

## Kinetic Theory of a Rarefied Gas of Rough Spheres

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**Abstract** A kinetic theory for the rarefied gas consisting of roughspherical molecules is developed, in which a macroscopic state is characterized by the 29 scalar fields of density, velocity, pressure tensor, temperature, translational heat flux, rotational heat flux, spin and spin flux. The relations of Navier-Stokes and Fourier are obtained by the use of an iteration method akin to the Maxwellian procedure.

### 1. INTRODUCTION

In this work a kinetic theory of a rarefied polyatomic gas consisting of spherical molecules with rotational energy is developed.

The model used is that of Bryan (see<sup>1</sup>) which assumes the spherical molecules as perfectly rough, elastic and rigid. This model states that the molecules grip to each other without slipping during a binary collision such that the relative velocity of points of contact is reversed.

We follow<sup>2</sup> and characterize a macroscopic state by the 29 scalar fields of density, linear momentum, pressure tensor, translational heat flux, temperature, rotational heat flux, density of spin and spin flux. The corresponding balance equations are obtained from a general equation of transfer derived from the Boltzmann equation.

In order to get the relations of Navier-Stokes and Fourier we use an iteration method akin to the Maxwellian procedure<sup>3</sup>. The resulting transport coefficients agree with those obtained from the Chapman-Enskog method<sup>1</sup>.

Cartesian notation for tensors is used and

i) angular parentheses around two indices denote the symmetric and traceless part of a tensor; for example

$$p_{\langle ij \rangle} = \frac{1}{2} (p_{ij} + p_{ji}) - \frac{1}{3} p_{rr} \delta_{ij},$$

$$p_{\langle i \langle j \rangle} \frac{\partial v_{\langle k \rangle}}{\partial x_n} = \frac{1}{2} \left( p_{\langle ij \rangle} \frac{\partial v_{\langle k \rangle}}{\partial x_n} + p_{\langle ik \rangle} \frac{\partial v_{\langle j \rangle}}{\partial x_n} \right) - \frac{1}{3} p_{\langle ir \rangle} \frac{\partial v_{\langle r \rangle}}{\partial x_n} \delta_{jk} .$$

ii) brackets indicate the antisymmetric part of a tensor; for example

$$\frac{\partial v_{[j]}}{\partial x_j} = \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i} \right)$$

## 2. THE DYNAMICS OF A BINARY COLLISION

We denote respectively by  $m$ ,  $a$  and  $I$  the mass, the diameter and the moment of inertia about an arbitrary axis, of a spherical molecule. Further we denote by  $(\vec{c}, \vec{c}_1)$  and  $(\vec{w}, \vec{w}_1)$  the linear and angular velocities of two molecules before collision while  $(\vec{c}', \vec{c}'_1)$  and  $(\vec{w}', \vec{w}'_1)$  are the same velocities after collision.

For a binary collision of perfectly rough, elastic and rigid spherical molecules, the equations which give the final velocities in terms of the initial ones are<sup>1</sup>

$$\begin{aligned} \vec{c}' &= \vec{c} + \vec{M}, \quad \vec{c}'_1 = \vec{c}_1 - \vec{M}, \quad \vec{w}'_1 = \vec{w}_1 - \vec{N}, \quad \vec{w}' = \vec{w} - \vec{N}, \\ \vec{M} &= \frac{K}{K+1} \left[ \vec{g} - \frac{a}{2} \vec{k} \times (\vec{w} + \vec{w}_1) + \frac{1}{K} (\vec{k} \cdot \vec{g}) \vec{k} \right], \quad \vec{N} = \frac{2}{aK} \vec{k} \times \vec{M}. \end{aligned} \quad (2.1)$$

In eq. (2.1)  $\vec{k}$  is the unit vector in the directions of the line which joint the two molecule centers at collision, pointing from the molecule labeled by 1 to the other;  $\vec{g} = \vec{c}_1 - \vec{c}$  is the relative linear velocity and  $K$  is the dimensionless moment of inertia defined by  $K = 4I/(ma^2)$ . The values of the dimensionless moment of inertia  $K$  may range from zero, which corresponds to a concentration of the mass at the center of the molecule, to  $2/3$  which corresponds to a uniform distribution of the mass on the surface of the spherical molecule.

For the case of smooth spheres, any direct collision taking  $(\vec{c}, \vec{c}_1)$  as the initial velocities,  $(\vec{c}', \vec{c}'_1)$  as the final velocities and  $\vec{k}$  as the direction of the apsidal line, allow an inverse collision taking  $(\vec{c}', \vec{c}'_1)$  as the initial velocities,  $(\vec{c}, \vec{c}_1)$  as the final velocities and  $-\vec{k}$

as the direction of the apsidal line.

For the case of rough spheres no such inverse collision exists and we denote by  $(\vec{c}^*, \vec{c}_1^*, \vec{w}^*, \vec{w}_1^*)$  the initial velocities which correspond to the final velocities  $(\vec{c}, \vec{c}_1, \vec{w}, \vec{w}_1)$  and to the direction of the apsidal line  $-\vec{k}$ .

### 3. THE GENERAL EQUATION OF TRANSFER

The state of the gas is characterized by the distribution function  $f(\vec{x}, \vec{c}, \vec{w}, t)$  such that  $f(\vec{x}, \vec{c}, \vec{w}, t) d\vec{x} d\vec{c} d\vec{w}$  gives at time  $t$  the number of molecules in the volume element between  $\vec{x}$  and  $\vec{x} + d\vec{x}$ , with linear velocities between  $\vec{c}$  and  $\vec{c} + d\vec{c}$  and angular velocities between  $\vec{w}$  and  $\vec{w} + d\vec{w}$ .

The distribution function  $f(\vec{x}, \vec{c}, \vec{w}, t)$  must satisfy the Boltzmann equation<sup>4</sup>

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + F_i \frac{\partial f}{\partial c_i} = \int (f^* f_1^* - f f_1) \alpha^2 (\vec{g} \cdot \vec{k}) d\vec{k} d\vec{c}_1 d\vec{w}_1. \quad (3.1)$$

In equation (3.1)  $F_i$  is the specific external body force and it has been assumed that there are no external torques. We have also introduced the abbreviations  $f_1 \equiv f(\vec{x}, \vec{c}_1, \vec{w}_1, t)$ ,  $f^* \equiv f(\vec{x}, \vec{c}^*, \vec{w}^*, t)$  and  $f_1^* \equiv f(\vec{x}, \vec{c}_1^*, \vec{w}_1^*, t)$ . Moreover  $d\vec{k} = \sin \theta d\Omega d\Sigma$ , and  $\Omega$  and  $\Sigma$  are polar coordinates specifying the direction of  $\vec{k}$ ;  $\Omega$  is the angle between  $\vec{g}$  and  $\vec{k}$  while  $\Sigma$  is the angle between the plane containing  $\vec{k}$  and  $\vec{g}$  and a reference plane through  $\vec{g}$ .

