The Boltzmann Equation for a Gas with Rotational Degrees of Freedom on the Basis of a Statistical Model

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Abstract. A new statistical model for the classical description of the collisions of molecules with rotational degrees of freedom based on a method of [1] is proposed. Two types of inelastic collisions are considered: the first moves closer to equilibrium, the second moves away from equilibrium. The appropriate collision integrals are written with a guarantee the conservation relations and the H-theorem. A detailed balancing relation is also valid that provides vanishing the collision integrals in equilibrium. The factorizing procedure which simplifies the calculations is introduced.

Keywords: Rotational degrees of freedom, Statistical collision model, the Boltzmann collision integrals.
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INTRODUCTION

A problem of the direct integration of the Boltzmann equation for the case of a gas with internal degrees of freedom is important. One of the main problems is that for a gas with internal degrees of freedom there is no inverse collision as in ordinary elastic collisions of simple atoms. One of the first integrals (where it has been taken into account that for some types of classical counteraction models there are no inverse collisions) has been suggested by Taxman in [2]. On the other hand, in models developed, e.g. by Larsen and Borgnakke [3] (which are widely applied in DSMC methods) the effects of internal degrees of freedom operate simply as a phenomenological internal-transitional energy exchange superimposed upon the otherwise monatomic collision dynamics.

In the present paper the statistical model of a continuum of inverse collisions corresponded to the direct collision is considered according to approach of the paper [1] where the model of interactions in gases with chemical reactions has been proposed. Some simple procedures are used. After averaging over the collision angles we can obtain the equation where the distribution function depends only on the inner energy and on the translational velocity as in the ordinary case. The collision integrals divided into two part satisfy the main physical principles. Then we introduce the supposition concerns dividing the distribution function into the part depends on the translational velocity and the part in which the inner energy only appears in the Maxwellian with temperature depended on the translational velocity. After averaging over the inner energy and discretization we obtain a scheme which is easy for numerical implementation.

A MODEL OF COLLISIONS FOR DIATOMIC GASES

The statistical model of interactions is characterized by the fact that each direct collision has many corresponding inverse collisions. Thus, the ordinary derivation of the Boltzmann equation is not valid in this case. Therefore we use the method of [1]. The distribution function has the form $f = f(\vec{\xi}, e)$, where $\vec{\xi}$ is the vector of translational velocity and e is the rotational energy of the molecule. The collision integral consists of two parts

$$I = I_{elast} + I_{inelast},$$

where the first term denotes the integral for traditional elastic collisions and the second term denotes the inelastic integral which consists of two types. Each inelastic integral is a sum of the gain and loss terms respectively

$$I_{\text{inelast}} = I_{(1)} + I_{(2)} = I^{+}{}_{(1)} - I^{-}_{(1)} + I^{+}{}_{(2)} - I^{-}{}_{(2)}. \quad (1)$$

For the first type inelastic integral energies after direct collisions are expressed as follows (a simple one parameter model of molecular interactions is proposed)

$$\begin{aligned} e_t^{'} &= e_t(1-\alpha)+\alpha e_t^0, \\ e^{'} &= e\,(1-\alpha)+\alpha e^0, \\ e_1^{'} &= e_1(1-\alpha)+\alpha e^0, \end{aligned} \quad (2)$$

where the parameter $0 \le \alpha \le 1$ (it can be found from experimental data), $e_t^0 = 3/7E$, $e^0 = 2/7E$, $E = e + e_1 + e_t = inv$ are the equilibrium translational, inner energies and a total energy respectively. One can see from (2) that post collision energies are closer to equilibrium. The Jacobian of the transformations (2) is

$$\frac{D(e_t^{'}, e_1^{'}, e^{'})}{D(e_t, e_1, e)} = (1-\alpha)^2 \le 1.$$

The probability of the type-I collisions is described by the following value

$$P_{(1)} = p_{(1)} \left| \frac{e_t}{3E} - \frac{e+e_1}{4E} \right|,$$

where $p_{(1)}$ is the steric (stereometric) factor. The energies in the interactions of type-II ("inverse collisions" for type-I) are expressed as follows

$$\begin{aligned} e_t^{'} &= e_t/(1-\alpha) - \alpha e_t^0/(1-\alpha), \\ e^{'} &= e/(1-\alpha) - \alpha e_t^0/(1-\alpha), \\ e_1^{'} &= e_1/(1-\alpha) - \alpha e^0/(1-\alpha). \end{aligned} \quad (3)$$

