BGK and Fokker-Planck models of the Boltzmann equation for gases with discrete levels of vibrational energy

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Abstract

We propose two models of the Boltzmann equation (BGK and Fokker-Planck models) for rarefied flows of diatomic gases in vibrational non-equilibrium. These models take into account the discrete repartition of vibration energy modes, which is required for high temperature flows, like for atmospheric re-entry problems. We prove that these models satisfy conservation and entropy properties (H-theorem), and we derive their corresponding compressible Navier-Stokes asymptotics.

Keywords: Fokker-Planck model, BGK model, H-theorem, Rarefied Gas Dynamics, vibrational molecules

1 Introduction

Numerical simulation of atmospheric reentry flows requires to solve the Boltzmann equation of Rarefied Gas Dynamics. The standard method to do so is the Direct Simulation Monte Carlo (DSMC) method [1, 2], which is a particle stochastic method. However, it is sometimes interesting to have alternative numerical methods, like, for instance, methods based on a direct discretization of the Boltzmann equation (deterministic approaches). This is hardly possible for the full Boltzmann equation (except for monatomic gases, see [3]), since this is still much too computationally expensive for real gases. But BGK like model equations [4] are very well suited for such deterministic codes: indeed, their complexity can be reduced by the well known reduced distribution technique [5], which leads to intermediate models between the full Boltzmann equation and moment models [6]. The Fokker-Planck model [7] is another model Boltzmann equation that can give very efficient stochastic particle methods, see [8].

These model equations have already been extended to polyatomic gases, so that they can take into account the internal energy of rotation of gas molecules. They contains correction terms that lead to correct transport coefficients: the ESBGK or Chekhov's models [9, 10, 11], and the cubic Fokker-Planck and ES-Fokker-Planck [8, 12, 13, 14].

For high temperature flows, like in space reentry problems, the vibrational energy of molecules is activated, and has a significant influence on energy transfers in the gas flow. It is therefore interesting to extend the model equations to take this vibrational modes into account. Several extended BGK models have been recently proposed to do so, for instance [15, 16, 17, 18], and a recent Fokker-Planck model has been proposed earlier in [19].

All these models assume a continuous vibrational energy repartition. However, while transitional and rotational energies in air can be considered as continuous for temperature larger than 1K and 10K, respectively, vibrational energy can be considered as continuous only for much larger temperatures (2000K for oxygen and 3300K for nitrogen). For flows up to 3000K around reentry vehicles, the discrete levels of vibrational energy must be used [20]. It seems that that the only BGK model that allows for this discrete repartition is the model of Morse [21].

In this paper, we consider a simpler version of this Morse BGK model for vibrating gases that allows for a discrete vibrational energy. We show that the complexity of this model can be reduced with the reduced distribution technique so that the discrete vibrational energy is eliminated. What is new here is that this construction allows us to prove that the corresponding reduced model satisfies the H-theorem. Moreover, the model is shown to give macroscopic Euler and Navier-Stokes equations in the dense regime, with temperature dependent heat capacities, as expected. This means that the reduced model is a good candidate for its implementation in a deterministic simulation code.

An equivalent reduced Fokker-Planck model is also proposed, that has the same properties. However, this model is not based on a non-reduced model, since we are not able so far to define diffusion process for the discrete vibrational energy. Up to our knowledge, this is the first time such a Fokker-Planck model for vibration energy is proposed.

Our paper is organized as follows. In section 2, we present the kinetic description of a gas with vibrating molecules, and we discuss the mathematical properties of the reduced distributions that will be used for our models. Our BGK and Fokker-Planck models are presented in sections 3 and 4, respectively. In section 5, the hydrodynamic limits of our models, obtained by a Chapman-Enskog procedure, are discussed. Section 6 gives some perspectives of this work.

2 Kinetic description of a vibrating diatomic gas

2.1 Distribution function and local equilibrium

We consider a diatomic gas. We define $f(t,x,v,\varepsilon,i)$ the mass density of molecules with position x, velocity v, internal energy ε, and in the ith vibrational energy level, such that the corresponding vibrational energy is iRT_0, where $T_0 = h\nu/k$ is a characteristic vibrational temperature of the molecule (h and k are the Planck and Boltzmann constant, while ν is the fundamental vibrational frequency of the molecule).

The corresponding local equilibrium distribution is defined by (see [1])

$$M_{vib}[f](v,\varepsilon,i) = \frac{\rho}{\sqrt{2\pi RT}^3}\frac{1-e^{-T_0/T}}{RT}\exp\left(-\frac{\frac{1}{2}|u-v|^2+\varepsilon+iRT_0}{RT}\right). \quad (1)$$

Here, ρ is the mass density of the gas, T its temperature of equilibrium and u its mean velocity, defined below.

2.2 Moments and entropy

The macroscopic quantities are defined by moments of f as follows:

$$\rho = \langle f \rangle_{v,\varepsilon,i}, \qquad \rho u = \langle v f \rangle_{v,\varepsilon,i}, \qquad \rho e = \left\langle \left(\frac{1}{2}|v-u|^2 + \varepsilon + iRT_0 \right) f \right\rangle_{v,\varepsilon,i}, \tag{2}$$

where we use the notation $\langle \phi \rangle_{v,\varepsilon,i} = \sum_{i=0}^{\infty} \iint \phi(t,x,v,\varepsilon,i)\, dv d\varepsilon$ for any function ϕ.

With standard Gaussian integrals and summation formula, it is easy to find that the moments of the equilibrium $M_{vib}[f]$ satisfy:

$$\langle M_{vib}[f] \rangle_{v,\varepsilon,i} = \rho, \qquad \langle v M_{vib}[f] \rangle_{v,\varepsilon,i} = \rho u.$$

At equilibrium, we can define the following energies of translation, rotation, and vibration

$$\rho e_{tr}(T) = \left\langle (\frac{1}{2}(v-u)^2) M_{vib}[f] \right\rangle_{v,\varepsilon,i} = \frac{3}{2}\rho RT, \tag{3}$$

$$\rho e_{rot}(T) = \langle \varepsilon M_{vib}[f] \rangle_{v,\varepsilon,i} = \rho RT, \tag{4}$$

$$\rho e_{vib}(T) = \langle (iRT_0) M_{vib}[f] \rangle_{v,\varepsilon,i} = \rho \frac{RT_0}{e^{T_0/T} - 1} = \frac{\delta(T)}{2}\rho RT, \tag{5}$$

where the number of degrees of freedom of vibrations is

$$\delta(T) = \frac{2T_0/T}{e^{T_0/T} - 1}, \tag{6}$$

which is a non integer and temperature dependent number, while the number of degrees of freedom is 3 for translation and 2 for rotation.

The temperature T is defined so that $M_{vib}[f]$ has the same energy as f:

$$\left\langle (\frac{1}{2}(v-u)^2 + \varepsilon + iRT_0) M_{vib}[f] \right\rangle_{v,\varepsilon,i} = \rho e,$$

which gives the non linear implicit definition of T:

$$e = \frac{5 + \delta(T)}{2} RT. \tag{7}$$

Since the function $T \to e$ is monotonic, T is uniquely defined by (7). Moreover, note that $\delta(T)$ is necessarily between 0 and 2, which means that vibrations add at most two degrees of freedom.

Finally, the entropy $\mathcal{H}(f)$ of f is defined by $\mathcal{H}(f) = \langle f \log f \rangle_{v,\varepsilon,i}$.

2.3 Reduced distributions

For computational efficiency, it is interesting to define marginal, or reduced, distributions F and G by

$$F(t,x,v,\varepsilon) = \sum_i f(t,x,v,\varepsilon,i), \quad \text{and} \quad G(t,x,v,\varepsilon) = \sum_i iRT_0 f(t,x,v,\varepsilon,i).$$

The macroscopic variables defined by f can be obtained through F and G only, as it is shown in the following proposition.

