

Boundary Conditions for the Distribution Function and for the Moments of a Gas at a Moving Wall

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As a slight generalization of previous work [1], boundary conditions for the distribution function of a monatomic gas at a moving solid or liquid wall are derived from the interfacial entropy production. The new scheme is compared with the conventional one. Boundary conditions for a set of moments of the distribution function are obtained by taking the corresponding moments of the new kinetic boundary condition. With a special set, the details are worked out. Finally, a simple two-parameter model for the interfacial kernel is designed and discussed.

In a recent paper [1], boundary conditions have been derived for the linearized Boltzmann equation using the concepts of reciprocity [2] and of interfacial entropy production [5]. With this method, the boundary conditions are obtained as a linear functional relation between “fluxes” and “forces” at the interface. Essentially, the flux and the force are given by the difference and the sum, respectively, of the distribution function itself and its motion-reversed counterpart, both taken for particles approaching the wall. The new form of the boundary conditions is well suited for applications, e.g. for the treatment of the heat transfer between parallel plates [3], or for the derivation of slip boundary conditions [1]. This is not surprising since the method originated from the study of boundary conditions for transport-relaxation equations [2], [4], [5].

Hitherto [1], the interface has been taken to be at rest. This restriction is dropped now and conditions are derived for the distribution function of a monatomic gas bounded by a moving solid or liquid wall. To this end, the interfacial entropy production is expressed by the components normal to the wall of the entropy fluxes in the gas and in the solid. From the beginning, the local conservation laws at the interface are incorporated. As a result, the interfacial entropy production is obtained as a bilinear expression in one “mixed” flux J_{IH} and one “mixed” force F_{IH} . This force-flux pair contains the distribution function, the motion-reversed distribution function, and the temperature and velocity of the wall. As in Ref. [1], the boundary condition is set up as a linear relation between the

flux and the force. The interfacial kernel which establishes this relation is the same as in Ref. [1] since it only depends on the particle momenta and on the equilibrium parameters of gas and wall. For a wall at rest, the previous result [1] is of course regained.

In the preceding literature, the boundary conditions have been stated as a relation between the distribution functions of the particles leaving and approaching the wall [6]. The interrelations between the different kernels occurring in the old [6] and in the new [1] method will be discussed in detail.

In practice, the linearized Boltzmann equation is frequently replaced by transport-relaxation equations for moments of the distribution function [7]. Boundary conditions for these moments are easily obtained from the new form of the boundary condition for the distribution function. First, the general procedure is described including Cartesian tensors up to rank three. Then the specialization to the small set of boundary conditions of Ref. [8] is made; in particular, their phenomenological surface coefficients are expressed as matrix elements of the interfacial kernel.

Finally, a simple but flexible model for the interfacial kernel is developed. Its two parameters characterize the fraction of particles which are reflected from the wall specularly and in backward direction. The remaining particles are scattered thermally. Explicit formulae for phenomenological surface coefficients in terms of the parameters are given.

1. Interfacial Entropy Production

The monatomic gas is described by the one-particle distribution function $f(t, \mathbf{x}, \mathbf{p})$ which depends on the time t , on the position \mathbf{x} and on the momen-

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tum $\mathbf{p} = m\mathbf{c}$ of the particle with mass m . Integration of f over momentum space gives the number density n ,

$$\int f(t, \mathbf{x}, \mathbf{p}) d^3p = n(t, \mathbf{x}). \quad (1.1)$$

The H-theorem of the quadratic Boltzmann equation for f states that the local non-equilibrium entropy density

$$s = -k \int f [\ln(fh^3) - 1] d^3p \quad (1.2)$$

changes according to the rate equation

$$\frac{\partial s}{\partial t} + \frac{\partial}{\partial \mathbf{x}_r} (s v_r + s_r) = \left(\frac{\delta s}{\delta t} \right)_{\text{irrev}}, \quad (1.3)$$

with a positive bulk entropy production rate $(\delta s / \delta t)_{\text{irrev}}$, see e.g. Ref. [9]. By k Boltzmann's constant is denoted, Planck's constant h is used to make the argument of the logarithm dimensionless in the correct way. In the divergence term of Eq. (1.3), $s v_r$ is the convective transport of entropy due to the local gas velocity

$$v_r = \frac{1}{n} \int c_r f d^3p, \quad (1.4)$$

and

$$s_r = -k \int (c_r - v_r) \ln(fh^3) f d^3p \quad (1.5)$$

is the (non-convective) entropy flux.

