k f_l)) \le 0. \quad (4.45)\end{aligned}$$

As in the monoatomic case, the equilibrium states, $\bar f^\infty$, for which $\frac{dH(t)}{dt} = 0$, are characterized by (see [9]):

Proposition 4.1 *The following properties are equivalent*

1. $\sum_{i\in E}\bar Q_\delta(\bar f^\infty,\bar f^\infty)_i\log(f_i^\infty) = 0$
2. $\bar Q_\delta(\bar f^\infty,\bar f^\infty)_i = 0\ \forall i\in E$
3. $\overline{\log f^\infty} = (\log f_i^\infty)_{i\in E}$ *is an invariant of collision that is* $\overline{\log f^\infty} \in \{\bar\varphi$ *such that* $\varphi_i+\varphi_j-\varphi_k-\varphi_l = 0$ *for all* i,j,k,l *such that* $A_{ij}^{kl}\neq 0\}$
4. $f_i^\infty f_j^\infty - f_k^\infty f_l^\infty = 0$ *if* $A_{ij}^{kl}\neq 0$

To see that these properties are equivalent one must recall that

$$(y-x)(\log x - \log y) = 0 \Leftrightarrow x = y$$

and use (4.43). Now, for the specific model given by (4.36) or by (4.40), it is noticeable that the reciprocal of (4.44) holds, like in the continuous case and so the only equilibrium states are discrete Maxwellians.

For a bounded domain we suppose that $\mathcal{D}_{v,I}$ is of the form $\mathcal{D}_{v,I} = B(0,R) \times [0,S]$ or $\mathcal{D}_{v,I} = [-R,R]^3 \times [0,S]$. For such bounded domains, the set E is

$$E = \{i \in L, 1_1^2 + i_2^2 + i_3^2 \leq M_1,\ i_4 \leq N\}$$

or

$$E = \{i \in L,\ i \sup_{p=1,3} i_p \leq M_2,\ i_4 \leq N\},$$

where M_1, M_2 and N are integers and we assume that $M_1 \geq 3$, $M_2 \geq 1$ and $N \leq M_2 - 2$. In the case of an unbounded domain for (v, I), we get $E = L$. We have

Lemma 4.3 *For the model given by (4.36) or by (4.40) the invariants of collisions are given by*

$$\varphi_i = A(v_i^2 + 2I_i^2) + < B, v_i > + C$$

with A and $C \in$ IR and $B \in$ IR^3 and the equilibrium states $\bar{f}^\infty$ have the form

$$f_i^\infty = \exp(A(v_i^2 + 2I_i^2) + < B, v_i > + C)$$

Proof. For $\varphi = (\varphi_i)_{i \in E}$, we let $\varphi(m)$ be the restriction of φ to the subset $E_m = \{i \in E,\ i_4 = m\}$ that is, $\varphi(m)$ is the restriction of φ at the level $m + \dfrac{1}{2}$. We note $\bar{i} = (i_1, i_2, i_3)$ for any element i of E_m. For $\varphi(m)$ we have the result

$$\varphi_i(m) = A(m)|\bar{i}|^2 + < B(m), \bar{i} > + C(m)$$

with $A(m)$ *and* $C(m) \in$ IR *and* $B(m) \in$ IR^3. We consider only elastics collisions between two elements of E_m. We consider first the case of $E_m = \mathbb{Z}^3$. We say that $(\bar{i}, \bar{j}) \to (\bar{k}, \bar{k})$ is a possible collision if $\mathcal{A}_{(\bar{i},m),(\bar{j},m)}^{(\bar{k},m),(\bar{k},m)} \neq 0$ that implies by the symmetry of $\mathbb{Z}^3$ that the collision $(-\bar{i}, -\bar{j}) \to (-\bar{k}, -\bar{l})$ is also admissible. Let $e_1 = (1,0,0),\ e_2 = (0,1,0),\ e_3 = (0,0,1)$ be the canonical basis of $\mathbb{Z}^3$. We search $\varphi(m)$ such that

$$\varphi_{\bar{i}}(m) + \varphi_{\bar{j}}(m) - \varphi_{\bar{k}}(m) - \varphi_{\bar{l}}(m) = 0 \quad for\ all\ \mathcal{A}_{(\bar{i},m),(\bar{j},m)}^{(\bar{k},m),(\bar{k},m)} \neq 0$$

