Upper and Lower Bounds for the Heat Flux in a Gas Between Parallel Plates

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Waldmann's result for heat transfer through a monatomic gas between parallel plates is the starting point for the derivation of upper and lower bounds for the heat flux as a function of Knudsen number. In order to obtain numerical results, one transport-relaxation eigenfunction and its eigenvalue are determined approximately, and a simple model for the interfacial kernel of the kinetic boundary condition for the distribution function is used.

For more than hundred years the particular behaviour of a rarefied gas near a solid is known: the gas does not stick, it slips along the interface, the temperature "jumps" across the boundary. Mechanical slip, discovered in 1860 [1], reduces the friction force on a particle [2] and increases the mass flow through a pipe [3], [4]. Thermal slip is responsible for thermal transpiration [3], [5] and for thermophoresis [6] which, for not too low pressure, explains the radiometer problem [7]. Temperature jump reduces heat transfer in a rarefied gas [8]. Finally, diffusion slip shows up in a pressure difference in a diffusing mixture in a capillary [9], and in a diffusiophoretic force [10]; see e.g. Ref. [11] for more recent work.

The basic ideas for an explanation of such slip effects are due to Maxwell [3] who used gas kinetic arguments to derive a boundary condition for the flow velocity and to calculate the slip coefficients. A lot of experimental work has been done since then [12] and is still going on, and the theoretical boundary value problem is of interest up to now [13]. Waldmann's engagement into this topic began in 1960 with experiments on diffusiophoresis [10] and on the Kramers-Kistemaker effect [14]; one of the results was an empirical expression for the diffusion slip constant. Following the ideas of Maxwell [3] and of Grad [15], Waldmann [16] derived hydrodynamical boundary conditions from kinetic theory by using a moments expansion of the velocity distribution function of the gas. A quite different approach was introduced [17] with the non-equilibrium thermodynamics of boundary conditions, where the interfacial entropy production plays a fundamental role. Starting from the ordinary hydrodynamical equations, the velocity slip and the temperature jump condition were obtained, and interfacial fluxes were postulated [17]. Furthermore, this method successfully was applied to the evaporation problem [18]. Later on, boundary conditions were derived for generalized hydrodynamics [19] and for linear transport-relaxation equations with arbitrarily many variables [20], [21]. This was the adequate basis for the treatment of thermal transpiration, thermal force and friction force [22], and for heat transfer between parallel plates [23]; in any case, the resulting formulae are valid over a wide pressure range.

Non-equilibrium thermodynamics together with singular interfacial densities was used by several authors for the derivation of boundary conditions for systems with surface tension [24], [25], [26] and for electrodynamics [27].

The interest in the "strange" behaviour of rarefied polyatomic gases in magnetic fields was stimulated by the discovery of Scott e.a. [28] of the thermomagnetic torque. The Scott effect partly could be explained by the Senftleben-Beenakker effect [29] of the thermal stresses [30]. But apart from these Burnett terms originating from the bulk of the gas, there is also a surface contribution due to the "thermomagnetic slip", as Waldmann pointed out [31]. According to Waldmann [31], this boundary layer effect should directly be measurable via the transverse pressure gradient occuring in a polyatomic gas in a rectangular box placed in a

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magnetic field. Indeed, with an ingeneous set up Hulsman e. a. [32] were able to measure this thermomagnetic pressure difference. A detailed theory [33] of this effect was obtained by the use of differential equations and boundary conditions for the angular momentum polarizations [34] present in a polyatomic gas in non-equilibrium, and again non-equilibrium thermodynamics led the way to the boundary conditions. In a further application Knudsen corrections were calculated for the Senftleben-Beenakker effect of viscosity [35] and for flow birefringence [36], stimulated by experimental data of Hulsman e. a. [37] and of Baas e. a. [38], respectively.

Another interesting experiment has been done by Eggermont e. a. [39] who measured, by application of a magnetic field, the transverse heat flux in a streaming polyatomic gas. The bulk contribution to this viscomagnetic heat flux is a Burnett term again and had been given already by Levi e. a. [30], the surface contributions were calculated [40] with the help of boundary conditions derived [34] according to Waldmann's thermodynamic method [17], [20], [21].

Crucial for all these effects in rarefied polyatomic gases is the boundary layer behaviour of polarizations, visualized in [41]. There should also be a possibility of directly detecting these polarizations through birefringence in the boundary layer of a heat conducting polyatomic gas [42].

In [21] boundary conditions had been derived for moments obeying transport-relaxation equations which in turn had been obtained from the linearized Boltzmann equation for the distribution function. The time reversal invariance of the linear collision operator of the kinetic equation led to Onsager symmetries in the boundary conditions by application of the universal postulate of reciprocity [43], [44], [45]. With all this in mind, Waldmann finally made the next step and used non-equilibrium thermodynamics to find boundary conditions for the linearized Boltzmann equation [46]. The result was a linear relation between a flux and a force which consist of the difference and the sum of the distributions of gas atoms approaching and of those leaving the interface, where the connecting interfacial kernel is symmetric and positive. This form of the boundary condition is particularly well suited for solving practical problems: for heat transfer between parallel plates [47], [48], [49], and for plane

Couette flow [49] formal solutions were found which are valid for all Knudsen numbers. The boundary conditions for all the moments are contained in the boundary condition for the distribution function, and the phenomenological slip coefficients are matrix elements of the interfacial kernel [50]. Also the conventional form of the boundary condition [13], [51], [52] as a relation between the distributions of incoming and of outgoing atoms is easily obtained from the new form [50]. Finally, the thermodynamical method has been used to derive new boundary conditions for the distribution operator of a diatomic gas of rotating molecules [53].

Recently, some new aspects of polyatomic Knudsen gases have been studied with the boundary condition in the conventional form, viz. heat transfer in a magnetic field [54], wall induced polarizations in plane Couette flow [55], and more general transport phenomena [56].