Since the gas (medium I) is bounded by a solid or liquid body (medium II), entropy is produced not only in the bulk media but also at the interface $\sigma_{\text{I II}}$. If we assume that the interface itself does not carry entropy, the interfacial entropy production is only due to the discontinuity of the normal entropy fluxes from the gas and from the wall [4, 5]:

$$\begin{aligned} \dot{S}_\sigma &= - \int_{\sigma_{\text{I II}}} d\sigma [\mathbf{n}_I \cdot \mathbf{s} + \mathbf{n}_{\text{II}} \cdot \mathbf{s}_{\text{II}}] \\ &= - \int_{\sigma_{\text{I II}}} d\sigma \mathbf{n}_I \cdot [\mathbf{s} - \mathbf{s}_{\text{II}}]; \end{aligned} \quad (1.6)$$

\mathbf{n}_I is the outer unit normal of the gas and $\mathbf{n}_{\text{II}} = -\mathbf{n}_I$ that of the wall. For the entropy flux in the wall the most simple expression is used, viz. the heat flux divided by the temperature,

$$\mathbf{s}_{\text{II}} = \mathbf{q}_{\text{II}} T_{\text{II}}^{-1}. \quad (1.7)$$

For the explicit calculation of \dot{S}_σ , the conservation laws at the interface $\sigma_{\text{I II}}$ have to be taken into account. These stem from the impenetrability for matter of $\sigma_{\text{I II}}$ and from the conservation of total energy and momentum [4]. In detail, this means i) the continuity of local normal velocities

$$\mathbf{n}_I \cdot \mathbf{v} + \mathbf{n}_{\text{II}} \cdot \mathbf{v}_{\text{II}} = 0, \quad (1.8)$$

the continuity of ii) the integrated fluxes of energy

$$\int_{\sigma_{\text{I II}}} d\sigma [\mathbf{n}_I \cdot \mathbf{q} + \mathbf{n}_I \cdot \mathbf{P} \cdot \mathbf{v} + \mathbf{n}_{\text{II}} \cdot \mathbf{q}_{\text{II}} + \mathbf{n}_{\text{II}} \cdot \mathbf{P}_{\text{II}} \cdot \mathbf{v}_{\text{II}}] = 0, \quad (1.9)$$

and iii) of momentum

$$\int_{\sigma_{\text{I II}}} d\sigma [\mathbf{n}_I \cdot \mathbf{P} + \mathbf{n}_{\text{II}} \cdot \mathbf{P}_{\text{II}}] = 0. \quad (1.10)$$

Here,

$$\mathbf{q} = \int \frac{m}{2} (\mathbf{c} - \mathbf{v})^2 (\mathbf{c} - \mathbf{v}) f d^3p \quad (1.11)$$

is the heat flux, and

$$\mathbf{P} = \int m (\mathbf{c} - \mathbf{v}) (\mathbf{c} - \mathbf{v}) f d^3p \quad (1.12)$$

is the pressure tensor in the gas. The integral relations (1.9), (1.10) have been derived under the assumption that the interface itself does not carry energy nor momentum. In the following, we will furthermore assume that no interfacial currents exist. Then, Eqs. (1.10), (1.9) reduce to the local conditions

$$\mathbf{n}_{\text{II}} \cdot \mathbf{P}_{\text{II}} = -\mathbf{n}_I \cdot \mathbf{P}, \quad (1.10a)$$

and

$$\mathbf{n}_{\text{II}} \cdot \mathbf{q}_{\text{II}} = -\mathbf{n}_I \cdot \mathbf{q} - \mathbf{n}_I \cdot \mathbf{P} \cdot (\mathbf{v} - \mathbf{v}_{\text{II}}). \quad (1.9a)$$

The interfacial entropy production (1.6) can be written in a very concise form if we use the local "wall Maxwellian"

$$f_{\text{II}} = n_{\text{II}} (2\pi m k T_{\text{II}})^{-3/2} \cdot \exp[-(\mathbf{p} - m \mathbf{v}_{\text{II}})^2 / 2 m k T_{\text{II}}] \quad (1.13)$$

with the local temperature T_{II} and local velocity \mathbf{v}_{II} of the wall at $\sigma_{\text{I II}}$. The value of the number density n_{II} is not relevant for the following considerations; it cancels in Equation (1.14). If we now use the definitions (1.5), (1.7) for the entropy fluxes, eliminate $\mathbf{n}_I \cdot \mathbf{v}$ and $\mathbf{n}_{\text{II}} \cdot \mathbf{q}_{\text{II}}$ with the help of Eqs. (1.8) and (1.9a), and finally insert the expressions (1.11), (1.12) for \mathbf{q} , \mathbf{P} we can easily prove for the local interfacial entropy production rate (1.6) per unit area