The general equation of transfer follows through the multiplication of the Boltzmann equation by an arbitrary function  $\psi \equiv \psi(\vec{x}, \vec{c}, \vec{w}, t)$  and the integration over all values of  $\vec{c}$  and  $\vec{w}$ .

$$\begin{aligned} & \frac{\partial}{\partial t} \int \psi f d\vec{c} d\vec{w} + \frac{\partial}{\partial x_i} \int c_i \psi f d\vec{c} d\vec{w} - \int \left[ \frac{\partial \psi}{\partial t} + c_i \frac{\partial \psi}{\partial x_i} + F_i \frac{\partial \psi}{\partial c_i} \right] f d\vec{c} d\vec{w} = \\ & = \int (\psi' - \psi) d\Gamma = \frac{1}{2} \int (\psi' - \psi + \psi_1' - \psi_1) d\Gamma. \end{aligned} \quad (3.2)$$

where

$$d\Gamma = f f_1 \alpha^2 (\vec{g} \cdot \vec{k}) d\vec{k} d\vec{c}_1 d\vec{w}_1 d\vec{c} d\vec{w}.$$

In order to get the two terms on the right-hand side of eq.(3.2) one must proceed as follows.

It is straightforward to prove from eq. (2.1) that

$$\vec{g} \cdot \vec{k} = -\vec{g}' \cdot \vec{k} = -\vec{g}^* \cdot \vec{k} = \vec{g}^* \cdot \vec{k}^*, \quad (3.3)$$

$$d\vec{c} d\vec{w} d\vec{c}_1 d\vec{w}_1 = d\vec{c}' d\vec{w}' d\vec{c}_1' d\vec{w}_1' = d\vec{c}^* d\vec{w}^* d\vec{c}_1^* d\vec{w}_1^*$$

In equations (3.3)  $\vec{g}'$ ,  $\vec{g}^*$  and  $\vec{k}^*$  are given by  $\vec{g}' = \vec{c}_1' - \vec{c}'$ ,  $\vec{g}^* = \vec{c}_1^* - \vec{c}^*$  and  $\vec{k}^* = -\vec{k}$ .

Further by taking into account equations (3.3) one can write the integral  $I$

$$I = \int \psi(\vec{x}, \vec{c}, \vec{w}, t) f^* f_1^* \alpha^2(\vec{g} \cdot \vec{k}) d\vec{k} d\vec{c}_1 d\vec{w}_1 d\vec{c} d\vec{w} \quad (3.4)$$

in the form of

$$I = \int \psi(\vec{x}, \vec{c}, \vec{w}, t) f^* f_1^* \alpha^2(\vec{g}^* \cdot \vec{k}^*) d\vec{k}^* d\vec{c}_1^* d\vec{w}_1^* d\vec{c}^* d\vec{w}^*. \quad (3.5)$$

Since  $(\vec{c}^*, \vec{w}^*, \vec{c}_1^*, \vec{w}_1^*)$  are initial velocities corresponding to the final velocities  $(\vec{c}, \vec{w}, \vec{c}_1, \vec{w}_1)$  and the direction of the apsidal line given by  $\vec{k}^* = -\vec{k}$ , we may relabel the initial velocities as  $(\vec{c}, \vec{w}, \vec{c}_1, \vec{w}_1)$ , the final velocities as  $(\vec{c}', \vec{w}', \vec{c}_1', \vec{w}_1')$  and the direction of the apsidal line as  $\vec{k}$ . Hence, equation (3.5) becomes

$$I = \int \psi(\vec{x}, \vec{c}', \vec{w}', t) f f_1 \alpha^2(\vec{g} \cdot \vec{k}) d\vec{k} d\vec{c}_1 d\vec{w}_1 d\vec{c} d\vec{w} \quad (3.6)$$

Then

$$\begin{aligned} & \int \psi(f^* f_1^* - f f_1) \alpha^2(\vec{g} \cdot \vec{k}) d\vec{k} d\vec{c}_1 d\vec{w}_1 d\vec{c} d\vec{w} = \\ & = \int (\psi - \psi') f f_1 \alpha^2(\vec{g} \cdot \vec{k}) d\vec{k} d\vec{c}_1 d\vec{w}_1 d\vec{c} d\vec{w}. \end{aligned} \quad (3.7)$$

Now the change of roles of the colliding molecules in eq. (3.7) implies

$$\begin{aligned} \int \psi (f^* f_1^* - f f_1) a^2 (\vec{g} \cdot \vec{k}) d\vec{k} d\vec{c}_1 d\vec{w}_1 d\vec{c} d\vec{w} = \\ = \int (\psi_1 - \psi_1) f f_1 a^2 (\vec{g} \cdot \vec{k}) d\vec{k} d\vec{c}_1 d\vec{w}_1 d\vec{c} d\vec{w}. \end{aligned} \quad (3.8)$$

The right-hand side of eq. (3.2) can be obtained now from equation (3.7) and (3.8).

#### 4. THE BALANCE EQUATIONS

The macroscopic state of a polyatomic gas can be described by the 29 scalar fields of density  $\rho$ , linear momentum  $\rho v_i$ , pressure tensor  $p_{ij}$ , temperature  $T$ , translational heat flux  $q_i$ , rotational heat flux  $h_i$ , density of spin  $\rho \gamma_i$  and spin flux  $m_{ij}$  defined by:

$$\begin{aligned} \rho &= \int m f d\vec{c} d\vec{w}, \quad \rho v_i = \int m c_i f d\vec{c} d\vec{w}, \quad p_{ij} = \int m c_i c_j f d\vec{c} d\vec{w} \\ T &= \frac{m}{3k\rho} \int \left[ \frac{m}{2} C^2 + \frac{I}{2} \Omega^2 \right] f d\vec{c} d\vec{w}, \quad q_i = \int \frac{m}{2} C^2 c_i f d\vec{c} d\vec{w}, \\ h_i &= \int \frac{I}{2} \Omega^2 c_i f d\vec{c} d\vec{w}, \quad \rho \gamma_i = \int I w_i f d\vec{c} d\vec{w}, \quad m_{ij} = \int I \Omega_i c_j f d\vec{c} d\vec{w}. \end{aligned} \quad (4.1)$$

In eq. (4.1)  $k$  is the Boltzmann constant,  $C_i = c_i - v_i$  the peculiar linear velocity and  $\Omega_i = w_i - s_i$  the peculiar angular velocity. Moreover  $s_i = (m/I)\gamma_z$  is the spin velocity.