Proposition 2.1 (Moments of the reduced distributions)**.** *The macroscopic variables ρ, u, and e, of f, defined by* (2)*, satisfy*

$$\rho = \langle F \rangle_{v,\varepsilon}\,, \qquad \rho u = \langle vF \rangle_{v,\varepsilon}\,, \qquad \rho e = \left\langle (\frac{1}{2}(v-u)^2 + \varepsilon)F \right\rangle_{v,\varepsilon} + \langle G \rangle_{v,\varepsilon}\,. \tag{8}$$

where we use the notation $\langle \psi \rangle_{v,\varepsilon} = \iint \psi(t,x,v,\varepsilon)\,dvd\varepsilon$ for any function ψ.

This reduction procedure can be extended to the entropy functional as follows. First, to simplify the following relations, we use the notation $f_i(v,\varepsilon)$ for $f(v,\varepsilon,i)$. Then, we define the reduced entropy by

$$\begin{aligned} &\mathcal{H}(F,G) = \langle H(F,G) \rangle_{v,\varepsilon}\,, \text{ where} \\ &H(F,G) = \inf_{f>0} \left\{ \sum_i f_i \log f_i \quad \text{such that} \quad \sum_i f_i = F, \quad \sum_i iRT_0 f_i = G \right\}. \end{aligned} \tag{9}$$

In other words, for a given couple of reduced distributions (F,G), we define the (non reduced) distribution that minimizes the marginal entropy $\sum_i f_i \log f_i$ among all the distributions that have the same marginal distributions F and G. Then the reduced entropy is the integral with respect to v and ε of the corresponding marginal entropy.

Now it is possible to write this reduced entropy as a function of F and G only, as it is shown in the following proposition.

Proposition 2.2 (Entropy)**.** *The reduced entropy $\mathcal{H}(F,G)$ defined by (9) is*

$$\mathcal{H}(F,G) = \left\langle F\log(F) + F\log\left(\frac{RT_0F}{RT_0F+G}\right) + \frac{G}{RT_0}\log\left(\frac{G}{RT_0F+G}\right)\right\rangle_{v,\varepsilon}. \tag{10}$$

Proof. The set $\{f>0 \text{ such that } \sum_i f_i = F, \quad \sum_i iRT_0 f_i = G\}$ is clearly convex, so that we can use a Lagrangian multiplier approach by finding a saddle point of the function $\mathcal{I}$ defined through :

$$\mathcal{I}(f,\alpha,\beta) = \sum_i f_i \log f_i - \alpha\left(\sum_i f_i - F\right) - \beta\left(\sum_i iRT_0 f_i - G\right),$$

where α and β are real numbers. The saddle point satisfies $\frac{\partial \mathcal{I}}{\partial f} = 0$, and it is easy to deduce that f can be written $f_i(v,\varepsilon) = A\exp(-iBRT_0)$, where $A := A(v,\varepsilon)$ and $B := B(v,\varepsilon)$ are functions that are still to be determined.

The linear constraints give:

$$\begin{aligned} F &= \sum_i f_i = \frac{A}{1-\exp(-BRT_0)}, \\ G &= \sum_i f_i iRT_0 = -\frac{1}{B}\frac{d}{dB}\sum_i f_i = \frac{ART_0\exp(-BRT_0)}{(1-\exp(-BRT_0))^2}. \end{aligned}$$

Solving this linear system gives

$$A = \frac{RT_0F^2}{RT_0F+G}, \qquad B = \frac{1}{RT_0}\log\left(1+\frac{RT_0F}{G}\right).$$

so that

$$H(F,G) = F\log(F) + F\log\left(\frac{RT_0F}{RT_0F+G}\right) + \frac{G}{RT_0}\log\left(\frac{G}{RT_0F+G}\right). \tag{11}$$

A final integration with respect to v and ε gives the final result. □

Now, we want to use this reduced entropy to define the corresponding reduced equilibrium. This is done by computing the minimum of the reduced entropy for the couple of reduced distributions (F_1, G_1) that have the same moments as f. It means that we look for the minimum of $\mathcal{H}(F_1, G_1)$ on the set $\mathcal{S} = \left\{(F_1, G_1) \text{ such that } \langle F_1\rangle_{v,\varepsilon} = \rho, \quad \langle vF_1\rangle_{v,\varepsilon} = \rho u, \quad \left\langle(\tfrac{1}{2}|v|^2+\varepsilon)F_1 + G_1\right\rangle_{v,\varepsilon} = \rho e\right\}$. The following proposition gives this minimum and other useful differential properties of the reduced entropy functional.

Proposition 2.3. *1. The partial derivatives of H computed at (F,G) are:*

$$D_1H(F,G) = 1 + \log\left(\frac{RT_0F^2}{RT_0F+G}\right), \quad D_2H(F,G) = \frac{1}{RT_0}\log\left(\frac{G}{RT_0F+G}\right). \tag{12}$$

2. *We note $\mathbb{H} = \begin{pmatrix} D_{11}H(F,G) & D_{12}H(F,G) \\ D_{12}H(F,G) & D_{22}H(F,G)\end{pmatrix}$ the Hessian matrix of H. The second order derivatives are*

$$D_{11}H(F,G) = \frac{2}{F} - \frac{RT_0}{RT_0F+G}, \qquad D_{12}H(F,G) = -\frac{1}{RT_0F+G},$$
$$D_{21}H(F,G) = D_{12}H(F,G), \qquad D_{22}H(F,G) = \frac{F}{G(RT_0F+G)},$$

and we have

$$\begin{aligned} FD_{11}H(F,G) + GD_{21}H(F,G) &= 1, \\ FD_{12}H(F,G) + GD_{22}H(F,G) &= 0. \end{aligned} \tag{13}$$

3. *The function $(F,G) \mapsto H(F,G)$ is convex.*

4. *The minimum of $\mathcal{H}$ on $\mathcal{S}$ is obtained for the couple $(M_{vib}(F,G), e_{vib}(T)M_{vib}(F,G))$ with*

$$M_{vib}[F,G] = \frac{\rho}{\sqrt{2\pi RT}^3}\exp\left(-\frac{|v-u|^2}{2RT}\right)\frac{1}{RT}\exp\left(-\frac{\varepsilon}{RT}\right) \tag{14}$$

where $e_{vib}(T)$ is the equilibrium vibrational energy defined by (5).

5. *For every (F_1, G_1) in $\mathcal{S}$, we have*

$$\begin{aligned} 0 &\geq H(M_{vib}(F,G), e_{vib}(T)M_{vib}(F,G)) - H(F_1,G_1) \\ &\geq D_1H(F,G)(M_{vib}(F,G) - F) + D_2H(F,G)(e_{vib}(T)M_{vib}(F,G) - G) \end{aligned}$$

Proof. Points 1 and 2 are given by direct calculations. For point 3, note that the determinant of the Hessian matrix $\mathbb{H}$, which is $\det \mathbb{H} = \frac{1}{G(RT_0F+G)}$ is positive. Moreover, its trace is positive too, so that the Hessian matrix is positive definite, and hence the function H is convex.

