Differential Equations and Boundary Conditions for Higher Gas Kinetic Moments. Heat Transfer Between Parallel Plates

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Transport-relaxation equations for seventeen moments are derived from the linearized Boltzmann equation for a monatomic gas. Besides the well-known thirteen moments (i. e. density n, temperature T, velocity $\boldsymbol{v}$, heat flux $\boldsymbol{q}$, friction pressure tensor $\overline{\mathsf{p}}$), one additional scalar A and one additional vector $\boldsymbol{A}$ are taken into account. In steady state, differential equations for T, $\boldsymbol{v}$, A and constitutive laws for $\boldsymbol{q}$, $\overline{\mathsf{p}}$, $\boldsymbol{A}$ follow from the transport-relaxation equations. Boundary conditions for T, $\boldsymbol{v}$, A are obtained by the thermodynamical method from the interfacial entropy production. The role of the higher moments A and $\boldsymbol{A}$ for heat transfer in a gas between parallel plates is discussed. The heat flux has the correct low pressure limit. Due to the presence of A and $\boldsymbol{A}$, exponential terms occur in the temperature profile near the boundary.

Approximate solutions of the linearized Boltzmann equation for a monatomic gas can be obtained by regarding a certain number of physically relevant quantities or moments. In the thirteen moments approximation [1] one takes into account the density, the temperature, the flow velocity, the heat flux and the friction pressure tensor. More generally, the Boltzmann equation is replaced by an arbitrarily large system of coupled linear differential equations, the transport-relaxation equations [2]. In steady state, linear partial differential equations ensue for some moments, like the temperature and the velocity vector, whereas for other moments constitutive laws are at hand, e. g. for the heat flux and the friction pressure tensor. The boundary conditions required for the solution of the differential equations can be derived by a thermodynamical method from the entropy production at the interface between the gas and a solid [3–9]. The treatment of special cases like thermal transpiration and thermal force with thirteen moments and suitable surface currents gives satisfactory results in a large pressure range from the hydrodynamical to the Knudsen regime [10].

In this paper, the role of higher moments which are usually neglected, will be studied for the heat transfer in a gas between parallel plates. A seventeen moments description is displayed, with one scalar A and one vector $\boldsymbol{A}$ in addition to the thirteen moments. The moment equations are given in the first section, in the second section they are specialized for the steady state. Differential equations are obtained for the velocity $\boldsymbol{v}$, the temperature T and the scalar A, and constitutive laws for the friction pressure tensor $\overline{\mathsf{p}}$, the heat flux $\boldsymbol{q}$ and the vector $\boldsymbol{A}$. By elimination of A one can get a fourth order equation for T and an ansatz for $\boldsymbol{q}$ which is different from the fourth order Chapman-Enskog expression.

Furthermore, boundary conditions are derived from the interfacial entropy production: Besides the velocity slip and the temperature jump conditions, there is also a boundary condition for the scalar A.

As an application of the general equations, the heat transfer in a rarefied gas between infinite parallel plates is studied. As in the old temperature-jump approximation, the heat flux has the correct limit for low pressures (Knudsen regime). In the bulk of the gas the temperature is linear in the x-coordinate, but close to the walls contributions exponential in x occur as a consequence of the higher moments A and $\boldsymbol{A}$. Due to the second law requirements for the surface coefficients, the value of the bulk temperature extrapolated linearly to the wall is always smaller (larger) than the actual temperature of the hot (cold) plate.

1. Moment Equations

A dilute monatomic gas is described by the one-particle distribution function $f(t, \boldsymbol{x}, \boldsymbol{c})$. For small relative deviations Φ of

$$f = f^{(0)}\,(1 + \Phi) \tag{1.1}$$

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from the equilibrium distribution

$$f^{(0)}(c) = n_0 \left(\frac{m}{2\pi k_B T_0} \right)^{3/2} \exp\left\{ - \frac{m c^2}{2 k_B T_0} \right\}, \qquad (1.2)$$

the linearized Boltzmann equation applies

$$\partial \Phi / \partial t + \boldsymbol{c} \cdot \boldsymbol{\nabla} \Phi + \omega(\Phi) = 0, \qquad (1.3)$$

where ω denotes the linearized collision operator. In Eq. (1.2), n_0, T_0 are the equilibrium values of number density and temperature, k_B is Boltzmann's constant, m and $\boldsymbol{c}$ are the particle mass and velocity.

In the moment method approach [2] for the solution of the linearized Boltzmann equation (1.3), the function Φ is expanded into a complete set of tensors in velocity space, so that the expansion coefficients, the "moments", depend on time t and position $\boldsymbol{x}$:

$$\Phi(t, \boldsymbol{x}, \boldsymbol{c}) = \sum_{l=0}^{\infty} \sum_{r=0}^{\infty} a^{(r)}_{\mu_1 \dots \mu_l}(t, \boldsymbol{x})\, \Phi^{(r)}_{\mu_1 \dots \mu_l}(\boldsymbol{c}) . \qquad (1.4)$$

With the normalization [2]

$$\langle \Phi^{(r)}_{\mu_1 \dots \mu_l} \Phi^{(r')}_{\mu_1' \dots \mu_{l'}'} \rangle_0 = \delta^{rr'} \delta_{ll'} \Delta^{(l)}_{\mu_1 \dots \mu_l, \mu_1' \dots \mu_{l'}'}, \qquad (1.5)$$

the moments are given by

$$a^{(r)}_{\mu_1 \dots \mu_l} = \langle \Phi^{(r)}_{\mu_1 \dots \mu_l} \rangle - \langle \Phi^{(r)}_{\mu_1 \dots \mu_l} \rangle_0 ;$$

for $\Phi^{(0)} = 1$ this gives in detail:

$$a^{(0)} = (n - n_0)/n_0, \qquad (1.6)$$

$$a^{(r)}_{\mu_1 \dots \mu_l} = \langle \Phi^{(r)}_{\mu_1 \dots \mu_l} \rangle, \quad (l, r) \neq (0, 0) .$$

The bracket $\langle \dots \rangle$ denotes the nonequilibrium integral, e. g.

$$\langle \Phi^{(r)}_{\mu_1 \dots \mu_l} \rangle = (1/n_0) \int f\, \Phi^{(r)}_{\mu_1 \dots \mu_l}\, d^3 c ;$$

similarly, $\langle \dots \rangle_0$ stands for the equilibrium integral taken with $f^{(0)}$ instead of f.

The quantity $\Phi^{(r)}_{\mu_1 \dots \mu_l}$ is a symmetric traceless tensor of rank l, multiplied with a Sonine-polynomial [11, 12] of degree r in c^2. In terms of the dimensionless velocity

$$\boldsymbol{W} \equiv \boldsymbol{c}\, (m/2 k_B T_0)^{1/2}$$

one has

$$\Phi^{(r)}_{\mu_1 \dots \mu_l} \qquad (1.7)$$
$$= \left[\frac{r!\,(2l+1)!!\, \frac{1}{2} \sqrt{\pi}}{l!\, \Gamma(l + r + \frac{3}{2})} \right]^{1/2} S^{(r)}_{l+\frac{1}{2}}(W^2)\, \overline{W_{\mu_1} \dots W_{\mu_l}} .$$

For practical use, the summations in the expansion (1.4) are extended over a small finite number of tensors. The moments corresponding to the most simple ones of these tensors are related to physical quantities, viz. to the "thirteen" moments density n, temperature T, flow velocity $\boldsymbol{v}$, heat flux $\boldsymbol{q}$, and friction pressure tensor $\overline{\mathbf{p}}$. In order to study the effect of "higher moments" on heat conduction, one additional scalar A and one more vector $\boldsymbol{A}$ are taken into account, i. e. we use a "seventeen" moments description with three scalars, three vectors and one symmetric traceless second rank tensor *:

$$\Phi^{(0)} = 1 \qquad a^{(0)} = (n - n_0)/n_0 \qquad \text{(a)}$$

$$\Phi^{(1)} = \sqrt{\tfrac{2}{3}} (\tfrac{3}{2} - W^2) \qquad a^{(1)} = -\sqrt{\tfrac{3}{2}} (T - T_0)/T_0 \qquad \text{(b)}$$

$$\Phi^{(2)} = \sqrt{\tfrac{2}{15}} (\tfrac{15}{4} - 5 W^2 + W^4) \qquad \text{(c)}$$
$$a^{(2)} = \sqrt{\tfrac{15}{8}} A/T_0$$

$$\boldsymbol{\Phi}^{(0)} = \sqrt{2}\, \boldsymbol{W} \qquad \boldsymbol{a}^{(0)} = \boldsymbol{v}/c_0 \qquad \text{(d)}$$

$$\boldsymbol{\Phi}^{(1)} = \sqrt{\tfrac{4}{5}} (\tfrac{5}{2} - W^2)\, \boldsymbol{W} \qquad \text{(e)}$$
$$\boldsymbol{a}^{(1)} = -\sqrt{\tfrac{2}{5}}\, \boldsymbol{q}/P_0 c_0 \qquad (1.8)$$

$$\boldsymbol{\Phi}^{(2)} = \sqrt{\tfrac{4}{35}} (\tfrac{35}{4} - 7 W^2 + W^4)\, \boldsymbol{W} \qquad \text{(f)}$$
$$\boldsymbol{a}^{(2)} = \sqrt{\tfrac{8}{35}}\, \boldsymbol{A}/P_0 c_0$$

$$\mathbf{\Phi}^{(0)} = \sqrt{2}\, \overline{\mathbf{W}\,\mathbf{W}} \qquad \mathbf{a}^{(0)} = \overline{\mathbf{p}}/P_0 \sqrt{2} . \qquad \text{(g)}$$