The balance equations for the 29 scalar fields (4.1) are obtained by choosing  $\psi$  in the general equation of transfer (3.2) equal to

i) Balance of mass:  $\psi = m$

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_i}{\partial x_i} = 0. \quad (4.2)$$

ii) Balance of linear momentum:  $\psi = m c_i$

$$\frac{\partial \rho v_i}{\partial t} + \frac{\partial}{\partial x_j} (p_{ij} + \rho v_i v_j) = \rho F_i. \quad (4.3)$$

iii) Balance of pressure tensor:  $\psi = m C_i C_j$

$$\frac{\partial p_{ij}}{\partial t} + \frac{\partial}{\partial x_k} (p_{i,j,k} + p_{i,j} v_k) + p_{ki} \frac{\partial v_j}{\partial x_k} + p_{kj} \frac{\partial v_i}{\partial x_k} = P_{ij} . \quad (4.4)$$

iv) Balance of translational heat flux:  $\psi = \frac{m}{2} C^2 C_i$

$$\frac{\partial q_i}{\partial t} + \frac{\partial}{\partial x_j} (q_{i,j} + q_i v_j) + p_{ijk} \frac{\partial v_j}{\partial x_k} + q_j \frac{\partial v_i}{\partial x_j} - \frac{p_{ki}}{\rho} \frac{\partial p_{kj}}{\partial x_j} + \frac{p_{rr}}{2\rho} \frac{\partial p_{i,j}}{\partial x_j} = Q_i . \quad (4.5)$$

v) Balance of energy:  $\psi = \frac{1}{2} (mc^2 + I w^2)$

$$\begin{aligned} \frac{\partial}{\partial t} (3 \frac{k}{m} \rho T + \frac{1}{2} \rho v^2 + \frac{m}{2I} \rho Y^2) + \frac{\partial}{\partial x_i} [q_i + h_i + p_{ij} v_j + \\ + \frac{m}{I} m_{ji} \gamma_j + (3 \frac{k}{m} \rho T + \frac{1}{2} \rho v^2 + \frac{m}{2I} \rho Y^2) v_i] = \rho F_i v_i . \end{aligned} \quad (4.6)$$

vi) Balance of rotational heat flux:  $\psi = \frac{I}{2} \Omega^2 C_i$

$$\begin{aligned} \frac{\partial h_i}{\partial t} + \frac{\partial}{\partial x_j} (h_{i,j} + h_i v_j) + \frac{m}{I} m_{kij} \frac{\partial \gamma_k}{\partial x_j} + h_j \frac{\partial v_i}{\partial x_j} - \frac{m}{I} \frac{m_{ji}}{\rho} \frac{\partial m_{jk}}{\partial x_k} \\ - (3 \frac{k}{m} T - \frac{p_{rr}}{2}) \frac{\partial p_{ij}}{\partial x_j} = H_i - \frac{m}{I} \frac{m_{ji}}{\rho} M_j . \end{aligned} \quad (4.7)$$

vii) Balance of density of spin:  $\psi = I w_i$

$$\frac{\partial \rho \gamma_i}{\partial t} + \frac{\partial}{\partial x_j} (m_{i,j} + \rho \gamma_i v_j) = M_i \quad (4.8)$$

viii) Balance of spin flux:  $\psi = I \Omega_i C_j$

$$\frac{\partial m_{ij}}{\partial t} + \frac{\partial}{\partial x_k} (m_{ijk} + m_{ij} v_k) + p_{jk} \frac{\partial \gamma_i}{\partial x_k} + m_{ik} \frac{\partial v_j}{\partial x_k} = M_{ij} . \quad (4.9)$$

In the derivation of eq. (4.5) and (4.7) we have used the eqs. (4.3) and (4.8). Moreover, we have defined

$$p_{ijk} = \int m C_i C_j C_k f d\vec{c} d\vec{w} \quad (4.10.1) \quad , \quad q_{ij} = \int \frac{m}{2} C^2 C_i C_j f d\vec{c} d\vec{w} \quad (4.10.2)$$

$$m_{ijk} = \int I \Omega_i C_j C_k f d\vec{c} d\vec{w} \quad (4.10.3) \quad , \quad h_{ij} = \int \frac{I}{2} \Omega^2 C_i C_j f d\vec{c} d\vec{w} \quad (4.10.4)$$

$$P_{ij} = \int m (C_i' C_j' - C_i C_j) d\Gamma \quad (4.10.5) \quad , \quad Q_i = \int \frac{m}{2} (C^{i2} C_i' - C^2 C_i) d\Gamma \quad (4.10.6)$$

$$M_i = \int I (\omega_i! - \omega_i) d\Gamma \quad (4.10.7) \quad , \quad M_{ij} = \int I (\Omega_i' C_j' - \Omega_i C_j) d\Gamma \quad (4.10.8)$$

$$H_i = \int \frac{I}{2} (\Omega^{i2} C_i' - \Omega^2 C_i) d\Gamma \quad (4.10.9)$$

$p_{ijk}$ ,  $q_{ij}$ ,  $m_{ijk}$  and  $h_{ij}$  are called the moments of the distribution function while  $P_{ij}$ ,  $Q_i$ ,  $M_i$ ,  $M_{ij}$  and  $H_i$  are the production terms.