We now compute the minimum of the reduced entropy. First, the set $\mathcal{S}$ is clearly convex, and it is non empty, since it is easy to see that $(M_{vib}, e_{vib}(T)M_{vib})$ realizes the moments ρ, ρu, and ρe, and hence belongs to $\mathcal{S}$. Now, we define the following Lagrangian

$$\begin{aligned}\mathcal{J}(F_1, G_1, \alpha, \beta, \gamma) = &\langle H(F_1, G_1)\rangle_{v,\varepsilon} - \alpha(\langle F_1\rangle_{v,\varepsilon} - \rho)\\ &- \beta \cdot (\langle vF_1\rangle_{v,\varepsilon} - \rho u) - \gamma \left(\left\langle (\frac{1}{2}|v|^2 + \varepsilon)F_1 + G_1 \right\rangle_{v,\varepsilon} - \rho e \right)\end{aligned}$$

for $(F_1, G_1) \in \mathcal{S}$, $\alpha \in \mathbb{R}$, $\beta \in \mathbb{R}^3$, $\gamma \in \mathbb{R}$. The reduced entropy has a minimum of $\mathcal{S}$ if, and only if, $\mathcal{J}$ has a saddle point. This saddle point, denoted by $(F_1, G_1, \alpha, \beta, \gamma)$ for the moment, is characterized by the fact that the partial derivatives of $\mathcal{J}$ vanish at $(F_1, G_1, \alpha, \beta, \gamma)$. This gives the following relations:

$$D_1H(F_1, G_1) = \alpha + \beta \cdot v + \gamma \frac{1}{2}|v|^2, \tag{15}$$

$$D_2H(F_1, G_1) = \gamma, \tag{16}$$

$$\langle F_1\rangle_{v,\varepsilon} - \rho = 0, \tag{17}$$

$$\langle vF_1\rangle_{v,\varepsilon} - \rho u = 0, \tag{18}$$

$$\left\langle (\frac{1}{2}|v|^2 + \varepsilon)F_1 + G_1 \right\rangle_{v,\varepsilon} - \rho e = 0, \tag{19}$$

where D_1H and D_2H are defined in (12). Combining equations (15) and (16), one gets that there exist four real numbers A, B, C, D and one vector $E \in \mathbb{R}^3$, independent of v and ε, such that:

$$\begin{aligned} F_1 &= A \exp\left(E \cdot v + B|v|^2 + C\varepsilon\right), \\ G_1 &= DF_1, \end{aligned}$$

where B and C are necessarily non positive to ensure the integrability of F_1 and G_1. It is then standard to use equations (17)–(19) to get $F_1 = M_{vib}(F, G)$ and $G_1 = e_{vib}(T)M_{vib}(F, G)$.

Finally point 5 is a direct consequence of the convexity of H and of the minimization property. □

3 A BGK model with vibrations

With the local equilibrium $M_{vib}[f]$ defined in (1), it is easy to derive the following BGK model:

$$\partial_t f + v \cdot \nabla f = \frac{1}{\tau}(M_{vib}[f] - f). \tag{20}$$

The macroscopic parameters ρ, u, and T are defined through the moments ρ, ρu and ρe of f (see (2)).

Like in the BGK model for monoatomic gases, it will be shown that the relaxation time of this BGK model is $\tau = \mu/p$, where $p = \rho RT$ is the pressure and μ the viscosity, that can be temperature dependent.

Now we have the following properties.

Property 3.1. • *Conservation: for BGK model* (20) *the mass, momentum and total energy are conserved:*

$$\partial_t \left\langle \begin{pmatrix} 1 \\ v \\ \frac{1}{2}|v|^2 \end{pmatrix} f \right\rangle_{v,\varepsilon,i} + \nabla_x \cdot \left\langle v \begin{pmatrix} 1 \\ v \\ \frac{1}{2}|v|^2 \end{pmatrix} f \right\rangle_{v,\varepsilon,i} = 0.$$

- *H-theorem: for the entropy* $\mathcal{H}(f) = \langle f \log f \rangle_{v,\varepsilon,i}$, *we have*

$$\partial_t \mathcal{H}(f) + \nabla_x \cdot \langle v f \log f \rangle_{v,\varepsilon,i} = \frac{1}{\tau} \langle (M_{vib}[f] - f) \log f \rangle_{v,\varepsilon,i} \leq 0.$$

The proof relies on standard arguments (definition of $M_{vib}[f]$ and convexity of $x \log x$) and is left to the reader.

3.1 A reduced BGK model with vibrations

For computational reasons, it is interesting to reduce the complexity of model (20) by using the usual reduced distribution technique [22]. We define the reduced distributions

$$F = \sum_i f(t, x, v, \varepsilon, i), \quad \text{and} \quad G = \sum_i iRT_0 f(t, x, v, \varepsilon, i),$$

and by summation of (20) on i we get the following closed system of two reduced equations:

$$\partial_t F + v \cdot \nabla_x F = \frac{1}{\tau} \left(M_{vib}[F, G] - F \right), \tag{21}$$

$$\partial_t G + v \cdot \nabla_x G = \frac{1}{\tau} \left(\frac{\delta(T)}{2} RT M_{vib}[F, G] - G \right), \tag{22}$$

where the reduced Maxwellian is

$$M_{vib}[F, G] = \frac{\rho}{\sqrt{2\pi RT}^3} \exp\left(-\frac{|v-u|^2}{2RT} \right) \frac{1}{RT} \exp\left(-\frac{\varepsilon}{RT} \right),$$

and the macroscopic quantities are defined by

$$\rho = \langle F \rangle_{v,\varepsilon}, \qquad \rho u = \langle v F \rangle_{v,\varepsilon}, \qquad \rho e = \left\langle \left(\frac{1}{2}(v-u)^2 + \varepsilon\right) F \right\rangle_{v,\varepsilon} + \langle G \rangle_{v,\varepsilon}, \tag{23}$$

and T is still defined by (7).

Note that this model can easily be reduced once again to eliminate the rotational energy variable. This gives a reduced system of three BGK equations, with three distributions (see [23] for such a reduction in a more complex ES-BGK model).

It is interesting to compare our new model to the work of [24] and [18]: in these recent papers, the authors also proposed, independently, BGK and ES-BGK models for temperature dependent δ, like in the case of vibrational energy. However, they are not based on an underlying discrete vibrational energy repartition, and the authors are not able to prove any H-theorem. Only a local entropy dissipation can be proved. The advantage of our new approach is that the reduced model, which is continuous in energy too, inherits the entropy property from the non-reduced model, and hence a H-theorem, as it is shown below.

3.2 Properties of the reduced model

System (21–22) naturally satisfies local conservation laws of mass, momentum, and energy. Moreover, the H-theorem holds with the reduced entropy $H(F, G)$ as defined in (9). Indeed, we have the

Proposition 3.1. *The reduced BGK system (21–22) satisfies the H-theorem*

$$\partial_t \mathcal{H}(F, G) + \nabla_x \cdot \langle vH(F, G)\rangle_{v,\varepsilon} \leq 0,$$

where $\mathcal{H}(F, G)$ is the reduced entropy defined in (9)*.*

Proof. By differentiation we get

$$\begin{aligned}
&\partial_t \mathcal{H}(F, G) + \nabla_x \cdot \langle vH(F, G)\rangle_{v,\varepsilon} \\
&= \langle D_1 H(F, G)(\partial_t F + v\nabla_x F) + D_2 H(F, G)(\partial_t G + v\nabla_x G)\rangle_{v,\varepsilon} \\
&= \frac{1}{\tau}\left\langle D_1 H(F, G)(M_{vib}[F, G] - F) + D_2 H(F, G)(\frac{\delta(T)}{2} RT M_{vib}[F, G] - G)\right\rangle_{v,\varepsilon} \\
&\leq 0
\end{aligned}$$

where we have used (21–22) to replace the transport terms by relaxation ones, and point 5 of proposition 2.3 to obtain the inequality. □

4 A Fokker-Planck model with vibrations

It is difficult to derive a Fokker-Planck model for the distribution function f with discrete energy levels. We find it easier to directly derive a reduced model, by analogy with the reduced BGK model (21–22) and by using our previous work [14] on a Fokker-Planck model for polyatomic gases.