One can see from (3) that post collision energies are farther from equilibrium. The Jacobian of (3) is

$$\frac{D(e_t^{'}, e_1^{'}, e^{'})}{D(e_t, e_1, e)} = (1-\alpha)^{-2}.$$

The probability of the II type of collisions is described by the following value

$$P_{(2)} = p_{(2)} \left| \frac{e_t}{3E} - \frac{e+e_1}{4E} \right| H\left(\mu \frac{(\vec{g}\vec{k})^2}{2} - \alpha e_t^0\right) H(e - \alpha e^0) H(e_1 - \alpha e^0),$$

where $H(\mu\frac{(\vec{g}\vec{k})^2}{2}-\alpha e_t^0)H(e-\alpha e^0)H(e_1-\alpha e^0)$ is the product of the Heaviside functions. The elastic collision integral has the ordinary form. The probability of the elastic collisions is equal 1-$P_{(1)}$ –$P_{(2)}$.

CONSTRUCTION OF COLLISION INTEGRALS

The direct inelastic collision integrals are defined by the traditional manner

$$I_{r1}^{-}=\frac{1}{2}d^2 f(\vec{\xi},e)\int f(\vec{\xi}_1,e_1)\,|\vec{g}\vec{k}|\,P_{(1)}d\vec{\xi}_1 de_1 d\vec{k}, \tag{4}$$

$$I_{r2}^{-}=\frac{1}{2}d^2 f(\vec{\xi},e)\int f(\vec{\xi}_1,e_1)\,|\vec{g}\vec{k}|\,P_{(2)}d\vec{\xi}_1 de_1 d\vec{k}\,. \tag{5}$$

Here *d* is the effective diameter of a molecule. The expression for the integral of "inverse" collisions of I type can be written using the technique which has been suggested in [1]

$$I_{r1}^{+}=\frac{1}{2}d^2\int f(\vec{\xi}',e')f(\vec{\xi}'_1,e'_1)\delta(\vec{\xi}-\vec{\xi}_*)\delta(e-e_*)\,|\vec{g}'\vec{k}|\,P_{(1)}(e_t',e_1',e')d\vec{\xi}_1'd\vec{\xi}'de_1'de'd\vec{k}\,\frac{d\vec{\omega}}{4\pi}, \tag{6}$$

where $\vec{\xi}_*=\vec{G}+\frac{1}{2}[\frac{2}{\mu}(e_t'(1-\alpha)+\alpha e_t^0)]^{1/2}\vec{\omega}$, $e_*=e'(1-\alpha)+\alpha e^0$, $e_t'=\mu(\vec{\xi}'_1-\vec{\xi}')^2/2$,

$\vec{G}=\vec{G}'=\frac{(\vec{\xi}+\vec{\xi}_1)}{2}=\frac{(\vec{\xi}'+\vec{\xi}'_1)}{2}$, $\vec{g}$ is the relative velocity, $\vec{\omega}$ is random isotropically distributed vector. The expression for the integral of "inverse" collisions of II type is written by a similar manner

$$I_{r2}^{+}=\frac{1}{2}d^2\int f(\vec{\xi}',e')f(\vec{\xi}'_1,e'_1)\delta(\vec{\xi}-\vec{\xi}_{**})\delta(e-e_{**})\,|\vec{g}'\vec{k}|\,P_{(2)}(e_t',e_1',e')d\vec{\xi}_1'd\vec{\xi}'de_1'de'd\vec{k}\,\frac{d\vec{\omega}}{4\pi}, \tag{7}$$