## 5. THE DISTRIBUTION FUNCTION

In order to get the distribution function close to equilibrium we seek the extremum of the entropy density  $\rho\eta$  under the constraints eq. (4.1) (see<sup>5</sup>). The entropy density is defined by

$$\rho\eta = -k \int f \ln f d\vec{c} d\vec{w}. \quad (5.1)$$

This problem is equivalent to finding the extremum of the functional

$$F = \int [-k \ln f - \Lambda_m - \Lambda_i^v m c_i - \Lambda_i^w I w_i - \lambda (\frac{m}{2} C^2 + \frac{I}{2} \Omega^2) - \Lambda_{ij}^m C_i C_j - \lambda_i^T \frac{m}{2} C^2 C_i - \lambda_i^R \frac{I}{2} \Omega^2 C_i - \lambda_{ij} I \Omega_i C_j] f d\vec{c} d\vec{w} \quad (5.2)$$

$\Lambda$ ,  $\Lambda_i^v$ ,  $\Lambda_i^w$ ,  $\Lambda_{ij}^m$ ,  $h$ ,  $\lambda_i^T$ ,  $\lambda_i^R$  and  $\lambda_{ij}$  are Lagrange multipliers which do not depend on the distribution function  $f$ .

Now we set the first derivative of eq. (5.2) with respect to  $f$  equal to zero and get the distribution function which maximizes the entropy density under the constraints (4.1).

$$f = \exp \left\{ \left( -\frac{m}{k} \left[ \frac{k}{m} + \Lambda + \Lambda_i^v v_i + \Lambda_i^w \gamma_i + \lambda^E \left( \frac{C^2}{2} + \frac{I}{m} \frac{\Omega^2}{2} \right) \right] \right) \right\}$$

$$\times \exp \left\{ \left( -\frac{m}{k} \left[ \Lambda_i^v c_i + \frac{I}{m} \Lambda_i^w \Omega_i + \Lambda_{ij} c_i c_j + \frac{I}{m} \lambda_{ij} \Omega_i \Omega_j \right. \right. \right.$$

$$\left. \left. \left. + \lambda_i^T \frac{C^2}{2} c_i + \frac{I}{m} \lambda_i^R \frac{\Omega^2}{2} c_i + \lambda^{NE} \left( \frac{C^2}{2} + \frac{I}{m} \frac{\Omega^2}{2} \right) \right] \right) \right\} . \quad (5.3)$$

In eq. (5.3) we have splitted the Lagrange multiplier  $\lambda$  into two parts  $\lambda^E$  and  $\lambda^{NE}$  corresponding respectively to the values of  $\lambda$  in equilibrium and in non-equilibrium.

Since we are interested in processes close to equilibrium we can use the approximation  $\exp(-x) \approx 1-x$  for the second exponential function and write  $f = f_0(1+\phi)$ .  $f_0$  is a Maxwellian distribution function and  $\phi$  its deviation.

$$f = \exp \left\{ \left( -\frac{m}{k} \left[ \frac{k}{m} + \Lambda + \Lambda_i^v v_i + \Lambda_i^w \gamma_i + \lambda^E \left( \frac{C^2}{2} + \frac{I}{m} \frac{\Omega^2}{2} \right) \right] \right) \left\{ 1 - \right. \right.$$

$$\left. \left. - \frac{m}{k} \left[ \Lambda_i^v c_i + \frac{I}{m} \Lambda_i^w \Omega_i + \Lambda_{ij} c_i c_j + \lambda_i^T \frac{C^2}{2} c_i + \frac{I}{m} \lambda_i^R \frac{\Omega^2}{2} c_i \right. \right. \right.$$

$$\left. \left. \left. + \frac{I}{m} \lambda_{ij}^R c_j + \lambda^{NE} \left( \frac{C^2}{2} + \frac{I}{m} \frac{\Omega^2}{2} \right) \right] \right\} . \quad (5.4)$$

In order to get the Maxwellian distribution function in equilibrium, we identify the Lagrange multiplier  $\lambda^E$  as the reciprocal of the absolute temperature, i.e.,  $\lambda^E = 1/T$ .

For the determination of the other Lagrange multipliers we insert the distribution function (5.4) into the definitions (4.1) and get after some calculations

$$\Lambda = -\frac{k}{m} \left\{ \ln \left[ \frac{\rho}{m} \frac{(mT)^{3/2}}{(2\pi kT)^3} \right] + 1 \right\} , \quad \Lambda_{ij} = -\frac{p_{ij}}{2\rho} \frac{m}{kT^2} ,$$

$$\Lambda_{rr} = -3 \frac{p}{\rho} \frac{m}{kT^2} , \quad \lambda_i^T = -\frac{2}{5} \frac{q_i}{\rho} \left( \frac{m}{k} \right)^2 \frac{1}{T^3} , \quad \lambda_i^R = -\frac{2}{3} \frac{h_i}{\rho} \left( \frac{m}{k} \right)^2 \frac{1}{T^3} , \quad (5.5)$$

$$\lambda^{NE} = \frac{p}{\rho} \frac{m}{kT^2} , \quad \lambda_{ij} = -\frac{m_{ij}}{\rho} \frac{m^2}{IkT^2} , \quad \Lambda_i^v = \frac{m}{\rho kT^2} (q_i + h_i) , \quad \Lambda_i^w = 0 .$$

Now it follows from eqs. (5.4) and (5.5), by neglecting all non-linear terms, that

$$f = \frac{\rho}{m} \frac{(mI)^{3/2}}{(2\pi kT)^3} \exp \left[ - \frac{m}{2kT} (C^2 + \frac{I}{m} \Omega^2) \right] \left\{ 1 + \frac{p_{ijj}}{2\rho} \left( \frac{m}{kT} \right)^2 C_i C_j + \frac{p^*}{2\rho} \left( \frac{m}{kT} \right)^2 (C^2 - \frac{I}{m} \Omega^2) + \frac{m_{ij}}{\rho} \left( \frac{m}{kT} \right)^2 \Omega_i C_j + \frac{q_i}{\rho} \left( \frac{m}{kT} \right)^2 \left( \frac{mC^2}{5kT} - 1 \right) C_i + \frac{h_i}{\rho} \left( \frac{m}{kT} \right)^2 \left( \frac{I\Omega^2}{3kT} - 1 \right) C_i \right\} . \quad (5.6)$$

In eqs. (5.5) and (5.6)  $p_{ijj}$  represents the pressure deviator (the traceless part of the pressure tensor), while  $p^* = p_{rr}/3 - k\rho T/m$  is the dynamic pressure.