4.1 A reduced Fokker-Planck model with vibrations

First, we remind the Fokker-Planck model for a diatomic gas (without vibration) obtained in [14]:

$$\partial_t f + v \cdot \nabla_x f = D(f), \tag{24}$$

where $f = f(t, x, v, \varepsilon)$ and the collision operator is

$$D(f) = \frac{1}{\tau}\left(\nabla_v \cdot \left((v - u)f + RT\nabla_v f\right) + 2\partial_\varepsilon(\varepsilon f + RT\varepsilon\partial_\varepsilon f)\right),$$

where the macroscopic values are

$$\rho = \langle f\rangle_{v,\varepsilon} \quad , \quad \rho u = \langle fv\rangle_{v,\varepsilon} \quad , \quad \rho e = \left\langle f\left(\frac{1}{2}(v-u)^2 + \varepsilon\right)\right\rangle_{v,\varepsilon} = \frac{5}{2}\rho RT.$$

The internal energy ε can be eliminated by the reduction technique (integration w.r.t $d\varepsilon$ and $\varepsilon d\varepsilon$) to get

$$\begin{aligned}
\partial_t \mathcal{F} + v \cdot \nabla_x \mathcal{F} &= D_1(\mathcal{F}, \mathcal{G}), \\
\partial_t \mathcal{G} + v \cdot \nabla_x \mathcal{G} &= D_2(\mathcal{F}, \mathcal{G}),
\end{aligned}$$

with the collision operators

$$D_{\mathcal{F}}(\mathcal{F},\mathcal{G}) = \frac{1}{\tau}\nabla_v \cdot \big((v-u)\mathcal{F} + RT\nabla_v\mathcal{F}\big),$$
$$D_{\mathcal{G}}(\mathcal{F},\mathcal{G}) = \frac{1}{\tau}\nabla_v \cdot \big((v-u)\mathcal{G} + RT\nabla_v\mathcal{G}\big) + \frac{2}{\tau}\left(RT\mathcal{F} - \mathcal{G}\right).$$

Note that the two velocity drift-diffusion terms in the two previous equations have exactly the same structure as the one in the non-reduced model (24). However, it is interesting to note that the energy drift-diffusion term of (24) gives, after reduction, a relaxation operator in the $\mathcal{G}$ equation.

By analogy, now we propose the following reduced Fokker-Planck model for a diatomic gas with vibrations. Note that now, the model is still with variables x, v, and ε: only the discrete energy levels i are eliminated. This model is

$$\partial_t F + v\cdot\nabla_x F = D_F(F,G), \tag{25}$$
$$\partial_t G + v\cdot\nabla_x G = D_G(F,G), \tag{26}$$

with

$$\begin{aligned} D_F(F,G) &= \frac{1}{\tau}\left(\nabla_v \cdot \big((v-u)F + RT\nabla_v F\big) + 2\partial_\varepsilon(\varepsilon F + RT\varepsilon\partial_\varepsilon F)\right), \\ D_G(F,G) &= \frac{1}{\tau}\left(\nabla_v \cdot \big((v-u)G + RT\nabla_v G\big) + 2\partial_\varepsilon(\varepsilon G + RT\varepsilon\partial_\varepsilon G)\right) + \frac{2}{\tau}\left(e_{vib}(T)F - G\right), \end{aligned} \tag{27}$$

where the macroscopic values are defined as in (23) and (7).

4.2 Properties of the reduced model

Using direct calculations and dissipation properties as in [14] we can prove the following proposition.

Proposition 4.1. *The collision operator conserves the mass, momentum, and energy:*

$$\langle (1,v)D_F(F,G)\rangle_{v,\varepsilon} = 0 \quad \textit{and} \quad \left\langle (\frac{1}{2}|v|^2+\varepsilon)D_F(F,G) + D_G(F,G)\right\rangle_{v,\varepsilon} = 0,$$

the reduced entropy $\mathcal{H}(F,G)$ satisfies the H-theorem:

$$\partial_t\mathcal{H}(F,G) + \nabla_x\cdot\langle vH(F,G)\rangle_{v,\varepsilon} = \mathcal{D}(F,G) \le 0,$$

and we have the equilibrium property

$$(D_F(F,G)=0 \textit{ and } D_G(F,G)=0) \Leftrightarrow (F = M_{vib}[F,G] \textit{ and } G = e_{vib(T)}M_{vib}[F,G]).$$

Proof. The conservation property is the consequence of direct integration of (27). The equilibrium property can be proved as follows. First, note that the Maxwellian $M_{vib}[F,G]$ can be written as

$$M_{vib}[F,G] = \frac{\rho}{(2\pi)^{3/2}(RT)^{5/2}}\exp\left(-\frac{1}{2}\begin{pmatrix} v-u \\ 2\varepsilon\end{pmatrix}^T \Omega^{-1}\begin{pmatrix} v-u \\ 2\varepsilon\end{pmatrix}\right),$$

with $\Omega = \begin{pmatrix} RT & 0 \\ 0 & 2\varepsilon RT \end{pmatrix}$. To shorten the notations, $M_{vib}[F,G]$ will be simply denoted by M_{vib} below, and $e_{vib}(T)$ will be simply denoted by e_{vib} as well. Then the collision operators can be written in the compact form

$$D_F(F,G) = \frac{1}{\tau}\nabla_{v,\varepsilon}\cdot\left(\Omega M_{vib}\nabla_{v,\varepsilon}\frac{F}{M_{vib}}\right),$$
$$D_G(F,G) = \frac{1}{\tau}\nabla_{v,\varepsilon}\cdot\left(\Omega M_{vib}\nabla_{v,\varepsilon}\frac{G}{M_{vib}}\right) + \frac{2}{\tau}\left(e_{vib}F - G\right).$$

Then an integration by part gives the following identity for $D_F(F,G)$:

$$\left\langle D_F(F,G)\frac{F}{M_{vib}}\right\rangle_{v,\varepsilon} = -\frac{1}{\tau}\left\langle\left(\nabla_{v,\varepsilon}\frac{F}{M_{vib}}\right)^T\Omega M_{vib}\nabla_{v,\varepsilon}\frac{F}{M_{vib}}\right\rangle_{v,\varepsilon}.$$

Consequently, if $D_F(F,G) = 0$, since the integrand in the previous relation is a definite positive form, the gradient is necessarily zero, and hence $F = M_{vib}$. For the equilibrium property of G, the proof is a bit more complicated. First, we have

$$\left\langle D_G(F,G)\frac{G}{e_{vib}M_{vib}}\right\rangle_{v,\varepsilon} = -\frac{1}{\tau e_{vib}}\left\langle\left(\nabla_{v,\varepsilon}\frac{G}{M_{vib}}\right)^T\Omega M_{vib}\nabla_{v,\varepsilon}\frac{G}{M_{vib}}\right\rangle_{v,\varepsilon} + \left\langle\frac{2}{\tau}\left(e_{vib}F - G\right)\frac{G}{e_{vib}M_{vib}}\right\rangle_{v,\varepsilon}.$$

Consequently, if $D_G(F,G) = 0$, and since $F = M_{vib}$, we have

$$\begin{aligned}
\frac{1}{e_{vib}}\left\langle\left(\nabla_{v,\varepsilon}\frac{G}{M_{vib}}\right)^T\Omega M_{vib}\nabla_{v,\varepsilon}\frac{G}{M_{vib}}\right\rangle_{v,\varepsilon} &= \frac{2}{\tau}\left\langle\left(e_{vib}M_{vib} - G\right)\frac{G}{e_{vib}M_{vib}}\right\rangle_{v,\varepsilon} \\
&= -\frac{2}{\tau}\left\langle\left(e_{vib}M_{vib} - G\right)^2\frac{1}{e_{vib}M_{vib}}\right\rangle_{v,\varepsilon} + \frac{2}{\tau}\left\langle e_{vib}M_{vib} - G\right\rangle_{v,\varepsilon} \\
&\leq \frac{2}{\tau}\left\langle e_{vib}M_{vib} - G\right\rangle_{v,\varepsilon} = \frac{2}{\tau}(\rho e_{vib} - \langle G\rangle_{v,\varepsilon}) = 0,
\end{aligned}$$

which comes from (8) and $F = M_{vib}$. Therefore, we obtain

$$\frac{1}{e_{vib}}\left\langle\left(\nabla_{v,\varepsilon}\frac{G}{M_{vib}}\right)^T\Omega M_{vib}\nabla_{v,\varepsilon}\frac{G}{M_{vib}}\right\rangle_{v,\varepsilon} \leq 0,$$

and again this gives $G = e_{vib}M_{vib}$, which concludes the proof of the equilibrium property.