New in comparison with the "thirteen" moments description are $\Phi^{(2)}$ and $\boldsymbol{\Phi}^{(2)}$. The abbreviations $P_0 = n_0 k_B T_0$ and

$$c_0 = (k_B T_0/m)^{1/2}$$

have been used. By insertion of this expansion for Φ into the linearized Boltzmann equation (1.3), the following set of transport-relaxation equations for the moments $a^{(0)}, \dots, \mathbf{a}^{(0)}$ is obtained:

$$\frac{\partial}{\partial t} a^{(0)} + c_0 \boldsymbol{\nabla} \cdot \boldsymbol{a}^{(0)} = 0 \qquad \text{(a)}$$

$$\frac{\partial}{\partial t} a^{(1)} + c_0 \boldsymbol{\nabla} \cdot \left(-\sqrt{\tfrac{2}{3}}\, \boldsymbol{a}^{(0)} + \sqrt{\tfrac{5}{3}}\, \boldsymbol{a}^{(1)} \right) = 0 \qquad \text{(b)}$$

$$\frac{\partial}{\partial t} a^{(2)} + c_0 \boldsymbol{\nabla} \cdot \left(-\sqrt{\tfrac{4}{3}}\, \boldsymbol{a}^{(1)} + \sqrt{\tfrac{7}{3}}\, \boldsymbol{a}^{(2)} \right) + \omega_0(22)\, a^{(2)} = 0 \qquad \text{(c)}$$

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* The numerical factors with A and $\boldsymbol{A}$, arbitrary to some extent, are chosen in such a way that in Eqs. (2.14), (2.15) no additional factors occur.

$$\frac{\partial}{\partial t}\boldsymbol{a}^{(0)} + c_0 \nabla (a^{(0)} - \sqrt{\tfrac{2}{3}}\, a^{(1)}) + c_0 \sqrt{2}\, \nabla \cdot \mathbf{a}^{(0)} = 0 \tag{d}$$

$$(1.9)$$

$$\frac{\partial}{\partial t}\boldsymbol{a}^{(1)} + c_0 \nabla (\sqrt{\tfrac{5}{3}}\, a^{(1)} - \sqrt{\tfrac{4}{3}}\, a^{(2)}) - c_0 \sqrt{\tfrac{4}{5}}\, \nabla \cdot \mathbf{a}^{(0)} + \sum_{r=1}^{2} \omega_1(1\, r)\, \boldsymbol{a}^{(r)} = 0 \tag{e}$$

$$\frac{\partial}{\partial t}\boldsymbol{a}^{(2)} + c_0 \nabla \sqrt{\tfrac{7}{3}}\, a^{(2)} + \sum_{r=1}^{2} \omega_1(2\, r)\, \boldsymbol{a}^{(r)} = 0 \tag{f}$$

$$\frac{\partial}{\partial t}\mathbf{a}^{(0)} + c_0 (\sqrt{2}\, \overline{\nabla \boldsymbol{a}}^{(0)} - \sqrt{\tfrac{4}{5}}\, \overline{\nabla \boldsymbol{a}}^{(1)}) + \omega_2(00)\, \mathbf{a}^{(0)} = 0\,. \tag{g}$$

The relaxation constants $\omega_l(r\, r')$ are matrix elements of the linearized collision operator ω:

$$\omega_l(r\, r') = \frac{1}{2l+1} \langle \Phi^{(r)}_{\mu_1 \ldots \mu_l}\, \omega\, (\Phi^{(r')}_{\mu_1 \ldots \mu_l}) \rangle_0\,; \tag{1.10}$$

the matrix $\omega_l(r\, r')$ is symmetric and positive definite [2, 12]. By introducing center of mass and relative velocities in the collision integral, one can easily prove the relations

$$\omega_0(22) = \omega_1(11) = \tfrac{2}{3}\, \omega_2(00)\,. \tag{1.11}$$

Accordingly, the Eqs. (1.9) contain only three independent relaxation constants, viz. $\omega_1(11)$, $\omega_1(12)$ and $\omega_1(22)$, which are expressed by Chapman-Cowling Ω-integrals [11] in the following way:

$$\omega_1(11) = n_0 \frac{16}{15}\, \Omega^{(2,2)}\,, \tag{1.12}$$

$$\omega_1(12) = \omega_1(21) = n_0 \frac{16}{15} \frac{1}{\sqrt{7}} \left(\frac{7}{2}\, \Omega^{(2,2)} - \Omega^{(2,3)} \right),$$

$$\omega_1(22) = n_0 \frac{16}{105} \left(\frac{77}{4}\, \Omega^{(2,2)} - 7\, \Omega^{(2,3)} + \Omega^{(2,4)} \right).$$

In particular, for Maxwell molecules the result is [12]

$$\omega_1(12) = 0\,, \quad \omega_1(22) = 1.5\, \omega_1(11)\,, \tag{1.13 a}$$

and for hard spheres of diameter σ

$$\omega_1(11) = \frac{8}{15}\, \omega_0\,, \quad \omega_1(12) = -\frac{4}{15} \frac{1}{\sqrt{7}}\, \omega_0\,,$$

$$\omega_1(22) = \frac{6}{7}\, \omega_0 = 1.61\, \omega_1(11)\,. \tag{1.13 b}$$

where ω_0 is an abbreviation for

$$\omega_0 = 4\, n_0\, c_0 \sqrt{\pi}\, \sigma^2\,.$$

The conservation equations for the particle density (1.9 a), energy density (1.9 b) and momentum density (1.9 d) of course do not contain relaxation terms. Linearization of the equation of state, $p = n\, k_B\, T$, leads to

$$a^{(0)} - \sqrt{\frac{2}{3}}\, a^{(1)} = \frac{p - P_0}{P_0}\,.$$

If the total pressure tensor, $\mathbf{p} = p\boldsymbol{\delta} + \bar{\mathbf{p}}$, is introduced, Eqs. (1.9 a, b, d) take the familiar form [12]:

$$\begin{aligned} \frac{\partial n}{\partial t} + \nabla \cdot \boldsymbol{v} &= 0\,, \\ \frac{3}{2}\, n_0\, k_B \frac{\partial T}{\partial t} + \nabla \cdot (P_0 \boldsymbol{v} + \boldsymbol{q}) &= 0\,, \\ n_0\, m \frac{\partial}{\partial t} \boldsymbol{v} + \nabla \cdot \mathbf{p} &= 0\,. \end{aligned} \tag{1.14}$$

2. The Steady State

The stationary transport-relaxation equations (1.9) lead to second order spatial differential equations for T, A, $\boldsymbol{v}$ (i. e. $a^{(1)}$, $a^{(2)}$, $\boldsymbol{a}^{(0)}$), and to constitutive laws for $\boldsymbol{q}$, $\boldsymbol{A}$, $\bar{\mathbf{p}}$ (i. e. $\boldsymbol{a}^{(1)}$, $\boldsymbol{a}^{(2)}$, $\mathbf{a}^{(0)}$).