We set

$$a_{\bar{i}}(m) = \varphi_{\bar{i}}(m) + \varphi_{-\bar{i}}(m)\ and\ b_{\bar{i}}(m) = \varphi_{\bar{i}}(m) - \varphi_{-\bar{i}}(m)$$

By construction we have $a_{-\bar{i}}(m) = a_{\bar{i}}(m)$, $b_{-\bar{i}}(m) = -b_{\bar{i}}(m)$ and then $b_0(m) = 0$. We show recursively on $L = |\bar{i}|_\infty = \max\limits_{n=1}^{3} |i_n|$ that

$$a_{\bar{i}} - a_0 = |\bar{i}|^2.(a_{e_1} - a_0),\ b_{\bar{i}} = i_1 b_{e_1} + i_2 b_{e_2} + i_3 b_{e_3}$$

This is evidently true for $a_{\bar{i}}$ when $|\bar{i}|_\infty = 1$ because $(e_\alpha, -e_\alpha) \to (e_\beta, -e_\beta)$ is an admissible collision. For $b_{\bar{i}}$ this is trivial. We suppose now that it is true until rank L. Let $\bar{i} \in \mathbb{Z}^3$ such that $|\bar{i}|_\infty = L + 1$. If $(\bar{i}, \bar{j}) \to (\bar{k}, \bar{l})$ is a possible collision then,

by construction, $a_{\bar{i}}+a_{\bar{j}} = a_{\bar{k}}+a_{\bar{l}}$ and $b_{\bar{i}}+b_{\bar{j}} = b_{\bar{k}}+b_{\bar{l}}$. Since the following collisions are admissible

$$(\bar{i},0) \to (i_1e_1 + i_2e_2, i_3e_3), \quad (i_1e_1 + i_2e_2, 0) \to (i_1e_1, i_2e_2)$$

we have

$$a_{\bar{i}} + a_0 = a_{i_1e_1+i_2e_2} + a_{i_3e_3} = a_{i_1e_1} + a_{i_2e_2} + a_{i_3e_3} - a_0$$

and then

$$a_{\bar{i}} - a_0 = (a_{i_1e_1} - a_0) + (a_{i_2e_2} - a_0) + (a_{i_3e_3} - a_0)$$

and for $b_{\bar{i}}$

$$b_{\bar{i}} = b_{i_1e_1} + b_{i_2e_2} + b_{i_3e_3}.$$

It suffices then to verify that

$$a_{(L+1)e_\alpha} - a_0 = (L+1)^2(a_{e_1} - a_0), \quad b_{(L+1)e_\alpha} = (L+1)b_{e_\alpha}. \tag{4.46}$$

We define $u = (L-1)e_\alpha$, $v = Le_\alpha + e_\beta$ and $w = Le_\alpha - e_\beta$. Since $|u|_\infty = L-1$ and $|v|_\infty = |w|_\infty = L$ the assumption holds for u, v, w. Since the following collision is possible

$$\Big((L+1)e_\alpha,\ u\Big) \ \to\ \Big(\ v,\ w\ \Big),$$

(4.46) is true: indeed we have for $a_{\bar{i}}$

$$a_{(L+1)e_\alpha} + a_u = a_v + a_w$$

and then

$$\begin{aligned}
a_{(L+1)e_\alpha} - a_0 &= a_w - a_0 + a_v - a_0 - (a_u - a_0)\\
&= (|w|^2 + |v|^2 - |u|^2)(a_{e_1} - a_0)\\
&= (L^2 + 1 + L^2 + 1 - (L-1)^2)(a_{e_1} - a_0)\\
&= (L+1)^2(a_{e_1} - a_0).
\end{aligned}$$

and for $b_{\bar{i}}$

$$b_{(L+1)e_\alpha} = b_v + b_w - b_u = Lb_{e_\alpha} + b_{e_\beta} + Lb_{e_\alpha} - b_{e_\beta} - (L-1)b_{e_\alpha} = (L+1)b_{e_\alpha}$$