The proof of the H-theorem is much longer. First, by differentiation one gets that the quantity $\mathcal{D}(F,G) = \partial_t\mathcal{H}(F,G) + \nabla_x\cdot\langle vH(F,G)\rangle_{v,\varepsilon}$ satisfies:

$$\begin{aligned}
\mathcal{D}(F,G) &= \langle D_1H(F,G)(\partial_t F + v\cdot\nabla_x F) + D_2H(F,G)(\partial_t G + v\cdot\nabla_x G)\rangle_{v,\varepsilon} \\
&= \langle D_1H(F,G)D_F(F,G) + D_2H(F,G)D_G(F,G)\rangle_{v,\varepsilon}, \qquad (28)
\end{aligned}$$

from (21–22). Then the proof is based on the convexity of $H(F,G)$: while for the BGK we only used the the first derivatives of H, we now use the positive-definiteness of the Hessian matrix of H.

To do so we integrate by parts $\mathcal{D}(F,G)$ and multiply by τ so that:

$$
\begin{aligned}
\tau\mathcal{D}(F,G) \quad = \quad & -\sum_{i=1}^{3}\left\langle \partial_{v_i}(F) D_{11}H(F,G)\left(F(v_i-u_i)+RT\partial_{v_i}F\right)\right\rangle_{v,\varepsilon} \\
& -2\left\langle \partial_{\varepsilon}(F) D_{11}H(F,G)\left(F\varepsilon+RT\varepsilon\partial_{\varepsilon}F\right)\right\rangle_{v,\varepsilon} \\
& -\sum_{i=1}^{3}\left\langle \partial_{v_i}(G) D_{21}H(F,G)\left(F(v_i-u_i)+RT\partial_{v_i}F\right)\right\rangle_{v,\varepsilon} \\
& -2\left\langle \partial_{\varepsilon}(G) D_{21}H(F,G)\left(F\varepsilon+RT\varepsilon\partial_{\varepsilon}F\right)\right\rangle_{v,\varepsilon} \\
& -\sum_{i=1}^{3}\left\langle \partial_{v_i}(F) D_{12}H(F,G)\left(G(v_i-u_i)+RT\partial_{v_i}G\right)\right\rangle_{v,\varepsilon} \\
& -2\left\langle \partial_{\varepsilon}(F) D_{12}H(F,G)\left(G\varepsilon+RT\varepsilon\partial_{\varepsilon}G\right)\right\rangle_{v,\varepsilon} \\
& -\sum_{i=1}^{3}\left\langle \partial_{v_i}(G) D_{22}H(F,G)\left(G(v_i-u_i)+RT\partial_{v_i}G\right)\right\rangle_{v,\varepsilon} \\
& -2\left\langle \partial_{\varepsilon}(G) D_{22}H(F,G)\left(G\varepsilon+RT\varepsilon\partial_{\varepsilon}G\right)\right\rangle_{v,\varepsilon} \\
& +2\left\langle (e_{vib}(T)F-G)\frac{1}{RT_0}\log\left(\frac{G}{RT_0F+G}\right)\right\rangle_{v,\varepsilon}
\end{aligned}
$$

To use the positive definiteness of the Hessian matrix $\mathbb{H}$ of H, we introduce the following vectors:

$$
\begin{aligned}
& V_i = (F(v_i-u_i)+RT\partial_{v_i}F, G(v_i-u_i)+RT\partial_{v_i}G) \\
& E = (F\varepsilon+RT\varepsilon\partial_{\varepsilon}F, G\varepsilon+RT\varepsilon\partial_{\varepsilon}G),
\end{aligned}
$$

and we decompose the partial derivatives of F and G in factor of $D_{11}F$, $D_{22}F$, $D_{12}F$ as follows:

$$
\begin{aligned}
& (\partial_{v_i}(F), \partial_{v_i}(G)) = \frac{1}{RT}V_i - (F\frac{v_i-u_i}{RT}, G\frac{v_i-u_i}{RT}) \\
& (\partial_{\varepsilon}(F), \partial_{\varepsilon}(G)) = \frac{1}{\varepsilon}E - (F\frac{1}{RT}, G\frac{1}{RT}).
\end{aligned}
$$

This gives

$$
\begin{aligned}
\tau\mathcal{D}(F,G) \;=\; & \sum_{i=1}^{3}\left\langle\left(F\frac{v_i-u_i}{RT}\right)D_{11}H(F,G)\left(F(v_i-u_i)+RT\partial_{v_i}F\right)\right\rangle_{v,\varepsilon} \\
& +2\left\langle\left(F\frac{1}{RT}\right)D_{11}H(F,G)\left(F\varepsilon+RT\varepsilon\partial_\varepsilon F\right)\right\rangle_{v,\varepsilon} \\
& +\sum_{i=1}^{3}\left\langle\left(G\frac{v_i-u_i}{RT}\right)D_{21}H(F,G)\left(F(v_i-u_i)+RT\partial_{v_i}F\right)\right\rangle_{v,\varepsilon} \\
& +2\left\langle\left(G\frac{1}{RT}\right)D_{21}H(F,G)\left(F\varepsilon+RT\varepsilon\partial_\varepsilon F\right)\right\rangle_{v,\varepsilon} \\
& +\sum_{i=1}^{3}\left\langle\left(F\frac{v_i-u_i}{RT}\right)D_{12}H(F,G)\left(G(v_i-u_i)+RT\partial_{v_i}G\right)\right\rangle_{v,\varepsilon} \\
& +2\left\langle\left(f\frac{1}{RT}\right)D_{12}H(F,G)\left(g\varepsilon+RT\varepsilon\partial_\varepsilon G\right)\right\rangle_{v,\varepsilon} \\
& +\sum_{i=1}^{3}\left\langle\left(G\frac{v_i-u_i}{RT}\right)D_{22}H(F,G)\left(G(v_i-u_i)+RT\partial_{v_i}G\right)\right\rangle_{v,\varepsilon} \\
& +2\left\langle\left(G\frac{1}{RT}\right)D_{22}H(F,G)\left(G\varepsilon+RT\varepsilon\partial_\varepsilon G\right)\right\rangle_{v,\varepsilon} \\
& -\sum_{i=1}^{3}\left\langle V_i^T\mathbb{H}V_i\right\rangle_{v,\varepsilon}-2\left\langle E^T\mathbb{H}E\right\rangle_{v,\varepsilon} \\
& +2\left\langle(e_{vib}(T)F-G)\frac{1}{RT_0}\log\left(\frac{G}{RT_0F+G}\right)\right\rangle_{v,\varepsilon}
\end{aligned}
$$

Now this expression can be considerably simplified by using property (13), and we get

$$
\begin{aligned}
\tau\mathcal{D}(F,G) \;=\; & \sum_{i=1}^{3}\left\langle\left(\frac{v_i-u_i}{RT}\right)\left(F(v_i-u_i)+RT\partial_{v_i}F\right)\right\rangle_{v,\varepsilon} \\
& +2\left\langle\frac{1}{RT}\left(F\varepsilon+RT\varepsilon\partial_\varepsilon F\right)\right\rangle_{v,\varepsilon} \\
& -\sum_{i=1}^{3}V_i^t\mathbb{H}V_i-E^t\mathbb{H}E \\
& -2\left\langle(e_{vib}(T)F-G)\frac{1}{RT_0}\log\left(\frac{G}{RT_0F+G}\right)\right\rangle_{v,\varepsilon}.
\end{aligned}
$$

