The BGK-model with velocity-dependent collision frequency

Henning Struchtrup
Technical University Berlin, Sekr. HF 2, Fasanenstr. 90, 10623 Berlin, Germany

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Abstract

We consider the BGK-model with velocity dependent collision frequency. By use of the Chapman-Enskog method we calculate thermal conductivity and viscosity. We show that a simple power law for the collision frequency may lead to the proper Prandtl number. Moreover we use Grad's moment method to calculate thermal conductivity and viscosity. We show that the results of both methods coincide if Grad's method is based on a large number of moments.

1 Introduction

Because of its simplicity compared to the Boltzmann equation the BGK equation is widely used in the kinetic theory of gases. This equation provides a good model in particular for the derivation of qualitatively good results. For quantitative results the model is less good; for instance the BGK equation with constant collision frequency is not able to derive the correct Prandtl number, i.e. the ratio of thermal conductivity and viscosity [2].

The aim of this paper is twofold. First we show that a velocity-dependent collision frequency may lead to the correct Prandtl number. We assume a simple power law for the collision frequency ν,

$$\nu = \zeta C^{\alpha},$$

and show that $\alpha = (\sqrt{21} - 1)/2 = 1.7913$ will lead to the Prandtl number $Pr = \frac{15}{4}\frac{k}{m}$.

Our second aim is to compare the Chapman-Enskog method with Grad's moment method. We use both methods for the calculation of the Prandtl number and show that the results of both agree, if the Grad method is based on a large number of moments.

2 Phase density and Boltzmann equation

The state of a mon-atomic ideal gas is completely described if the phase density $f(x_i, t, c_i)$ is known[2]. f is the phase density such that $f d\mathbf{c}$ gives the number density of atoms with velocity in $(c_i, c_i + dc_i)$ at place x_i and time t.

The macroscopic quantities density ϱ, velocity v_i and temperature T of the gas are given by moments of the phase density, viz.

$$\varrho = \int m f d\mathbf{c} \quad , \quad \varrho v_i = \int m c_i f d\mathbf{c} \quad , \quad \varrho\varepsilon = \frac{3}{2}\varrho\frac{k}{m}T = \int \frac{m}{2}\left(c_i - v_i\right)^2 f d\mathbf{c} \tag{1}$$

where m is the mass of one particle, k is Boltzmann's constant and $\varrho\varepsilon$ denotes the density of internal energy. The entropy of the gas is given by

$$\varrho s = -k \int f \ln f d\mathbf{c}.$$

For later use we define arbitrary moments of the phase density by

$$u^r_{i_1 i_2 \cdots i_n} = \int m C^r C_{i_1} C_{i_2} \cdots C_{i_n} f d\mathbf{c} \tag{2}$$

with $C_i = c_i - v_i$ as the peculiar velocity. Only 13 of this moments have a macroscopic interpretation, namely

$$u^0 = \varrho \quad , \quad u^0_i = 0 \quad , \quad u^2 = 2\varrho\varepsilon \quad , \quad u^0_{\langle ij \rangle} = p_{\langle ij \rangle} \quad , \quad u^2_i = 2q_i$$

with the pressure deviator $p_{\langle ij \rangle}$ and the heat flux q_i.

The phase density $f(x_i, t, c_i)$ is governed by the Boltzmann equation [2],

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = \mathcal{S} = \int \left(f' f'^1 - f f^1 \right) \sigma g \sin\theta d\theta d\varepsilon d\mathbf{c}_1. \tag{3}$$

The collision term on the right hand side has the following four properties [2]

i.) It guarantees the conservation of mass, momentum and energy, which may be written as

$$\int m\mathcal{S} d\mathbf{c} = 0 \quad , \quad \int m c_i \mathcal{S} d\mathbf{c} = \int m C_i \mathcal{S} d\mathbf{c} = 0 \quad , \quad \int \tfrac{m}{2} c^2 \mathcal{S} d\mathbf{c} = \int \tfrac{m}{2} C^2 \mathcal{S} d\mathbf{c} = 0 \tag{4}$$

ii.) The production of entropy is always positive (H-Theorem),

$$-k \int \ln f \mathcal{S} d\mathbf{c} \geqslant 0 \tag{5}$$

iii.) Due to the specific Form of $\mathcal{S}$ the phase density in equilibrium is a Maxwellian, i.e.