Since $\varphi_{\bar{i}} = \dfrac{a_{\bar{i}} + b_{\bar{i}}}{2}$ we have the result for $\varphi_{\bar{i}}$ with

$$A(m) = \frac{a_{e_1} - a_0}{2},\ C(m) = \frac{a_0}{2},\ B(m) = (\frac{b_{e_1}}{2}, \frac{b_{e_2}}{2}, \frac{b_{e_3}}{2}).$$

Recall that $E_m = \{\bar{i} \in \mathbb{Z}^3 \ / \ i_1^2 + i_2^2 + i_3^2 \le M_1\}$ or $E_m = \{\bar{i} \in \mathbb{Z}^3 \ / \sup_{k=1}^{3} i_k \le M_2\}$. It is then easy to check, from the above analysis, that the result for the form of $\varphi(m)$ remains valid provided $M_1 \ge 3$ and $M_2 \ge 1$.

Let us consider the case of inelastic collisions. For a given m such that $m \leq M_1 - 2$ or $m \leq M_2 - 2$ in the case of bounded domain, we consider the following collisions

$$z_i = \Delta v(0,0,0,m+\frac{1}{2}), z_j = \Delta v(1,0,0,\frac{1}{2}) \to z_k = \Delta v(m+1,0,0,\frac{1}{2}), \quad z_l = \Delta v(-m,0,0,\frac{1}{2})$$

$$z_i = \Delta v(1,0,0,m+\frac{1}{2}), z_j = \Delta v(0,0,0,\frac{1}{2}) \to z_k = \Delta v(m+1,0,0,\frac{1}{2}), \quad z_l = \Delta v(-m,0,0,\frac{1}{2})$$

$$z_i = \Delta v(0,1,0,m+\frac{1}{2}), z_j = \Delta v(0,0,0,\frac{1}{2}) \to z_k = \Delta v(m+1,0,0,\frac{1}{2}), \quad z_l = \Delta v(-m,0,0,\frac{1}{2})$$

$$z_i = \Delta v(0,0,1,m+\frac{1}{2}), z_j = \Delta v(0,0,0,\frac{1}{2}) \to z_k = \Delta v(m+1,0,0,\frac{1}{2}), \quad z_l = \Delta v(-m,0,0,\frac{1}{2})$$

$$z_i = \Delta v(2,0,0,m+\frac{1}{2}), z_j = \Delta v(0,0,0,\frac{1}{2}) \to z_k = \Delta v(m+2,0,0,\frac{1}{2}), \quad z_l = \Delta v(1-m,0,0,\frac{1}{2})$$

For these collisions we have $\mathcal{A}_{ij}^{kl} \neq 0$ and then for φ we must have

$$\varphi_i + \varphi_j = \varphi_k + \varphi_l$$

By using the result for φ at the levels $\frac{1}{2}$ and $m+\frac{1}{2}$ of internal energy we derive the following set of equations

$$\begin{cases} C(m) = 2A(0)((m+\frac{1}{2})^2 - \frac{1}{4}) + C(0) \\ A(m) + B_1(m) = A(0) + B_1(0) \\ A(m) + B_2(m) = A(0) + B_2(0) \\ A(m) + B_3(m) = A(0) + B_3(0) \\ 4A(m) + 2B_1(m) = 4A(0) + 2B_1(0) \end{cases}$$

for which the solution is

$$\begin{cases} C(m) = 2A(0)((m+\frac{1}{2})^2 - \frac{1}{4}) + C(0) \\ A(m) = A(0) \\ B_1(m) = B_1(0) \\ B_2(m) = B_2(0) \\ B_3(m) = B_3(0) \end{cases}$$

and then for each m

$$\varphi_{\bar{i}}(m) = A(0)|\bar{i}|^2 + < B(0), \bar{i} > + 2A(0)((m + \frac{1}{2})^2 - \frac{1}{4}) + C(0)$$

We have indeed for any $i \in E$, using the definition of $z_i = (v_i, I_i)$

$$\varphi_i = A(|v_i|^2 + 2I_i^2) + < B, v_i > + C.$$

Since to say that $\bar{f}^\infty$ is an equilibrium state is equivalent to say that $\overline{\log f^\infty}$ is an invariant of collisions we have indeed

$$\bar{f}_i^\infty = \exp(A(|v_i|^2 + 2I_i^2) + < B, v_i > + C),$$

which ends the proof. □

Since the only invariants of collisions are $(1)_{i\in E}, (v_i)_{i\in E}, (|v_i|^2 + 2I_i^2)_{i\in E}$ the constants A, B, C are functions of the density, mean velocity, and temperature of $\bar{f}$. All these properties show that our discrete collision operator for polyatomic gases behaves like the continuous one as we have claimed.