In this paper, an addition to Waldmann's solution of heat transfer through a monatomic gas between parallel plates [47], [48], [49] is made. Typical for Waldmann's approach are, firstly, the expansion of the velocity distribution function in terms of special solutions of the linearized Boltzmann equation, the "transport-relaxation eigenfunctions", and, secondly, the use of the new form of the boundary condition for the distribution function [46]. By application of this boundary condition in its original and in its inverse form [49], two different expressions for the heat flux are obtained. This is the basis for giving upper and lower bounds for the heat flux, where the upper bound leads to the exact Knudsen limit. Here, numerical results are stated with the help of one transport-relaxation eigenfunction and its eigenvalue, which are determined approximately. The upper bound obtained in this way is identical with the moment method solution [23] including two "higher moments". For a simple model for the interfacial kernel a detailed numerical study of the bounds is performed. A survey of the literature and a discussion of theoretical methods for solving the heat transfer problem in monatomic gases is found in Cercignani's book [13].

1. Recollection of Waldmann's Results

In this section, the most important results from Waldmann's recent papers [47], [48], [49] on heat transfer are summarized.

Expansion

A monatomic gas (medium I) is confined between two parallel plates made of the same material (medium II). The plates are at rest at $x = \pm d/2$ and have the temperatures

$$T_{\mathrm{II}}(\pm d/2) = T_0 \pm \tfrac{1}{2} \Delta T. \tag{1.1}$$

For small values of $|\Delta T|/T_0 \ll 1$, the relative deviation $\Phi(x, \boldsymbol{p})$ of the distribution function

$$f = f_0(1 + \Phi)$$

of the gas from the Maxwellian

$$f_0 = n_0(2\pi m k_{\mathrm{B}} T_0)^{-3/2}$$
$$\cdot \exp(-\boldsymbol{p} \cdot \boldsymbol{p}/2 m k_{\mathrm{B}} T_0)$$

will be "small" and hence will obey the linearized Boltzmann equation

$$c_x \,\partial \Phi/\partial x + \omega(\Phi) = 0. \tag{1.2}$$

Here, $\boldsymbol{p} = m\,\boldsymbol{c}$ is the momentum of a gas atom with mass m and velocity $\boldsymbol{c}$, k_{B} is Boltzmann's constant, and n_0, T_0 are the equilibrium values of density and temperature, respectively; the equilibrium pressure will be denoted by $P_0 = n_0 k_{\mathrm{B}} T_0$. The solution of the kinetic equation (1.2) with the required symmetry [49] is written as

$$\Phi = \frac{\Delta T}{T_0} \frac{q^*}{d} [-\sqrt{\tfrac{3}{2}} \chi_2 + x(W^2 - \tfrac{5}{2})]$$
$$+ \frac{\Delta T}{T_0} \sum_{i=5}^{\infty} [\tfrac{1}{2}(\psi_i - \psi_{i\mathrm{T}}) \cosh k_i x \tag{1.3}$$
$$- \tfrac{1}{2}(\psi_i + \psi_{i\mathrm{T}}) \sinh k_i x] \frac{C_i}{\sinh(k_i d/2)}.$$

The first two terms represent the Chapman-Enskog solution valid in the bulk of the gas; the function χ_2 which determines thermal conductivity,

$$\lambda = \tfrac{3}{2}(P_0/T_0) \int \chi_2 \,\omega(\chi_2) \,d\gamma,$$

is a solution of the integral equation

$$\omega(\chi_2) = c_x \sqrt{\tfrac{2}{3}} (W^2 - \tfrac{5}{2}). \tag{1.4}$$

The abbreviations

$$d\gamma = (f_0/n_0) \,d^3 p, \quad \boldsymbol{W} = \boldsymbol{p}/\sqrt{2}\,m\,c_0,$$
$$c_0 = (k_{\mathrm{B}} T_0/m)^{1/2}$$

have been introduced above. In Eq. (1.3), the sum extends over all transport-relaxation eigenfunctions [48] $\psi_i(\boldsymbol{p})$ with finite $k_i > 0$; $\psi_{i\mathrm{T}}(\boldsymbol{p}) = \psi_i(-\boldsymbol{p})$. The ψ_i originate from particular solutions

$$\Phi_i(x, \boldsymbol{p}) = \psi_i(\boldsymbol{p}) \exp\{-k_i x\}$$

of the linearized Boltzmann equation (1.2), i.e. they obey the "eigenvalue equation"

$$- k_i c_x \psi_i + \omega(\psi_i) = 0, \tag{1.5}$$

with the "eigenvalues" k_i which are inverse free paths. Hence, these contributions to Φ only play a role close to the walls in a boundary layer with a thickness of several mean free paths.

Here we are mainly interested in the heat flux

$$q_x = P_0 \int c_x (W^2 - \tfrac{5}{2}) \Phi \,d\gamma = - \lambda \frac{\Delta T}{d} q^*, \tag{1.6}$$

i.e. in the constant q^*. The coefficients q^* and C_i have to be determined from the boundary condition for the Boltzmann equation.

Boundary Condition

In Waldmann's formulation, the boundary condition consists of a linear relation

$$\mathscr{J} = \mathfrak{L}\mathscr{F} \tag{1.7}$$

or

$$\mathscr{F} = \mathfrak{L}^{-1} \mathscr{J} \tag{1.8}$$

between the "flux"

$$\mathscr{J} = \frac{1}{\sqrt{2}} P_+(c)(\Phi_{\mathrm{I}\,\mathrm{II}} - \Phi_{\mathrm{I}\,\mathrm{II}\,\mathrm{T}}) \tag{1.9}$$

and the "force"

$$\mathscr{F} = \hat{\mathscr{F}} - v_1(v_1, \hat{\mathscr{F}}),$$
$$\hat{\mathscr{F}} = \frac{1}{\sqrt{2}} P_+(c)(\Phi_{\mathrm{I}\,\mathrm{II}} + \Phi_{\mathrm{I}\,\mathrm{II}\,\mathrm{T}}) \tag{1.10}$$

which are combinations of

$$\Phi_{\mathrm{I}\,\mathrm{II}} = \Phi - \Phi_{\mathrm{II}} = \Phi - \frac{P_{\mathrm{II}} - P_0}{P_0}$$
$$- (W^2 - \tfrac{5}{2}) \frac{T_{\mathrm{II}} - T_0}{T_0} - \boldsymbol{p} \cdot \boldsymbol{v}_{\mathrm{II}}/k_{\mathrm{B}} T_0$$

and of the motion-reversed distribution

$$\Phi_{\mathrm{I}\,\mathrm{II}\,\mathrm{T}}(x, \boldsymbol{p}) = \Phi_{\mathrm{I}\,\mathrm{II}}(x, -\boldsymbol{p}).$$