$$\mathcal{S} = 0 \Longrightarrow f = f_M = \frac{\varrho}{m} \sqrt{\frac{m}{2\pi kT}}^3 \exp -\frac{m}{2kT} C^2 \tag{6}$$

iv.) The Prandtl number Pr, defined as the ratio of thermal conductivity and viscosity μ, is close to $\frac{15}{4}\frac{k}{m}$ for all collision factors σ,

$$Pr = \frac{\kappa}{\mu} \simeq \frac{15}{4} \frac{k}{m} \tag{7}$$

3 The BGK equation

Because of its complex non-linearity, the Boltzmann collision term $\mathcal{S}$ is difficult to handle. Therefore one is interested in model equations which are easier to handle than the Boltzmann equation but which should also have the properties i.) through iv.).

In the literature one finds many collision models but none is as popular as the one due to Bhatnagar, Gross and Krook [1]. We briefly recall the motivation of the BGK collision term in Appendix A, here only the result is given.

The BGK equation reads

$$\frac{\partial f}{\partial t}+c_i\frac{\partial f}{\partial x_i}=\mathcal{S}_\gamma=-\nu\left(f-f_\gamma\right), \tag{8}$$

where

$$\nu=\nu\left(x_i,t,C_i\right)$$

is a mean collision frequency, which depends on C_i, and f_γ is a phase density, given by

$$f_\gamma=a\exp\left(-\Gamma c^2+\gamma_i c_i\right).$$

The coefficients a,Γ,γ_i follow from the conservation conditions (4), which now read

$$\textstyle\int\nu m\left(f-f_\gamma\right)d\mathbf{c}=0\quad,\qquad\int\nu mC_i\left(f-f_\gamma\right)d\mathbf{c}=0\quad,\qquad\int\nu\frac{m}{2}C^2\left(f-f_\gamma\right)d\mathbf{c}=0. \tag{9}$$

Note, that in general f_γ is *not* a Maxwellian. From (9) and (1) follows that f_γ is a Maxwellian only if ν does not dependent on the peculiar velocity C_i.

It should be emphasized that - because of the conditions (9) - the BGK equation (8) is a non-linear integro-differential equation, just like the Boltzmann equation. So one will not expect analytical solutions. But as we will show, the standard procedures of Chapman-Enskog and Grad are much easier to perform for the BGK equation thanfor the Boltzmann equation.

We proceed to discuss the properties of the BGK model which we should like to be the same ones as those of the Boltzmann equation.

i.) The conservation of mass, momentum and energy is ensured by the proper choice of a,Γ,γ_i according to (9)

ii.) Since, with (9),

$$k\int\ln f_\gamma\mathcal{S}_\gamma d\mathbf{c}=k\int\left(\ln a-\Gamma c^2+\gamma_i c_i\right)\mathcal{S}_\gamma d\mathbf{c}=0$$

we may write the entropy production as

$$\begin{aligned}-k\int\ln f\mathcal{S}_\gamma d\mathbf{c}&=-k\int\ln f\mathcal{S}_\gamma d\mathbf{c}+k\int\ln f_\gamma\mathcal{S}_\gamma d\mathbf{c}\\&=k\int\nu\ln\frac{f}{f_\gamma}\left(f-f_\gamma\right)d\mathbf{c}\geqslant0,\end{aligned}$$

the H-theorem is fulfilled.

iii.) In thermodynamic equilibrium (characterized by the subscript E) the BGK collision term must vanish

$$\mathcal{S}_{|E}=0\Longrightarrow-\nu\left(f_{|E}-f_{\gamma|E}\right)=0,$$

i.e. in equilibrium both phase densities are equal, $f_{|E}=f_{\gamma|E}$. Moreover both functions must have the same moments. Since the first five moments of f define density, velocity and temperature we have to conclude, that both functions are Maxwellians in equilibrium

$$f_{|E}=f_{\gamma|E}=f_M.$$

iv.) The calculation of the Prandtl number will be performed in the remainder of the paper. But one may conjecture sees easily that the extension of the ordinary BGK model to the case where ν is a function of C offers an additional degree of freedom which may be used to adjust both, viscosity and thermal conductivity, to their measured values.

In summary we conclude, that the BGK model with a velocity-dependent collision frequency may be formulated so as to have the properties i.)-iv.) just like the Boltzmann equation. Thus it may be a good substitute for the Boltzmann equation. What remains to be done is an explicit demonstration of the conjecture issued in item iv.).