## 6. THE EVALUATION OF THE PRODUCTION TERMS AND OF THE MOMENTS OF THE DISTRIBUTION FUNCTION

The moments of the distribution function  $p_{ijk}$ ,  $q_{ij}$ ,  $m_{ijk}$  and  $h_{ij}$  can be determined by insertion of the distribution function (5.6) into the eqs. (4.10.1)-(4.10.4) and integration:

$$\begin{aligned} p_{ijk} &= \frac{2}{5} (\delta_{ij} q_k + \delta_{ik} q_j + \delta_{jk} q_i) , \\ q_{ij} &= \left[ \frac{5}{2} \rho \left( \frac{kT}{m} \right)^2 + 5p^* \frac{kT}{m} \right] \delta_{ij} + \frac{7}{2} \frac{kT}{m} p_{ijj} , \\ m_{ijk} &= 0 , \quad h_{ij} = \frac{3}{2} \rho \left( \frac{kT}{m} \right)^2 \delta_{ij} + \frac{3}{2} \frac{kT}{m} p_{ijj} . \end{aligned} \quad (6.1)$$

In the derivation of eq.(6.1) we have used eqs. (A.1) and (A.2).

The evaluation of the production terms  $P_{ijj}$ ,  $Q_i$ ,  $M_i$ ,  $M_{ij}$  and  $H_i$  is a routine but laborious work, and a scheme of the calculation is given in the appendix.

$$P_{ijj} = \frac{4\rho T^{1/2}}{(K+1)^2} \left[ - \frac{32}{2} K p^* \delta_{ij} - \frac{8}{15} (13K+6) p_{ijj} \right] , \quad (6.2)$$

$$Q_i = \frac{4\rho T^{1/2}}{(K+1)^2} \left[ -\frac{8}{15} (4+17K) q_i + \frac{40}{9} K h_i \right], \quad M_i = \frac{4\rho T^{1/2}}{(K+1)} \left[ -\frac{16}{3} \gamma_i \right],$$

$$M_{ij} = \frac{4\rho T^{1/2}}{(K+1)} \left[ -\frac{16}{3} (K+1) m_{ij} + \frac{2K\alpha}{9} \left( \frac{m\pi}{kT} \right)^{1/2} \epsilon_{ijk} h_k \right]$$

$$H_i = \frac{4\rho T^{1/2}}{(K+1)^2} \left[ \frac{8}{3} K q_i - \frac{8}{3} (2K^2 + 2K + 1) h_i \right]. \quad (6.2)$$

In eq. (6.2)  $A = (\alpha^4 \pi k / m^3)^{1/2}$  is a constant.

## 7. THE FIELD EQUATIONS

Without loss of generality, we may take the spin velocity  $s_i$  equal to zero since we have made the assumption that the rarefied gas under study is free of external torques. For this reason we shall not take into account the balance of the density of spin eq.(4.8) and of the spin flux eq.(4.9) in the following analysis.

Hence, insertion of the production terms (6.2) and of the moments of the distribution function (6.1) into the balance equations (4.2) through (4.7) leads to the following field equations for the 17 scalar fields  $\rho, v_i, T, p^*, p_{<ij>}, q_i, h_i$ :

$$\dot{\rho} + \rho \frac{\partial v_i}{\partial x_i} = 0, \quad (7.1.1)$$

$$\dot{v}_i + \frac{\partial p_{ij}}{\partial x_j} = \rho F_i, \quad (7.1.2)$$

$$\left( \frac{k}{m} \rho T + p^* \right)^* + \frac{5}{3} \left( \frac{k}{m} \rho T + p^* \right) \frac{\partial v_i}{\partial x_i} + \frac{2}{3} \frac{\partial q_i}{\partial x_i} + \frac{2}{3} p_{<ij>} \frac{\partial v_i}{\partial x_j} = \frac{A \rho T^{1/2}}{(K+1)^2} \left[ -\frac{32}{3} K p^* \right], \quad (7.1.3)$$

$$\begin{aligned} \dot{p}_{<ij>} &+ \frac{5}{3} p_{<ij>} \frac{\partial v_k}{\partial x_k} + \frac{4}{5} \frac{\partial q_{<i>}}{\partial x_j} + 2 p_{<k<i>} \frac{\partial v_{<j>}}{\partial x_k} + p_{<ki>} \frac{\partial v_{<j>}}{\partial x_k} + p_{<kj>} \frac{\partial v_{<i>}}{\partial x_k} \\ &+ 2 \left( \frac{k}{m} \rho T + p^* \right) \frac{\partial v_{<i>}}{\partial x_j} = \frac{A \rho T^{1/2}}{(K+1)^2} \left[ -\frac{8}{15} (13K + 6) p_{<ij>} \right], \quad (7.1.4) \end{aligned}$$

$$\begin{aligned}
\dot{q}_i + \frac{7}{5} q_i \frac{\partial v_j}{\partial x_j} + \frac{1}{5} q_j \frac{\partial v_i}{\partial x_j} + \frac{2}{5} q_j \frac{\partial v_j}{\partial x_i} + \frac{5}{2} \left( \frac{kT}{m} - \frac{p^*}{\rho} \right) \frac{\partial p^*}{\partial x_i} + \frac{5}{2} p^* \frac{kT}{m} \left( \frac{1}{T} \frac{\partial T}{\partial x_i} \right. \\
\left. - \frac{1}{\rho} \frac{\partial \rho}{\partial x_i} \right) + \frac{5}{2} \left( \frac{k}{m} \right)^2 \rho T \frac{\partial T}{\partial x_i} - \frac{p_{<ki>}}{\rho} \frac{\partial p_{<ki>}}{\partial x_j} + \left( \frac{kT}{m} - \frac{5}{2} \frac{p^*}{\rho} \right) \frac{\partial p_{<ij>}}{\partial x_j} \\
- \frac{p_{<ij>}}{\rho} \left( \frac{\partial p^*}{\partial x_j} + \frac{k}{m} \frac{\partial \rho T}{\partial x_j} \right) + \frac{1}{2} p_{<ij>} \frac{k}{m} \frac{\partial T}{\partial x_j} = \frac{A \rho T^{1/2}}{(K+1)^2} \left[ -\frac{8}{15} (4+17K) q_i + \frac{40}{9} K h_i \right] \\
(7.1.5)
\end{aligned}$$