Here, T_{II} and $\boldsymbol{v}_{\mathrm{II}} = 0$ are the temperature and velocity of the plates, and the "pressure" P_{II} may be determined by [50]

$$\frac{P_{\mathrm{II}} - P_0}{P_0} = \frac{n_{\mathrm{II}} - n_0}{n_0} + \frac{T_{\mathrm{II}} - T_0}{T_0} \tag{1.11}$$
$$= (\Phi, v_1) + \frac{1}{2} \frac{T_{\mathrm{II}} - T_0}{T_0} - \frac{1}{2\hat{c}_0} \boldsymbol{n} \cdot \boldsymbol{v}_{\mathrm{II}}.$$

As the Heaviside function

$$P_+(c) = \begin{cases} 1 \\ 0 \end{cases} \quad \text{for} \quad c \begin{matrix} > 0 \\ < 0 \end{matrix}$$

indicates, the force and flux are functions on the half space with positive normal velocity

$$c = \boldsymbol{c} \cdot \boldsymbol{n}, \quad \boldsymbol{n}: \text{outer unit normal of the gas.}$$

In Eqs. (1.10), (1.11) the function

$$v_1 = P_+(c)$$

occurs, and a half space scalar product has been used:

$$(\boldsymbol{\Phi}, \psi) = \int \boldsymbol{\Phi}\psi \, d\Gamma, \quad (v_1, v_1) = 1,$$

$$d\Gamma = P_+(c) \frac{c}{\hat{c}_0} \, d\gamma, \qquad \hat{c}_0 = c_0/\sqrt{2\pi}.$$

Furthermore, the boundary conditions (1.7), (1.8) have been written in a formal operator notation [50]

$$(\mathfrak{L}\mathscr{F})(x, \boldsymbol{p}) = \int \mathfrak{L}(\boldsymbol{p}, \boldsymbol{p}') \mathscr{F}(x, \boldsymbol{p}') \, d\Gamma'.$$

The operator $\mathfrak{L}$ is symmetric and positive, but, due to the impenetrability of the interface

$$(\mathscr{J}, v_1) = 0,$$

is not definite:

$$\mathfrak{L} v_1 = 0.$$

Therefore, $\mathfrak{L}$ has an "inverse" $\mathfrak{L}^{-1}$ only on the subspace of all half space functions v which are orthogonal to v_1,

$$(v, v_1) = 0.$$

Consequently, the operators $\mathfrak{L}$ and $\mathfrak{L}^{-1}$ obey the relation

$$\mathfrak{L}\mathfrak{L}^{-1} = \mathfrak{L}^{-1}\mathfrak{L} = \mathfrak{E} = \mathfrak{U} - v_1 v_1,$$

where $\mathfrak{U}$ is the half space unity operator. Accordingly, $\mathfrak{L}^{-1}$ also is a symmetric*, positive operator with

$$\mathfrak{L}^{-1} v_1 = 0.$$

If P_{II} is determined from Eq. (1.11), $(\hat{\mathscr{F}}, v_1) = 0$ applies and one has $\mathscr{F} = \hat{\mathscr{F}}$.

Formal Solution

For the evaluation of the boundary condition Eq. (1.7) or Eq. (1.8), the flux and the force with

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* In Ref. [49] this is not the case, however, the results used here are still valid.

Eqs. (1.9), (1.10) and the ansatz (1.3) at $x = d/2$ are rewritten as

$$\mathscr{J} = \frac{1}{\sqrt{2}\,\hat{c}_0} \frac{\varDelta T}{T_0} \tag{1.12}$$

$$\cdot \left\{ -q^* \frac{\lambda T_0}{d P_0} v^2 + \sum_{i=5}^{\infty} v^i \frac{C_i}{k_i \tanh(k_i\, d/2)} \right\},$$

$$\mathscr{F} = -\frac{1}{\sqrt{2}} \frac{\varDelta T}{T_0} \left\{ (1 - q^*)\,[v_2 - v_1(v_1, v_2)] \right.$$

$$\left. + \sum_{i=5}^{\infty} C_i\,[v_i - v_1(v_1, v_i)] \right\}. \tag{1.13}$$

Here, instead of the transport-relaxation eigenfunctions ψ_i, the half space functions v_i, v^i, orthogonalized according to [49]

$$(v_i, v^{i'}) = \delta_i^{i'} \tag{1.14}$$

have been used:

$$v_i = P_+(c)\,(\psi_i + \psi_{i\mathrm{T}}), \tag{1.15}$$
$$v^i = P_+(c)\,\hat{c}_0\,k_i(\psi_i - \psi_{i\mathrm{T}}), \quad i \geqq 5,$$

and

$$v_1 = P_+(c), \qquad v^1 = P_+(c)\,2\hat{c}_0\,p_x/k_\mathrm{B}T_0,$$

$$v_2 = P_+(c)\,(W^2 - \tfrac{5}{2}), \quad v^2 = P_+(c)\,\sqrt{6}\,\frac{P_0\,\hat{c}_0}{\lambda T_0}\,\chi_2,$$

$$v_3 = P_+(c)\,\frac{P_0}{\eta\,c_0}\,\chi_4, \qquad v^3 = P_+(c)\,2\hat{c}_0\,p_y/k_\mathrm{B}T_0,$$

$$v_4 = P_+(c)\,\frac{P_0}{\eta\,c_0}\,\chi_5, \qquad v^4 = P_+(c)\,2\hat{c}_0\,p_z/k_\mathrm{B}T_0;$$

$$\tag{1.16}$$

by η the shear viscosity is denoted, and χ_4, χ_5 are the viscosity Chapman-Enskog functions [49].