For explicit calculations one has to know the collision frequency as a function of C. For the calculations in the next sections we have chosen the simplest possible dependence of ν on velocity, namely a polynominal dependence,

$$\nu = \zeta C^{\alpha} \quad \text{with } \zeta = \varrho \cdot h\left(T\right), \; \alpha \geq 0. \tag{10}$$

The choice of a positive α reflects our expectation, that the collision frequency should increase with the speed of the particle; the linear dependence on ϱ follows from (A.1); the function $h\left(T\right)$ must be fitted to measurements of the thermal conductivity.

We restrict ourselves to processes close to equilibrium. Then f_γ will be close to a Maxwellian and we may expand as

$$f_\gamma \simeq f_M \left(1 + \hat{a} + \hat{\gamma}_i C_i - \hat{\Gamma} C^2\right);$$

$\hat{a}, \hat{\gamma}_i, \hat{\Gamma}$ follow from (9) as

$$\hat{a} = \frac{\alpha+5}{2}\frac{\Delta^{\alpha}}{u^{\alpha}_{|E}} - \frac{\alpha+3}{2}\frac{\Delta^{\alpha+2}}{u^{\alpha+2}_{|E}}$$

$$\hat{\gamma}_i = \frac{3}{u^{\alpha+2}_{|E}} u^{\alpha}_i$$

$$\hat{\Gamma} = \frac{m}{2kT}\left(\frac{\Delta^{\alpha+2}}{u^{\alpha+2}_{|E}} - \frac{\Delta^{\alpha}}{u^{\alpha}_{|E}}\right)$$

where we have introduced the abbreviations

$$\Delta^r = u^r - u^r_{|E},$$

$$u^r_{|E} = \varrho \left(\frac{2kT}{m}\right)^{\frac{r}{2}} \frac{\Gamma\left(\frac{r+3}{2}\right)}{\Gamma\left(\frac{3}{2}\right)}.$$

$u^{\alpha}, u^{\alpha+2}$ and u^{α}_i are moments (2) of the phase density f; we must know f before we are able to determine them.

For use in subsequent sections we present some moments of f_γ as functions of u^α, $u^{\alpha+2}$ and u_i^α,

$$\Delta^{r+\alpha}_{|\gamma} = u^{r+\alpha}_{|E}\left(\frac{r}{2}\frac{\Delta^{\alpha+2}}{u^{\alpha+2}_{|E}} - \left(\frac{r-2}{2}\right)\frac{\Delta^{\alpha}}{u^{\alpha}_{|E}}\right)$$

$$u^{r+\alpha}_{i|\gamma} = \left(\frac{2kT}{m}\right)^{\frac{r}{2}}\frac{\Gamma\left(\frac{\alpha+r+5}{2}\right)}{\Gamma\left(\frac{\alpha+5}{2}\right)}u_i^\alpha\,, \tag{11}$$

$$u^{r+\alpha}_{\langle ij\rangle|\gamma} = 0.$$

4 Chapman-Enskog method

We proceed by calculating the phase density f from (8) by means of the Chapman-Enskog method [2]. In case of the BGK model the Chapman-Enskog method turns out to be very simple: We insert the Maxwell phase density on the right hand side of (8) and eliminate all time derivatives by means of the Euler equations for mon-atomic gases,

$$\dot{\varrho} + \varrho\frac{\partial v_k}{\partial x_k} = 0 \quad , \quad \dot{v}_i + \frac{1}{\varrho}\frac{\partial \varrho\frac{k}{m}T}{\partial x_i} = 0 \quad , \quad \left(\frac{T^{\frac{3}{2}}}{\varrho}\right)^{\bullet} = 0. \tag{12}$$

After some rearrangement of the resulting equation we find for the phase density

$$f = f_\gamma - \frac{1}{\zeta}f_M\left\{\frac{m}{kT}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\frac{C_iC_j}{C^\alpha} + \frac{1}{T}\frac{\partial T}{\partial x_i}\left(\frac{m}{2kT}C^2 - \frac{5}{2}\right)\frac{C_i}{C^\alpha}\right\}.$$

Now it is an easy task to calculate the pressure deviator $p_{\langle ij\rangle}$ and the heat flux vector q_i. Of course, we rederive the laws of Navier-Stokes and Fourier with explicit expressions for viscosity μ and thermal conductivity κ, viz.