4.2. A second discrete velocity and energy model

We propose a discrete collision operator which mimics the discrete-velocity collision dynamics described in [11] for polyatomic gases. We show that this discrete collision operator, which uses a finer discretization of the internal energy than the previously described one, has also the same properties as the continuous one. Now we uses the expression of Q_δ given by (3.17) and for simplicity, we restrict ourselves to the case of VHS models.

4.2.1. *Discretization*

We again take a regular discretization of $\mathbb{R}^3 \times \mathbb{R}^+$: Let $\Delta v > 0$,

$$(v_i, e_i) = (i_1\Delta v, i_2\Delta v, i_3\Delta v, (i_4 + \frac{1}{2})\Delta v^2), \tag{4.47}$$

with $i = (i_1, i_2, i_3, i_4) \in L = \mathbb{Z}^3 \times \mathbb{N}$, and we let $f_i(t) \simeq (\Delta v)^5 f(v_i, e_i, t)$. We introduce a particle approximation of the problem (4.18). Given any test function $\varphi(v, e)$ we have

$$\begin{aligned}
&\int_{\mathbb{R}^3\times\mathbb{R}^+} \frac{df}{dt}\varphi(v,e)e^{\frac{\delta}{2}-1}dvde \\
&= \frac{1}{4}\int_{\mathbb{R}^3\times\mathbb{R}^+} Q_\delta(\varphi(v,e) + \varphi(v_*,e_*) - \varphi(v_*^{'},e_*^{'}) - \varphi(v^{'},e^{'}))e^{\frac{\delta}{2}-1}dvde \\
&= \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^+\times\mathbb{R}^+\times S^2\times[0,1]^2} B(\varphi + \varphi_* - \varphi' - \varphi_*^{'})(f'f_*' - ff_*)d\sigma
\end{aligned} \tag{4.48}$$

with the measure and B of the form

$$d\sigma = dv_*dve_*^{\frac{\delta}{2}-1}de_*e^{\frac{\delta}{2}-1}ded\omega R^2(1-R^2)^{\delta-1}dR[r(1-r)]^{\frac{\delta}{2}-1}dr$$

$$B := B(E, |g|.|g'|, |g.g'|, ee', e_*e'_*) > 0$$

We derive an approximation of the two terms of the equality (4.48) by using quadrature formulaes for the integrals. For the left hand side, we obtain

$$\int_{\mathbb{R}^3 \times \mathbb{R}^+} \frac{df(v,e)}{dt} \varphi(v,e) e^{\frac{\delta}{2}-1} dvde \simeq \sum_{i \in L} \frac{df_i}{dt} \varphi(v_i, e_i) e_i^{\frac{\delta}{2}-1}. \tag{4.49}$$

For the right hand side term of (4.48) we make some transformations. We set

$$U = \frac{v + v_*}{2}$$

and

$$dvdv_* = 8dUdg.$$

Let us define the domain of admissible parameters

$$D_{g,e,e_*} = \{(g', e') \in \mathbb{R}^3 \times \mathbb{R}^+ \text{ such that } |g'|^2 + e' \leq E(g, e, e_*) = |g|^2 + e + e_*\}$$

and we use the following change of variables for fixed (g, e, e_*)

$$\begin{cases} \omega = \dfrac{g'}{|g'|} \\[2ex] R = \dfrac{|g'|}{\sqrt{E(g,e,e_*)}} \\[2ex] r = \dfrac{e'}{E(g,e,e_*) - |g'|^2} \end{cases}$$

where $(g', e') \in D_{g,e,e_*}$. We have

$$d\omega [r(1-r)]^{\frac{\delta}{2}-1} dr R^2 (1-R^2)^{\delta-1} dR = \frac{(e'e'_*)^{\frac{\delta}{2}-1}}{E(g,e,e_*)^{\delta+\frac{1}{2}}} dg'de'$$

