The P_N Method in the Kinetic Theory of Gases

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An expansion of the velocity distribution function in a series of spherical harmonics is used to transform the nonlinear Boltzmann equation into a system of moment equations. The close connection between the moment equations of zeroth and first order with the transport equations for mass, momentum and energy is pointed out. By comparing the order of magnitude of the various moments it is shown that the P_2 approximation is adequate for systems with small mean free path. Simplifications of the collision terms of the moment equations are discussed, where attention is payed to the conservation laws and the H theorem.

Key words: Kinetic theory, Nonlinear Boltzmann equation, Spherical harmonics method, Moment equations.

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1. Introduction

The Boltzmann equation is the basic equation in the kinetic theory of gases. It governs the velocity distribution function of the atoms or molecules of the gas. Due to the complicated structure of the collision term, the Boltzmann equation can in general not be solved analytically. This means that approximate methods must be developed.

Moment methods are known as the most flexible procedures for approximately solving the Boltzmann equation. They are based on an expansion of the velocity distribution function in terms of orthogonal polynomials to transform the Boltzmann equation into a system of moment equations for easier solution. For spatially homogeneous gases, expansions in generalized Laguerre polynomials [1–3] proved to be efficient. For the more interesting case of inhomogeneous systems, tensorial Hermite polynomials [4] and Burnett functions [5, 6] were applied as basic functions. A common feature of the various techniques is that the moments of low order are closely connected to the hydrodynamical variables. Therefore, a special advantage of moment methods is that they can be used to derive the basic equations of gas dynamics from the Boltzmann equation (Grad's 13 moment method [4]).

A further technique in this context is the spherical harmonics method or P_N method, where the distribution function is expanded in a series of spherical harmonics in terms of the solid angle of the particle velocity vector. Here, the moments of expansion depend on space, time and the particle speed. This is in contrast to Grad's or Burnett's method where the moments depend on space and time alone. The P_N method has been used very efficiently in neutron transport theory, where a linear form of the Boltzmann equation applies [7]. In the nonlinear case, less attention has been payed to the spherical harmonics method. Jaffé [8] was the first to apply this particular method in kinetic theory. He confined himself to terms up to second order, to obtain solutions of the Boltzmann equation for the case of small Knudsen numbers. Jaffé showed that the spherical harmonics method leads to the same results as Enskog's famous technique. In a more recent paper [9], the spherical harmonics method has been generalized to arbitrary order. This has been done by including the Boltzmann collision term into the expansion scheme.

In this paper, the P_N^{KLM} method proposed in [9] is adapted to the central idea of Jaffé's work, viz., to perform the expansion of the distribution function for a moving reference system in velocity space. Furthermore, we investigate some collision models which allow a simplification of the collision terms of the moment equations.

In Chapt. 2, the Boltzmann equation is presented in the scattering kernel formulation, and its transformation to the moving reference system is given. Chapter 3 is devoted to the P_N method in nonlinear transport theory. The moment equations of arbitrary order

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are derived. In Chapt. 4, we point out the link between the moment equations of zeroth and first order and the transport equations for mass, momentum and energy. The limiting case of small Knudsen numbers is of special importance in the kinetic theory of gases. We investigate this case in Chapter 5. Finally, in Chapter 6 (see [10]) possible simplifications of the collision terms are discussed, where special attention is paid to the conservation laws and the H theorem.

2. The Boltzmann Equation

In kinetic theory, the state of a simple, monatomic gas is described by the velocity distribution function $f(\boldsymbol{r}, \boldsymbol{v}, t)$. It is defined in such a way that $f(\boldsymbol{r}, \boldsymbol{v}, t)\, \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{v}$ represents the number of molecules (of mass m) in the volume element $\mathrm{d}\boldsymbol{r}$ located at $\boldsymbol{r}$, whose velocities lie in $\mathrm{d}\boldsymbol{v}$ about $\boldsymbol{v}$ at time t. Given the distribution function, the macroscopic properties of the gas are obtained as certain integrals over f with respect to $\boldsymbol{v}$ [11].

The velocity distribution function is taken to satisfy the nonlinear integro-differential Boltzmann equation [12] which can be written in the form

$$D[f] = J[f, f] \tag{1}$$

with the streaming operator

$$D[f] = \left(\frac{\partial}{\partial t} + \boldsymbol{v}\, \nabla_r\right) f(\boldsymbol{r}, \boldsymbol{v}, t) \tag{2}$$

and the collision operator

$$J[f, f] = \int \mathrm{d}\boldsymbol{v}' \int \mathrm{d}\boldsymbol{v}'_1\, S(\boldsymbol{v}' \to \boldsymbol{v}; \boldsymbol{v}'_1)\, f(\boldsymbol{v}')\, f(\boldsymbol{v}'_1) - f(\boldsymbol{v}) \int \mathrm{d}\boldsymbol{v}_1\, f(\boldsymbol{v}_1) \int \mathrm{d}\boldsymbol{v}'\, S(\boldsymbol{v} \to \boldsymbol{v}'; \boldsymbol{v}_1)\,. \tag{3}$$

In (3), the dependence of f on $\boldsymbol{r}$ and t has been omitted for brevity.