$$p_{\langle ij\rangle} = -\underbrace{\frac{\varrho}{\zeta}\left(\frac{2kT}{m}\right)^{\frac{2-\alpha}{2}}\frac{\Gamma\left(\frac{7-\alpha}{2}\right)}{\Gamma\left(\frac{7}{2}\right)}}_{2\mu}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}$$

$$q_i = -\underbrace{\frac{k}{m}\frac{\varrho}{\zeta}\left(\frac{2kT}{m}\right)^{\frac{2-\alpha}{2}}\frac{10-2\alpha+\alpha^2}{8}\frac{\Gamma\left(\frac{5-\alpha}{2}\right)}{\Gamma\left(\frac{5}{2}\right)}}_{\kappa}\frac{\partial T}{\partial x_i}$$

As expected, the Prandtl number depends on the power of C in the collision frequency

$$Pr = \frac{\kappa}{\mu} = \frac{15}{4}\frac{k}{m}\frac{10-2\alpha+\alpha^2}{15-3\alpha}. \tag{13}$$

Since we are interested in positive values of α only, we find one value of α for each measured Prandtl number. $\alpha = 0$ gives $Pr = \frac{5}{2}\frac{k}{m}$ while $\alpha = \frac{1}{2}\left(-1+\sqrt{21}\right) = 1.7913$ provides the desired Prandtl number $Pr = \frac{15}{4}\frac{k}{m}$.

5 Grad Method

5.1 Moment equations

In Grad's moment method the Boltzmann equation is replaced by moment equations [4]. Crucial is the choice of the moments on which the theory is based. Here we assume that the state of the gas is sufficiently well described by the knowledge of the moments

$$u^{2n} = \int mC^{2n} f d\mathbf{C} \quad , \quad u_i^{2n} = \int mC^{2n} C_i f d\mathbf{C} \quad , \quad u_{\langle ij\rangle}^{2n} = \int mC^{2n} C_{\langle i} C_{j\rangle} f d\mathbf{C} \tag{14}$$

with $n = 0, 1, \ldots, N$. Here N is a number, which takes into account isotropic deviations from the Maxwell distribution. Its value will be discussed in the sequel.

With this choice of moments we imply that deviations from isotropy are small; if we were interested in highly anisotropic processes we should have to consider moments $u^{2n}_{\langle i_1 \cdots i_m\rangle} = \int mC^{2n} C_{\langle i_1} \cdots C_{i_m\rangle} f d\mathbf{C}$ with $m = 0, 1, \ldots, M; M > 2$ also.

The moment equations follow by multiplication of the BGK equation (8) with mC^{2n}, $mC^{2n}C_i$, $mC^{2n}C_{\langle i}C_{j\rangle}$ and subsequent integration over velocity space.

With the assumption (10) for the collision frequency we obtain

$$\begin{aligned}
\dot{u}^{2n} - 2nu_k^{2n-2}\frac{1}{\varrho}\frac{\partial p_{kl}}{\partial x_l} + \frac{\partial u_k^{2n}}{\partial x_k} + 2nu_{kl}^{2n-2}\frac{\partial v_k}{\partial x_l} + u^{2n}\frac{\partial v_k}{\partial x_k} &= -\zeta\left(u^{2n+\alpha} - u_{|\gamma}^{2n+\alpha}\right) \\[2ex]
\dot{u}_i^{2n} - u^{2n}\frac{1}{\varrho}\frac{\partial p_{ik}}{\partial x_k} - 2nu_{ik}^{2n-2}\frac{1}{\varrho}\frac{\partial p_{kl}}{\partial x_l} + \frac{\partial u_{ik}^{2n}}{\partial x_k} + & \\
2nu_{ikl}^{2n-2}\frac{\partial v_k}{\partial x_l} + u_i^{2n}\frac{\partial v_k}{\partial x_k} + u_k^{2n}\frac{\partial v_i}{\partial x_k} &= -\zeta\left(u_i^{2n+\alpha} - u_{i|\gamma}^{2n+\alpha}\right) \\[2ex]
\dot{u}_{\langle ij\rangle}^{2n} - 2nu_{\langle ij\rangle k}^{2n-2}\frac{1}{\varrho}\frac{\partial p_{kl}}{\partial x_l} - 2u_{\langle i}^{2n}\frac{1}{\varrho}\frac{\partial p_{j\rangle k}}{\partial x_k} + \frac{\partial u_{\langle ij\rangle k}^{2n}}{\partial x_k} & \\
+2nu_{\langle ij\rangle kl}^{2n-2}\frac{\partial v_k}{\partial x_l} + 2u_{k\langle i}^{2n}\frac{\partial v_{j\rangle}}{\partial x_k} + u_{\langle ij\rangle}^{2n}\frac{\partial v_k}{\partial x_k} &= -\zeta u_{\langle ij\rangle}^{2n+\alpha}
\end{aligned}\tag{15}$$