Then the first two terms are simplified by using an integration by parts and relations (8) and (7) to get

$$\begin{aligned}
\tau\mathcal{D}(F,G) &= \frac{2}{RT}(\rho e_{vib}(T) - \langle G\rangle_{v,\varepsilon}) \\
&\quad -\sum_{i=1}^{3} V_i^t \mathbb{H} V_i - 2E^t\mathbb{H}E \\
&\quad +2\left\langle (e_{vib}(T)F - G)\frac{1}{RT_0}\log\left(\frac{G}{RT_0F+G}\right)\right\rangle_{v,\varepsilon}.
\end{aligned}$$

The terms with the Hessian are clearly negative, since $\mathbb{H}$ is positive definite. Then we have

$$\begin{aligned}
\tau\mathcal{D}(F,G) &\leq \frac{2}{RT}(\rho e_{vib}(T) - \langle G\rangle_{v,\varepsilon}) \\
&\quad +2\left\langle (e_{vib}(T)F - G)\frac{1}{RT_0}\log\left(\frac{G}{RT_0F+G}\right)\right\rangle_{v,\varepsilon}.
\end{aligned}$$

Note that from (8) the first term can be written as

$$\frac{2}{RT}(\rho e_{vib}(T) - \langle G\rangle_{v,\varepsilon}) = \frac{2}{RT}\langle e_{vib}(T)F - G\rangle_{v,\varepsilon},$$

and can be factorized with the second term to find

$$\tau\mathcal{D}(F,G) \leq 2\left\langle (e_{vib}(T)F - G)\left(\frac{1}{RT_0}\log\left(\frac{G}{RT_0F+G}\right) + \frac{1}{RT}\right)\right\rangle_{v,\varepsilon}.$$

We can now prove that the integrand of the right-hand side is non-positive. Indeed, assume for instance that the first factor is non-positive, that is to say $e_{vib}(T)F - G \leq 0$. By using $e_{vib}(T) = \frac{RT_0}{e^{T_0/T}-1}$ (see definition (5)), it is now very easy to prove the following relations

$$e_{vib}(T)F - G \leq 0 \Leftrightarrow \frac{1}{T_0}\log\left(\frac{G}{RT_0F+G}\right) \geq -\frac{R}{T}$$

that is to say the second factor of the integrand is non-negative.

Consequently, we have proved $\tau\mathcal{D}(F,G) \leq 0$, which concludes the proof. □

5 Hydrodynamic limits for reduced models

With a convenient scaling, the relaxation time τ of the reduced BGK model (21)–(22) and the Fokker-Planck model (25)-(26) is replaced by $\mathrm{Kn}\,\tau$, where Kn is the Knudsen number, which can be defined as a ratio between the mean free path and a macroscopic length scale. It is then possible to look for macroscopic models derived from BGK and Fokker-Planck reduced models, in the asymptotic limit of small Knudsen numbers.

For convenience, these models are re-written below in non-dimensional form. The BGK model is

$$\partial_t F + v\cdot\nabla_x F = \frac{1}{\mathrm{Kn}\,\tau}\left(M_{vib}[F,G] - F\right), \tag{29}$$

$$\partial_t G + v\cdot\nabla_x G = \frac{1}{\mathrm{Kn}\,\tau}\left(\frac{\delta(T)}{2}TM_{vib}[F,G] - G\right), \tag{30}$$

where $M_{vib}[F,G]$ can be defined by (14) with $R=1$. Similarly, the relations (3)–(7) between the translational, internal, and total energies and the temperature, have to be read with $R=1$ in non-dimensional variables. The Fokker-Planck model is

$$\partial_t F + v\cdot\nabla_x F = D_F(F,G), \tag{31}$$
$$\partial_t G + v\cdot\nabla_x G = D_G(F,G), \tag{32}$$

with

$$\begin{aligned} D_F(F,G) &= \frac{1}{\mathrm{Kn}\,\tau}\left(\nabla_v\cdot\big((v-u)F+T\nabla_v F\big)+2\partial_\varepsilon(\varepsilon F+T\varepsilon\partial_\varepsilon F)\right),\\ D_G(F,G) &= \frac{1}{\mathrm{Kn}\,\tau}\left(\nabla_v\cdot\big((v-u)G+T\nabla_v G\big)+2\partial_\varepsilon(\varepsilon G+T\varepsilon\partial_\varepsilon G)\right)+\frac{2}{\mathrm{Kn}\,\tau}\left(e_{vib}(T)F-G\right). \end{aligned} \tag{33}$$

5.1 Euler limit

In this section, we prove the following proposition:

Proposition 5.1. *The mass, momentum, and energy densities $(\rho,\rho u,E=\frac{1}{2}\rho u^2+\rho e)$ of the solutions of the reduced BGK and the Fokker-Planck models satisfy the equations*

$$\begin{aligned} &\partial_t\rho+\nabla_x\cdot\rho u=0,\\ &\partial_t\rho u+\nabla_x\cdot(\rho u\otimes u)+\nabla p=O(\mathrm{Kn}),\\ &\partial_t E+\nabla_x\cdot(E+p)u=O(\mathrm{Kn}), \end{aligned} \tag{34}$$

which are the Euler equations, up to $O(\mathrm{Kn})$. The non-conservative form of these equations is

$$\begin{aligned} &\partial_t\rho+\nabla_x\cdot\rho u=0,\\ &\rho(\partial_t u+(u\cdot\nabla_x)u)+\nabla p=O(\mathrm{Kn}),\\ &\partial_t T+u\cdot\nabla_x T+\frac{T}{c_v(T)}\nabla_x\cdot u=O(\mathrm{Kn}), \end{aligned} \tag{35}$$

where $c_v(T)=\frac{d}{dT}e(T)$ is the heat capacity at constant volume.

Proof. The reduced BGK model (21)–(22) is multiplied by 1, v, and $\frac{1}{2}|v|^2+\varepsilon$ and integrated with respect to v and ε, which gives the following conservation laws:

$$\begin{aligned} &\partial_t\rho+\nabla_x\cdot\rho u=0,\\ &\partial_t\rho u+\nabla_x\cdot(\rho u\otimes u)+\nabla_x\sigma(F)=0,\\ &\partial_t E+\nabla_x\cdot Eu+\nabla_x\cdot\sigma(F)u+\nabla_x\cdot q(F,G)=0, \end{aligned} \tag{36}$$

where $\sigma(F)=\langle(v-u)\otimes(v-u)F\rangle_{v,\varepsilon}$ is the stress tensor, and $q(F,G)=\left\langle(v-u)(\frac{1}{2}|v-u|^2+\varepsilon)F\right\rangle_{v,\varepsilon}+\langle(v-u)G\rangle_{v,\varepsilon}$ is the heat flux.

When Kn is very small, if all the time and space derivatives of F and G are $O(1)$ with respect to Kn, then (29)–(30) imply $F=M_{vib}[F,G]+O(\mathrm{Kn})$ and $G=e_{vib}(T)M_{vib}[F,G]+O(\mathrm{Kn})$. Then it is easy to find that $\sigma(F)=\sigma(M_{vib}[F,G])+O(\mathrm{Kn})=pI+O(\mathrm{Kn})$, where I is the unit tensor, and $q(F,G)=q(M_{vib}[F,G],e_{vib}(T)M_{vib}[F,G])+O(\mathrm{Kn})=O(\mathrm{Kn})$, which gives the Euler equations (35). The same analysis can be applied for the reduced Fokker-Planck model (31)–(33).