Equation (3) is the so-called scattering kernel formulation of the Boltzmann collision operator [13, 14]. Here, the scattering kernel S is defined as the product of the relative speed of the colliding particles, the integral cross section σ and the differential scattering probability w:

$$S(\boldsymbol{v}' \to \boldsymbol{v}; \boldsymbol{v}'_1) = |\boldsymbol{v}' - \boldsymbol{v}'_1|\, \sigma(|\boldsymbol{v}' - \boldsymbol{v}'_1|)\, w(\boldsymbol{v}' \to \boldsymbol{v}; \boldsymbol{v}'_1)\,. \tag{4}$$

The quantity $w(\boldsymbol{v}' \to \boldsymbol{v}; \boldsymbol{v}'_1)\, \mathrm{d}\boldsymbol{v}$ is the probability that if a test particle of velocity $\boldsymbol{v}'$ and a target particle of velocity $\boldsymbol{v}'_1$ collide, then the former is scattered to $\mathrm{d}\boldsymbol{v}$ about $\boldsymbol{v}$, while the latter is scattered to any velocity-space element. The differential scattering probability obeys the normalization condition

$$\int \mathrm{d}\boldsymbol{v}\, w(\boldsymbol{v}' \to \boldsymbol{v}; \boldsymbol{v}'_1) = 1\,. \tag{5}$$

As is well-known, the collision term of the Boltzmann equation conserves mass, momentum and energy:

$$\int \mathrm{d}\boldsymbol{v} \begin{pmatrix} 1 \\ m\boldsymbol{v} \\ \frac{1}{2} m v^2 \end{pmatrix} J[f, f] = 0\,. \tag{6}$$

Furthermore, it leads to the H theorem [12], showing the irreversible trend of the distribution function towards the equilibrium (Maxwellian) distribution.

The idea of the P_N method is to expand the distribution function in velocity space in a series of spherical harmonics and to derive a set of equations governing the moments of expansion. It would be unfavourable to perform this expansion for a fixed coordinate system, i.e. the laboratory system, because then in general a large number of terms in the spherical harmonics expansion would have to be considered for a good series approximation, owing to the anisotropy of the velocity distribution. A series truncation is much more promising if the particle velocity is measured in a reference system moving at the mean velocity of the gas, $\boldsymbol{u}(\boldsymbol{r}, t)$. Therefore we introduce the intrinsic velocity

$$\boldsymbol{c} = \boldsymbol{v} - \boldsymbol{u}(\boldsymbol{r}, t) \tag{7}$$

as the independent velocity variable. Correspondingly we transform

$$f(\boldsymbol{r}, \boldsymbol{v}, t) \to f(\boldsymbol{r}, \boldsymbol{c}, t) \tag{8}$$

with

$$\mathrm{d}\boldsymbol{c} = \mathrm{d}\boldsymbol{v}\,.$$

The connection between the distribution function and the hydrodynamical variables is now given by (cf. [11])

$$\begin{pmatrix} n \\ n\boldsymbol{u}' \\ e \\ P \\ \boldsymbol{q} \end{pmatrix} = \int \mathrm{d}\boldsymbol{c}\, f(\boldsymbol{r}, \boldsymbol{c}, t) \begin{pmatrix} 1 \\ \boldsymbol{c} \\ \frac{m}{2} c^2 \\ m\boldsymbol{c}\boldsymbol{c} \\ \frac{m}{2} c^2 \boldsymbol{c} \end{pmatrix}, \tag{9}$$

with $\boldsymbol{u}' = 0$. Here, n, $\boldsymbol{u}'$, e, P and $\boldsymbol{q}$ are the number density, mean velocity, energy density, pressure tensor and heat flux measured with respect to the mean. Note that in the following the mean velocity of the gas, $\boldsymbol{u}$, has to be determined self-consistently so that $\boldsymbol{u}' = 0$.

In our new reference system, the equilibrium distribution $M(\boldsymbol{c})$ is isotropic:

$$M(c) = n\left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{mc^2}{2kT}\right). \tag{10}$$

Here, k is the Boltzmann constant, and T is the temperature defined by

$$\tfrac{3}{2} n kT = e, \tag{11}$$

with n and e given by (9).

In order to adjust the Boltzmann equation to the transformation (8), the derivations in (2) have to be substituted according to

$$\frac{\partial f}{\partial t} \to \frac{\partial f}{\partial t} - \frac{\partial u_i}{\partial t}\frac{\partial f}{\partial c_i} \tag{12}$$

and

$$\frac{\partial f}{\partial x_i} \to \frac{\partial f}{\partial x_i} - \frac{\partial u_j}{\partial x_i}\frac{\partial f}{\partial c_j}. \tag{13}$$

The streaming operator (2) then reads

$$D[f] = \frac{\mathrm{d}f}{\mathrm{d}t} + c_i \frac{\partial f}{\partial x_i} - \frac{\partial f}{\partial c_i}\left(\frac{\mathrm{d}u_i}{\mathrm{d}t} + c_j \frac{\partial u_i}{\partial x_j}\right) \tag{14}$$

with

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + u_i \frac{\partial}{\partial x_i}. \tag{15}$$

In (12) to (15), Cartesian tensor notation has been used.

As a result of the Galilean-invariance of the scattering kernel of the Boltzmann equation [12],

$$S(\boldsymbol{c}' + \boldsymbol{u} \to \boldsymbol{c} + \boldsymbol{u}; \boldsymbol{c}_1' + \boldsymbol{u}) = S(\boldsymbol{c}' \to \boldsymbol{c}; \boldsymbol{c}_1'), \tag{16}$$

the structure of the collision term is not affected by the transformation to a moving reference system for measuring the particle velocities.