$$\vec{\xi}_{**}=\vec{G}'-\frac{1}{2}[\frac{2}{\mu}(e_t'-\alpha e_t^0/(1-\alpha))]^{1/2}\vec{\omega}\,,\ e_{**}=(e'-\alpha e_0)/(1-\alpha),$$

$$P_{(2)}(e_t',e_1',e')=p_{(2)}\,|\frac{e'_t}{3E}-\frac{e'+e'_1}{4E}|\,X(\mu\frac{(\vec{g}'\vec{k})^2}{2}-\alpha e_t^0)X(e_1'-\alpha e^0)X(e'-\alpha e^0).$$

After transformations of variables and integration of the delta-functions the integrals of inverse collisions are reduced to the following simple form:

$$I_{r1}^{+}=\frac{1}{2}d^2\int\frac{p_1}{p_2(1-\alpha)^3}f(\vec{\xi}',e')f(\vec{\xi}'_1,e'_1)\,|\vec{g}\vec{k}|\,P_{(2)}(e_t,e_1,e\ )d\vec{\xi}_1 de_1\,d\vec{k}\,\frac{d\vec{\omega}}{4\pi},$$

where

$$\vec{\xi}'=\vec{G}+\frac{1}{2}[\frac{2}{\mu}(e_t-\alpha e_t^0)/(1-\alpha))]^{1/2}\vec{\omega}\,,\ \vec{\xi}_1'=\vec{G}-\frac{1}{2}[\frac{2}{\mu}(e_t-\alpha e_t^0)/(1-\alpha))]^{1/2}\vec{\omega}\,, \tag{8}$$

$$e'_1=(e_1-\alpha e_0)/(1-\alpha),\ e'=(e-\alpha e_0)/(1-\alpha),$$

$$I_{r2}^{+}=\frac{1}{2}d^2\int\frac{p_2(1-\alpha)^3}{p_1}f(\vec{\xi}',e')f(\vec{\xi}'_1,e'_1)\,|\vec{g}\vec{k}|\,P_{(1)}(e_t,e_1,e\ )d\vec{\xi}_1 de_1\,d\vec{k}\,\frac{d\vec{\omega}}{4\pi},$$

where

$$\vec{\xi}' = \vec{G} + \frac{1}{2}[\frac{2}{\mu}(e_t\,(1-\alpha)+\alpha e_t^0)]^{1/2}\vec{\varpi}\ ,\quad \vec{\xi}'_1 = \vec{G} - \frac{1}{2}[\frac{2}{\mu}(e_t\,(1-\alpha)+\alpha e_t^0)]^{1/2}\vec{\varpi}\ , \tag{9}$$

$$e'_1 = e_1\,(1-\alpha)+\alpha e^0,\ \ e' = e(1-\alpha)+\alpha e^0\,.$$

Taking $p_1 = p_2(1-\alpha)^3$ to satisfy a detailed balancing principle, the full inelastic collision integral can be written as follows (one can note that the importance of a detailed balancing relation for DSMC approaches has been discussed by Pullin [4]):

$$I_r = (I_{r2}^+ - I_{r1}^-) + (I_{r1}^+ - I_{r2}^-),$$

where

$$I_{r2}^+ - I_{r1}^- = \frac{1}{2}d^2\int\ (f'f'_1 - ff_1)\,|\vec{g}\vec{k}|\,P_{(1)}(e_t, e_1, e\ )\,d\vec{\xi}_1 de_1\,d\vec{k}\,\frac{d\vec{\omega}}{4\pi},$$

$$I_{r1}^+ - I_{r2}^- = \frac{1}{2}d^2\int\ (f'f'_1 - ff_1)\,|\vec{g}\vec{k}|\,P_{(2)}(e_t, e_1, e\ )\,d\vec{\xi}_1 de_1\,d\vec{k}\,\frac{d\vec{\omega}}{4\pi}\,.$$

Here, in the first integral primed values are computed by relations (9), and in the second integral they are computed by the relations (8). We recombined the expressions in the collision integral using Eq. (1) to emphasize the separate operation of two parts of the appropriate integrals to provide the H-theorem.