The scalar equations (1.9 a, b, c) reduce to

$$\nabla \cdot \boldsymbol{a}^{(r)} = -\,\delta_{r2} \frac{\omega_0(22)}{c_0} \sqrt{\frac{3}{7}}\, a^{(2)}\,, \quad r = 0, 1, 2\,,$$

i. e. in detail

$$\nabla \cdot \boldsymbol{v} = 0\,, \tag{2.1}$$

$$\nabla \cdot \boldsymbol{q} = 0\,, \tag{2.2}$$

$$\nabla \cdot \boldsymbol{A} = -\frac{15}{8} \frac{P_0}{T_0}\, \omega_0(22)\, A\,. \tag{2.3}$$

Taking the second derivative $\nabla\nabla:$ of Eq. (1.9 g), the first derivative $\nabla\cdot$ of Eq. (1.9 d) and employing also Eqs. (1.9 a, b), we find

$$\nabla \cdot (\nabla \cdot \mathbf{a}^{(0)}) = 0\,, \quad \Delta (a^{(0)} - \sqrt{\tfrac{2}{3}}\, a^{(1)}) = 0\,,$$

or

$$\Delta p = 0\,. \tag{2.4}$$

A differential equation for $a^{(2)}$ is obtained by applying the operator $\nabla\cdot$ to Eq. (1.9 f),

$$c_0 \sqrt{\tfrac{7}{3}}\, \Delta a^{(2)} - \omega_1(22)\, \omega_0(22) \sqrt{\tfrac{3}{7}}\, c_0^{-1}\, a^{(2)} = 0\,,$$

which gives

$$A - L^2 \Delta A = 0\,, \tag{2.5}$$

with

$$L^2 = \frac{7}{3} \frac{c_0^2}{\omega_0(22)\, \omega_1(22)} > 0\,. \tag{2.6 a}$$

In terms of the "viscosity free path" l_η,

$$l_\eta = c_0/\omega_2(00) \, ,$$

the length L is given by

$$L = \sqrt{\tfrac{7}{2}}\, l_\eta = 1.87\, l_\eta \quad \text{for Maxwell molecules,} \qquad (2.6\,\text{b})$$

and

$$L = 1.81\, l_\eta \qquad \text{for hard spheres.} \qquad (2.6\,\text{c})$$

Similarly, a differential equation for $a^{(1)}$ is obtained by taking $\boldsymbol{\nabla} \cdot$ (1.9 e) and using Eq. (2.3):

$$\Delta[T + (1+\varepsilon) A] = 0 \, . \qquad (2.7)$$

Here, ε is an abbreviation for the ratio

$$\varepsilon = \sqrt{\frac{7}{4} \frac{\omega_1(12)}{\omega_1(22)}} \, , \qquad (2.8\,\text{a})$$

with

$$\varepsilon = 0 \qquad (2.8\,\text{b})$$

for Maxwell molecules, and

$$\varepsilon = -7/45 = -0.156 \qquad (2.8\,\text{c})$$

for hard spheres.

With the help of Eqs. (2.5), (2.7) the scalar A can be expressed by ΔT:

$$A = -L^2 (1+\varepsilon)^{-1} \Delta T \, ; \qquad (2.9\,\text{a})$$

hence Eq. (2.7) leads to a fourth order equation for T,

$$\Delta T - L^2 \Delta^2 T = 0 \, . \qquad (2.9\,\text{b})$$

Finally, a differential equation for the velocity $\boldsymbol{v}$ is obtained from the steady state momentum equation (1.9 d) or (1.14)

$$\boldsymbol{\nabla} p + \boldsymbol{\nabla} \cdot \overline{\mathbf{p}} = 0 \, , \qquad (2.10)$$

by insertion of the constitutive law (1.9 g) for the friction pressure tensor

$$\overline{\mathbf{p}} = -2\eta [\overline{\boldsymbol{\nabla} \boldsymbol{v}} + \tfrac{2}{5} P_0{}^{-1} \overline{\boldsymbol{\nabla} \boldsymbol{q}}] \, , \qquad (2.11)$$

viz.

$$\boldsymbol{\nabla} p = \eta [\Delta \boldsymbol{v} + \tfrac{2}{5} P_0{}^{-1} \Delta \boldsymbol{q}] \, . \qquad (2.12)$$

The shear viscosity η is determined by the relaxation constant for $\overline{\mathbf{p}}$:

$$\eta = P_0/\omega_2(00) > 0 \, . \qquad (2.13)$$

With the help of Eqs. (2.10) and (1.9 e), (1.9 f), the vectors $\boldsymbol{q}$ and $\boldsymbol{A}$ can be expressed by gradients of p, T and A:

$$\boldsymbol{q} = -\lambda \left[\boldsymbol{\nabla} T + (1+\varepsilon) \boldsymbol{\nabla} A - \frac{2}{5} \frac{T_0}{P_0} \boldsymbol{\nabla} p \right] , \qquad (2.14)$$

$$\boldsymbol{A} = \varepsilon \boldsymbol{q} - \lambda' \boldsymbol{\nabla} A \, . \qquad (2.15)$$

If the scalar A is replaced by ΔT via Eq. (2.9 a), an alternative formulation of Eqs. (2.14), (2.15) is obtained:

$$\boldsymbol{q} = -\lambda \left[\boldsymbol{\nabla} T - \frac{2}{5} \frac{T_0}{P_0} \boldsymbol{\nabla} p - L^2 \boldsymbol{\nabla} \Delta T \right] , \qquad (2.14\,\text{a})$$

$$\boldsymbol{A} = \varepsilon \boldsymbol{q} + \lambda' (1+\varepsilon)^{-1} L^2 \boldsymbol{\nabla} \Delta T \, . \qquad (2.15\,\text{a})$$

As a consequence of the constitutive law (2.14) for $\boldsymbol{q}$ and of Eqs. (2.4), (2.7) we note

$$\Delta \boldsymbol{q} = 0 \, .$$

Hence, Eq. (2.12) reduces to the well-known Navier-Stokes equation for an incompressible fluid:

$$\boldsymbol{\nabla} p = \eta \Delta \boldsymbol{v} \, . \qquad (2.16)$$

The thermal conductivity λ and the quantity λ' occurring in Eqs. (2.14), (2.15) are given by

$$\lambda = \frac{5}{2} P_0 \frac{k_\text{B}}{m} [\omega_1(11) - \omega_1(12)^2/\omega_2(22)]^{-1} > 0 \, , \qquad (2.17)$$

$$\lambda' = \frac{35}{8} P_0 \frac{k_\text{B}}{m} \frac{1}{\omega_1(22)} > 0 \, . \qquad (2.18\,\text{a})$$

In the case of Maxwell molecules one has

$$\lambda = \frac{5}{2} P_0 \frac{k_\text{B}}{m} \frac{1}{\omega_1(11)} \, , \quad \frac{\lambda'}{\lambda} = \frac{7}{6} = 1.167 \, . \qquad (2.18\,\text{b})$$

For other models of the intermolecular potential, this simple expression for λ is only valid in the thirteen moments approximation. With additional vectors (besides $\boldsymbol{v}$ and $\boldsymbol{q}$), the theoretical value for λ is more complicated than the one in Eq. (2.18 b); e. g. in our seventeen moments approximation (with the vectors $\boldsymbol{v}$, $\boldsymbol{q}$ and $\boldsymbol{A}$) of Eq. (2.17) the correction factor

$$[1 - \omega_1(12)^2/\omega_1(11)\, \omega_1(22)]^{-1}$$

occurs, which is equal to $45/44 = 1.023$ in the case of hard spheres. The hard sphere value for λ'/λ is

$$\lambda'/\lambda = 1.065 \, . \qquad (2.18\,\text{c})$$

Now, the constitutive laws for $\overline{\mathbf{p}}$ and $\boldsymbol{q}$ are rewritten so that only derivatives of T, p and $\boldsymbol{v}$ occur. First, Eq. (2.14 a) for $\boldsymbol{q}$ is inserted into Eq. (2.11):

$$\overline{\mathbf{p}} = -2\eta [\overline{\boldsymbol{\nabla} \boldsymbol{v}} - \tfrac{2}{5} P_0{}^{-1} \lambda\, \overline{\boldsymbol{\nabla} \boldsymbol{\nabla}} T + \tfrac{4}{25} T_0 P_0{}^{-2} \lambda\, \overline{\boldsymbol{\nabla} \boldsymbol{\nabla}} p + \tfrac{2}{5} P_0{}^{-1} \lambda L^2 \overline{\boldsymbol{\nabla} \boldsymbol{\nabla}} \Delta T] \, . \qquad (2.19\,\text{a})$$

Then the pressure gradient is eliminated from Eq. (2.14 a) with the help of the Navier-Stokes equation (2.16):

$$\boldsymbol{q} = -\lambda [\boldsymbol{\nabla} T - \tfrac{2}{5} T_0 P_0{}^{-1} \eta \Delta \boldsymbol{v} - L^2 \boldsymbol{\nabla} \Delta T] \, . \qquad (2.19\,\text{b})$$

These are the results of the moment method.