From the positivity of the interfacial entropy production

$$d\dot{S}_\sigma/d\sigma = \frac{P_0}{T_0}\,\hat{c}_0(\mathscr{J}, \mathscr{F}) = \frac{P_0}{T_0}\,\frac{1}{2}\left(\frac{\varDelta T}{T_0}\right)^2$$

$$\cdot \left\{ q^*(1 - q^*)\frac{\lambda T_0}{d P_0} - \sum_{i=5}^{\infty} \frac{C_i^2}{k_i \tanh(k_i\, d/2)} \right\}$$

one easily gets the inequality

$$q^*(1 - q^*) > 0$$

or

$$0 < q^* < 1, \tag{1.17}$$

i.e. for any Knudsen number l/d, the heat flux q_x has the same sign as the hydrodynamic limit

$$q_x{}^h = -\lambda \varDelta T/d,$$

and its magnitude is smaller than that of $q_x{}^h$. According to Eq. (1.17), q^* is written as

$$q^* = 1 \Big/ \left[1 + 2\frac{l}{d} g\left(\frac{l}{d}\right) \right], \quad g > 0, \qquad (1.18)$$

with the mean free path l defined by thermal conductivity via

$$\lambda = \frac{15}{4} \frac{P_0}{T_0} c_0 l.$$

The quantity

$$g_0 \equiv g(l/d = 0)$$

is the temperature jump coefficient for heat transfer through a gas between parallel plates. This becomes clear from a discussion of the temperature profile in the gas:

$$T(x) = T_0 + \tfrac{2}{3} T_0 \int (W^2 - \tfrac{3}{2}) \Phi(x, p) \, d\gamma$$
$$= T_0 + q^* \frac{\Delta T}{d} x - \Delta T \sum_{i=5}^{\infty} C_i \frac{\sinh k_i x}{\sinh(k_i d/2)} \frac{2}{3}$$
$$\cdot \int (W^2 - \tfrac{3}{2}) \psi_i \, d\gamma.$$

For small Knudsen numbers l/d, the terms in the sum only play a role at the plates $x = \pm d/2$ and in a small boundary layer of thickness l. Several free paths away from the walls, the temperature profile is identical with the linear bulk profile

$$T_b(x) = T_0 + q^* \frac{\Delta T}{d} x.$$

Since q^* is smaller than unity, the effective temperature gradient $q^* \Delta T/d$ in the bulk of the gas is smaller than the applied gradient $\Delta T/d$. Hence, the value of the bulk temperature extrapolated up to the wall is smaller than the wall temperature or, in other words, the relative temperature jump

$$\frac{T_{\mathrm{II}}(d/2) - T_b(d/2)}{T_{\mathrm{II}}(d/2) - T_{\mathrm{II}}(-d/2)} = \frac{1}{2} (1 - q^*)$$
$$= \frac{l}{d} \frac{g}{1 + 2(l/d)g} > 0$$

is positive. In lowest order in l/d, the right hand side of this relation can be replaced by $(l/d)g_0$, so that g_0 may be called the temperature jump coefficient. Further discussions are found in Waldmann's papers [48], [49].

From the boundary condition (1.7) linear equations

$$(v_i, \mathcal{J}) = (v_i, \mathfrak{L}\mathcal{F}), \quad i = 2, \quad i \geq 5,$$

for q^* and C_i are obtained which can easily be solved [48] for q^*, respectively g:

$$g = [L_{22} - \sum_{i=5}^{\infty} \sum_{i'=5}^{\infty} L_{2i} M_{ii'}^{-1} L_{i'2}]^{-1}. \qquad (1.19)$$

Hence, the heat flux is determined by the **matrix** elements

$$L_{ii'} = \frac{8}{15} \frac{1}{\sqrt{2\pi}} (v_i, \mathfrak{L} v_{i'}),$$
$$i, i' = 2 \quad \text{and} \quad \geq 5, \qquad (1.20)$$

of the $\mathfrak{L}$-operator, and by the inverse (in the usual sense) of the symmetric, positive definite matrix

$$M_{ii'} = L_{ii'} + \delta_{ii'} \left(\frac{15}{8} c_0 k_i \tanh \frac{k_i d}{2} \right)^{-1},$$
$$i, i' \geq 5. \qquad (1.21)$$

From the positivity of $M_{ii'}^{-1}$ and from the symmetry $L_{i'2} = L_{2i'}$ one easily gets an upper bound for q^*:

$$q^* \leq 1 \Big/ \left[1 + 2\frac{l}{d} \frac{1}{L_{22}} \right] \equiv q^*_{\max}. \qquad (1.22)$$

Now, the boundary condition in the inverse form (1.8) is transformed into another set of linear equations

$$(v^i, \mathcal{F}) = (v^i, \mathfrak{L}^{-1} \mathcal{J}), \quad i = 2, \quad i \geq 5,$$

for q^* and C_i which yields an alternative expression for g:

$$g = K_{22} - \sum_{i=5}^{\infty} \sum_{i'=5}^{\infty} K_{2i} N_{ii'}^{-1} K_{i'2}. \qquad (1.23)$$

Here, the matrix elements

$$K_{ii'} = \frac{15}{8} \sqrt{2\pi} (v^i, \mathfrak{L}^{-1} v^{i'}),$$
$$i, i' = 2 \quad \text{and} \quad \geq 5 \qquad (1.24)$$

of the operator $\mathfrak{L}^{-1}$, and the inverse of the symmetric, positive definite matrix

$$N_{ii'} = K_{ii'} + \delta_{ii'} \frac{15}{8} c_0 k_i \tanh \frac{k_i d}{2},$$
$$i, i' \geq 5, \qquad (1.25)$$

occur. The positivity of $N_{ii'}^{-1}$ and the symmetry $K_{i'2} = K_{2i'}$ now lead to a lower bound for q^*:

$$q^*_{\min} \equiv \frac{1}{1 + 2(l/d) K_{22}} \leq q^*. \qquad (1.26)$$

The lower bound $1/L_{22}$ and the upper bound K_{22} for the temperature jump coefficient g_0 have already been given by Waldmann and Vestner [49].

In the next section, more refined bounds for q^* will be derived.

2. Refined Upper and Lower Bounds for the Heat Flux

The simple bounds (1.22) and (1.26) for q^* have been obtained from Eq. (1.19), resp. Eq. (1.23), by completely neglecting the infinite sum. Now, in a better approximation we replace the sum by one term, i.e. we take into account one of the transport-relaxation eigenfunctions ψ_i, $i \geq 5$, with positive eigenvalue k_i; this one function is called ψ_5. The inequality

$$\sum_{i=5}^{\infty} \sum_{i'=5}^{\infty} L_{2i} M_{ii'}^{-1} L_{2i'} \geq L_{25}^2 / M_{55} \qquad (2.1)$$

is the basis for the following estimates. For a symmetric, positive definite $n \times n$ matrix $M_{ii'}$ of finite dimension n this relation derives from the fact that the matrix

$$\hat{M}_{ii'} \equiv M_{ii'}^{-1} - \delta_{ii_o} \delta_{i'i_o} (1/M_{i_o i_o})$$

is symmetric and positive semi-definite (and has rank $n-1$). We assume that Eq. (2.1) also applies for matrices of infinite dimension.