It is obvious that substitution of a local Maxwellian into integrals provides zero for both collision integrals. It can be proved the H-theorem for this kinetic equation in a similar way as in [1]. We emphasize that to guarantee the conservation relationships, the collision integrals have to be recombined in the following manner: (4) and (6), (5) and (7), then we obtain

$$\int (I_{r1}^+ - I_{r1}^-)\psi_m d\vec{\xi}\ de = 0,$$

$$\int (I_{r2}^+ - I_{r2}^-)\psi_m d\vec{\xi}\ de = 0,$$

where m=0,1,2,3,4; $\psi_0 = 1,\ \psi_i = \xi_i (i = 1,2,3),\ \psi_4 = (1/2)m\vec{\xi}^2 + e.$

AVERAGING THE KINETIC EQUATION OVER THE ROTATIONAL ENERGY

For simplification of the kinetic equation let us consider two distribution functions dependent only on the translational velocity $\vec{\xi}$ (which allows us find all necessary moments, including the rotational temperature and flux of the rotational energy):

$$f_0(\vec{\xi}) = \int f(\vec{\xi}, e)de\,,$$

$$f_1(\vec{\xi}) = \int ef(\vec{\xi}, e)de\,.$$

The ratio of the first and second functions is proportional to the rotational temperature dependent on the translational velocity (and of course, on time and space coordinate). Let us denote it as

$$\varphi(\vec{\xi}) = f_1(\vec{\xi})/f_0(\vec{\xi})\,.$$

The next assumption is that the distribution function is factorized: it can be represented in the form of the product of the function only dependent on the translational velocity and the equilibrium function dependent on the rotational energy and the mentioned temperature $\varphi(\vec{\xi})$

$$f(\vec{\xi},e) = f_0(\vec{\xi}) f_M(e,\varphi), \tag{10}$$

where

$$f_M(e,\varphi) = (\pi\varphi(\vec{\xi}))^{-1} \exp(-e/\varphi(\vec{\xi})). \tag{11}$$

One can remark that such a representation of the distribution function describes two important limit cases. The first one is related to the local equilibrium. The second one is related to a free-molecular flow: if we consider a flow around a solid body the function from (11) corresponds to the reflected particles with full accommodation and this function is the same for the trajectory of a particle. The collision integral is simplified and we derive the system of equations dependent only on the translational velocities. For this purpose the original equation is integrated over the inner energy with the weights 1 and the inner energy e. The first integration yields

$$\int_0^\infty I_{r1}^+ de = \frac{1}{2} d^2 \int f(\vec{\xi}', e') f(\vec{\xi}'_1, e'_1) \delta(\vec{\xi} - \vec{\xi}_*) \delta(e - e_*) |\vec{g}'\vec{k}| P_{(1)}(e'_t, e'_1, e') d\xi'_1 d\xi' de'_1 de' d\vec{k} \frac{d\vec{\omega}}{4\pi} de.$$

Here the form of the distribution function is given by (10). As the integration of the delta-function over the inner energy is equal to unity, we obtain

$$A_1 = \int_0^\infty I_{r1}^+ de = \frac{1}{2} d^2 \int f_0' f'_{01} \frac{\exp(-e'/(k\varphi'))}{k\varphi'} \frac{\exp(-e'_1/(k\varphi'_1))}{k\varphi'_1} \delta(\vec{\xi} - \vec{\xi}_*) |\vec{g}'\vec{k}| \times$$

$$\times P_{(1)}(e'_t, e'_1, e') d\vec{\xi}' d\xi'_1 de'_1 de' d\vec{k} \frac{d\vec{\omega}}{4\pi},$$

where $\vec{\xi}_* = \vec{G}' + \frac{1}{2}[\frac{2}{\mu}(e'_t(1-\alpha) + \alpha e_t^0)]^{1/2} \varpi$, $e_* = e'(1-\alpha) + \alpha e^0$, $e'_t = \mu(\vec{\xi}'_1 - \vec{\xi}')^2/2$.