Finally, the non conservative form is readily obtained from the conservative form. Note another formulation of the energy equation that will be useful below:

$$\partial_t e_{vib}(T) + u \cdot \nabla_x e_{vib}(T) + \frac{T e'_{vib}(T)}{c_v(T)} \nabla_x \cdot u = O(\mathrm{Kn}\,), \tag{37}$$

where $e'_{vib}(T) = \frac{d}{dT} e_{vib}(T)$. □

5.2 Compressible Navier-Stokes limit

In this section, we shall prove the following proposition:

Proposition 5.2. *The moments of the solution of the BGK and Fokker-Planck kinetic models* (21)-(22) *and* (25)-(26) *satisfy, up to $O(\mathrm{Kn}^2)$, the Navier-Stokes equations*

$$\begin{aligned} &\partial_t \rho + \nabla \cdot \rho u = 0, \\ &\partial_t \rho u + \nabla \cdot (\rho u \otimes u) + \nabla p = -\nabla \cdot \sigma, \\ &\partial_t E + \nabla \cdot (E + p) u = -\nabla \cdot q - \nabla \cdot (\sigma u), \end{aligned} \tag{38}$$

where the shear stress tensor and the heat flux are given by

$$\sigma = -\mu\big(\nabla u + (\nabla u)^T - \alpha \nabla \cdot u\big), \quad \text{and} \quad q = -\kappa \nabla \cdot T, \tag{39}$$

and where the following values of the viscosity and heat transfer coefficients (in dimensional variables) are

$$\begin{aligned} &\mu = \tau p, \quad \text{and} \quad \kappa = \mu c_p(T) \quad \text{for BGK}, \\ &\mu = \frac{1}{2}\tau p, \quad \text{and} \quad \kappa = \frac{2}{3}\mu c_p(T) \quad \text{for Fokker-Planck}, \end{aligned} \tag{40}$$

while the volumic viscosity coefficient is $\alpha = \frac{c_p(T)}{c_v(T)} - 1$ for both models, and $c_p(T) = \frac{d}{dT}(e(T) + p/\rho) = c_v(T) + R$ is the heat capacity at constant pressure. Moreover, the corresponding Prandtl number is

$$\mathrm{Pr} = \frac{\mu c_p(T)}{\kappa} = 1 \quad \text{for BGK}, \quad \text{and} \quad \frac{3}{2} \quad \text{for Fokker-Planck}. \tag{41}$$

5.2.1 Proof for the BGK model

The usual Chapman-Enskog method is applied as follows. We decompose F and G as $F = M_{vib}[F,G] + \mathrm{Kn}\, F_1$ and $G = e_{vib}(T) M_{vib}[F,G] + \mathrm{Kn}\, G_1$, which gives

$$\sigma(F) = pI + \mathrm{Kn}\, \sigma(F_1), \qquad \text{and} \qquad q(F,G) = \mathrm{Kn}\, q(F_1, G_1).$$

Then we have to approximate $\sigma(F_1)$ and $q(F_1, G_1)$ up to $O(\mathrm{Kn}\,)$. This is done by using the previous expansions and (21) and (22) to get

$$\begin{aligned} F_1 &= -\tau(\partial_t M_{vib}[F,G] + v \cdot \nabla_x M_{vib}[F,G]) + O(\mathrm{Kn}\,), \\ G_1 &= -\tau(\partial_t e_{vib}(T) M_{vib}[F,G] + v \cdot \nabla_x e_{vib}(T) M_{vib}[F,G]) + O(\mathrm{Kn}\,). \end{aligned}$$

This gives the following approximations

$$\sigma(F_1) = -\tau \left\langle (v-u)\otimes(v-u)(\partial_t M_{vib}[F,G] + v\cdot\nabla_x M_{vib}[F,G])\right\rangle_{v,\varepsilon} + O(\mathrm{Kn}\,), \tag{42}$$

and

$$\begin{aligned} q(F_1,G_1) = &-\tau\left\langle (v-u)(\frac{1}{2}|v-u|^2+\varepsilon)(\partial_t M_{vib}[F,G] + v\cdot\nabla_x M_{vib}[F,G])\right\rangle_{v,\varepsilon} \\ &-\tau\left\langle (v-u)(\partial_t e_{vib}(T)M_{vib}[F,G] + v\cdot\nabla_x e_{vib}(T)M_{vib}[F,G])\right\rangle_{v,\varepsilon} + O(\mathrm{Kn}\,). \end{aligned} \tag{43}$$

Now it is standard to write $\partial_t M_{vib}[F,G]$ and $\nabla_x M_{vib}[F,G]$ as functions of derivatives of ρ, u, and T, and then to use Euler equations (34) to write time derivatives as functions of the space derivatives only. After some algebra, we get

$$\partial_t\left(M_{vib}(F,G)\right) + v\cdot\nabla_x\left(M_{vib}(F,G)\right) = \frac{\rho}{T^{\frac{5}{2}}}M_0(V)e^{-J}\left(A\cdot\frac{\nabla T}{\sqrt{T}} + B:\nabla u\right) + O(\mathrm{Kn}\,), \tag{44}$$

where

$$\begin{aligned} &V = \frac{v-u}{\sqrt{T}}, \qquad J = \frac{\varepsilon}{T}, \qquad M_0(V) = \frac{1}{(2\pi)^{\frac{3}{2}}}\exp(-\frac{|V|^2}{2}) \\ &A = \left(\frac{|V|^2}{2} + J - \frac{7}{2}\right)V, \qquad B = V\otimes V - \left(\frac{1}{c_v}\left(\frac{1}{2}|V|^2 + J\right) + \frac{e'_{vib}(T)}{c_v(T)}\right)I. \end{aligned}$$

Then we introduce (44) into (42) to get

$$\sigma_{ij}(F_1) = -\tau\rho T\left\langle V_iV_jB_{kl}M_0e^{-J}\right\rangle_{V,J}\partial_{x_l}u_k + O(\mathrm{Kn}\,),$$

where we have used the change of variables $(v,\varepsilon)\mapsto(V,J)$ in the integral (the term with A vanishes due to the parity of M_0). Then standard Gaussian integrals (see appendix A) give

$$\sigma(F_1) = -\mu\left(\nabla u + (\nabla u)^T - \alpha\nabla\cdot u\, I\right) + O(\mathrm{Kn}\,),$$

with $\mu = \tau\rho T$ and $\alpha = \frac{c_p}{c_v} - 1$, which is the announced result, in a non-dimensional form.

For the heat flux, we use the same technique. First for $e_{vib}(T)M_{vib}[F,G]$ we obtain

$$\partial_t\left(e_{vib}M_{vib}(F,G)\right) + v\cdot\nabla_x\left(e_{vib}M_{vib}(F,G)\right) = \frac{\rho}{T^{\frac{3}{2}}}M_0(V)\left(\tilde{A}\cdot\frac{\nabla T}{\sqrt{T}} + \tilde{B}:\nabla u\right) + O(\mathrm{Kn}\,), \tag{45}$$

where

$$\begin{aligned} \tilde{A} &= \left(\frac{|V|^2}{2} + J - \frac{7}{2} + \frac{Te'_{vib}(T)}{e_{vib}}\right)V, \\ \tilde{B} &= V\otimes V - \left(\frac{1}{c_v}\left(\frac{1}{2}|V|^2 + J\right) + \frac{e'_{vib}(T)}{c_v(T)} + \frac{Te'_{vib}(T)}{c_v(T)e_{vib}}\right)I. \end{aligned}$$

Then $q(F_1,G_1)$ as given in (43) can be reduced to

$$\begin{aligned} q_i(F_1,G_1) = &-\tau\rho T\left(\left\langle\frac{1}{2}|V|^2V_iA_jM_0e^{-J}\right\rangle_{V,J} + \left\langle V_iJA_jM_0e^{-J}\right\rangle_{V,J}\right)\partial_{x_j}T \\ &-\tau\rho\left\langle V_i\tilde{A}_jM_0e^{-J}\right\rangle_{V,J}\partial_{x_j}T. \end{aligned}$$

Using again Gaussian integrals , we get

$$q(F_1, G_1) = -\kappa \nabla_x T,$$

where $\kappa = \mu c_p(T)$ with $c_p(T) = \frac{d}{dT}(e(T) + \frac{p}{\rho}) = \frac{7}{2} + e'_{vib}(T) = 1 + c_v(T)$ in a non-dimensional form.