3. P_N Method

In the following we confine ourselves to systems which depend on only one space dimension, i.e. z. Denoting the spherical polar coordinates of the particle velocity vector $\boldsymbol{c}$ by (c, ϑ, ω), it is also assumed that the velocity distribution is symmetric about the polar axis ($\equiv z$-axis):

$$f(\boldsymbol{r}, \boldsymbol{c}, t) = f(z, c, \cos\vartheta, t). \tag{17}$$

The streaming operator (14) then reads

$$D[f] = \frac{\partial}{\partial t} f(z, c, \mu, t) + (u + c\mu)\frac{\partial f}{\partial z} - \left[\frac{\partial u}{\partial t} + (u + c\mu)\frac{\partial u}{\partial z}\right]\left[\mu\frac{\partial f}{\partial c} + \frac{(1-\mu^2)}{c}\frac{\partial f}{\partial \mu}\right], \tag{18}$$

where $\mu = \cos\vartheta$ and $u = u_z$. We expand the velocity distribution function in a series of Legendre polynomials P_n

$$f(z, c, \mu, t) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} f_n(z, c, t)\, P_n(\mu). \tag{19}$$

As a result of the orthogonality of the Legendre polynomials [15], the moments of expansion of a given distribution function are obtained by

$$f_n(z, c, t) = 2\pi \int_{-1}^{1} \mathrm{d}\mu\, P_n(\mu)\, f(z, c, \mu, t). \tag{20}$$

Before going on with the derivation of a set of equations governing the moments of expansion, we point out the close connection between the Legendre moments of the distribution function and the hydrodynamical variables. From (9) and (20) one finds for a one-dimensional flow

$$n = \int_0^\infty \mathrm{d}c\, c^2 f_0(z, c, t), \tag{21}$$

$$nu' = \int_0^\infty \mathrm{d}c\, c^3 f_1 = 0, \tag{22}$$

$$e = \frac{m}{2}\int_0^\infty \mathrm{d}c\, c^4 f_0, \tag{23}$$

$$P_{xx} = P_{yy} = \frac{m}{3}\int_0^\infty \mathrm{d}c\, c^4 f_0 - \frac{m}{3}\int_0^\infty \mathrm{d}c\, c^4 f_2, \tag{24}$$

$$P_{zz} = \frac{m}{3}\int_0^\infty \mathrm{d}c\, c^4 f_0 + \frac{2m}{3}\int_0^\infty \mathrm{d}c\, c^4 f_2, \tag{25}$$

$$q = \frac{m}{2}\int_0^\infty \mathrm{d}c\, c^5 f_1, \tag{26}$$

where u' and q stand for u_z' and q_z, respectively. As can be seen from (21) to (26), the moments of zeroth, first and second order completely determine the macroscopic state of the gas.

For the derivation of the moment equations we project the Boltzmann equation to the Legendre polynomial system. To this end we substitute the expansion (19) into (1) with D from (18), multiply by $P_m(\mu)$

and integrate with respect to the solid angle in velocity space. The result can be written in the form

$$D_n[f_{n-2}, f_{n-1}, f_n, f_{n+1}, f_{n+2}] = J_n[f_i, f_j], \quad n=0,1,2,\dots . \tag{27}$$

The left hand side of the moment equations (27) can be obtained by applying the orthogonality of the Legendre polynomials, as well as the recurrence relations [15]

$$(2n+1)\,x\,P_n(x) = (n+1)\,P_{n+1}(x) + n\,P_{n-1}(x), \tag{28}$$

$$(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}P_n(x) = n\,P_{n-1}(x) - n\,x\,P_n(x). \tag{29}$$

One finds

$$\begin{aligned}
D_n = {} & \frac{\mathrm{d}}{\mathrm{d}t} f_n(z,c,t) + \frac{n+1}{2n+1}\left(c\frac{\partial f_{n+1}}{\partial z} - \frac{du}{dt}\frac{\partial f_{n+1}}{\partial c}\right) + \frac{n}{2n+1}\left(c\frac{\partial f_{n-1}}{\partial z} - \frac{\mathrm{d}u}{\mathrm{d}t}\frac{\partial f_{n-1}}{\partial c}\right) \\
& - \left[\frac{n^2}{(2n-1)(2n+1)} + \frac{(n+1)^2}{(2n+1)(2n+3)}\right] c\frac{\partial u}{\partial z}\frac{\partial f_n}{\partial c} - \frac{(n+1)(n+2)}{(2n+1)(2n+3)} c\frac{\partial u}{\partial z}\frac{\partial f_{n+2}}{\partial c} \\
& - \frac{n(n-1)}{(2n-1)(2n+1)} c\frac{\partial u}{\partial z}\frac{\partial f_{n-2}}{\partial c} - \frac{(n+1)(n+2)}{2n+1}\frac{1}{c}\frac{\mathrm{d}u}{\mathrm{d}t} f_{n+1} + \frac{n(n-1)}{2n+1}\frac{1}{c}\frac{\mathrm{d}u}{\mathrm{d}t} f_{n-1} \\
& - \frac{(n+1)(n+2)(2n+5) - (n+1)(n+2)^2}{(2n+1)(2n+3)}\frac{\partial u}{\partial z} f_{n+2} \\
& + \frac{n(n+1)^2(2n-1) + n^3(2n+3) - n^2(2n+1)(2n+3)}{(2n-1)(2n+1)(2n+3)}\frac{\partial u}{\partial z} f_n + \frac{n(n-1)(n-2)}{(2n-1)(2n+3)}\frac{\partial u}{\partial z} f_{n-2}
\end{aligned} \tag{30}$$

with

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial z}. \tag{31}$$

Provided that u is given self-consistently, so that $u'=0$ with u' defined by (22), D_n is a linear differential operator containing first order derivatives with respect to z, t and c. It affects on Legendre moments of order $n-2$ to $n+2$ ($f_{-2} = f_{-1} = 0$).