If we choose $n = 0, 1$ in the scalar equation $(15)_1$ we obtain the balance laws of mass and energy,

$$\dot{\varrho} + \varrho\frac{\partial v_k}{\partial x_k} = 0 \quad , \quad \varrho\dot{\varepsilon} + \frac{\partial q_k}{\partial x_k} = -p_{kl}\frac{\partial v_k}{\partial x_l}. \tag{16}$$

In (15) all time derivatives of the macroscopic velocity v_i were eliminated by means of the balance of momentum,

$$\varrho\dot{v}_i - \frac{\partial p_{ik}}{\partial x_k} = 0, \tag{17}$$

which has therefore to replace equation $(15)_2$ with $n = 0$.

5.2 Closure Problem

The set of moment equations (15) is not a system of field equations for the moments (14) because it contains additional moments, such as $u^{2n}_{\langle ij\rangle k}$, $u^{2n}_{\langle ij\rangle kl}$, $u^{2n+\alpha}$, $u_i^{2n+\alpha}$, $u^{2n+\alpha}_{\langle ij\rangle}$. Constitutive equations are needed for these additional quantities. The Grad method proceeds on the assumption that the phase density is a function of the moments (14); thus the constitutive equations will be of the form

$$u^{2n}_{\langle ij\rangle k}, u^{2n}_{\langle ij\rangle kl}, u^{2n+\alpha}, u_i^{2n+\alpha}, u^{2n+\alpha}_{\langle ij\rangle}, \ldots = \mathcal{F}\left(u^{2n}, u_i^{2n}, u^{2n}_{\langle ij\rangle}; n = 0, 1 \ldots N\right). \tag{18}$$

The phase density is assumed to be a power series of C_i of the following form

$$f = f_M \left(1 + \sum_{k=0}^{N} \lambda^k C^{2k} + \sum_{k=0}^{N} \lambda_i^k C^{2k} C_i + \sum_{k=0}^{N} \lambda^k_{\langle ij\rangle} C^{2k} C_i C_j\right). \tag{19}$$

The coefficients $\lambda^k, \lambda_i^k, \lambda^k_{\langle ij\rangle}$ follow from the requirements (14):

$$\lambda^k = \frac{\sqrt{\pi}}{2\varrho} \sum_{n=2}^{N} \mathcal{A}^{-1}_{kn} \left(\frac{m}{2kT}\right)^{n+k} \Delta^{2n}, \text{ with } \mathcal{A}_{kn} = \Gamma\left(n + k + \frac{3}{2}\right);$$

$$\lambda_i^k = \frac{3\sqrt{\pi}}{2\varrho} \sum_{n=1}^{N} \mathcal{B}^{-1}_{kn} \left(\frac{m}{2kT}\right)^{n+k+1} u_i^{2n}, \text{ with } \mathcal{B}_{kn} = \Gamma\left(n + k + \frac{5}{2}\right); \tag{20}$$

$$\lambda^k_{\langle ij\rangle} = \frac{15\sqrt{\pi}}{4\varrho} \sum_{n=0}^{N} \mathcal{C}^{-1}_{kn} \left(\frac{m}{2kT}\right)^{n+k+2} u^{2n}_{\langle ij\rangle}, \text{ with } \mathcal{C}_{kn} = \Gamma\left(n + k + \frac{7}{2}\right).$$