They can be compared with the Chapman-Enskog approximations for $\overline{\mathbf{p}}$ and $\boldsymbol{q}$ which are obtained successively according to the order of the derivatives [11]: the r-th approximation contains derivatives of T, p, $\boldsymbol{v}$ up to the order $r-1$. In fourth order one gets:

$$\overline{\mathbf{p}}_{\mathrm{CE}} = -2\,\eta\,[\overline{\nabla \boldsymbol{v}} - \alpha P_0^{-1}\lambda\,\overline{\nabla\nabla} T + \beta T_0 P_0^{-2}\lambda\,\overline{\nabla\nabla}\,p + l_v^2\,\overline{\nabla \Delta \boldsymbol{v}}]\,, \tag{2.20 a}$$

$$\boldsymbol{q}_{\mathrm{CE}} = -\lambda\,[\nabla T - \alpha T_0 P_0^{-1}\eta\,\Delta \boldsymbol{v} + l_T^2\,\nabla \Delta T + l_p^2\,T_0 P_0^{-1}\,\nabla \Delta p]\,, \tag{2.20 b}$$

with

$$\alpha = \tfrac{2}{5}\,,\quad \beta = \tfrac{4}{15}\,,\quad l_v = \sqrt{\tfrac{2}{3}}\,l_\eta\,,\quad l_T = \sqrt{\tfrac{49}{20}}\,l_\eta\,,\quad l_p = \sqrt{\tfrac{1}{6}}\,l_\eta$$

in the case of Maxwell molecules [11, 13].

The first two terms in $\overline{\mathbf{p}}$ and $\boldsymbol{q}$ are the same in Eqs. (2.19 a, b) and (2.20 a, b). But there is a difference in the $\overline{\nabla\nabla}\,p$ terms occurring in the friction pressure tensor: the numerical factors are 4/25 and $\beta = 4/15$, respectively. The terms discussed so far are present in the thirteen moments treatment and in the third order Chapman-Enskog approximation. The seventeen moments ansatz for $\boldsymbol{q}$, full Eq. (2.19 b), is different from the fourth order Chapman-Enskog expression (2.20 b) in two respects: the $\nabla \Delta T$ terms have different sign and magnitude; furthermore, no $\nabla \Delta p$ term occurs in (2.19 b) since $\Delta p = 0$ according to Eq. (2.4), whereas $\Delta p \neq 0$ in the Chapman-Enskog approach. The seventeen moments ansatz for $\overline{\mathbf{p}}$, full Eq. (2.19 a), is rewritten by means of Eq. (2.16) so that the first three terms are identical with those in the Chapman-Enskog expression (2.20 a):

$$\overline{\mathbf{p}} = -2\,\eta\,[\overline{\nabla \boldsymbol{v}} - \tfrac{2}{5} P_0^{-1}\lambda\,\overline{\nabla\nabla}\,T + \tfrac{4}{15} T_0 P_0^{-2}\lambda\,\overline{\nabla\nabla}\,p - \tfrac{2}{5} l_\eta^2\,\overline{\nabla \Delta \boldsymbol{v}} + \tfrac{2}{5} P_0^{-1}\lambda L^2\,\overline{\nabla\nabla}\,\Delta T]\,. \tag{2.19 c}$$

However, the following $\overline{\nabla \Delta \boldsymbol{v}}$-term has different sign and magnitude in both approximations. The fourth order derivative of T occurs only in the seventeen moments expression.

Hence, the moment method and the Chapman-Enskog theory give different constitutive laws for the friction pressure tensor and the heat flux (and consequently also different differential equations for p, T, $\boldsymbol{v}$) if one goes beyond the hydrodynamical limits

$$\overline{\mathbf{p}} = -2\,\eta\,\overline{\nabla \boldsymbol{v}}\,,\quad \boldsymbol{q} = -\lambda\,\nabla T\,.$$

For the study of Knudsen effects, where the higher order derivatives become important, the moment method seems to be simpler and more physical than the Chapman-Enskog theory since the inclusion of only two new quantities, A and $\boldsymbol{A}$, leads to quite a number of higher order derivatives of T, p and $\boldsymbol{v}$. Furthermore, the resulting differential equations are much simpler in the moment method treatment, in particular if the coupled equations for T, A and $\boldsymbol{v}$ are used. Another argument in favour of the moment method is the possibility to derive boundary conditions for the relevant quantities (viz. T, A, $\boldsymbol{v}$ in the present approximation) in quite a simple way from the interfacial entropy production.

3. Boundary Conditions

Starting point for the derivation of boundary conditions for the transport-relaxation equations (1.9) is the interfacial (kinetic) entropy production $\dot{S}_\sigma$ which is due to a discontinuity of the normal entropy fluxes $\boldsymbol{s}$ and $\boldsymbol{s}_s$ in the gas and in the solid at the interface σ [3, 5, 6]:

$$\dot{S}_\sigma = -\int_\sigma \mathrm{d}\sigma\,\boldsymbol{n}\cdot(\boldsymbol{s} - \boldsymbol{s}_s)\,. \tag{3.1}$$

Here, $\boldsymbol{n}$ denotes the outer unit normal of the gas. In the following, $\dot{S}_\sigma$ will be transformed into a quadratic form of deviations from equilibrium.

For the entropy flux in the solid we simply take

$$\boldsymbol{s}_s = \boldsymbol{q}_s T_s^{-1}\,, \tag{3.2}$$

and immediately decompose it:

$$\boldsymbol{s}_s = \boldsymbol{s}_s^{(0)} + \boldsymbol{s}_s^{(1)} \tag{3.3}$$

with

$$\boldsymbol{s}_s^{(0)} = \boldsymbol{q}_s T_0^{-1}\,, \tag{3.4}$$

$$\boldsymbol{s}_s^{(1)} \approx -\boldsymbol{q}_s (T_s - T_0)/T_0^2\,. \tag{3.5}$$

The first part is simply proportional to the energy (heat) flux.

A similar decomposition automatically ensues from the Boltzmann equation for the entropy flux of the gas, see Eq. (1.25) of Ref. [8]:

$$\boldsymbol{s} = \boldsymbol{s}^{(0)} + \boldsymbol{s}^{(1)} \tag{3.6}$$

with

$$\boldsymbol{s}^{(0)} = [(\mathbf{p} - P_0\boldsymbol{\delta})\cdot\boldsymbol{v} + \boldsymbol{q}]\,T_0^{-1}\,, \tag{3.7}$$

$$\begin{aligned} \boldsymbol{s}^{(1)} &\approx -P_0 T_0^{-1} \langle \tfrac{1}{2} \boldsymbol{c}\, \Phi^2 \rangle_0 \\ &= -P_0 T_0^{-1} \sum_l \sum_r \sum_s a^{(s)}_{\nu_1 \ldots \nu_{l+1}} \langle \Phi^{(s)}_{\nu_1 \ldots \nu_{l+1}} \\ &\qquad \boldsymbol{c}\, \Phi^{(r)}_{\mu_1 \ldots \mu_l} \rangle_0\, a^{(r)}_{\mu_1 \ldots \mu_l} . \end{aligned} \tag{3.8}$$

Again, the first part is simply proportional to the energy flux. In particular, with the finite expansion from Eq. (1.8) the entropy flux of the gas is

$$\begin{aligned} \boldsymbol{s}^{(1)} &\approx -P_0 T_0^{-1} c_0 [\boldsymbol{a}^{(0)} (a^{(0)} - \sqrt{\tfrac{2}{3}}\, a^{(1)}) \\ &\quad + \boldsymbol{a}^{(1)} (\sqrt{\tfrac{5}{3}}\, a^{(1)} - \sqrt{\tfrac{4}{3}}\, a^{(2)}) + \boldsymbol{a}^{(2)} \sqrt{\tfrac{7}{3}}\, a^{(2)} \\ &\quad + \mathbf{a}^{(0)} \cdot (\sqrt{2}\, \boldsymbol{a}^{(0)} - \sqrt{\tfrac{4}{5}}\, \boldsymbol{a}^{(1)})] \qquad (3.9) \\ &= -T_0^{-1} [\boldsymbol{v} (p - P_0) + \boldsymbol{q} (T - T_0 + A) T_0^{-1} \\ &\quad + \boldsymbol{A} A T_0^{-1} + \overline{\mathbf{p}} \cdot (\boldsymbol{v} + \tfrac{2}{5} P_0^{-1} \boldsymbol{q})] . \end{aligned}$$