and with

$$e'_* = E(g, e, e_*) - |g'|^2 - e'$$

The right hand side of (4.48) can be written

$$\begin{aligned} &\frac{1}{4} \int_{\mathbb{R}^4} Q_\delta (\varphi + \varphi_* - \varphi' - \varphi'_*) e^{\frac{\delta}{2}-1} dvde \\ = 2 \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^+ \times \mathbb{R}^+} &\left\{ \int_{D_{g,e,e_*}} B(\varphi + \varphi_* - \varphi' - \varphi'_*)(f'f'_* - ff_*) \right. \\ &\left. \frac{(e'e'_*)^{\frac{\delta}{2}-1}}{E(g,e,e_*)^{\delta+\frac{1}{2}}} dg'de' \right\} dUdgdede_*. \end{aligned} \tag{4.50}$$

We first discretize with respect to U. The quadrature points are the elements of $\frac{\Delta v}{2}.\mathbb{Z}^3$. We have

$$\begin{aligned}
&\frac{1}{4}\int_{\mathbb{R}^4} Q_\delta(\varphi+\varphi_*-\varphi'-\varphi'_*)e^{\frac{\delta}{2}-1}dvde \\
\simeq \frac{\Delta v^3}{4} &\sum_{U_m\in\frac{\Delta v}{2}.\mathbb{Z}^3}\int_{\mathbb{R}^3\times\mathbb{R}^+\times\mathbb{R}^+}\Bigg\{\int_{D_{g,e,e_*}} B(\varphi(U_m+g,e)+\varphi(U_m-g,e_*) \\
&-\varphi(U_m+g',e')-\varphi(U_m-g',e_*^{'}))(f(U_m+g',e')f(U_m-g',e_*^{'}) \\
&-f(U_m+g,e)f(U_m-g,e_*))\frac{(e'e_*^{'})^{\frac{\delta}{2}-1}}{E(g,e,e_*)^{\delta+\frac{1}{2}}}dg'de'\Bigg\}dgdede_*. \quad (4.51)
\end{aligned}$$

By discretizing now with respect to g,e,e_* with the quadrature points in $(U_m+\Delta v\mathbb{Z}^3)\times(\Delta v^2(\mathbb{N}+\frac{1}{2}))^2$, and by setting

$$U_{ij}=\frac{v_i+v_j}{2},\ g_{ij}=\frac{v_i-v_j}{2},\ D_{ij}=D_{g_{ij},e_i,e_j},\ E_{ij}=E_{g_{ij},e_i,e_j}$$

we obtain the approximation

$$\begin{aligned}
&\frac{1}{4}\int_{\mathbb{R}^4} Q_\delta(\varphi+\varphi_*-\varphi'-\varphi'_*)e^{\frac{\delta}{2}-1}dvde \\
\simeq \frac{\Delta v^{10}}{4} &\sum_{i,j\in L} e_i^{\frac{\delta}{2}-1}e_j^{\frac{\delta}{2}-1}\Bigg\{\int_{D_{ij}} B(\varphi(v_i,e_i)+\varphi(v_j,e_j)-\varphi(U_{ij}+g',e') \\
&-\varphi(U_{ij}-g',e_*^{'}))(f(U_{ij}+g',e')f(U_{ij}-g',e_*^{'}) \\
&-f(v_i,e_i)f(v_j,e_j))\frac{(e'e_*^{'})^{\frac{\delta}{2}-1}}{E_{ij}^{\delta+\frac{1}{2}}}dg'de'\Bigg\} \quad (4.52)
\end{aligned}$$