With (19, 20) we are able to compute all constitutive equations (18). Especially we obtain

$$\Delta^p = \sum_{\substack{k=0\\n=2}}^{N} \Gamma\left(\frac{p}{2} + k + \frac{3}{2}\right) \mathcal{A}^{-1}_{kn} \left(\frac{m}{2kT}\right)^{n-\frac{p}{2}} \Delta^{2n},$$

$$u_i^p = \sum_{\substack{k=0\\n=1}}^{N} \Gamma\left(\frac{p}{2} + k + \frac{5}{2}\right) \mathcal{B}^{-1}_{kn} \left(\frac{m}{2kT}\right)^{n-\frac{p}{2}} u_i^{2n}, \tag{21}$$

$$u^p_{\langle ij\rangle} = \sum_{k,n=0}^{N} \Gamma\left(\frac{p}{2} + k + \frac{7}{2}\right) \mathcal{C}^{-1}_{kn} \left(\frac{m}{2kT}\right)^{n-\frac{p}{2}} u^{2n}_{\langle ij\rangle}.$$

5.3 Maxwellian iteration

We do not want to set up the complete system of moment equations. Rather we proceed by an simple iteration procedure, known as Maxwellian iteration [7, 6].

The first step is to introduce the equilibrium values of the moments (calculated by Maxwell's phase density f_M) on the lefthand side of the moment equations. The moment equations thus reduce to the Euler equations (12) and

$$
\begin{aligned}
&n\left(\ln\frac{T}{\varrho^{\frac{2}{3}}}\right)^{\bullet} u_{|E}^{2n} = 0 = -\zeta\left(\Delta^{2n+\alpha} - \Delta_{|\gamma}^{2n+\alpha}\right) &, \qquad & n = 2,3,\dots,N \\
&\frac{n}{3}u_{|E}^{2n+2}\frac{1}{T}\frac{\partial T}{\partial x_i} = -\zeta\left(u_i^{2n+\alpha} - u_{i|\gamma}^{2n+\alpha}\right) &, \qquad & n = 1,2,\dots,N \qquad (22) \\
&2\frac{2n+5}{15}u_{|E}^{2n+2}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\zeta u_{\langle ij\rangle}^{2n+\alpha} &, \qquad & n = 0,1,\dots,N
\end{aligned}
$$

Now we introduce (21, 11) in the right-hand sides of (22). This gives $3N$ linear equations for the non-conserved moments u^{2n}, $n = 2,3,\dots,N$; u_i^{2n}, $n = 1,2,\dots,N$; $u_{\langle ij\rangle}^{2n+\alpha}$, $n = 0,1,\dots,N$. We obtain

$$
\begin{aligned}
\Delta^{2s} &= u^{2s} - u_{|E}^{2s} = 0, \\
u_i^{2s} &= -\frac{k}{m}\frac{\varrho}{\zeta}\left(\frac{2kT}{m}\right)^{s-\frac{\alpha}{2}}\sum_{n=1}^{N}\theta_{sn}^{-1}n\frac{\Gamma\left(n+\frac{5}{2}\right)}{\Gamma\left(\frac{5}{2}\right)}\frac{\partial T}{\partial x_i}, \qquad (23) \\
u_{\langle ij\rangle}^{2s} &= -\frac{\varrho}{\zeta}\left(\frac{2kT}{m}\right)^{s+1-\frac{\alpha}{2}}\sum_{n=0}^{N}\vartheta_{sn}^{-1}\frac{\Gamma\left(n+\frac{7}{2}\right)}{\Gamma\left(\frac{7}{2}\right)}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}},
\end{aligned}
$$

with the matrices

$$
\theta_{nr} = \sum_{k=0}^{N}\left(\Gamma\left(n+k+\frac{\alpha+5}{2}\right) - \frac{\Gamma\left(n+\frac{\alpha+5}{2}\right)\Gamma\left(k+\frac{5+\alpha}{2}\right)}{\Gamma\left(\frac{\alpha+5}{2}\right)}\right)\mathcal{B}_{kr}^{-1},
$$

$$
\vartheta_{nr} = \sum_{k=0}^{N}\Gamma\left(n+k+\frac{\alpha+7}{2}\right)\mathcal{C}_{kn}^{-1}.
$$

With the computation of the moments the first step of the Maxwellian iteration is finished. The next step of the iteration is to insert the moments (23) on the left hand side of the moment equations (15) and to solve for the moments on the right hand side again.