On insertion of the decompositions (3.3), (3.6) into the integral (3.1), their first parts give zero

$$\int_\sigma \mathrm{d}\sigma\, \boldsymbol{n} \cdot [(\mathbf{p} - P_0 \boldsymbol{\delta}) \cdot \boldsymbol{v} + \boldsymbol{q} - \boldsymbol{q}_s] = 0 . \tag{3.10}$$

Indeed, as

$$\boldsymbol{n} \cdot \boldsymbol{v} = 0 \quad \text{at} \quad \sigma , \tag{3.11}$$

the integral (3.10) is the total energy entering the interface per unit time and vanishes for the system gas/solid which has no surface tension. So, the rate of interfacial entropy production is given by the second parts alone

$$\dot{S}_\sigma = -\int_\sigma \mathrm{d}\sigma\, \boldsymbol{n} \cdot (\boldsymbol{s}^{(1)} - \boldsymbol{s}_s^{(1)}) . \tag{3.12}$$

Inserting (3.5) and (3.9) gives

$$\begin{aligned} \dot{S}_\sigma &= \int_\sigma \mathrm{d}\sigma\, T_0^{-1} [\boldsymbol{n} \cdot \boldsymbol{q} (\tilde{T} - T_0) T_0^{-1} \qquad (3.13) \\ &\quad - \boldsymbol{n} \cdot \boldsymbol{q}_s (T_s - T_0) T_0^{-1} + \boldsymbol{n} \cdot \boldsymbol{A} A T_0^{-1} + \tilde{\boldsymbol{v}}^{\tan} \cdot \boldsymbol{k}^{\tan}] . \end{aligned}$$

The abbreviations

$$\begin{aligned} \boldsymbol{k} &= \boldsymbol{n} \cdot \mathbf{p} , \quad \tilde{\boldsymbol{v}} = \boldsymbol{v} + \tfrac{2}{5} P_0^{-1} \boldsymbol{q} , \\ \tilde{T} &= T + A + \tfrac{2}{5} T_0 P_0^{-1} \boldsymbol{n} \cdot \overline{\mathbf{p}} \cdot \boldsymbol{n} \end{aligned} \tag{3.14}$$

have been used. The superscript "tan" in (3.13) denotes the tangential vector component.

Equation (3.13) has not yet the final shape desirable for the interfacial entropy production. This should be given by an expression bilinear in "fluxes and forces". But the temperature differences $T - T_0$, $T_s - T_0$ are not the desired "forces" because the choice of T_0 is arbitrary, of course within the restrictions of the linearized theory. To achieve the said bilinearity one has to eliminate one of the normal heat fluxes by means of the local linearized energy equation at the interface[3]

$$\boldsymbol{n} \cdot (\boldsymbol{q} - \boldsymbol{q}_s) = \boldsymbol{\nabla}^{\tan} \cdot \mathbf{Q} , \tag{3.15}$$

where $\mathbf{Q}$ is the surface heat flux first introduced in Reference[3]. Using the identity

$$\begin{aligned} &\boldsymbol{n} \cdot \boldsymbol{q} (\tilde{T} - T_0) - \boldsymbol{n} \cdot \boldsymbol{q}_s (T_s - T_0) \\ &= \boldsymbol{n} \cdot (\boldsymbol{q} - \boldsymbol{q}_s) [\tfrac{1}{2} (\tilde{T} + T_s) - T_0] \\ &\quad + \tfrac{1}{2} \boldsymbol{n} \cdot (\boldsymbol{q} + \boldsymbol{q}_s) (\tilde{T} - T_s) \end{aligned}$$

we obtain the final form of the interfacial entropy production,

$$\begin{aligned} \dot{S}_\sigma &= \int_\sigma \mathrm{d}\sigma\, T_0^{-1} [\tfrac{1}{2} \boldsymbol{n} \cdot (\boldsymbol{q} + \boldsymbol{q}_s) (\tilde{T} - T_s) T_0^{-1} \\ &\quad + \boldsymbol{n} \cdot \boldsymbol{A} A T_0^{-1} - T_0^{-1} \mathbf{Q} \cdot \boldsymbol{\nabla}^{\tan} \tfrac{1}{2} (\tilde{T} + T_s) \\ &\quad + \tilde{\boldsymbol{v}}^{\tan} \cdot \boldsymbol{k}^{\tan}] , \end{aligned} \tag{3.16}$$

which now is bilinear in fluxes and forces.

Linear relations set up between the "fluxes and forces" of Eq. (3.16) are the boundary conditions[3]. Under the assumption that there is no coupling between scalars and vectors at the interface σ, one gets a generalized temperature-jump condition and a condition for the normal component of the vector $\boldsymbol{A}$:

$$\tfrac{1}{2} \boldsymbol{n} \cdot (\boldsymbol{q} + \boldsymbol{q}_s) = l_{qq} (\tilde{T} - T_s) + l_{qA} A , \tag{3.17}$$

$$\boldsymbol{n} \cdot \boldsymbol{A} = l_{Aq} (\tilde{T} - T_s) + l_{AA} A . \tag{3.18}$$

Furthermore, the well-known velocity slip condition and an ansatz for the surface heat flux $\mathbf{Q}$ are obtained[3, 6, 10]:

$$\tilde{\boldsymbol{v}}^{\tan} = L_{vv} \boldsymbol{k}^{\tan} + L_{vQ} \boldsymbol{\nabla}^{\tan} \tfrac{1}{2} (\tilde{T} + T_s) , \tag{3.19}$$

$$-T_0^{-1} \mathbf{Q} = L_{Qv} \boldsymbol{k}^{\tan} + L_{QQ} \boldsymbol{\nabla}^{\tan} \tfrac{1}{2} (\tilde{T} + T_s) . \tag{3.20}$$

Due to Onsager relations, the matrices l_{ik} and L_{ik} are symmetric[3, 7]:

$$l_{Aq} = l_{qA} , \quad L_{Qv} = L_{vQ} . \tag{3.21}$$

Since the second law requires a positive surface entropy production, the l_{ik} and L_{ik} form positive matrices, i. e.

$$\begin{aligned} l_{qq} &\geqq 0 , \quad l_{qq} l_{AA} - l_{Aq}^2 \geqq 0 ; \\ L_{vv} &\geqq 0 , \quad L_{vv} L_{QQ} - L_{Qv}^2 \geqq 0 . \end{aligned} \tag{3.22}$$

For the symmetry and positivity of the coefficient matrices l_{ik} and L_{ik} it is crucial to use the force-flux pairs occurring in the surface entropy production. This fact has to be kept in mind if boundary conditions are derived on a more microscopic basis. In particular, in Eqs. (3.17), (3.18) the fluxes have been chosen as $\tfrac{1}{2} \boldsymbol{n} \cdot (\boldsymbol{q} + \boldsymbol{q}_s)$, $\boldsymbol{n} \cdot \boldsymbol{A}$, and in Eqs. (3.19), (3.20) we wanted to have $\boldsymbol{k}^{\tan}$ as a force and $-T_0^{-1} \mathbf{Q}$ as a flux. As a consequence of this choice the tilded quantities $\tilde{T}$, $\tilde{\boldsymbol{v}}$ from Eq. (3.14) occur in the boundary conditions. A different choice of fluxes and forces would be obtained by a linear transformation which lets the surface entropy production invariant.

The boundary conditions (3.11) and (3.19) for the velocity, the conditions (3.15) and (3.20) for the discontinuity of the normal heat flux and for the interfacial heat flux, the conditions (3.17) for the temperature-jump and (3.18) for the scalar A, all of them are necessary and sufficient for the solution of the differential equations for $\boldsymbol{v}$, T and A.