The Legendre moments of the collision operator are defined by

$$J[f,f] = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} J_n(z,c,t)\,P_n(\mu) \tag{32}$$

with

$$J_n(z,c,t) = 2\pi \int_{-1}^{1} \mathrm{d}\mu\, P_n(\mu)\, J(z,c,\mu,t). \tag{33}$$

As already mentioned above, the structure of the collision operator is not affected by the transformation (7). Hence, for J_n we can take over the result from a previous work [9], in which we considered a fixed coordinate system for measuring the particle velocities. The moments of the collision term can thus be written in the form

$$\begin{aligned}
J_n = {} & \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\int_0^{\infty} \mathrm{d}c'\, c'^2 \int_0^{\infty} \mathrm{d}c_1'\, c_1'^2 A_{ijn}(c', c_1', c)\, f_i(c')\, f_j(c_1') \\
& - \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} f_i(c) \int_0^{\infty} \mathrm{d}c_1\, c_1^2 B_{ijn}(c,c_1)\, f_j(c_1),
\end{aligned} \tag{34}$$

where the coefficients A_{ijn} and B_{ijn} are defined by

$$A_{ijn}(c', c_1', c) = \frac{(2i+1)(2j+1)}{(4\pi)^2} \int_{4\pi} \mathrm{d}^2\Omega' \int_{4\pi} \mathrm{d}^2\Omega_1' \int_{4\pi} \mathrm{d}^2\Omega \cdot S(\mathbf{c}' \to \mathbf{c}; \mathbf{c}_1')\, P_i(\mu')\, P_j(\mu_1')\, P_n(\mu) \tag{35}$$

and

$$B_{ijn}(c, c_1) = \frac{(2i+1)(2j+1)}{(4\pi)^2} \int_{4\pi} \mathrm{d}^2\Omega \int_{4\pi} \mathrm{d}^2\Omega_1 \int_{4\pi} \mathrm{d}^2\Omega' \int_0^{\infty} \mathrm{d}c'\, c'^2 \cdot S(\mathbf{c} \to \mathbf{c}'; \mathbf{c}_1)\, P_i(\mu)\, P_j(\mu_1)\, P_n(\mu). \tag{36}$$

In (35) and (36), $\int_{4\pi} \mathrm{d}^2\Omega$ denotes integration over the solid angle in velocity space:

$$\int_{4\pi} \mathrm{d}^2\Omega = \int_0^{2\pi} \mathrm{d}\omega \int_{-1}^{1} \mathrm{d}\mu. \tag{37}$$

For brevity, the dependence of f_n on z and t has been omitted in (34).

The moment equations (27) are an infinite set of integro-differential equations determining the Legendre coefficients f_n. Note in particular that through the collision term J_n, moments of arbitrary order enter the equation of a given order n.

The P_N approximation to the transport problem is now obtained if we truncate the series expansion (19) after $N+1$ terms:

$$f(z, c, \mu, t) \sim \sum_{n=0}^{N} \frac{2n+1}{4\pi} f_n(z, c, t)\, P_n(\mu)\,. \tag{38}$$

Note that for a low order approximation it is not required that the distribution function is close to a local Maxwellian, but only that the angular distribution is weakly anisotropic in the moving reference system.

According to the truncation (38), the system of moment equations is now of finite dimension:

$$D_n[f_{n-2}, f_{n-1}, f_n, f_{n+1}, f_{n+2}] = J_n[f_i, f_j]\,, \quad n=0, 1, 2, \ldots, N, \tag{39}$$

with $f_{-2}=f_{-1}=f_{N+1}=f_{N+2}=0$.

4. Transport Equations

The close connection between the Legendre moments of the distribution function and the hydrodynamical variables allows the derivation of the macroscopic conservation equations for mass, momentum and energy from the moment equations (27) of order zero and one. To this end, we start with the implication of the condition (6) on the Legendre moments of the collision operator. According to (32) we find

$$\int_0^\infty \mathrm{d}c\, c^2 J_0 = 0\,, \tag{40}$$

$$\int_0^\infty \mathrm{d}c\, c^3 J_1 = 0\,, \tag{41}$$

$$\int_0^\infty \mathrm{d}c\, c^4 J_0 = 0\,. \tag{42}$$

For the derivation of the transport equation for mass, we multiply the moment equation of zeroth order

$$\frac{\mathrm{d}f_0}{\mathrm{d}t} + c\frac{\partial f_1}{\partial z} - \frac{\mathrm{d}u}{\mathrm{d}t}\frac{\partial f_1}{\partial c} - \frac{1}{3}c\frac{\partial u}{\partial z}\frac{\partial f_0}{\partial c} - \frac{2}{3}c\frac{\partial u}{\partial z}\frac{\partial f_2}{\partial c} - \frac{2}{c}\frac{\mathrm{d}u}{\mathrm{d}t}f_1 - 2\frac{\partial u}{\partial z}f_2 = J_0 \tag{43}$$

by c^2 and integrate over the whole range of c. For those terms in (43), which contain derivatives of f with respect to c, we integrate by parts and consider that f vanishes for $c\to\infty$. Using (9) and (40) we find the continuity equation

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial z}(n\,u) = 0\,. \tag{44}$$

Multiplying (43) by $\frac{1}{4}mc^4$, integrating with respect to c and considering (42), we obtain the energy transport equation

$$\frac{\mathrm{d}e}{\mathrm{d}t} + \frac{\partial q}{\partial z} + (e+P_{zz})\frac{\partial u}{\partial z} = 0\,, \tag{45}$$

with $\mathrm{d}/\mathrm{d}t$ given by (31).