$$3 \frac{k}{m} \rho \dot{T} + \frac{\partial h_i}{\partial x_i} + \frac{\partial q_i}{\partial x_i} + \left( \frac{k}{m} \rho T + p^* \right) \frac{\partial v_i}{\partial x_i} + p_{<ij>} \frac{\partial v_i}{\partial x_j} = 0 \quad (7.1.6)$$

$$\begin{aligned}
\dot{h}_i + h_i \frac{\partial v_k}{\partial x_k} + h_j \frac{\partial v_i}{\partial x_j} + \frac{3}{2} \frac{p^*}{\rho} \left[ \frac{\partial p^*}{\partial x_i} + \frac{\partial p_{<ij>}}{\partial x_j} + \frac{k}{m} T \frac{\partial \rho}{\partial x_i} + \frac{k}{m} \rho \frac{\partial T}{\partial x_i} \right] \\
+ \frac{3}{2} \frac{k}{m} \left[ \frac{k}{m} \rho T \delta_{ij} + p_{<ij>} \right] \frac{\partial T}{\partial x_j} - \frac{3}{2} \frac{k}{m} T \frac{\partial p^*}{\partial x_i} = \frac{A \rho T^{1/2}}{(K+1)^2} \left[ \frac{8}{3} K q_i \right. \\
\left. - \frac{8}{3} (2K^2 + 2K + 1) h_i \right]. \quad (7.1.7)
\end{aligned}$$

Eqs. (7.1.3), (7.1.4) are respectively the trace and the traceless part of eq. (2.4). Moreover, a dot denotes the material time derivative.

## 8. THE RELATIONS OF NAVIER-STOKES AND FOURIER

The system of eqs. (7.1) represents the field equations of extended thermodynamics of an ideal gas with an internal variable in the absence of external torques<sup>6</sup>.

In ordinary thermodynamics this system reduces to the field equations of balance of mass (7.1.1), linear momentum (7.1.2) and internal energy (7.1.6). Moreover, the fields  $p^*$ ,  $p_{<ij>}$ ,  $q_i$  and  $h_i$  are related to the basic fields,  $\rho$ ,  $T$  and  $v_i$  by constitutive functions.

(\*) For an ideal gas the thermodynamic pressure  $\tilde{p}$  and the specific internal energy  $\epsilon$  are related by  $\tilde{p} = k\rho T/m = 2\rho\epsilon/3$ .

In order to get constitutive equations for the fields  $p^*$ ,  $p_{<i,j>}^{*}$ ,  $q_i$  and  $h_i$  we use the remaining eqs. (7.1.3), (7.1.4), (7.1.5) and (7.1.7) and an iteration method akin to the Maxwellian procedure<sup>3</sup>.

We begin with the elimination of  $T$  from eq. (7.1.3) by the use of eq. (7.1.6):

$$\dot{p}^* + \left( \frac{1}{3} \frac{k}{m} \rho T + \frac{4}{3} p^* \right) \frac{\partial v_i}{\partial x_i} + \frac{1}{3} \frac{\partial}{\partial x_i} (q_i - h_i) + \frac{1}{3} p_{<i,j>} \frac{\partial v_i}{\partial x_j} = \frac{A \rho T^{1/2}}{(K+1)^2} \left[ - \frac{32}{3} K p^* \right] \quad (8.1)$$

Now we insert the equilibrium values  $p^*(0) = 0$ ,  $p_{<i,j>}^{(0)} = 0$ ,  $q_i^{(0)}$  = 0 and  $h_i^{(0)} = 0$  into the left hand side of eqs. (7.1.4), (7.1.5), (7.1.7) and (8.1). By neglecting all non-linear terms we get the first iterated values  $p^*(1)$ ,  $p_{<i,j>}^{(1)}$ ,  $q_i^{(1)}$  and  $h_i^{(1)}$  on the right hand side:

$$2 \frac{k}{m} \rho T \frac{\partial v_{<i>}}{\partial x_j} = \frac{A \rho T^{1/2}}{(K+1)^2} \left[ - \frac{8}{15} (13K + 6) p_{<i,j>}^{(1)} \right],$$

$$\frac{5}{2} \left( \frac{k}{m} \right)^2 \rho T \frac{\partial T}{\partial x_i} = \frac{A \rho T^{1/2}}{(K+1)^2} \left[ - \frac{8}{15} (4 + 17K) q_i^{(1)} + \frac{40}{9} K h_i^{(1)} \right],$$

$$\frac{3}{2} \left( \frac{k}{m} \right) \rho T \frac{\partial T}{\partial x_i} = \frac{A \rho T^{1/2}}{(K+1)^2} \left[ \frac{8}{3} K q_i^{(1)} - \frac{8}{3} (2K^2 + 2K + 1) h_i^{(1)} \right],$$

$$\frac{1}{3} \frac{k}{m} \rho T \frac{\partial v_i}{\partial x_i} = \frac{A \rho T^{1/2}}{(K+1)^2} \left[ - \frac{32}{3} K p^*(1) \right] \quad (8.2)$$

From eq. (8.2) it follows that:

$$p_{<i,j>}^{(1)} = - 2\mu \frac{\partial v_{<i>}}{\partial x_j} \quad (8.3.1), \quad p^*(1) = - \eta \frac{\partial v_i}{\partial x_i}, \quad (8.3.2)$$

$$q_i^{(1)} = - \lambda^T \frac{\partial T}{\partial x_i} \quad (8.3.3), \quad h_i^{(1)} = - \lambda^R \frac{\partial T}{\partial x_i}. \quad (8.3.4)$$

Eqs. (8.3.1), (8.3.2) represent the Navier-Stokes relations while eqs. (8.3.3), (8.3.4) represent the Fourier relation. Hence we identify  $\mu$  as the shear viscosity,  $\eta$  as the volume viscosity,  $\lambda^T$  as the

translational thermal conductivity and  $\lambda^R$  as the rotational thermal conductivity. Moreover we have

$$\begin{aligned} \mu &= \frac{15}{8} \frac{k}{m} \frac{T^{1/2}}{A} \frac{(K+1)^2}{(13K+6)} \quad , \quad \eta = \frac{1}{32} \frac{k}{m} \frac{T^{1/2}}{A} \frac{(K+1)^2}{K} \\ \lambda^T &= \frac{225}{16} \left(\frac{k}{m}\right)^2 \frac{T^{1/2}}{A} \frac{(1+2K)(1+K)^3}{(102K^3 + 101K^2 + 75K + 12)} \quad , \quad (8.4) \\ \lambda^R &= \frac{9}{4} \left(\frac{k}{m}\right)^2 \frac{T^{1/2}}{A} \frac{(3+19K)(1+K)^2}{(102K^3 + 101K^2 + 75K + 12)} \quad . \end{aligned}$$