4. Heat Transfer Between Parallel Plates

The influence of the higher moments A and $\boldsymbol{A}$ on the heat transfer in a monatomic gas between infinite parallel plates of distance $2\,d$ is now studied[14, 15]. The plates are located at $x = \pm d$, and have the temperatures $T_{\pm}$:

$$T_s(\pm d) = T_{\pm} \,. \tag{4.1}$$

According to the Navier-Stokes equation (2.16) the pressure is constant in a gas at rest:

$$\boldsymbol{v} = 0 \,, \quad p = \text{const} = P_0 \,. \tag{4.2}$$

The two scalars T and A depend on x only, hence also the two vectors $\boldsymbol{q}$ and $\boldsymbol{A}$ depend on x only and are parallel to $\boldsymbol{e}$, the unit vector in x-direction. Because of Eq. (2.2), $\boldsymbol{\nabla}\cdot\boldsymbol{q} = 0$, the heat flux is constant, so that the ansatz (2.11) for the friction pressure tensor gives

$$\overline{\mathsf{p}} = 0 \,. \tag{4.3}$$

The differential equation (2.5) for the scalar A has the two solutions $\exp(x/L)$ and $\exp(-x/L)$ which, due to the symmetry of the problem, combine to $\sinh x/L$,

$$A(x) = \frac{T_+ - T_-}{2} F \frac{\sinh x/L}{\sinh d/L} \,, \tag{4.4}$$

where F is a numerical factor, still to be determined. From Eq. (2.7) one sees that $T + (1+\varepsilon) A$ is a linear function of x. Consequently the solution for the temperature can be written as

$$T(x) = \frac{T_+ + T_-}{2} + \frac{T_+ - T_-}{2} G \frac{x}{d} - (1+\varepsilon) A(x) \,. \tag{4.5}$$

The numerical factor G is still to be determined. With the expressions (4.2), (4.4) and (4.5) for p, A and T, the heat flux and the vector $\boldsymbol{A}$ follow from the constitutive laws (2.14), (2.15):

$$\boldsymbol{q} = -\lambda \frac{T_+ - T_-}{2\,d} \boldsymbol{e}\, G \,, \tag{4.6}$$

$$\boldsymbol{A}(x) = -\lambda \frac{T_+ - T_-}{2\,d} \boldsymbol{e} \left[\varepsilon G + \frac{\lambda'}{\lambda} \frac{d}{L} F \frac{\cosh x/L}{\sinh d/L} \right] . \tag{4.7}$$

Due to the symmetry of the problem there exists no surface heat flux $\boldsymbol{Q}$ in this case; the boundary conditions (3.19), (3.20) are void. Again, due to symmetry, the two factors F and G are determined by the boundary conditions (3.17), (3.18) at one plate, e.g. at $x = +d$ where $\boldsymbol{n} = +\boldsymbol{e}$. Using Eqs. (4.3) – (4.5) we write down the temperature $\tilde{T}$ from Eq. (3.14) in the form:

$$\tilde{T}(d) = T_+ + \frac{T_+ - T_-}{2} (G-1) - \varepsilon A(d) \,.$$

The boundary conditions (3.17), (3.18) for $x = +d$ now are:

$$-G = l_{qq} \frac{d}{\lambda} (G-1) + (l_{qA} - \varepsilon\, l_{qq}) \frac{d}{\lambda} F \,, \tag{4.8 a}$$

$$-\left(\varepsilon G + \frac{\lambda'}{\lambda} \frac{d}{L} F \coth d/L \right) = l_{Aq} \frac{d}{\lambda} (G-1) + (l_{AA} - \varepsilon\, l_{Aq}) \frac{d}{\lambda} F \,. \tag{4.8 b}$$

These are two linear inhomogeneous equations for F and G. For convenience, the dimensionless coefficients C_{ik} are introduced instead of the l_{ik},

$$l_{ik} = \frac{\lambda}{l} C_{ik} = \frac{15}{4} n_0 k_{\mathrm{B}} c_0 C_{ik} \,, \tag{4.9}$$

with

$$l = l_\eta \left[1 - \omega_1(12)^2 / \omega_1(11)\, \omega_1(22) \right]^{-1} .$$

Furthermore, we will use the abbreviation δ for the ratio

$$\delta = \frac{\lambda'}{\lambda} \frac{l}{L} = \frac{1}{2} \sqrt{\frac{7}{3} \frac{\omega_1(11)}{\omega_1(22)}} \tag{4.10 a}$$

which has the numerical values

$$\delta = 0.624 \quad \text{for Maxwell molecules} \,, \tag{4.10 b}$$

and

$$\delta = 0.602 \quad \text{for hard spheres} \,. \tag{4.10 c}$$

Now, the solution of Eqs. (4.8 a, b) can be expressed in the form:

$$F = \frac{l}{d} G \frac{C_{Aq} - \varepsilon C_{qq}}{C_{qq} C_{AA} - C_{Aq}^2 + C_{qq}\, \delta \coth d/L}, \tag{4.11}$$

$$G = 1/[1 + (l/d) g], \tag{4.12}$$

where g is a function of L/d and herewith of pressure P_0,

$$g(L/d) = \frac{C_{AA} - 2\,\varepsilon C_{Aq} + \varepsilon^2 C_{qq} + \delta \coth d/L}{C_{qq} C_{AA} - C_{Aq}^2 + C_{qq}\, \delta \coth d/L}. \tag{4.13}$$

In writing down Eqs. (4.11), (4.13), we have used the symmetry $C_{Aq} = C_{qA}$. According to Eq. (3.22), the matrix C_{ik} is positive. Hence the quantity g contains the positive terms

$$C_{AA} - 2\,\varepsilon C_{Aq} + \varepsilon^2 C_{qq} > 0,$$
$$C_{qq} C_{AA} - C_{Aq}^2 > 0, \quad C_{qq} > 0,$$

so that g, as well as G from Eq. (4.12), are positive:

$$g > 0, \quad G > 0. \tag{4.14}$$

Via l, g and G, the heat flux $\boldsymbol{q}$ from Eq. (4.6) becomes pressure dependent; actually, the function G is always smaller than its high pressure limit 1.

In the special case

$$C_{Aq} = \varepsilon C_{qq} \tag{4.15 a}$$

our seventeen moments method reduces to the thirteen moments scheme. Indeed, the constant F then is zero so that the scalar A vanishes everywhere, and the vector $\boldsymbol{A}$ is proportional to the heat flux:

$$A = 0, \quad \boldsymbol{A} = \varepsilon \boldsymbol{q}. \tag{4.15 b}$$

In this case the quantity g is independent of the pressure,

$$g = 1/C_{qq} > 0. \tag{4.15 c}$$

Now, the pressure dependence of the moments T, A, $\boldsymbol{q}$ and $\boldsymbol{A}$ is discussed. In the near-hydrodynamic regime, i. e. for $L/d \ll 1$, the heat flux decreases with increasing Knudsen number l/d according to

$$G \approx 1 - (l/d)\, g(0), \tag{4.16 a}$$

where

$$g(0) = \frac{C_{AA} - 2\,\varepsilon C_{Aq} + \varepsilon^2 C_{qq} + \delta}{C_{qq} C_{AA} - C_{Aq}^2 + C_{qq}\, \delta}. \tag{4.16 b}$$

In the same limit the function F is linear in l/d,

$$F \approx F' = \frac{l}{d} \frac{C_{Aq} - \varepsilon C_{qq}}{C_{qq} C_{AA} - C_{Aq}^2 + C_{qq}\, \delta}. \tag{4.16 c}$$

Therefore, after Eq. (4.4), the boundary value of A,

$$A(d) \approx \tfrac{1}{2}(T_+ - T_-)\, F',$$

is of the order l/d. With increasing distance from the walls, $A(x)$ decreases exponentially to zero with the characteristic length L. Consequently, in the bulk of the gas, the temperature [after (4.5)] varies linearly with x,

$$T(x) \approx T_b(x) = \frac{T_+ + T_-}{2} + x \frac{T_+ - T_-}{2\,d} \left(1 - \frac{l}{d} g(0)\right)$$
$$\text{for } |d - x| \gg L. \tag{4.17}$$

But in a boundary layer of thickness L there are small exponential contributions, e. g. near the plate $x = +d$:

$$T(x) \approx T_b(x) - (1 + \varepsilon) \frac{T_+ - T_-}{2} F' \cdot \exp\{-(d - x)/L\}.$$

According to Eq. (4.17), the constant $g(0)$ characterizes the difference between the temperature of the wall $T_s(d) = T_+$ and the extrapolated value of the bulk-temperature

$$T_s(d) - T_b(d) \approx \frac{T_+ - T_-}{2} \frac{l}{d} g(0). \tag{4.18 a}$$

Thus it is reasonable to identify $g(0)$ with the measured temperature-jump coefficient C_t:

$$g(0) = C_t; \tag{4.18 b}$$

e. g. for argon an experimental value of $C_t = 3.6$ has been used in Reference [10]. Whereas $g(0)$ is positive from thermodynamical reasons, this is not necessarily the case for the constant g' which characterizes the jump of the temperature itself:

$$T_s(d) - T(d) \approx \frac{T_+ - T_-}{2} \frac{l}{d} g',$$

with

$$g' = \frac{C_{AA} + (1 - \varepsilon) C_{Aq} - \varepsilon C_{qq} + \delta}{C_{qq} C_{AA} - C_{Aq}^2 + C_{qq}\, \delta}.$$