$$\begin{aligned} d\dot{S}_\sigma / d\sigma &\equiv -\mathbf{n}_I \cdot (\mathbf{s} - \mathbf{s}_{\text{II}}) \\ &= k \int \mathbf{n}_I \cdot (\mathbf{c} - \mathbf{v}_{\text{II}}) \ln(f/f_{\text{II}}) f d^3p. \end{aligned} \quad (1.14)$$

It should be noted that this expression, together with the boundary condition (3.14), is the starting point for Cercignani's proof [6] of the positivity of the interfacial entropy production. With the definition of $\Phi_{\text{I II}}$ through

$$f = f_{\text{II}} (1 + \Phi_{\text{I II}}), \quad (1.15)$$

and by use of the relation equivalent to (1.8),

$$\int (\mathbf{c} - \mathbf{v}_{II}) \cdot \mathbf{n}_I \Phi_{III} f_{II} d^3p = 0, \quad (1.8a)$$

Eq. (1.14) can be written in the alternative form

$$\begin{aligned} d\dot{S}_\sigma/d\sigma &= k \int \mathbf{n}_I \cdot (\mathbf{c} - \mathbf{v}_{II}) \\ &\quad \cdot [(1 + \Phi_{III}) \ln(1 + \Phi_{III}) - \Phi_{III}] \\ &\quad \cdot f_{II} d^3p. \end{aligned} \quad (1.16)$$

In the following, the gas as well as the solid or liquid shall be *close to an absolute equilibrium*. Hence, the relative deviations Φ and Φ_{II} of the distributions

$$f = f_0(1 + \Phi), \quad f_{II} = f_0(1 + \Phi_{II}) \quad (1.17)$$

from f_0 are "small". In Eq. (1.17), f_0 is a resting Maxwellian with number density n_0 and temperature T_0 ,

$$\begin{aligned} f_0 &= n_0 (2\pi m k T_0)^{-3/2} \\ &\quad \cdot \exp[-p^2/2mkT_0]. \end{aligned} \quad (1.18)$$

The small deviation Φ_{III} of f from the wall Maxwellian f_{II} is given by

$$\Phi_{III} = \Phi - \Phi_{II}, \quad (1.19)$$

whereas for the wall Maxwellian itself in linear approximation one has

$$\begin{aligned} \Phi_{II} &= \frac{n_{II} - n_0}{n_0} + \left(\frac{p^2}{2mkT_0} - \frac{3}{2} \right) \frac{T_{II} - T_0}{T_0} \\ &\quad + \mathbf{p} \cdot \mathbf{v}_{II}/kT_0. \end{aligned} \quad (1.20)$$

The linearized version of the impenetrability condition (1.8a) reads

$$\int c \Phi_{III} d\gamma = 0. \quad (1.21)$$

Here, the abbreviation

$$c \equiv \mathbf{n}_I \cdot \mathbf{c} \quad (1.22)$$

and the dimensionless integration element

$$d\gamma \equiv \frac{1}{n_0} f_0 d^3p, \quad \int d\gamma = 1 \quad (1.23)$$

have been introduced. The local conservation laws for energy and momentum, Eqs. (1.9a), (1.10a), do not lead to an integral condition for Φ_{III} similar to Equation (1.21). They just can be used to express the normal components of the heat flux and of the pressure tensor in the wall through non-equilibrium integrals in the gas. In linear approximation one finds:

$$\mathbf{n}_{II} \cdot \mathbf{q}_{II} = -\mathbf{n}_I \cdot \mathbf{q} = -P_0 \int c \frac{p^2}{2mkT_0} \Phi_{III} d\gamma,$$

$$\begin{aligned} \mathbf{n}_{II} \cdot \mathbf{P}_{II} &= -\mathbf{n}_I P_0 \left[1 + \frac{n_{II} - n_0}{n_0} + \frac{T_{II} - T_0}{T_0} \right] \\ &\quad - n_0 \int c \mathbf{p} \Phi_{III} d\gamma. \end{aligned}$$

The ideal gas law for the equilibrium pressure

$$P_0 = n_0 k T_0$$

has been used.