From Eqs. (1.19) and (2.1) we get a lower bound g_L

$$g \geq g_L \equiv [L_{22} - L_{25}^2 / M_{55}]^{-1} \geq 1/L_{22} \qquad (2.2)$$

for the function g, i.e. an upper bound q_L^* for the heat flux, which is smaller than q_{max}^* from Eq. (1.22):

$$q^* \leq q_L^* \equiv \frac{1}{1 + 2(l/d)g_L} \leq q_{max}^* . \qquad (2.3)$$

Similarly, Eqs. (1.23) and (2.1), via

$$g \leq g_K \equiv K_{22} - K_{25}^2 / N_{55} \leq K_{22} , \qquad (2.4)$$

lead to a lower bound q_K^*

$$q^* \geq q_K^* \equiv \frac{1}{1 + 2(l/d)g_K} \geq q_{min}^* \qquad (2.5)$$

for q^*, which is larger than q_{min}^* from Eq. (1.26). Consequently, the new bounds q_K^*, q_L^* for q^* are narrower than the simple bounds q_{min}^*, q_{max}^*.

By insertion of the expressions (1.21) for M_{55} and (1.25) for N_{55} into Eqs. (2.2) and (2.4), respectively, explicit results are obtained for

$$g_L = \frac{1}{C_{22}} \frac{C_{55} + 1/G_5}{C_{55} - C_{25}^2 / C_{22} + 1/G_5} \qquad (2.6)$$

and for

$$g_K = D_{22} \frac{D_{55} - D_{25}^2 / D_{22} + G_5}{D_{55} + G_5} . \qquad (2.7)$$

Instead of $L_{ii'}$, $K_{ii'}$ the dimensionless coefficients $C_{ii'}$, $D_{ii'}$ have been introduced,

$$C_{22} = L_{22} , \quad C_{25} = \sqrt{\frac{5 c_0}{8 l}} L_{25} ,$$

$$C_{55} = \frac{5 c_0}{8 l} L_{55} , \qquad (2.8)$$

$$D_{22} = K_{22} , \quad D_{25} = \sqrt{\frac{8 l}{5 c_0}} K_{25} ,$$

$$D_{55} = \frac{8 l}{5 c_0} K_{55} ; \qquad (2.9)$$

the function G_5 contains the dependence on the Knudsen number l/d of g_L, g_K:

$$G_5 = 3 k_5 l \tanh \frac{k_5 d}{2} . \qquad (2.10)$$

Since the quantities k_5, ψ_5, χ_2 depend on the mean free path l like [48]

$$k_5 \propto l^{-1} , \quad \psi_5 \propto l^{1/2} , \quad \chi_2 \propto l ,$$

the coefficients $C_{ii'}$ and $D_{ii'}$ are independent of l. It should be noted that upper and lower bound coincide,

$$g_L = g_K ,$$

if the 2×2 matrices

$$\begin{pmatrix} C_{22} & C_{25} \\ C_{25} & C_{55} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} D_{22} & D_{25} \\ D_{25} & D_{55} \end{pmatrix}$$

are inverse to each other.

In the Knudsen limit $l/d \to \infty$, with

$$G_5 \approx \tfrac{3}{2} k_5 l k_5 d \propto d/l \to 0 ,$$

the lower bounds q_K^* and q_{min}^* tend towards

$$q_{K\infty}^* = \frac{d}{2 l} [D_{22} - D_{25}^2 / D_{55}]^{-1} ,$$

$$q_{min\infty}^* = \frac{d}{2 l} \frac{1}{D_{22}} , \qquad (2.11)$$

whereas the upper bounds q_L^* and q_{max}^* get identical,

$$q_{L\infty}^* = q_{max\infty}^* = \frac{d}{2 l} C_{22} \equiv q_{\infty}^* , \qquad (2.12)$$

and lead to the correct limit [49]

$$q_{x\infty} = -P_0 c_0 \frac{\Delta T}{T_0} \frac{15}{8} L_{22} \qquad (2.13)$$

of the heat flux.

In the hydrodynamic limit $l/d \to 0$, with a constant value

$$G_5 \approx 3 k_5 l$$

for G_5, the functions g_L and g_K become independent of l and give bounds for the temperature jump coefficient g_0,

$$1/C_{22} \leqq g_L(l/d = 0) \leqq g_0$$
$$\leqq g_K(l/d = 0) \leqq D_{22}, \qquad (2.14)$$

which are narrower than those given earlier [49].

3. Approximate Determination of a Transport-Relaxation Eigenfunction

The transport-relaxation eigenfunction ψ_5, like the distribution Φ, is rotationally symmetrical about the W_x-axis [49], hence it has the form

$$\psi_5 = \psi^{(0)}(W_x{}^2, W^2) + W_x \psi^{(1)}(W_x{}^2, W^2). \qquad (3.1)$$

For any ψ_i and its eigenvalue k_i the "Boltzmann equation"

$$-k_i c_x \psi_i + \omega(\psi_i) = 0 \qquad (3.2)$$

and the ortho-normalization properties [49]

$$\int \psi_i c_x \psi_{i'} \, d\gamma = (1/k_i) \delta_{ii'} \qquad (3.3)$$

have to be fulfilled.