We stop the iteration with the first step and calculate those moments wich have a physical interpretation, namely $q_i = \frac{1}{2}u_i^2$ and $p_{\langle ij\rangle} = u_{\langle ij\rangle}^0$. Again we find the laws of Fourier and Navier-Stokes,

$$
2q_i = \underbrace{-\frac{k}{m}\frac{\varrho}{\zeta}\left(\frac{2kT}{m}\right)^{1-\frac{\alpha}{2}}\sum_{n}^{N}\theta_{1n}^{-1}n\frac{\Gamma\left(n+\frac{5}{2}\right)}{\Gamma\left(\frac{5}{2}\right)}}_{2\kappa}\frac{\partial T}{\partial x_i},
$$

$$
p_{\langle ij\rangle} = \underbrace{-\frac{\varrho}{\zeta}\left(\frac{2kT}{m}\right)^{1-\frac{\alpha}{2}}\sum_{n}^{N}\vartheta_{0n}^{-1}\frac{\Gamma\left(n+\frac{7}{2}\right)}{\Gamma\left(\frac{7}{2}\right)}}_{2\mu}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}.
$$

Now thermal conductivity and viscosity do not only depend on the exponent α in the collision frequency ν but also on the number N of moments. For the Prandtl number we find

$$Pr = \frac{\kappa}{\mu} = \frac{15}{4}\frac{k}{m}\frac{2}{3}\frac{\sum_n^N \theta_{1n}^{-1} n\Gamma\left(n+\frac{5}{2}\right)}{\sum_n^N \vartheta_{0n}^{-1}\Gamma\left(n+\frac{7}{2}\right)} \tag{24}$$

5.4 Comparison with Chapman-Enskog method

The main difference between the two methods - Grad and Chapman-Enskog - is, that in the latter one equilibrium values are inserted on the left hand side of the BGK equation first and afterwards the moments are calculated. In the Grad method one first calculates the moment equations and inserts equilibrium afterwards.

The ratio of the Prandtl numbers (13, 24) gives

$$F\left(\alpha,N\right) = 2\frac{5-\alpha}{10-2\alpha+\alpha^2}\frac{\sum_n^N \theta_{1n}^{-1} n\Gamma\left(n+\frac{5}{2}\right)}{\sum_n^N \vartheta_{0n}^{-1}\Gamma\left(n+\frac{7}{2}\right)}.$$

In the case $\alpha = 0$ we have $F\left(0,N\right) = 1$ for all N and the Prandtl numbers obtained from the Chapman-Enskog and the Grad methods agree.

If $\alpha \neq 0$ holds, the Grad method gives the same result as the Chapman-Enskog method only when the number N is sufficiently big.

Figure 1 shows $F\left(\alpha = 1, N\right)$; F increases with increasing N and reaches the value $F = 1$ for $N = 11$. Figure 2 shows $F\left(\alpha = 1.79129, N\right)$. Here, the convergence towards the value $F = 1$ is slower then in the case $\alpha = 1$. For $N = 11$ we find only $F \simeq 0.96$[1]. We expect that F will tend to 1 with increasing N. An agreement between both methods is only possible if in the Grad

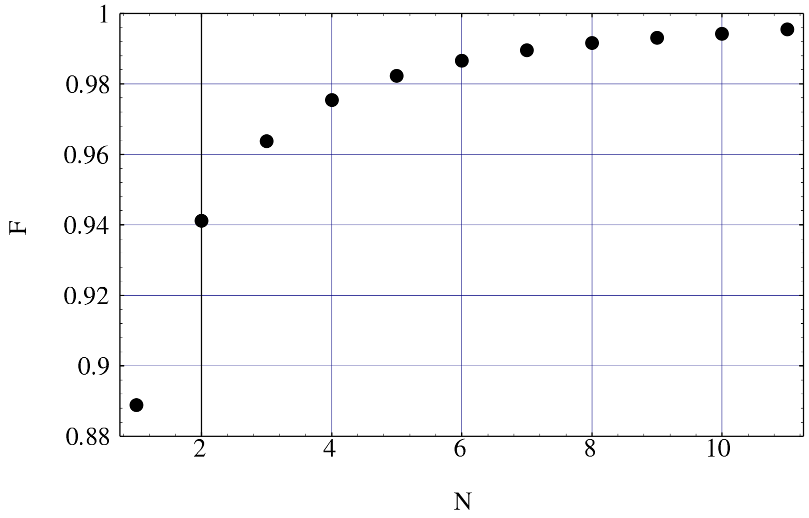

Figure 1: $F\left(\alpha,N\right)$ *for* $\alpha = 1$ *as a function of the number of moments* N.

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[1] Due to accuracy problems in the numerical inversion of the matrices, we cannot present results with $N > 11$.