Now, the logarithm in the integral (1.16) is expanded for small Φ_{III} . In lowest order one gets

$$(1 + \Phi_{III}) \ln(1 + \Phi_{III}) - \Phi_{III} \approx \frac{1}{2} \Phi_{III}^2.$$

If no terms higher than quadratic in deviations from equilibrium are taken into account in the interfacial entropy production, the wall Maxwellian f_{II} in Eq. (1.16) can be replaced by f_0 , and the term proportional to $\mathbf{v}_{II} \cdot \mathbf{n}_I$ can be dropped:

$$d\dot{S}_\sigma/d\sigma \approx \frac{P_0}{T_0} \int c \frac{1}{2} \Phi_{III}^2 d\gamma.$$

In this approximation, the *interfacial entropy production rate* from Eq. (1.6) reduces to

$$\dot{S}_\sigma = \int_{\sigma_{II}} d\sigma \frac{P_0}{T_0} \int \frac{1}{2} c \Phi_{III}^2 d\gamma. \quad (1.24)$$

Due to the condition (1.21), \dot{S}_σ is independent of the density n_{II} .

2. Boundary Condition for the Distribution Function

In the bulk of the gas, the distribution function Φ shall obey the linearized Boltzmann equation. The kinetic equation has to be supplemented by a boundary condition for Φ at the interface σ_{II} . According to the procedure described in Ref. [1], boundary conditions for Φ are derived from the interfacial entropy production by rewriting \dot{S}_σ from Eq. (1.24) in the form

$$\dot{S}_\sigma = \int_{\sigma_{II}} d\sigma \frac{P_0}{T_0} \int F_{III} J_{III} d\gamma. \quad (2.1)$$

This is achieved by transforming the momentum integral in (1.24) into an integral over the half space $c > 0$ with the "surface force"

$$F_{III} \equiv \frac{1}{\sqrt{2}} P_+(c) (\Phi_{III} + \Phi_{IIIT}), \quad (2.2)$$

and the "surface flux"

$$J_{III} \equiv \frac{1}{\sqrt{2}} P_+(c) c (\Phi_{III} - \Phi_{IIIT}). \quad (2.3)$$

The motion-reversed distribution has been denoted by

$$\Phi_{\text{IIIT}}(t, \mathbf{x}, \mathbf{p}) = \Phi_{\text{II}}(t, \mathbf{x}, -\mathbf{p}), \quad (2.4)$$

and the Heaviside function by P_+ :

$$\begin{aligned} P_+(c) &= 0 \quad \text{for } c < 0, \\ &= 1 \quad \text{for } c > 0. \end{aligned} \quad (2.5)$$

In the formula (1.24) for the interfacial entropy production, the local conservation of energy and momentum at σ_{II} is already incorporated by the use of Eq. (1.9a). Insofar, the pertinent subsidiary conditions are eliminated. But the continuity of normal velocities, Eq. (1.8), still leads to a restriction for the surface flux J_{II} . Indeed, by rewriting Eq. (1.21) as a half space integral, one has

$$\int P_+(c) c (\Phi_{\text{II}} - \Phi_{\text{IIIT}}) d\gamma = 0.$$

Hence,

$$\int J_{\text{II}} d\gamma = 0 \quad (2.6)$$

is the only remaining subsidiary condition. Consequently, terms in F_{II} which are independent of momentum \mathbf{p} do not contribute to \dot{S}_σ .

In view of the form (2.1) for the interfacial entropy production \dot{S}_σ , the *boundary conditions at the gas/wall interface* are set up as an instantaneous linear relation between the flux J_{II} and the force F_{II} :

$$J_{\text{II}}(t, \mathbf{x}, \mathbf{p}) = \int L(\mathbf{p}, \mathbf{p}') F_{\text{II}}(t, \mathbf{x}, \mathbf{p}') d\gamma'. \quad (2.7)$$

The present L coincides with the former L_{II} . Indeed, in a steady state, for a wall at rest ($\mathbf{v}_{\text{II}} = 0$), Eq. (2.7) reduces to the "elaborate" boundary condition (5.9) of Ref. [1]. With the linear law (2.7), the interfacial entropy production (2.1) is rewritten as a quadratic expression in the force F_{II} . The second law requires that

$$\begin{aligned} \dot{S}_\sigma &= \int d\sigma \frac{P_0}{T_0} \iint d\gamma d\gamma' F_{\text{II}}(t, \mathbf{x}, \mathbf{p}) \\ &\quad \cdot L(\mathbf{p}, \mathbf{p}') F_{\text{II}}(t, \mathbf{x}, \mathbf{p}') d\gamma' \end{aligned} \quad (2.8)$$

is positive for arbitrary F_{II} , i.e. $L(\mathbf{p}, \mathbf{p}')$ has to be a positive operator. On the other hand, "particle conservation" (2.6) leads to the condition

$$\iint d\gamma d\gamma' L(\mathbf{p}, \mathbf{p}') F_{\text{II}}(t, \mathbf{x}, \mathbf{p}') d\gamma' = 0.$$