The quantity g' can be negative, e. g. with the hard sphere parameters for ε and δ, and the allowed values

$$C_{AA} = 2, \quad C_{qq} = 5, \quad C_{Aq} = -3,$$

one finds a very small negative g' and a small positive $g(0)$:

$$g' = -0.02, \quad g(0) = 0.44.$$

By the way, in all recent attempts to establish a microscopic theory of slip phenomena, the temperature jump coefficient $g(0)$ was calculated, see e. g. the work of Loyalka [16]. It should be noted that the value of $g(0)$ is in practice essentially determined by C_{qq} alone. The parameter ε is small. If one puts $\varepsilon=0$, which is true for Maxwell molecules, cf. Eqs. (2.8 a, b, c), and assumes

$$C_{Aq}^2 \ll C_{AA}\, C_{qq}\,,$$

one has indeed

$$g(0) \approx 1/C_{qq}\,.$$

The theory presented here is reliable only for not too large values of L/d, but for curiosity let us look for the Knudsen limit. For large Knudsen numbers, $L/d \gg 1$, one can replace $\coth d/L$ by L/d; then the quantity g approaches a constant value and the function G is proportional to d/l:

$$g \rightarrow g(\infty) = 1/C_{qq}\,, \quad G \rightarrow (d/l)\, C_{qq}\,. \qquad (4.19)$$

Since $\sinh x/L$ can be replaced by x/L and $\cosh x/L$ by 1, the scalars A and T, after Eqs. (4.4), (4.5), are linear functions of x,

$$A(x) \rightarrow \frac{x}{l}\, \frac{T_+ - T_-}{2}\, (C_{Aq} - \varepsilon\, C_{qq})\, \frac{\lambda}{\lambda'}\,,$$

$$T(x) \rightarrow \frac{T_+ + T_-}{2} + \frac{x}{l}\, \frac{T_+ - T_-}{2} \cdot \left[C_{qq} - (1+\varepsilon)(C_{Aq} - \varepsilon\, C_{qq})\, \frac{\lambda}{\lambda'} \right],$$

whereas the vector $\boldsymbol{A}$ is constant:

$$\boldsymbol{A}(x) \rightarrow \boldsymbol{q}_\infty\, C_{Aq}/C_{qq}\,.$$

The limiting value $\boldsymbol{q}_\infty$ of the heat flux is proportional to the gas pressure

$$\boldsymbol{q} \rightarrow \boldsymbol{q}_\infty = -\boldsymbol{e}(T_+ - T_-)\, \frac{P_0}{T_0}\, c_0\, \frac{15}{8}\, C_{qq}\,, \qquad (4.20)$$

and is identical with the correct value $\boldsymbol{q}_K$ for $\boldsymbol{q}$ in the Knudsen regime. Indeed, the coefficient C_{qq} and the heat flux $\boldsymbol{q}_K$ can be expressed[17] by the gas-wall collision operator $L_{\text{II}}(\boldsymbol{p}, \boldsymbol{p}')$ which occurs in the boundary condition for the distribution function[8]. In particular, with a simple model for L_{II} the coefficient C_{qq} is given in terms of the accommodation coefficient a by

$$C_{qq} = \frac{8}{15} \sqrt{\frac{2}{\pi}}\, \frac{a}{2-a}\,, \qquad (4.21)$$

so that the well-known expression[18]

$$\boldsymbol{q}_\infty = \boldsymbol{q}_K = -\boldsymbol{e}(T_+ - T_-)\, \frac{P_0}{T_0}\, c_0 \sqrt{\frac{2}{\pi}}\, \frac{a}{2-a} \qquad (4.22)$$

is found. It should be noted that the correct Knudsen limit (4.22) for the heat flux is already obtained with the old temperature-jump approximation (where no higher moments are taken into account) by using Eqs. (4.15 c), (4.18 b) and (4.21):

$$g \equiv g(0) = C_t = 1/C_{qq}\,.$$

Finally, a remark on the variation of g and G with the Knudsen number L/d is made. With the help of Eqs. (4.16 b) and (4.19), we can rewrite the expression (4.13) for $g(L/d)$ in the following way:

$$\begin{aligned} g(L/d) &= g(\infty) + \frac{1}{C_{qq}}\, \frac{(C_{Aq} - \varepsilon\, C_{qq})^2}{C_{qq}\, C_{AA} - C_{Aq}^2 + C_{qq}\, \delta \coth d/L} \\ &= g(0) - \frac{(C_{Aq} - \varepsilon\, C_{qq})^2\, \delta(\coth d/L - 1)}{(C_{qq}\, C_{AA} - C_{Aq}^2 + C_{qq}\, \delta)\,(C_{qq}\, C_{AA} - C_{Aq}^2 + C_{qq}\, \delta \coth d/L)}\,. \end{aligned}$$

Hence, $g(L/d)$ is bound by $g(\infty)$ and $g(0)$,

$$g(\infty) \leqq g(L/d) \leqq g(0)\,,$$

and due to the relation

$$\partial g/\partial(L/d) = -\delta \left[\frac{d}{L}\, \frac{C_{Aq} - \varepsilon\, C_{qq}}{\sinh d/L\, (C_{qq}\, C_{AA} - C_{Aq}^2 + C_{qq}\, \delta \coth d/L)} \right]^2 \leqq 0\,,$$

$g(L/d)$ is a monotonously decreasing function of L/d. Similarly, with

$$\sinh 2\, d/L - 2\, d/L \geqq 0$$

and

$$\partial\left(\frac{L}{d}\, g\right) / \partial(L/d) = g(\infty) + \frac{1}{C_{qq}} \left[\frac{C_{Aq} - \varepsilon\, C_{qq}}{\sinh d/L\, (C_{qq}\, C_{AA} - C_{Aq}^2 + C_{qq}\, \delta \coth d/L)} \right]^2 \cdot \left[\sinh^2 d/L\, (C_{qq}\, C_{AA} - C_{Aq}^2) + \tfrac{1}{2}\, C_{qq}\, \delta(\sinh 2\, d/L - 2\, d/L) \right] \geqq g(\infty) > 0\,,$$

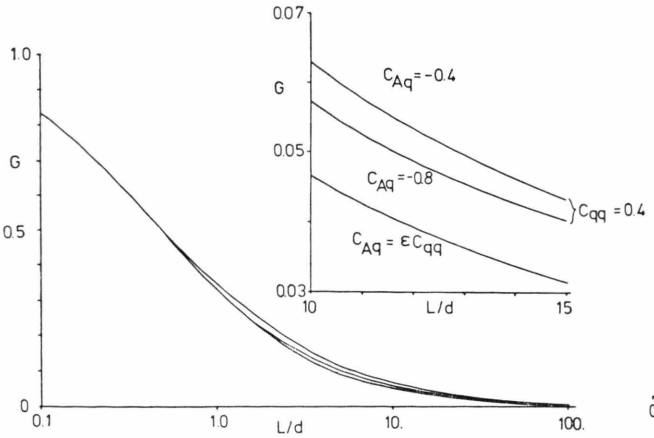

Fig. 1. Dependence of the dimensionless heat flux G on the Knudsen number L/d according to Eqs. (4.6), (4.12), (4.13) calculated with $g(0)=3.6$ and some values of C_{qq}, C_{Aq}. The lower curve corresponds to the thirteen moments approximation, and is characterized by $C_{Aq}=\varepsilon C_{qq}=-0.043$, $C_{qq}=1/g(0)=0.278$.

one can easily prove that G also is a monotonously decreasing function of L/d, varying between the values 1 and $C_{qq}\,d/l$.

In Figs. 1 – 4 some quantitative results are shown, with the underlying hard sphere values $\varepsilon=-0.156$, $\delta=0.602$, $l/L=0.566$ and the fixed "temperature jump coefficient" $g(0)=3.6$.