If we finally multiply the moment equation of first order

$$\frac{\mathrm{d}f_1}{\mathrm{d}t} + \frac{2}{3}c\frac{\partial f_2}{\partial z} - \frac{2}{3}\frac{\mathrm{d}u}{\mathrm{d}t}\frac{\partial f_2}{\partial c} + \frac{1}{3}c\frac{\partial f_0}{\partial z} - \frac{1}{3}\frac{\mathrm{d}u}{\mathrm{d}t}\frac{\partial f_0}{\partial c} - \frac{3}{5}c\frac{\partial u}{\partial z}\frac{\partial f_1}{\partial c} - \frac{2}{5}c\frac{\partial u}{\partial z}\frac{\partial f_3}{\partial c} - \frac{2}{c}\frac{\mathrm{d}u}{\mathrm{d}t}f_2 - \frac{8}{5}\frac{\partial u}{\partial z}f_3 - \frac{2}{5}\frac{\partial u}{\partial z}f_1 = J_1 \tag{46}$$

by mc^3, integrate over the whole range of c and consider (41), we find the transport equation for momentum:

$$mn\frac{\mathrm{d}u}{\mathrm{d}t} + \frac{\partial P_{zz}}{\partial z} = 0\,. \tag{47}$$

It is well-known that the system of the conservation equations (44), (45) and (47) is underdetermined in the sense that we only have three equations for the five unkowns n, u, e, P_{zz}, and q. From the moment equations of first and second order, one can derive governing equations for q and P_{zz}. However, these equations contain higher order terms which have no direct physical meaning. Moreover, the corresponding collision integrals do not vanish, as is the case in the conservation equations for mass, momentum and energy. One is therefore led to suitable approximations in order to derive additional equations combining the hydrodynamical variables ("closure relations").

5. Small Mean Free Paths and P_2 Approximation

We now investigate under which circumstances the series expansion (19) can be truncated after only a few terms. This is the case if the velocity distribution is only weakly anisotropic. In order to justify a series truncation, the magnitude of the moments $f_0, f_1, f_2, \ldots$ has to be estimated.

We begin with the investigation of the order of magnitude of the various terms appearing in the Boltzmann equation. To this end, we approximate the collision term by the BGK model [16], so that the Boltzmann equation reads

$$\varepsilon D[f] = -\frac{\nu}{\nu_r}(f-M)\,. \tag{48}$$

In the nondimensional representation (48), ν is the collision frequency and M is the local Maxwellian distribution (10) expressed in terms of the local mean density and temperature. In (48), length is measured in units of a characteristic length L required for a significant change in f, and speed is measured in units of a typical molecular velocity c_r. The time unit is chosen to be L/c_r. The quantity $\nu_r = c_r/\lambda_r$ stands for a typical value of the collision frequency, with λ_r denoting a characteristic value of the mean free path. The ratio $\varepsilon = \lambda_r/L$ is the Knudsen number. Finally, the nondimensional distribution function is defined through the transformation $c_r^3 f/n_r \to f$, where n_r is a characteristic reference density. It is assumed that the reference quantities L, c_r, ν_r, and n_r can be chosen in such a way that each term in (48) with the exception of the Knudsen number ε, is at most of order unity [17].

In this section we are interested in the special case of small mean free paths, $\varepsilon \ll 1$. Here, the gas can be said to be collision dominated. As can be seen from (48), for $\varepsilon \ll 1$ the distribution function is close to the (local) equilibrium distribution. In particular we expect that for systems with $\varepsilon \ll 1$, an observer moving at the mean velocity of the gas will detect an "almost" isotropic velocity distribution. To quantify this statement, we write the moment equations (27) in a nondimensional form. Using the BGK collision model and applying (32) we obtain

$$\varepsilon D_n[f_{n-2}, f_{n-1}, f_n, f_{n+1}, f_{n+2}] = -\frac{\nu}{\nu_r}(f_n - 4\pi\,\delta_{n,0} M), \quad n = 0, 1, 2, \dots\,, \tag{49}$$

with D_n given by (30). The term $\delta_{i,j}$ is the Kronecker delta. According to the assumption made above, the various terms appearing in D_n are at most of order unity. In particular we suppose that f_0 is of order unity. Furthermore it is assumed that all derivatives of f_n are at most of the same order of magnitude as f_n.

The order of magnitude of the moments f_n can now be obtained as follows. From the moment equation of first order we see that f_1 is smaller by the factor ε than the largest term in D_1 which is of order unity. Hence we have $f_1 = O(\varepsilon)$. The same applies for f_2 as can be seen by using the moment equation of second order. In general, the order of magnitude of the moment f_n is obtained by considering that f_n is smaller by the factor ε than the term with the lowest index in the streaming operator D_n. This term has the index $n-2$ (for $n \geq 2$). Therefore we find in the case $\varepsilon \ll 1$:

$$f_0 = O(1); \quad f_1, f_2 = O(\varepsilon); \quad f_3, f_4 = O(\varepsilon^2); \dots\,. \tag{50}$$

Thus for systems with small mean free paths, we can restrict ourselves to the first three terms in the expansion (19), or equivalently, the P_2 approximation is adequate for $\varepsilon \ll 1$.