In the following, a function ψ_5 of the type (3.1) will be determined such that Eq. (3.3) applies for $i = \pm 5$ and $1 \leqq |i'| \leqq 5$, and that Eq. (3.2) is „fulfilled on the average". This will be done for Maxwell molecules since the eigenfunctions $\Phi_{\mu_1 \ldots \mu_l}^{(r)}$ and eigenvalues ω_{lr} of the linearized collision operator ω

$$\omega(\Phi_{\mu_1 \ldots \mu_l}^{(r)}) = \omega_{lr} \Phi_{\mu_1 \ldots \mu_l}^{(r)} \qquad (3.4)$$

are known in this case: the eigenfunctions are the product of a Sonine-polynomial and a symmetric traceless tensor of rank l [57], [58]

$$\Phi_{\mu_1 \ldots \mu_l}^{(r)} = \left[\frac{r!(2l+1)!! \frac{1}{2} \sqrt{\pi}}{l! \, \Gamma(l+r+\frac{3}{2})} \right]^{1/2} \cdot S_{l+\frac{1}{2}}^{(r)}(W^2) \overline{W_{\mu_1} \ldots W_{\mu_l}}. \qquad (3.5)$$

Hence, the Chapman-Enskog function χ_2 is proportional to $\Phi_x^{(1)}$ and is given by

$$\chi_2 = l\sqrt{3}\, W_x(W^2 - \tfrac{5}{2}).$$

The transport constants η, λ are expressed by the relaxation coefficients ω_{20}, ω_{11},

$$\eta = \frac{P_0}{\omega_{20}}, \quad \lambda = \frac{5}{2} \frac{P_0}{T_0} \frac{c_0{}^2}{\omega_{11}},$$

and, due to

$$\omega_{11} = \tfrac{2}{3}\, \omega_{20},$$

l is identical with the viscosity free path

$$l = c_0/\omega_{20}.$$

First, it is noted that the orthogonality (3.3) for $i = \pm 5$ and $1 \leqq |i'| \leqq 4$ is fulfilled if the relations

$$\int \varphi\, c_x \psi_5 \, d\gamma = 0$$

apply for

$$\varphi = \Phi^{(0)}, \Phi^{(1)}, \Phi_\mu^{(0)}, \chi_2, \chi_4, \chi_5.$$

With Eq. (3.1) this leads to the conditions

$$\int \Phi_x^{(r)} W_x \psi^{(s)} \, d\gamma = 0, \quad r, s = 0, 1. \qquad (3.6)$$

For $i = i' = \pm 5$, Eq. (3.3) yields

$$\int W_x \psi^{(0)} W_x \psi^{(1)} \, d\gamma = 1/2 \sqrt{2}\, c_0 k_5. \qquad (3.7)$$

If we assume that $\psi^{(0)}$ and $\psi^{(1)}$ only depend on W^2, and if we then choose

$$W_x \psi^{(s)} = \sum_{r \geqq 2} a_r^{(s)} \Phi_x^{(r)}, \quad s = 0, 1, \qquad (3.8)$$

as trial functions, Eqs. (3.6) are trivially fulfilled due to the orthogonality of the eigenfunctions $\Phi_x^{(r)}$. From Eq. (3.7) and the ortho-normalization of the $\Phi_x^{(r)}$ the relation

$$\sum_{r \geqq 2} a_r^{(0)} a_r^{(1)} = 1/2 \sqrt{2}\, c_0 k_5 \qquad (3.9)$$

is obtained. According to Eqs. (3.1) and (3.8) the transport-relaxation eigenfunction ψ_5 is written as

$$\psi_5 = \sqrt{\frac{8}{15}}\, a_2 \left(\frac{5}{2} - W^2 \right) + \sum_{r \geqq 2} [a_r \Phi^{(r)} + a_r^{(1)} \Phi_x^{(r)}], \qquad (3.10)$$

where the coefficients $a_r^{(0)}$ and a_r are simply inter-related, e.g.

$$a_2^{(0)} = \sqrt{\frac{7}{6}}\, a_2 - a_3, \quad a_3^{(0)} = \sqrt{\frac{3}{2}}\, a_3 - \sqrt{\frac{4}{3}}\, a_4. \qquad (3.11)$$

Next, the left hand side of Eq. (3.2) is evaluated for $i = 5$. For the "streaming term" the relations (3.1) and (3.8) are used, and for the collision term the ansatz (3.10) is inserted. With the choice

$$a_r^{(1)} = \frac{k_5 c_0 \sqrt{2}}{\omega_{1r}} a_r^{(0)}, \quad r \geqq 2, \qquad (3.12)$$

still two non-compensating functions of momentum remain in the sum,

$$- k_5 c_x \psi_5 + \omega(\psi_5) \qquad (3.13)$$
$$= \sum_{r \geqq 2} [a_r \omega_{0r} \Phi^{(r)} - a_r^{(1)} k_5 c_0 \sqrt{2} W_x \Phi_x^{(r)}].$$

As can be easily seen, the right hand side of Eq. (3.13) is orthogonal to $\Phi^{(0)}$ and $\Phi^{(1)}$; we now require that this is true also for the higher order scalar functions $\Phi^{(2)}, \Phi^{(3)}, \ldots$:

$$\int \mathrm{d}\gamma \, \Phi^{(s)} \sum_{r \geqq 2} [a_r \omega_{0r} \Phi^{(r)} - a_r^{(1)} k_5 c_0 \sqrt{2} W_x \Phi_x^{(r)}] = 0,$$
$$s \geqq 0. \qquad (3.14)$$

With the ansatz (3.10) for ψ_5, Eq. (3.2) cannot be fulfilled exactly, we instead postulate the validity of the integral conditions (3.14), so that the "Boltzmann equation" is fulfilled on the average:

$$\int \mathrm{d}\gamma \, \Phi^{(s)} [- k_5 c_x \psi_5 + \omega(\psi_5)] = 0, \quad s \geqq 0.$$

From Eqs. (3.14) another set of relations between the coefficients a_r and $a_r^{(1)}$ is obtained,

$$a_r = \frac{k_5 c_0 \sqrt{2}}{\omega_{0r}} \sum_{s \geqq 2} a_s^{(1)} \int \mathrm{d}\gamma \, \Phi_x^{(s)} W_x \Phi^{(r)}, \quad r \geqq 2; \quad (3.15)$$

in particular for $r = 2$ one gets

$$a_2 = \sqrt{\frac{7}{3}} \frac{k_5 c_0}{\omega_{02}} a_2^{(1)}. \qquad (3.16)$$

Now, with the help of Eq. (3.12), the coefficient $a_s^{(1)}$ in Eq. (3.15) is replaced by $a_s^{(0)}$, and by relations of the type (3.11), $a_s^{(0)}$ is expressed by a linear combination of a_r. As a result one gets eigenvalue equations for the a_r with eigenvalue $1/k_5^2$.