In Fig. 1, the dependence of the reduced heat flux G [see Eq. (4.6)] on the Knudsen number L/d is plotted. The lower curve refers to the thirteen moments approximation; according to Eqs. (4.15 a, c) it is characterized by $C_{Aq}=\varepsilon C_{qq}$, $C_{qq}=1/g(0)$, i.e. by the value of the parameter $g(0)$. In the seventeen moments approximation, there are two additional free parameters besides $g(0)$, viz. C_{qq} and C_{Aq}. The two upper curves in Fig. 1 refer to $C_{Aq}=-0.4$, $C_{Aq}=-0.8$, respectively, and to the same value of $C_{qq}=0.4$ (the corresponding C_{AA} values are $C_{AA}=0.45$ and $C_{AA}=4.09$). For very large Knudsen numbers, these two curves coincide according to Eq. (4.20). The difference in the C_{Aq} values only plays a role for moderate L/d. Below $L/d=0.5$, the three curves are practically again coincident since $g(L/d)$ can here be replaced by $g(0)=3.6$.

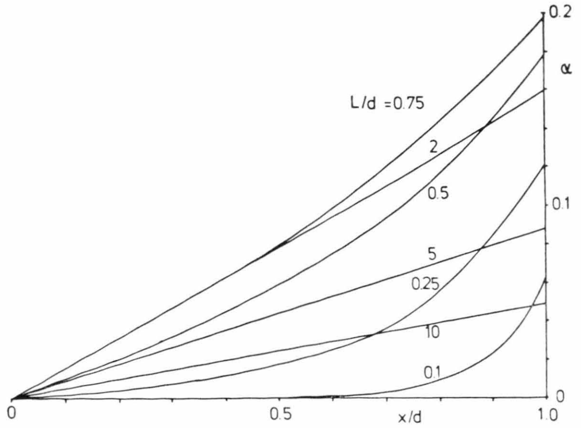

Fig. 2. Profile of the dimensionless scalar $\alpha\propto A$ according to Eqs. (4.23) and (4.11) – (4.13), calculated for $g(0)=3.6$, $C_{qq}=0.4$, $C_{Aq}=-0.4$ and some values of L/d.

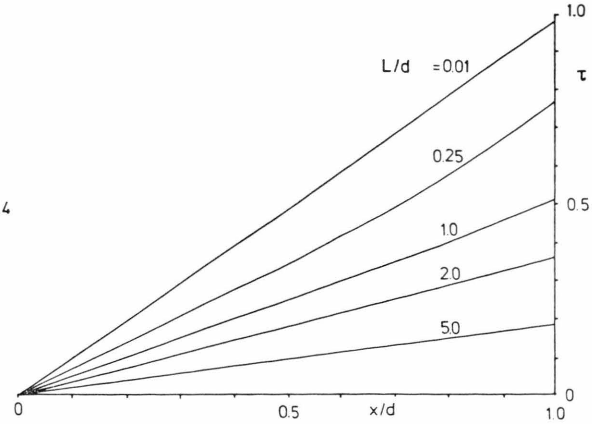

Fig. 3. Profile of the dimensionless temperature $\tau\propto T-(T_+ + T_-)/2$ according to Eqs. (4.24) and (4.12), (4.13), calculated for $g(0)=3.6$, $C_{qq}=0.4$, $C_{Aq}=-0.4$ and some values of L/d.

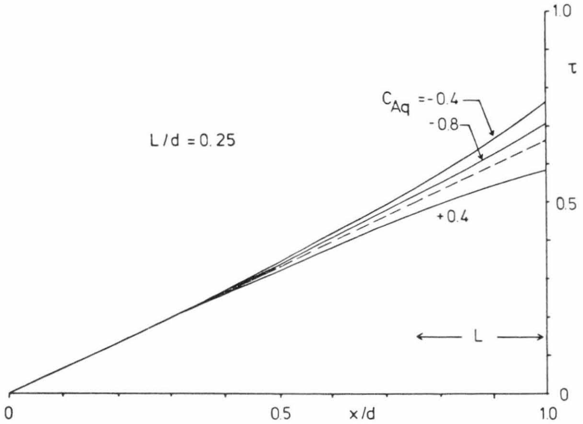

Fig. 4. Profile of the dimensionless temperature $\tau\propto T-(T_+ + T_-)/2$ for $L/d=0.25$, $g(0)=3.6$, $C_{qq}=0.4$ and some values of C_{Aq}. The dotted line is the linear bulk profile $(x/d)\,G$.

In Fig. 2, the scalar $A(x)$ is plotted in form of the dimensionless quantity

$$\begin{aligned}\alpha(x/d) &= -2\,A(x)/(T_+ - T_-)\\ &= -F\sinh x/L/\sinh d/L \qquad (4.23)\end{aligned}$$

for the parameters $C_{qq}=0.4$, $C_{Aq}=-0.4$ and some values of L/d. Up to about $L/d=1$, α is essentially an exponential of $(d-x)/L$, and the boundary value $\alpha(1)$ increases with increasing L/d. For $L/d \gg 1$, however, α is linear in x/d, and $\alpha(1)$ decreases with increasing L/d.

In Figs. 3, 4 the temperature profile is plotted in terms of the dimensionless function τ:

$$\tau(x/d)=2\left(T(x)-\frac{T_+ + T_-}{2}\right)\Big/(T_+ - T_-)= \\ =\frac{x}{d}\,G+(1+\varepsilon)\,\alpha(x/d)\,. \qquad (4.24)$$

The dependence of $\tau(x/d)$ on the Knudsen number is shown in Fig. 3 for the parameters $C_{qq}=0.4$, $C_{Aq}=-0.4$. For very small and very large L/d, τ is practically a linear function of x/d. The exponential contributions to τ only play a role for intermediate Knudsen numbers. This is demonstrated with Fig. 4 where τ is plotted versus x/d for $L/d=0.25$, $g(0)=3.6$, $C_{qq}=0.4$ and three values of C_{Aq}. In the bulk of the gas, all three curves approach the linear "bulk temperature" (dotted line).

In this paper, the heat transfer in a monatomic gas between parallel plates has been treated with constitutive laws, differential equations and boundary conditions for a few macroscopic variables, including moments of higher powers of particle energy. A complete formal solution of the heat transfer problem is obtained[17] directly from the linearized Boltzmann equation and the boundary condition for the distribution function[8].

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[1] H. Grad, Comm. Pure Appl. Math. **2,** 331 [1949]; Handbuch der Physik, Vol. 12, ed. S. Flügge, Springer-Verlag, Berlin 1958.

[2] L. Waldmann, Z. Naturforsch. **18 a**, 1033 [1963]; S. Hess and L. Waldmann, Z. Naturforsch. **21 a**, 1529 [1966].

[3] L. Waldmann, Z. Naturforsch. **22 a**, 1269 [1967].

[4] L. Waldmann and R. Rübsamen, Z. Naturforsch. **27 a**, 1025 [1972].

[5] L. Waldmann, Rarefied Gas Dynamics, 8th Symposium 1972, Academic Press, New York 1974, p. 431.

[6] L. Waldmann and H. Vestner, Physica **80 A,** 523 [1975].

[7] L. Waldmann, Z. Naturforsch. **31 a,** 1029, 1439 [1976].

[8] L. Waldmann, Z. Naturforsch. **32 a,** 521 [1977].

[9] D. Bedeaux, A. M. Albano, and P. Mazur, Physica **82 A,** 438 [1976].

[10] H. Vestner and L. Waldmann, Physica **86 A,** 303 [1977].

[11] S. Chapman and T. G. Cowling, The mathematical theory of non-uniform gases, Cambridge University Press 1970.

[12] L. Waldmann, in Handbuch der Physik, Vol. 12, ed. S. Flügge, Springer-Verlag, Berlin 1958.

[13] For special geometry and Maxwell molecules the fourth order terms are found in J. D. Foch, Acta Physica Austriaca, Suppl. X, 123 [1973].

[14] Theoretical work has been done by e. g. S. K. Hsu and T. F. Morse, Phys. Fluids **15,** 584 [1972]; B. T. Yeh and A. Frohn, Phys. Fluids **16,** 330 [1973].

[15] Experiments have been performed by e. g. W. P. Teagan and G. S. Springer, Phys. Fluids **11,** 497 [1968]; D. Braun and A. Frohn, Int. J. Heat Mass Transfer **19,** 1329 [1976].

[16] S. K. Loyalka, Z. Naturforsch. **26 a**, 964 [1971].

[17] L. Waldmann, Phys. Letters **61 A,** 433 [1977].

[18] E. H. Kennard, Kinetic Theory of Gases, McGraw-Hill, New York 1938.