Now we define the total heat flux  $q_i^*$  as the sum of the translational and rotational heat flux:

$$q_i^* = q_i + h_i = - (\lambda^T + \lambda^R) \frac{\partial T}{\partial x_i} = - \lambda \frac{\partial T}{\partial x_i} \quad . \quad (8.5)$$

In eq.(8.5) the thermal conductivity  $h$  is given by:

$$\lambda = \frac{9}{16} \left(\frac{k}{m}\right)^2 \frac{T^{1/2}}{A} \frac{(37+151K+50K^2)(1+K)^2}{(102K^3 + 101K^2 + 75K + 12)} \quad . \quad (8.6)$$

The results in eqs. (8.4) and (8.6) are the same as those obtained by the use of the Chapman-Enskog method (see ref.1).

## APPENDIX

### A.1 - Some results on integration

If  $\vec{c}$  is a vector in a 3-dimensional vector-space  $V$ , then (see for example ref.7):

$$\int_V c_i c_j f(c^2) d\vec{c} = \frac{1}{3} \delta_{ij} \int_V c^2 f(c^2) d\vec{c} \quad , \quad (A.1)$$

$$\int_V c_i c_j c_r c_s f(c^2) d\vec{c} = \frac{1}{15} (\delta_{ij}\delta_{rs} + \delta_{ir}\delta_{js} + \delta_{is}\delta_{jr}) \int_V c^4 f(c^2) d\vec{c} \quad .$$

The following definite integrals can be found in standard tables of integrals:

$$\int_0^\infty e^{2n} e^{-\alpha c^2} dc = \frac{\sqrt{\pi}}{2} \frac{(2n-1)!!}{2^n} \left(\frac{1}{\alpha}\right)^{\frac{2n+1}{2}},$$

$$\int_0^\infty e^{2n+1} e^{-\alpha c^2} dc = \frac{n!}{2} \left(\frac{1}{\alpha}\right)^{n+1}.$$
(A.2)

On the other hand, the following formulae are valid for all  $n = 0, 1, 2, 3, \dots$ :

$$\int (\vec{g} \cdot \vec{k})^n d\vec{k} = \frac{2\pi}{(n+1)} g^n,$$

$$\int k_i (\vec{g} \cdot \vec{k})^n d\vec{k} = \frac{2\pi}{(n+2)} g^{n-1} g_i,$$

$$\int k_i k_j (\vec{g} \cdot \vec{k})^n d\vec{k} = \frac{2\pi}{(n+1)(n+3)} g^{n-2} (g^2 \delta_{ij} + n g_i g_j),$$

$$\begin{aligned} \int k_i k_j k_k (\vec{g} \cdot \vec{k})^n d\vec{k} &= \frac{2\pi}{(n+2)(n+4)} g^{n-3} \left[ g^2 (g_i \delta_{jk} + g_j \delta_{ik} + g_k \delta_{ij}) \right. \\ &\quad \left. + (n-1) g_i g_j g_k \right], \end{aligned}$$

$$\begin{aligned} \int k_i k_j k_r k_s (\vec{g} \cdot \vec{k}) d\vec{k} &= \frac{2\pi}{(n+1)(n+3)(n+5)} g^{n-4} \left[ g^4 (\delta_{ij} \delta_{rs} + \delta_{ir} \delta_{js} + \delta_{is} \delta_{jr}) \right. \\ &\quad \left. + n g^2 (g_i g_j \delta_{rs} + g_i g_r \delta_{js} + g_i g_s \delta_{jr} + g_r g_j \delta_{is} + g_s g_j \delta_{ir} + g_r g_s \delta_{ij}) \right. \\ &\quad \left. + n(n-2) g_i g_j g_r g_s \right]. \end{aligned}$$
(A.3)

One can derive the formulae (A.3) using the method described on pages 319-321 of ref.1.

#### A.2 - The calculation of the production terms

First we build from eq.(5.6) the product  $ff^1$  and neglect all

non-linear terms:

$$\begin{aligned}
 ff^1 = & \left( \frac{\rho}{m} \right)^2 \frac{(mI)^3}{(2\pi kT)^6} \exp \left[ - \frac{m}{kT} G^2 - \frac{m}{4kT} g^2 - \frac{I}{kT} Z^2 - \frac{I}{4kT} z^2 \right] \left\{ 1 + \right. \\
 & + \frac{p_{ij}}{2\rho} \left( \frac{m}{kT} \right)^2 (2G_i G_j + \frac{1}{2} g_i g_j) + \frac{p_{ij}^*}{2\rho} \left( \frac{m}{kT} \right)^2 \left[ 2G^2 + \frac{1}{2} g^2 \right. \\
 & \left. - \frac{2I}{m} Z^2 - \frac{I}{2m} z^2 \right] + \frac{m_{ij}}{\rho} \left( \frac{m}{kT} \right)^2 (2Z_i G_j + \frac{1}{2} z_i g_j) \\
 & + \frac{q_{ij}}{\rho} \left( \frac{m}{kT} \right)^2 \left\{ 2G_i \left[ \frac{m}{kT} (G^2 + \frac{1}{4} g^2) - 1 \right] + \frac{5m}{2kT} g_i g_r G_r \right\} \\
 & \left. + \frac{h_{ij}}{\rho} \left( \frac{m}{kT} \right)^2 \left\{ 2G_i \left[ \frac{I}{3kT} (Z^2 + \frac{1}{4} z^2) - 1 \right] + \frac{I}{3kT} g_i z_r z_r \right\} \right\}. \quad (A.4)
 \end{aligned}$$

In eq.(A.4)  $\vec{g}$  is the linear relative velocity,  $\vec{G}$  the linear mean velocity,  $\vec{z}$  the angular relative velocity and  $\vec{Z}$  the angular mean velocity, which are defined by

$$\vec{g} = \vec{C}_1 - \vec{C}, \quad 2\vec{G} = \vec{C}_1 + \vec{C}, \quad \vec{z} = \vec{\Omega}_1 - \vec{\Omega}, \quad 2\vec{Z} = \vec{\Omega}_1 + \vec{\Omega}. \quad (A.5)$$