We must now discretize the collision integral with respect to g' and e'. For fixed i and j we take the quadrature points for g',e' in $L_{ij}=(U_{ij}+\Delta v\mathbb{Z}^3)\times\Delta v^2(\mathbb{N}+\frac{1}{2})$. One can verify that for $(g',e')\in L_{ij}\cap D_{ij}$ we have $e_*^{'}\in\Delta v^2(\mathbb{N}+\frac{1}{2})$ and $U_{ij}\pm g'\in\Delta v.\mathbb{Z}^3$. We use the same kind of quadrature formula as for the other variables U,g,e,e_*. First we remark that

$$\int_{D_{ij}} B\frac{(e'e_*^{'})^{\frac{\delta}{2}-1}}{E_{ij}^{\delta+\frac{1}{2}}}dg'de'=C_{\alpha\delta}|g_{ij}|^{1-2\alpha} \quad (4.53)$$

where $C_{\alpha\delta}$ is a constant just depending of δ and α. In the same manner as for the first discrete model, by defining

$$S_{ij}=\{k,l\in L \text{ such that } g_{kl}\in L_{ij}\cap D_{ij} \text{ and } U_{kl}=U_{ij}\}$$

we obtain the following approximation

$$C_{\alpha\delta}|g_{ij}|^{1-2\alpha} \simeq \Delta v^5 \sum_{k,l\in S_{ij}} \frac{C}{E_{ij}^{1+\delta-\alpha}} (e_k e_l)^{\frac{\delta}{2}-1} |g_{kl}|^{1-2\alpha} |g_{ij}|^{1-2\alpha} \tag{4.54}$$

and

$$\begin{aligned}
&\int_{D_{ij}} B(\varphi(v_i,e_i) + \varphi(v_j,e_j) - \varphi(U_{ij}+g',e') - \varphi(U_{ij}-g',e_*^{'})) \\
&(f(U_{ij}+g',e')f(U_{ij}-g',e_*^{'}) - f(v_i,e_i)f(v_j,e_j)) \frac{(e'e_*^{'})^{\frac{\delta}{2}-1}}{E_{ij}^{\delta+\frac{1}{2}}} dg'de' \\
&\simeq \Delta v^5 \sum_{k,l\in S_{ij}} \frac{C}{E_{ij}^{1+\delta-\alpha}} (e_k e_l)^{\frac{\delta}{2}-1} |g_{kl}|^{1-2\alpha} |g_{ij}|^{1-2\alpha} \\
&(\varphi(v_i,e_i) + \varphi(v_j,e_j) - \varphi(v_k,e_k) - \varphi(v_l,e_l)) \\
&(f(v_k,e_k)f(v_l,e_l) - f(v_i,e_i)f(v_j,e_j)),
\end{aligned} \tag{4.55}$$

where the constant C comes from the definition of the VHS cross section (2.10). We can remark that for $(k,l) \in S_{ij}$ we have $S_{kl} = S_{ij}$. (4.53), (4.54) and (4.55) gives the approximation

$$\begin{aligned}
&\int_{D_{ij}} B(\varphi(v_i,e_i) + \varphi(v_j,e_j) - \varphi(U_{ij}+g',e') - \varphi(U_{ij}-g',e_*^{'})) \\
&(f(U_{ij}+g',e')f(U_{ij}-g',e_*^{'}) - f(v_i,e_i)f(v_j,e_j)) \frac{(e'e_*^{'})^{\frac{\delta}{2}-1}}{E_{ij}^{\delta+\frac{1}{2}}} dg'de' \\
&\simeq C_{\alpha\delta}|g_{ij}|^{1-2\alpha} \sum_{k,l\in S_{ij}} p_{kl}(\varphi(v_i,e_i) + \varphi(v_j,e_j) - \varphi(v_k,e_k) - \varphi(v_l,e_l)) \\
&(f(v_k,e_k)f(v_l,e_l) - f(v_i,e_i)f(v_j,e_j))
\end{aligned} \tag{4.56}$$

with the weight p_{kl} defined by

$$p_{kl} = \frac{(e_k e_l)^{\frac{\delta}{2}-1} |g_{kl}|^{1-2\alpha}}{\sum_{k,l\in S_{ij}} (e_k e_l)^{\frac{\delta}{2}-1} |g_{kl}|^{1-2\alpha}}.$$