5.2.2 Proof for the Fokker-Planck model

Here, we rather use the decomposition $F = M_{vib}(1 + \mathrm{Kn}\, F_1)$ and $G = e_{vib} M_{vib}(1 + \mathrm{Kn}\, G_1)$, which gives

$$\sigma(F) = pI + \mathrm{Kn}\, \sigma(M_{vib} F_1) \quad \text{and} \quad q(F, G) = \mathrm{Kn}\, q(M_{vib} F_1, e_{vib} M_{vib} G_1),$$

in which, for clarity, the dependence of M_{vib} on F and G has been omitted, and the dependence of e_{vib} on T as well. Finding F_1 and G_1 is less simple than for the BGK model: however, the computations are very close to what is done in the standard monatomic Fokker-Planck model (see [13] for instance), so that we only give the main steps here (see appendix A for details).

First, the decomposition is injected into (33) to get

$$\begin{aligned} D_F(F, G) &= \frac{1}{\tau} M_{vib} L_F(F_1) + O(\mathrm{Kn}\,), \\ D_G(F, G) &= \frac{1}{\tau} e_{vib} M_{vib} L_G(F_1, G_1) + O(\mathrm{Kn}\,), \end{aligned}$$

where L_F and L_G are linear operators defined by

$$\begin{aligned} L_F(F_1) &= \frac{1}{M_{vib}} \Big(\nabla_v \cdot (T M_{vib} \nabla_v F_1) + \partial_\varepsilon \left(2T\varepsilon M_{vib} \partial_\varepsilon F_1 \right) \Big), \\ L_G(F_1, G_1) &= \frac{1}{e_{vib} M_{vib}} \Big(\nabla_v \cdot (T e_{vib} M_{vib} \nabla_v G_1) + 2\partial_\varepsilon \left(T\varepsilon e_{vib} M_{vib} \partial_\varepsilon G_1 \right) + 2(F_1 - G_1) \Big). \end{aligned} \tag{46}$$

Then the Fokker-Planck equations (31)-(32) suggest to look for an approximation of F_1 and G_1 up to $O(\mathrm{Kn}\,)$ as solutions of

$$\begin{aligned} \partial_t M_{vib} + v \cdot \nabla_x M_{vib} &= \frac{1}{\tau} M_{vib}(F, G) L_F(F_1) \\ \partial_t e_{vib} M_{vib} + v \cdot \nabla_x e_{vib} M_{vib} &= \frac{1}{\tau} e_{vib} M_{vib}(F, G) L_G(F_1, G_1). \end{aligned}$$

By using (44)-(45), these relations are equivalent, up to another $O(\mathrm{Kn}\,)$ approximation, to

$$L_F(F_1) = \tau \left(A \cdot \frac{\nabla T}{\sqrt{T}} + B : \nabla u \right), \quad \text{and} \quad L_G(F_1, G_1) = \tau \left(\tilde{A} \cdot \frac{\nabla T}{\sqrt{T}} + \tilde{B} : \nabla u \right), \tag{47}$$

where A, B, $\tilde{A}$, and $\tilde{B}$ are the same as for the BGK equation in the previous section.

Now, we rewrite $L_F(F_1)$ and $L_G(F_1, G_1)$, defined in (46), by using the change of variables $V = \frac{v-u}{\sqrt{T}}$ and $G = \frac{\varepsilon}{T}$ to get

$$\begin{aligned} L_F(F_1) &= -V \cdot \nabla_V F_1 + \nabla_V \cdot (\nabla_V F_1) + 2\left((1 - J)\partial_J F_1 + J \partial_{JJ} F_1\right), \\ L_G(F_1, G_1) &= L_F(G_1) + 2(F_1 - G_1). \end{aligned}$$

Then simple calculation of derivatives show that A, B, $\tilde{A}$, and $\tilde{B}$ satisfy the following properties

$$L_F(A) = -3A, \qquad L_F(B) = -2B,$$
$$L_G(A, \tilde{A}) = -3\tilde{A}, \qquad L_G(B, \tilde{B}) = -2\tilde{B}.$$

Therefore, we look for F_1 and G_1 as solution of (47) under the following form

$$F_1 = aA \cdot \frac{\nabla T}{\sqrt{T}} + bB : \nabla u \quad \text{and} \quad G_1 = \tilde{a}\tilde{A} \cdot \frac{\nabla T}{\sqrt{T}} + \tilde{b}\tilde{B} : \nabla u,$$

and we find $\tilde{a} = a = -1/3$ and $\tilde{b} = b = 1/2$.

Finally, using these relations into σ and q and using some Gaussian integrals (see appendix A) give

$$\sigma(M_{vib}F_1) = -\mu\left(\nabla u + (\nabla u)^T - \alpha \nabla \cdot u\, I\right) \quad \text{and} \quad q(M_{vib}F_1, e_{vib}M_{vib}G_1) = -\kappa \nabla_x T,$$

where $\alpha = \frac{c_p}{c_v} - 1$, $\mu = \frac{\tau}{2}\rho T$, and $\kappa = \frac{2}{3}\mu c_p(T)$, which is the announced result, in a non-dimensional form.

6 Conclusion

In this paper, we have proposed to different models (BGK and Fokker-Planck) of the Boltzmann equation that allow for vibrational energy discrete modes. These models satisfy the conservation and entropy property (H-theorem), and the vibration energy variable can be eliminated by the usual reduced distribution function. The low complexity of the reduced BGK model can make it attractive to be implemented in a deterministic code, while the Fokker-Planck model can be easily simulated with a stochastic method.

Of course, since these models are based on a single time relaxation, they cannot allow for multiple relaxation times scales. This is not physically correct, since it is known that the relaxation times for translational, rotational, and vibrational energies are very different. However, standard procedures can be used to extend our model, like the ellipsoidal-statistical approach, already used to correct the Prandtl number of the BGK model [10] and Fokker-Plank models [13, 14]. Indeed, such an extension for our BGK model will be presented soon [23].

A Gaussian integrals and other summation formula

In this section, we give some integrals and summation formula that are used in the paper.

First, we remind the definition of the absolute Maxwellian $M_0(V) = \frac{1}{(2\pi)^{\frac{3}{2}}} \exp(-\frac{|V|^2}{2})$. We denote by $\langle \phi \rangle = \int_{\mathbb{R}^3} \phi(V)\, dV$ for any function ϕ. It is standard to derive the following integral relations (see [25], for instance), written with the Einstein notation:

$$\begin{aligned}
&\langle M_0 \rangle_V = 1, \\
&\langle V_i V_j M_0 \rangle_V = \delta_{ij}, \qquad \langle V_i^2 M_0 \rangle_V = 1, \qquad \langle |V|^2 M_0 \rangle_V = 3, \\
&\langle V_i^2 V_j^2 M_0 \rangle_V = 1 + 2\,\delta_{ij}, \qquad \langle V_i V_j V_k V_l M_0 \rangle_V = \delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} \\
&\langle V_i V_j |V|^2 M_0 \rangle_V = 5\,\delta_{ij}, \qquad \langle |V|^4 M_0 \rangle_V = 15, \\
&\langle V_i V_j |V|^4 M_0 \rangle_V = 35\,\delta_{ij}, \qquad \langle |V|^6 M_0 \rangle = 105,
\end{aligned}$$

while all the integrals of odd power of V are zero. From the previous Gaussian integrals, it can be shown that for any 3×3 matrix C, we have

$$\langle V_i V_j C_{kl} V_k V_l M_0 \rangle_V = C_{ij} + C_{ji} + C_{ii}\delta_{ij}.$$

Finally, we have also used the following relations:

$$\int_0^{+\infty} J e^{-J}\, dJ = \int_0^{+\infty} e^{-J}\, dJ = 1,$$

and also

$$\sum_{i=0}^{+\infty} e^{-iT_0/T} = \frac{1}{1 - e^{-T_0/T}} \quad \text{and} \quad \sum_{i=0}^{+\infty} i e^{-iT_0/T} = \frac{e^{-T_0/T}}{(1 - e^{-T_0/T})^2}.$$

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