From equations (A.5) it follows that

$$d\vec{c} d\vec{w} d\vec{c}_1 d\vec{w}_1 = d\vec{g} d\vec{G} d\vec{z} d\vec{Z}. \quad (A.6)$$

Since the scheme of the calculation for all production terms eq.(6.2) is the same, we shall illustrate it by the calculation of  $P_{ij}$ . According to eq.(4.10.5)  $P_{ij}$  is given by

$$P_{ij} = \int m(C_i^! C_j^! - C_i^! C_j^!) ff^1 \alpha^2 (\vec{g} \cdot \vec{k}) d\vec{k} d\vec{c} d\vec{c}_1 d\vec{w}_1. \quad (A.7)$$

On the other hand it follows from equation (2.1):

$$\begin{aligned}
 C_i^! C_j^! = & \left\{ C_i + \frac{K}{K+1} \left[ g_i - \alpha \epsilon_{irs} k_r z_s - \frac{am}{I} \epsilon_{irs} k_r \gamma_s + \frac{1}{K} (\vec{k} \cdot \vec{g}) k_i \right] \right\} \left\{ C_j \right. \\
 & \left. + \frac{K}{K+1} \left[ g_j - \alpha \epsilon_{jmn} k_m z_n - \frac{am}{I} \epsilon_{jmn} k_m \gamma_n + \frac{1}{K} (\vec{k} \cdot \vec{g}) k_j \right] \right\} \quad (A.8)
 \end{aligned}$$

Now we insert eqs. (A.6) and (A.8) into eq. (A.7) and integrate with respect to the angles  $\Theta$  and  $C$  using eqs. (A.3)

$$\begin{aligned}
 P_{ij} = & \int \pi m a^2 f f^1 d\vec{g} d\vec{\alpha} d\vec{z} d\vec{Z} \left\{ \frac{K}{(K+1)} \left[ g_i^G j^G - \frac{2}{3} \alpha \epsilon_{irs} g_r^Z s^G j^G \right. \right. \\
 & - \frac{2}{3} \frac{\alpha m}{I} \epsilon_{irs} g_r^Y s^G j^G + \frac{1}{2K} g g_i^G j^G + g_j^G i^G - \frac{2}{3} \alpha \epsilon_{jrs} g_r^Z s^G i^G \\
 & - \frac{2}{3} \frac{\alpha m}{I} \epsilon_{jrs} g_r^Y s^G i^G + \frac{1}{2K} g g_j^G i^G - g g_i^G j^G + \frac{\alpha}{3} \epsilon_{irs} g_r^Z s^G j^G \\
 & + \frac{\alpha m}{3I} \epsilon_{irs} g_r^Y s^G j^G - \frac{1}{2K} g_i^G j^G + \frac{\alpha}{3} \epsilon_{jrs} g_r^Z s^G i^G + \frac{\alpha m}{3I} \epsilon_{jrs} g_r^Y s^G i^G \\
 & + \frac{K^2}{(K+1)^2} \left[ g_i^G j^G - \frac{2}{3} \alpha g_j^G \epsilon_{irs} g_r^Z s^G - \frac{2}{3} \frac{\alpha m}{I} \epsilon_{irs} g_r^Y s^G j^G + \frac{1}{K} g g_i^G j^G \right. \\
 & - \frac{2}{3} \alpha \epsilon_{jrs} g_r^Z s^G i^G - \frac{1}{4} g^{-1} \epsilon_{irs}^Z s^G \epsilon_{jmn}^Z n^G (g^2 \delta_{rm} + g_r^G g_m^G) \\
 & + \frac{1}{4} \frac{\alpha^2 m}{I} \epsilon_{irs}^Y s^G \epsilon_{jmn}^Z n^G g^{-1} (g^2 \delta_{rm} + g_r^G g_m^G) - \frac{2}{15} \frac{\alpha}{K} \epsilon_{jrs}^Z s^G (g^2 \delta_{ir} \\
 & + 2g_r^G g_i^G) - \frac{2}{3} \frac{\alpha m}{I} g_i^G \epsilon_{jrs} g_r^Y s^G + \frac{1}{4} \frac{\alpha^2 m}{I} \epsilon_{irs}^Z s^G \epsilon_{jmn}^Y n^G g^{-1} (g^2 \delta_{rm} \\
 & + g_r^G g_m^G) + \frac{1}{4} \frac{\alpha^2 m^2}{I^2} \epsilon_{irs}^Y s^G \epsilon_{imn}^Y n^G g^{-1} (g^2 \delta_{rm} + g_r^G g_m^G) \\
 & - \frac{2}{15} \frac{\alpha m}{IK} \epsilon_{jrs}^Y s^G (g^2 \delta_{ir} + 2g_r^G g_i^G) - \frac{2}{15} \frac{\alpha}{K} \epsilon_{irs}^Z s^G (g^2 \delta_{jr} + 2g_j^G g_r^G) \\
 & \left. \left. - \frac{2}{15} \frac{\alpha m}{IK} \epsilon_{irs}^Y s^G (g^2 \delta_{jr} + 2g_j^G g_r^G) + \frac{1}{12K^2} g (g^2 \delta_{ij} + 3g_i^G g_j^G) \right] \right\}. \quad (\text{A.9})
 \end{aligned}$$

Finally we insert eq. (A.4) into eq. (A.9) and integrate by making use of eq. (A.1) and eq. (A.2), and neglecting all non-linear terms leads to:

$$P_{ij} = \frac{a^2}{m} \left( \frac{\pi k T}{m} \right)^{1/2} \frac{\rho}{(K+1)^2} \left[ -\frac{32}{3} K p^* \delta_{ij} - \frac{8}{15} (13K+6) p_{\langle ij \rangle} \right]. \quad (\text{A.10})$$

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## Resumo

Desenvolve-se uma teoria cinética para um gás rarefeito, constituído de moléculas esféricas e rugosas, caracterizada por 29 campos escalares: densidade, velocidade, tensor pressão, temperatura, fluxo de calor translacional, fluxo de calor rotacional, spin e fluxo de spin. As relações de Navier-Stokes e Fourier são obtidas através da utilização de um método de iteração semelhante ao método de iteração de Maxwell.