Within the scope of the P_2 approximation, the closure relations mentioned above can be derived from the moment equations of first and second order. Using the estimation (50), Jaffé [8] showed that the spherical harmonics method leads to the same results as the celebrated Enskog method. We note that for the BGK collision model, the closure relations (Fourier's law and Newton's law) can be derived immediately from the moment equations [18].

6. Higher Order Approximations

For many situations in rarefied gas dynamics, approximations of higher order than the P_2 approximation are required. A systematic approach to the moment equations of arbitrary order and arbitrary collision laws is given in the form of the P_N^{KLM} method [9]. The problem in dealing with higher order approximations lies in the evaluation of the collision integrals A_{ijn} [see (35)]. There, on the one hand, natural angular variables (scattering angles) entering the scattering kernel S are involved. On the other hand, angular variables depending on the special choice of the coordinate system appear (for a more detailed discussion see [9]). In the framework of the P_N^{KLM} method, this involvement is disentangled by a triple expansion of the scattering kernel in terms of Legendre polynomials. However, this expansion creates a complicated algebraic structure of the collision terms. We are therefore led to scattering models for which we can obtain simple expressions for the collision terms of the moment equations.

The simplest model in this sense is the BGK model [16], where

$$J[f] = -\nu(f-M)\,. \tag{51}$$

Here, the moments of the collision operator read

$$J_n[f_n] = -\nu(f_n - 4\pi\,\delta_{n,0} M), \quad n = 0, 1, 2, \dots, \tag{52}$$

as can be seen by inserting (51) into (33). The density and the temperature appearing in the local equilibrium distribution M and in the local collision frequency ν have to be determined self-consistently according to (11), (21), and (23).

If the P_N method is applied to the BGK model Boltzmann equation, the resulting moment equations are conserving, as can be seen by substituting J_n from (52) into (40), (41) and (42), and using (22). To investigate the effect of the collision terms on the moments of the distribution function, we confine ourselves to spatially homogeneous gases,

$$\frac{\partial f_n}{\partial t} = J_n\,, \quad n=0, 1, 2, \ldots\,. \tag{53}$$

We note that moments f_n of order $n \geq 1$ are damped as a result of collisions, while f_0 is forced towards the (isotropic) equilibrium distribution. This equilibration can be expressed by an H theorem. Within the framework of the P_N approximation, we have to solve $N+1$ moment equations. We therefore define the $(N+1)$ H functions

$$H_n = \begin{cases} \int\limits_0^\infty \mathrm{d}c\, c^2 f_0 \log f_0 & \text{for} \quad n=0 \\ \frac{1}{2} f_n^2 & \text{for} \quad 1 \leq n \leq N. \end{cases} \tag{54}$$

It is easy to prove that the inequality (H theorem)

$$\frac{\mathrm{d}H_n}{\mathrm{d}t} \leq 0\,, \quad n=0, 1, 2, \ldots, N, \tag{55}$$

holds. Equations (55) show that the result of the collisions is an irreversible trend of the distribution function towards the local Maxwellian distribution.

As a further example for a collision model allowing simple expressions for the collision terms, we consider that the scattering is isotropic in a coordinate system moving at the mean velocity of the gas:

$$w(\boldsymbol{c}' \to \boldsymbol{c}; \boldsymbol{c}'_1) = \frac{1}{4\pi}\, \Pi(c' \to c; c'_1)\,. \tag{56}$$

Here, the scattering probability is independent of the orientation of the velocity vectors $\boldsymbol{c}, \boldsymbol{c}'$ and $\boldsymbol{c}'_1$. According to (5), Π is normalized to unity:

$$\int\limits_0^\infty \mathrm{d}c\, c^2\, \Pi(c' \to c; c'_1) = 1\,. \tag{57}$$

It is important to note that for this kind of scattering, momentum conservation is in general violated in the binary collision events. For a stationary gas, the assumption (56) means isotropic scattering in the laboratory system, as investigated by Boffi and Spiga [10].

The collision term of the Boltzmann equation now reads

$$\begin{aligned} J[f,f] = &\frac{1}{4\pi} \int\limits_0^\infty \mathrm{d}c'\, c'^2 \int\limits_0^\infty \mathrm{d}c'_1\, c_1'^2 \int\limits_0^{2\pi} \mathrm{d}\omega' \int\limits_0^{2\pi} \mathrm{d}\omega'_1 \\ &\cdot \int\limits_{-1}^1 \mathrm{d}(\cos\zeta') \int\limits_{-1}^1 \mathrm{d}(\cos\zeta'_1)\, g'\sigma(g')\, \Pi(c' \to c; c'_1) \\ &\cdot f(c', \cos\zeta')\, f(c'_1, \cos\zeta'_1) - f(c, \cos\zeta) \\ &\cdot \int\limits_0^\infty \mathrm{d}c_1\, c_1^2 \int\limits_0^{2\pi} \mathrm{d}\omega_1 \int\limits_{-1}^1 \mathrm{d}(\cos\zeta_1)\, f(c_1, \cos\zeta_1)\, g\,\sigma(g), \end{aligned} \tag{58}$$

where g' denotes the relative velocity of particles colliding with speeds $\boldsymbol{c}'$ and $\boldsymbol{c}'_1$,

$$g' = (c'^2 + c_1'^2 - 2c'c'_1 \cos\theta')^{1/2}; \tag{59}$$

θ' is the collision angle defined through

$$\cos\theta' = \cos\zeta' \cos\zeta'_1 + \sin\zeta' \sin\zeta'_1 \cos(\omega' - \omega'_1); \tag{60}$$

(g is defined as g' but in terms of unprimed quantities). In (58) the dependence of f_n on z and t has been omitted.