Here, we make the most simple approximation by taking into account only one scalar and one vector in the sum of Eq. (3.10), viz. $\Phi^{(2)}$ and $\Phi_x^{(2)}$. From Eqs. (3.11), (3.12) one gets

$$a_2^{(0)} = \sqrt{\frac{7}{6}} a_2, \quad a_2^{(1)} = \sqrt{\frac{7}{3}} \frac{k_5 c_0}{\omega_{12}} a_2,$$

and from Eq. (3.16),

$$a_2 = \frac{7}{3} \frac{(k_5 c_0)^2}{\omega_{02} \omega_{12}} a_2,$$

the eigenvalue k_5 is obtained as

$$k_5 = \frac{1}{c_0} \sqrt{\frac{3}{7} \omega_{02} \omega_{12}} = \sqrt{\frac{2}{7}} / l; \qquad (3.17)$$

the relations

$$\omega_{02} = \tfrac{2}{3} \omega_{12} = \tfrac{2}{3} \omega_{20}$$

for Maxwell molecules have been used. With all these results, Eq. (3.9) finally leads to an expression for a_2:

$$a_2 = \sqrt{3/4 \, \omega_{20}}.$$

According to Eq. (3.10), the approximate transport-relaxation eigenfunction ψ_5 is given by

$$\psi_5 = \frac{1}{\sqrt{10 \, \omega_{20}}} \qquad (3.18)$$
$$\cdot \left(W^4 - 7 W^2 + \frac{35}{4} \right) \left(1 + \sqrt{\frac{4}{7}} W_x \right),$$

and from Eqs. (1.15) the following expressions for the half space functions v_5 and v^5 are derived:

$$v_5 = P_+(c) \sqrt{\frac{2}{5 \, \omega_{20}}} \left(W^4 - 7 W^2 + \frac{35}{4} \right), \qquad (3.19)$$

$$v^5 = P_+(c) \frac{4}{7} \sqrt{\frac{\omega_{20}}{10 \, \pi}} W_x \left(W^4 - 7 W^2 + \frac{35}{4} \right). \qquad (3.20)$$

The coefficients $C_{ii'}$ and $D_{ii'}$ can now be calculated from Eqs. (1.16), (1.20), (2.8), (3.19) and (1.24), (2.9), (3.20) as matrix elements of the operators $\mathfrak{L}$ and $\mathfrak{L}^{-1}$, respectively. Then, the upper bound q_L^* for the heat flux, as obtained from Eqs. (2.3) and (2.6), is identical with the higher moments solution derived earlier [23], where the coefficients C_{qq}, C_{qA}, C_{AA} are equal to the present C_{22}, C_{25}, C_{55} [50]. In contradistinction to the moment method approach [23] which gives one approximate expression for the heat flux q^*, the kinetic treatment of the heat transfer problem leads to two approximate expressions q_L^*, q_K^* which are upper (q_L^*) and lower bounds (q_K^*, see Eqs. (2.5), (2.7)) for the exact q^*.

4. Numerical Results

Numerical results are presented for the special model for the interfacial kernel

$$\mathfrak{L} = \frac{\alpha}{2 - \alpha} \mathfrak{P}^{(1)} + \frac{\alpha_{\mathrm{odd}}}{2 - \alpha_{\mathrm{odd}}} \mathfrak{P}^{(-1)}, \qquad (4.1)$$

$$\mathfrak{L}^{-1} = \frac{2-\alpha}{\alpha}\,\mathfrak{P}^{(1)} + \frac{2-\alpha_{\text{odd}}}{\alpha_{\text{odd}}}\,\mathfrak{P}^{(-1)}\,, \qquad (4.2)$$

containing two accommodation coefficients α and α_{odd} [50]. The projection operators

$$\mathfrak{P}^{(1)}(\boldsymbol{p},\boldsymbol{p}') = P_+(c)\,P_+(c') \qquad\qquad (4.3)$$

$$\cdot\left\{\frac{1}{2}[\delta(\boldsymbol{p},\boldsymbol{p}')+\delta(\boldsymbol{p},-\boldsymbol{p}'+2\boldsymbol{n}\boldsymbol{n}\cdot\boldsymbol{p}')]\frac{\dot{c}_0\,\mathrm{d}^3p'}{c'\,\mathrm{d}\gamma'}-1\right\},$$

$$\mathfrak{P}^{(-1)}(\boldsymbol{p},\boldsymbol{p}') = P_+(c)\,P_+(c') \qquad\qquad (4.4)$$

$$\cdot\tfrac{1}{2}[\delta(\boldsymbol{p},\boldsymbol{p}')-\delta(\boldsymbol{p},-\boldsymbol{p}'+2\boldsymbol{n}\boldsymbol{n}\cdot\boldsymbol{p}')]\frac{\dot{c}_0\,\mathrm{d}^3p'}{c'\,\mathrm{d}\gamma'}$$

have the properties

$$\mathfrak{P}^{(m)}\,\mathfrak{P}^{(m')} = \delta_{mm'}\,\mathfrak{P}^{(m)}\,, \quad m,m' = \pm 1\,, \quad (4.5)$$

$$\mathfrak{P}^{(1)} + \mathfrak{P}^{(-1)} = \mathfrak{E} = \mathfrak{U} - v_1 v_1\,. \qquad (4.6)$$

Since the functions v_2, v_5, v^2, v^5 are even in the tangential velocity, only the operator $\mathfrak{P}^{(1)}$ plays a role in the matrix elements $C_{ii'}$ and $D_{ii'}$. With

$$\mathfrak{P}^{(1)}\,v_2 = v_2 + v_1\,, \quad \mathfrak{P}^{(1)}\,v_5 = v_5 - \frac{3}{4}\sqrt{\frac{2}{5\,\omega_{20}}}\,v_1\,,$$

$$\mathfrak{P}^{(1)}\,v^2 = v^2\,, \qquad\quad \mathfrak{P}^{(1)}\,v^5 = v^5$$

one easily finds the following results:

$$C_{22} = \frac{8}{15}\sqrt{\frac{2}{\pi}}\frac{\alpha}{2-\alpha}\,, \quad C_{25} = -\frac{4}{15}\sqrt{\frac{2}{\pi}}\frac{\alpha}{2-\alpha}\,,$$

$$C_{55} = \frac{14}{15}\sqrt{\frac{2}{\pi}}\frac{\alpha}{2-\alpha}\,, \qquad\qquad (4.7)$$

$$D_{22} = \frac{39}{10}\sqrt{\frac{2}{\pi}}\frac{2-\alpha}{\alpha}\,, \quad D_{25} = \frac{69}{70}\sqrt{\frac{2}{\pi}}\frac{2-\alpha}{\alpha}\,,$$

$$D_{55} = \frac{1299}{490}\sqrt{\frac{2}{\pi}}\frac{2-\alpha}{\alpha}\,. \qquad\qquad (4.8)$$