For the direct collision integral we have

$$B_1 = \int_0^\infty I_{r1}^- de = \frac{1}{2} d^2 \int f_0 f_{01} \frac{\exp(-e/(k\varphi))}{k\varphi} \frac{\exp(-e/(k\varphi))}{k\varphi} |\vec{g}\vec{k}| P_{(1)}(e_t, e_1, e) d\xi_1 de_1 de d\vec{k}.$$

One can write in a similar way the appropriate expressions for the II type integrals

$$A_2 = \int_0^\infty I_{r2}^+ de, \quad B_2 = \int_0^\infty I_{r2}^- de.$$

After integration of the collision integrals over energy with the weight e we obtain the analogous relationships.

DISCRETISATION IN VELOCITY SPACE

Discretization in velocity space is performed in an ordinary manner. We consider a bounded domain beyond of which the distribution function is taken as zero. The area is divided into equal cells of the parallelepipedal form. Let us $\vec{\xi}_i$ denote a center of the *i-th* cell. The functions have the following forms

$$f_0 = \sum_i n_i \delta(\vec{\xi} - \vec{\xi}_i),$$

$$\varphi(\vec{\xi}) = \sum_i \chi_i(\vec{\xi}) \varphi_i,$$

where n_i is the amount of particles in the *i*-th cell, φ_i is the average rotational energy of particles of the *i*-th cell and χ_i is the appropriate characteristic function. For deriving the discrete analog of the equation let us multiply the equation on the characteristic function and integrate this expression over velocity space

$$\frac{\partial n_i}{\partial t} + \vec{\xi}_i \frac{\partial n_i}{\partial x} = \sum_{m,s} n_m n_s A_{ms}^{1i} - n_i \sum_j n_j B_{ij}^1 + \sum_{m,s} n_m n_s A_{ms}^{2i} - n_i \sum_j n_j B_{ij}^2 \cdot$$

Here the inelastic collision integral is only approximated, elastic collisions are not given because the discretization of it can be performed by an ordinary manner. From this equation relations of conservation of number of particles and momentum are derived. Expressions for coefficients A_{ms}^{1i} of the inverse collision integral of the I-st type are obtained by the appropriate integration (these large formulas are not presented here). Coefficients in the direct collision integral are defined as following integral sums

$$B_{ms}^1 = \sum_i A_{ms}^{1i}, \quad B_{ms}^2 = \sum_i A_{ms}^{2i} \cdot$$

One can see that these expressions correspond (with an accuracy of approximation in velocity space) to sums for evaluation of the direct collision integrals. Expressions for the II type integrals are presented similarly. The second equation obtained after integration with the appropriate weight

$$\frac{\partial E_i}{\partial t} + \vec{\xi}_i \frac{\partial E_i}{\partial x} = \sum_{m,s} n_m n_s C_{ms}^{1i} - n_i \sum_j n_j D_{ij}^1 + \sum_{m,s} n_m n_s C_{ms}^{2i} - n_i \sum_j n_j D_{ij}^2 \cdot$$

Here $\mathrm{E}_i = n_i(m\vec{\xi}^2/2 + \varphi_i)$ is energy of the *i*-th cell. One can see that from the last equation the relation of conservation of energy can be obtained.

CONCLUSION

The Boltzmann kinetic equation for diatomic gas with rotational degrees of freedom is constructed on the basis of the statistical model of counteractions. Discretization is performed due to the procedure of averaging kinetic equations over the rotational energy. A simple numerical scheme can be realized in the same way as for the Boltzmann equation for elastic collisions using the 8-fold integral [5].

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