We expand

$$g'\sigma(g') = \sum_{n=0}^\infty \frac{2n+1}{4\pi}\, \sigma_n(c', c'_1)\, P_n(\cos\theta')\,, \tag{61}$$

with

$$\sigma_n(c', c'_1) = 2\pi \int\limits_{-1}^1 \mathrm{d}(\cos\theta')\, g'\sigma(g')\, P_n(\cos\theta')\,. \tag{62}$$

By applying the addition theorem for Legendre polynomials [15],

$$\begin{aligned} P_n(\cos\theta') = &P_n(\cos\zeta')\, P_n(\cos\zeta'_1) \\ &+ 2\sum_{\varrho=1}^n \frac{(n-\varrho)!}{(n+\varrho)!}\, P_n^\varrho(\cos\zeta')\, P_n^\varrho(\cos\zeta'_1) \cos[\varrho(\omega' - \omega'_1)], \end{aligned} \tag{63}$$

we obtain for the first term on the right hand side of (58)

$$\begin{aligned} J^{\mathrm{in}}[f_i, f_j] = &\sum_{k=0}^\infty \frac{2k+1}{(4\pi)^2} \int\limits_0^\infty \mathrm{d}c'\, c'^2 \int\limits_0^\infty \mathrm{d}c'_1\, c_1'^2 \\ &\cdot \sigma_k(c', c'_1)\, \Pi(c' \to c; c'_1)\, f_k(c')\, f_k(c'_1)\,. \end{aligned} \tag{64}$$

Since this term is independent of $\mu = \cos\zeta$, the Legendre moments of the in-scattering term (64) are simply given by [see (32)]

$$J_n^{\mathrm{in}} = 4\pi\, J^{\mathrm{in}}\, \delta_{n,0}\,. \tag{65}$$

Hence, as a result of the isotropic scattering, only the moment equation of zeroth order possesses an in-scattering term.

Inserting the expansions (19) and (61) into the out-scattering term of the collision operator (58) and carrying out the angular integrations by considering the addition theorem (63), one finally obtains

$$J_n[f_i, f_j] = \delta_{n,0} \sum_{k=0}^{\infty} \frac{2k+1}{4\pi} \int_0^{\infty} \mathrm{d}c'\, c'^2 \int_0^{\infty} \mathrm{d}c'_1\, c_1'^2 \cdot \sigma_k(c', c'_1)\, \Pi(c' \to c; c'_1)\, f_k(c')\, f_k(c'_1) - \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{(2i+1)(2j+1)}{8\pi} \alpha_{ijn}\, f_i(c) \cdot \int_0^{\infty} \mathrm{d}c_1\, c_1^2\, \sigma_j(c, c_1)\, f_j(c_1), \quad (66)$$

with

$$\alpha_{ijn} = \int_{-1}^{1} \mathrm{d}x\, P_i(x)\, P_j(x)\, P_n(x). \quad (67)$$

A comparison of the collision term (66) with the result for arbitrary scattering [9] shows that the assumption (56) results in a remarkable simplification. However, it is not clear whether the isotropic scattering here under consideration is compatible with the conservation of mass, momentum and energy, and with an H theorem. In fact, as already mentioned, momentum conservation is violated on the microscopic scale.

In order to bring a further simplification to the collision terms of the moment equations, we confine ourselves to Maxwellian molecules,

$$\sigma(g) = \frac{4\pi\varkappa}{g}, \quad (68)$$

where $\varkappa$ is a constant. Here, the only non-vanishing moment of the term $g\sigma(g)$ is [see (61)]

$$\sigma_0 = (4\pi)^2 \varkappa, \quad (69)$$

so that we find by applying (21)

$$J_n = 4\pi\varkappa\, \delta_{n,0} \int_0^{\infty} \mathrm{d}c'\, c'^2 \int_0^{\infty} \mathrm{d}c'_1\, c_1'^2\, \Pi(c' \to c; c'_1) \cdot f_0(c')\, f_0(c'_1) - 4\pi\varkappa\, n' f_n(c), \quad (70)$$

with n' denoting the local particle density. The simplification of the collision terms is now advanced to a stage where only moments of order n contribute to the collision term J_n. However, (70) retains all the challenging nonlinear features of the original problem.

The moments defined by (70) bear the advantage that the conservation laws and an H theorem can be proven. First we note that as a result of (22), momentum conservation (41) is guaranteed. To prove that mass and energy are conserved, we assume that Π possesses the properties of a well-defined scattering kernel of the scalar (or space homogeneous) Boltzmann equation [2]

$$\Pi(c' \to c; c'_1) = \Pi(c'_1 \to c_1; c'), \quad (71)$$

$$c'_1\, \Pi(c' \to c; c'_1) = c_1\, \Pi(c \to c'; c_1), \quad (72)$$

where

$$c_1 = (c'^2 + c_1'^2 - c^2)^{1/2}. \quad (73)$$

To be well-defined, the scattering kernel must vanish if the velocity triple (c, c', c'_1) is not compatible with energy conservation:

$$\Pi(c' \to c; c'_1) = 0 \quad \text{if} \quad c'^2 + c_1'^2 - c^2 < 0. \quad (74)$$

In order to give an example for the scattering kernel of the scalar Boltzmann equation, we quote the result for Maxwellian molecules [19]

$$\Pi(c' \to c; c'_1) = \frac{8\pi\varkappa}{c\, c'\, c'_1}\, \Theta(c'^2 + c_1'^2 - c^2) \arcsin \frac{\mathrm{Min}(c, c_1, c', c'_1)}{(c'^2 + c_1'^2)^{1/2}}. \quad (75)$$

Here, Θ denotes Heaviside's step function.