According to Eq. (2.11), the Knudsen limit for the lower bound q_{K}^* is still about $17\,^0/_0$ smaller than the exact value,

$$q_{\text{K}\infty}^* = \frac{25\,\pi}{104}\frac{5629}{5100}\,q_\infty^* = 0.834\,q_\infty^*\,, \qquad (4.9)$$

but is closer to q_∞^* than the limit of the simple bound

$$q_{\text{min}\,\infty}^* = \frac{25\,\pi}{104}\,q_\infty^* = 0.755\,q_\infty^*\,. \qquad (4.10)$$

After insertion of the values (4.7), (4.8) for $C_{ii'}$, $D_{ii'}$ into the expressions (2.6), (2.7) for g_{L} and g_{K}, re-

spectively, it can easily be proven that the ratio

$$r\!\left(\frac{k_5\,d}{2}\,,\alpha\right) \equiv g_{\text{L}}/g_{\text{K}}$$

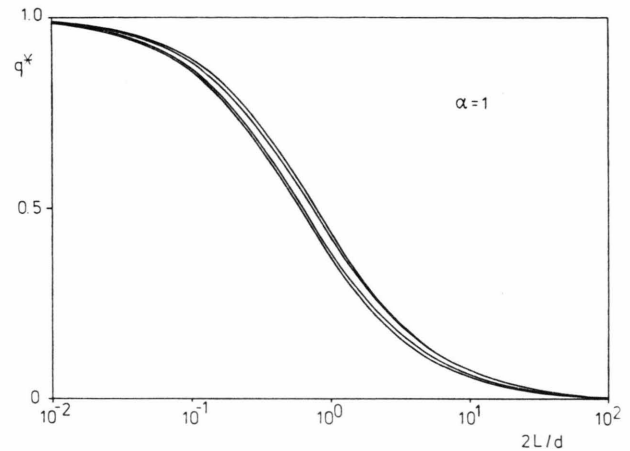is a monotonously increasing function of the inverse Knudsen number $k_5 d/2$ and of the accommodation

Fig. 1. Reduced heat flux q^*, see Eq. (1.6), for complete accommodation ($\alpha = 1.0$) as a function of $(k_5 d/2)^{-1} \equiv 2\,L/d$. The curves represent, from below, the successive approximations

$$q_{\text{min}}^* < q_{\text{K}}^* < q_{\text{L}}^* < q_{\text{max}}^*$$

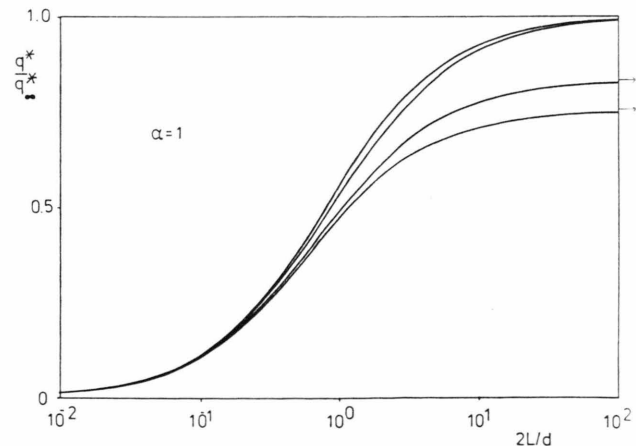for q^*, cf. Eqs. (1.26), (2.5), (2.3), (1.22) together with Eqs. (2.6), (2.7) and (4.7), (4.8).

Fig. 2. Heat flux scaled with the Knudsen limit q_∞^* from Eq. (2.12) for complete accommodation ($\alpha = 1.0$) as a function of $2\,L/d$. The curves are in the same order as in Figure 1. The arrows on the right indicate the Knudsen limits $q_{\text{min}\,\infty}^*/q_\infty^* = 0.755$ and $q_{\text{K}\,\infty}^*/q_\infty^* = 0.834$, respectively.

coefficient α ($0 \leqq \alpha \leqq 1$). Thus, r lies between rather narrow bounds:

$$0.834 = r(0, \alpha) \leqq r\left(\frac{k_5 d}{2}, \alpha\right)$$
$$\leqq r(\infty, \alpha) \leqq r(\infty, 1) = 0.865 . \qquad (4.11)$$

The value for the temperature jump coefficient g_0 can now be estimated with Eq. (2.14); for $\alpha = 1.0$ and $\alpha = 0.85$ inequalities are noted, including numbers for $1/C_{22}$, $g_{\mathrm{L}}(l/d = 0)$, $g_{\mathrm{K}}(l/d = 0)$ and D_{22}:

$$2.350 < 2.548 < g_0 < 2.945 < 3.111 \quad \text{for } \alpha = 1.0 ,$$

and

$$3.179 < 3.408 < g_0 < 3.956 < 4.210 \quad \text{for } \alpha = 0.85 .$$

For $\alpha = 1.0$, the reduced heat flux q^* (i.e. the heat flux scaled with the hydrodynamic limit) is plotted versus the Knudsen number

$$(k_5 d/2)^{-1} \equiv 2 L/d$$

in Figure 1. The four curves are the upper bounds $q_{\max}^*$, q_{L}^* and the lower bounds q_{K}^*, $q_{\min}^*$. The true value of q^* lies between the two inner curves, and for large Knudsen numbers will be close to the upper bound q_{L}^* which contains the exact Knudsen limit. In Fig. 2, the plot of the heat flux scaled with the Knudsen limit more clearly reveals, for large $2 L/d$, the quality of the different approximations.

It should be possible to find a suitable transport-relaxation eigenfunction that leads to bounds for the heat flux which are narrower than those given above.

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