We set $\bar{f} = (f_i)_{i\in L}$. Using (4.49), (4.52), (4.56) and the definition of the f_i we deduce a particle approximation of the continuous homogeneous problem of the form

$$\sum_{i\in L} \frac{df_i}{dt} e_i^{\frac{\delta}{2}-1} \delta(v-v_i) \otimes \delta(e-e_i) = \sum_{i\in L} \bar{Q}_\delta(\bar{f},\bar{f})_i e_i^{\frac{\delta}{2}-1} \delta(v-v_i) \otimes \delta(e-e_i) \tag{4.57}$$

with

$$\bar{Q}_\delta(\bar{f},\bar{f})_i = \sum_{j\in L} \sum_{(k,l)\in S_{ij}} (A_{kl}^{ij} f_k f_l - A_{ij}^{kl} f_i f_j) \tag{4.58}$$

or

$$\bar{Q}_\delta(\bar{f},\bar{f})_i = \sum_{(j,k,l)\in(L)^3} (A_{k,l}^{i,j} f_k f_l - A_{ij}^{kl} f_i f_j), \tag{4.59}$$

with

$$A_{ij}^{kl} = \frac{\mathcal{A}_{ij}^{kl}}{e_i^{\frac{\delta}{2}-1}} = \begin{cases} C_{\alpha\delta} e_j^{\frac{\delta}{2}-1} p_{kl} |g_{ij}|^{1-2\alpha} & \text{if} \quad (k,l)\in S_{ij} \\ 0 \quad \text{otherwise.} \end{cases} \tag{4.60}$$

4.2.2. *Properties of the discrete collision operator*

As for the first model, by construction the tensor $\mathcal{A}_{ij}^{kl}$ is non negative, and satisfies the symmetry properties

$$\mathcal{A}_{ij}^{kl} = \mathcal{A}_{ji}^{kl} = \mathcal{A}_{ij}^{lk} \tag{4.61}$$

and the so called microreversibility property

$$\mathcal{A}_{ij}^{kl} = \mathcal{A}_{kl}^{ij}. \tag{4.62}$$

We can write a discrete analogue of identity (2.5): let $\bar{\varphi} = (\varphi_i)_{i\in L}$ be a test sequence, then

$$\sum_{i\in L} \bar{Q}_\delta(\bar{f},\bar{f})_i \varphi_i e_i^{\frac{\delta}{2}-1} = \frac{1}{4} \sum_{(i,j,k,l)\in(L)^4} \mathcal{A}_{ij}^{kl} (f_k f_l - f_i f_j)(\varphi_i + \varphi_j - \varphi_k - \varphi_l). \tag{4.63}$$

Using the definition of tensor $\mathcal{A}_{ij}^{kl}$ and equality (4.63) we write the discrete analogue of conservation of mass, momentum and energy according to

$$\sum_{i\in L} \bar{Q}_\delta(\bar{f},\bar{f})_i e_i^{\frac{\delta}{2}-1} \begin{pmatrix} 1 \\ v_i \\ \frac{|v_i|^2}{2} + e_i \end{pmatrix} = 0. \tag{4.64}$$

For a global positive solution the discrete H-theorem, that is the dissipation of entropy

$$H(t) = \sum_{i\in L} f_i(t) \log(f_i(t)) e_i^{\frac{\delta}{2}-1},$$

hold:

$$\frac{dH(t)}{dt} = \frac{1}{4} \sum_{(i,j,k,l)\in(L)^4} \mathcal{A}_{ij}^{kl} (f_k f_l - f_i f_j)(\log(f_i f_j) - \log(f_k f_l) \leq 0. \tag{4.65}$$

As in the first model, the equilibrium states $\bar{f}^\infty$, are characterized by the same properties (see proposition 1). For this model the equilibrium states are still discrete Maxwellians:

Lemma 4.4 *For the discrete collision operator defining by (4.58) and (4.60) the invariants of collisions are given by*

$$\varphi_i = A(v_i^2 + 2e_i) + < B, v_i > + C$$

with A and $C \in \mathrm{I\!R}$ and $B \in \mathrm{I\!R}^3$ and the equilibrium states $\bar{f}^\infty$ have the form

$$f_i^\infty = \exp(A(v_i^2 + 2e_i) + < B, v_i > + C)$$

Proof. For $\varphi = (\varphi_i)_{i \in L}$, we let $\varphi(m)$ be the restriction of φ to the subset $L_m = \{i \in L,\ i_4 = m\}$ that is, $\varphi(m)$ is the restriction of φ at the level $m + \dfrac{1}{2}$ of internal energy. We set $\bar{i} = (i_1, i_2, i_3)$ for an element i of L_m. For $\varphi(m)$ we have already proved, (see proof of lemma 3), that