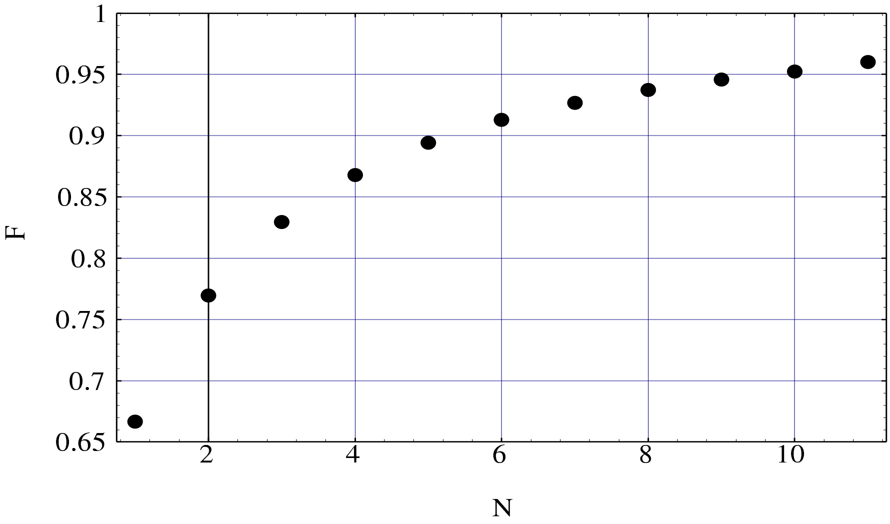

Figure 2: $F(\alpha, N)$ *for* $\alpha = 1.79129$ *as a function of the number of moments* N.

method a large number N of moments is taken into account. Grad's well known 13 moment distribution [6],

$$f = f_M\left(1 + \frac{p_{\langle ij\rangle}}{\varrho}\left(\frac{m}{kT}\right)^2 C_{\langle i}C_{j\rangle} - \frac{q_i}{\varrho}\left(\frac{m}{kT}\right)^2 C_i\left(1 - \frac{1}{5}\frac{m}{kT}C^2\right)\right)$$

gives $Pr = \frac{5}{2}\frac{k}{m}$ for all values of α.

Appendix A: Motivation of BGK equation

For motivation of the BGK equation we simplify the Boltzmann collision term in three steps [5].

Step 1: Because of the collisions the phase density will tend to a phase density f_γ for which the Boltzmann collision term vanishes. Thus $\ln f_\gamma$ must be a linear combination of the collisional invariants $m, mc_i, \frac{m}{2}c^2$,

$$f_\gamma = a\exp\left(-\Gamma c^2 + \gamma_i c_i\right). \tag{25}$$

The phase densities $f'f'^1$ in the collision term (3) refer to the velocities after the collision - they may be replaced by $f'_\gamma f'^1_\gamma$,

$$\mathcal{S} \to \widehat{\mathcal{S}}_\gamma = \int \left(f'_\gamma f'^1_\gamma - ff^1\right)\sigma g \sin\theta d\theta d\varepsilon d\mathbf{c}_1$$

Step 2: Since $\ln f_\gamma$ is a linear combination of the collisional invariants we may replace $f'_\gamma f'^1_\gamma$ by $f_\gamma f^1_\gamma$,

$$\widehat{\mathcal{S}}_\gamma \to \widetilde{\mathcal{S}}_\gamma = f_\gamma \int f^1_\gamma \sigma g \sin\theta d\theta d\varepsilon d\mathbf{c}_1 - f\int f^1 \sigma g \sin\theta d\theta d\varepsilon d\mathbf{c}_1$$

Step 3: The difference between the two integrals may be neglected. This last step leads to the BGK collision term (8)

$$\widetilde{\mathcal{S}}_\gamma \to \mathcal{S}_\gamma = -\nu\left(f - f_\gamma\right)$$

and we are able to identify the collision frequency as

$$\nu\left(x_i,t,C_i\right)=\int f_\gamma^1\sigma g\sin\theta d\theta d\varepsilon d\mathbf{c}_1. \qquad (A.1)$$

Since σ and g depend on C this is true also for ν. This function is evaluated for the case of hard spheres and equilibrium in [3]. One should not rely on (A.1) as the exact value for ν because all the assumptions will lead to errors. It is possible, however, to choose the function ν so as to fit thermal conductivity and viscosity (or Prandtl number) to measurements.

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