Using the properties (71), (72) and (74) together with (21), it can be shown that J_0 defined by (70) can also be written in the form

$$J_0 = 4\pi\varkappa \int_0^{\infty} \mathrm{d}c'\, c'^2 \int_0^{\infty} \mathrm{d}c'_1\, c_1'^2\, \Pi(c' \to c; c'_1) \cdot [f_0(c')\, f_0(c'_1) - f_0(c)\, f_0(c_1)], \quad (76)$$

with c_1 defined by (73). Using the symmetries (71) and (72) we can deduce from (76) that

$$\int_0^{\infty} \mathrm{d}c\, c^2\, \psi(c)\, J_0 = \pi\varkappa \int_0^{\infty} \mathrm{d}c'\, c'^2 \int_0^{\infty} \mathrm{d}c'_1\, c_1'^2\, \Pi(c' \to c; c'_1) \cdot [f_0(c')\, f_0(c'_1) - f_0(c)\, f_0(c_1)] \cdot [\psi(c) + \psi(c_1) - \psi(c') - \psi(c'_1)], \quad (77)$$

where ψ is an arbitrary molecular property. By inserting $\psi = 1$ and $\psi = \frac{1}{2} m c^2$ into (77), one immediately sees that the collision terms of the moment equations conserve mass and energy.

In order to prove that the collision terms result in an equilibration of the distribution function, we first note that

$$f_n = \begin{cases} 4\pi M & \text{for} \quad n=0 \\ 0 & \text{for} \quad n \geq 1 \end{cases}, \tag{78}$$

is the equilibrium solution to the collision terms (70). This is obvious in the case of $n \geq 1$. For $n=0$, one can easily verify (78) by considering the representation (76). Using the $(N+1)$ H functions defined by (54), we find that for spatially homogeneous gases the H theorem (55) is valid. The proof is trivial for $n \geq 1$. To prove the H theorem for $n=0$, we insert

$$\psi = 1 + \log f_0 \tag{79}$$

into (77). It then follows that $\mathrm{d}H_0/\mathrm{d}t \leq 0$, where equality is given if and only if $f_0 \propto M$.

Hence, we have shown that for a gas composed of "artificial" Maxwell molecules as defined by (56) and (68), the collision terms (70) of the moment equations are conserving and obey an H theorem. It is interesting to note that for the special case of Maxwellian molecules we have momentum conservation on the macroscopic scale. Remember that for the isotropic scattering here under consideration, momentum conservation is in general violated in the binary encounters.

7. Concluding Remarks

By means of the P_N method, the angular dependence of the particle velocity vector has been separated from the velocity distribution function. Hence, the basis is laid out for a multigroup treatment of the nonlinear transport problem. In this formalism, by means of a discretization of the velocity range, the integro-differential moment equations are transformed into a set of differential equations which can be solved by using a computer. This technique has been efficiently used in nuclear reactor theory for solving the (linear) neutron transport equation [20]. The multigroup method has also been applied to nonlinear problems [21], but only for the special case of homogeneous gases. The numerical solutions hereby obtained are in excellent agreement with an exact solution of the nonlinear Boltzmann equation.

In developing the P_N method, we confined ourselves to one-dimensional geometry, as well as to systems without external forces. The generalizations necessary to describe more complex situations in this respect, create a more complicated algebraic structure of the moment equations without requiring substantial alterations of the method itself. The P_N method can also be extended to gas mixtures and to systems with inelastic or reactive scattering. In the latter case, the scattering kernel for inelastic scattering [22] has to be used in the collision integrals of the form (35) and (36). We expect that, compared to other moment methods, the P_N method is especially applicable to reactive gases or to systems whose particles possess internal degrees of freedom. Inelastic collisions may severely disturb the distribution function without causing a substantial anisotropy, if the particle velocities are measured in a reference system moving at the mean velocity of the gas. In this case, the transport problem can be described by a low order approximation (e.g. P_2 approximation), whereby the term f_0 may deviate strongly from the local Maxwellian distribution. Hence, in the framework of the P_N method, a low order approximation can be used even for systems which deviate from local equilibrium. We point out that this is not the case for other moment methods.

A final point concerns the boundary conditions. The problem in dealing with boundary conditions in the context of moment methods lies in the fact that they can in general not be satisfied exactly by a truncated series expansion of the distribution function (see also the work of Grad [4]). To impose the boundary conditions in the P_N approximation, the ideas and methods can be used which proved to be efficient in neutron transport theory (Mark's and Marshak's boundary conditions [7]). A possible way to satisfy the boundary conditions exactly is a half range expansion of the distribution function. This technique has also already been applied in neutron transport theory (Double-P_N method [23]). It can certainly be adopted to the non-linear problem here under consideration. A special case being of interest in kinetic theory is given if the molecules are specularly reflected at the boundary. If the latter is situated at $z=L$, the boundary condition for the distribution function reads $f(L, c, \mu, t) = f(L, c, -\mu, t)$. In the framework of the P_N method, this boundary condition can be satisfied by considering that f is an even function in μ. Hence, specular reflection imposes no restriction on any moment of the expansion (19) which is of even order and requires that all odd moments vanish at the boundary.

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