$$\varphi_i(m) = A(m)|\bar{i}|^2 + < B(m), \bar{i} > + C(m)$$

with $A(m)$ *and* $C(m) \in \mathrm{I\!R}$ *and* $B(m) \in \mathrm{I\!R}^3$. We set $A(0) = A$, $C(0) = C$, $B(0) = B$. We have now to show that for any m, we have

$$A(m) = A,\ B(m) = B,\ C(m) = 2mA + C. \tag{4.66}$$

It is readily seen that (4.66) implies lemma 4 from the equivalence properties given in proposition 1. The idea to prove (4.66) is to show that all the levels of internal energy are sufficiently coupled. We prove (4.66) inductively on m. Assume the result holds for $m \leq m_0$. Let m be an integer in $[0, m_0 + 2]$ such that m can be written as a sum of three squares of integers a, b, c that is $m = a^2 + b^2 + c^2$. In all the cases the largest possible m is greater or equal to 2 . Consequently for any m_0 we have $m_0 + 2 - m \leq m_0$. The inelastic collisions can be characterized by a relation on the multiindices (i, j) and (k, l) for the velociies and internal energies as defined in (4.47). Among the many collisions processes, we shall consider the following cases:

$$i = (0,0,0,m_0{+}1), j = (2,0,0,0) \to k = (a{+}1, b, c, m_0{+}2{-}m), l = (1{-}a, -b, -c, 0)$$

$$i = (2,0,0,m_0{+}1), j = (0,0,0,0) \to k = (a{+}1, b, c, m_0{+}2{-}m), l = (1{-}a, -b, -c, 0)$$

$$i = (0,2,0,m_0{+}1), j = (0,0,0,0) \to k = (a, b{+}1, c, m_0{+}2{-}m), l = (-a, 1{-}b, -c, 0)$$

$$i = (0,0,2,m_0{+}1), j = (0,0,0,0) \to k = (a, b, c{+}1, m_0{+}2{-}m), l = (-a, -b, 1{-}c, 0)$$

$$i = (4,0,0,m_0{+}1), j = (2,0,0,0) \to k = (a{+}3, b, c, m_0{+}2{-}m), l = (3{-}a, -b, -c, 0)$$

One can verify that, for these collision processes, we have $\mathcal{A}_{ij}^{kl} \neq 0$, which implies that the invariants of collision satisfy

$$\varphi_i(m_0 + 1) + \varphi_j(0) = \varphi_k(m_0 + 2 - m) + \varphi_l(0).$$

By the use of the result (4.66) for m_0+2-m, we have then the set of equations

$$\left\{\begin{array}{c} C(m_0+1) = 2(m_0+1)A + C \\ 4A(m_0+1) + 2B_1(m_0+1) = 4A + 2B_1 \\ 4A(m_0+1) + 2B_2(m_0+1) = 4A + 2B_2 \\ 4A(m_0+1) + 2B_3(m_0+1) = 4A + 2B_3 \\ 16A(m_0+1) + 4B_1(m_0+1) = 16A + 4B_1 \end{array}\right.$$

for which the unique solution is

$$\left\{\begin{array}{c} C(m_0+1) = 2(m_0+1)A + C \\ A(m_0+1) = A \\ B_1(m_0+1) = B_1 \\ B_2(m_0+1) = B_2 \\ B_3(m_0+1) = B_3. \end{array}\right.$$

This proves (4.66) at order m_0+1. Using the integrability requirements, that is

$$\sum_{i\in L} f_i^\infty e_i^{\frac{\delta}{2}-1} < +\infty,$$

we necessarily have $A<0$. $\square$

As for the first model, we can bound the velocity-energy domain by a straightforward adaptation of the analysis presented for the first model. We mention that if the resulting set for the multiindices i is of the form

$$\{i \in L, \imath_1^2 + i_2^2 + i_3^2 \leq M,\ i_4 \leq N\}$$

or

$$\{i \in L,\ i \sup_{p=1,3} i_p \leq M,\ i_4 \leq N\},$$

with $M \geq 4$, then all the properties of the collision operators are still satisfied except for the sign of the coefficient of A in the equilibrium state (see the dicussion of this problem in the first case).

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