This is fulfilled for arbitrary F_{II} only if L has the property

$$\int d\gamma L(\mathbf{p}, \mathbf{p}') = 0 \quad \text{for any } \mathbf{p}'. \quad (2.9)$$

Hence, L is a positive semi-definite operator.

The boundary condition (2.7) is local in time t and in the space coordinate \mathbf{x} , i.e. the absorption and the migration of particles at the interface have been neglected. As indicated, the interfacial kernel L depends on the particle momenta \mathbf{p}, \mathbf{p}' , but tacitly L also depends on the equilibrium values P_0, T_0 , and on the unit normal \mathbf{n}_{I} . It is emphasized that the system is assumed to be at rest in global equilibrium: $\mathbf{v}_0 = 0$. This is no restriction, it can always be achieved by a Galilean transformation. According to Ref. [1], the interfacial kernel

$$L(\mathbf{p}, \mathbf{p}') = L(\mathbf{p}', \mathbf{p}) \quad (2.10)$$

is symmetric.

The combination of Eqs. (2.9) and (2.10) leads to

$$\int L(\mathbf{p}, \mathbf{p}') d\gamma' = 0 \quad \text{for any } \mathbf{p}. \quad (2.11)$$

Therefore, terms in F_{II} which are independent of the momentum \mathbf{p} don't contribute to the L -integral (2.7). This means that the number density n_{II} can be chosen freely. — If the gas is in thermal equilibrium with the wall, it must have the velocity \mathbf{v}_{II} and the temperature T_{II} . The choice

$$n_{\text{II}} = n$$

then yields the simple property

$$\Phi_{\text{II}} = 0 \quad \text{in equilibrium.} \quad (2.12)$$

As a consequence, the flux J_{II} and the force F_{II} both vanish in thermal equilibrium, the boundary condition (2.7) is trivially fulfilled.

Inserting the meanings (1.19) and (1.20) into the definitions (2.2) and (2.3) of the interfacial force and flux yields the following *explicit form of the boundary condition* (2.7)

$$\begin{aligned} P_+(c) c (\Phi - \Phi_{\text{T}} - 2\mathbf{p} \cdot \mathbf{v}_{\text{II}}/kT_0) \\ = \int L(\mathbf{p}, \mathbf{p}') \left(\Phi' + \Phi_{\text{T}}' - \frac{p'^2}{m k T_0} \frac{T_{\text{II}} - T_0}{T_0} \right) d\gamma'. \end{aligned} \quad (2.13)$$

Terms of F_{II} which don't contribute to the integral because of the property (2.11), have been omitted. The projection behaviour

$$P_+(c) L(\mathbf{p}, \mathbf{p}') = L(\mathbf{p}, \mathbf{p}') P_+(c') = L(\mathbf{p}, \mathbf{p}') \quad (2.14)$$

of the L -operator has been utilized. Indeed, L establishes a mapping between the two momentum half spaces $c > 0$ and $c' > 0$.

Another comment, from the physicists point of view, may still be welcome. Boundary condition

(2.13) for the moving wall is simply obtained from that one for the resting wall [1] by a *Galilean transformation of the function Φ* . Indeed, an observer moving with the wall in his frame sees the function

$$\Phi_w(\mathbf{p}) = \Phi(\mathbf{p}) - \mathbf{p} \cdot \mathbf{v}_{II} / k T_0 \quad (2.15)$$

and inserts his Φ_w into formula (5.9) of Ref. [1], which then at once is Equation (2.13). The transformation (2.15) follows immediately from the invariance of the full distribution function under a Galilean transformation (which in momentum space merely amounts to a shift of the origin):

$$f_w(\mathbf{p}) = f(\mathbf{p} + m \mathbf{v}_{II}). \quad (2.16)$$

Only has this to be rewritten by use of the consistent definitions

$$f_w(\mathbf{p}) = f_0(p) [1 + \Phi_w(\mathbf{p})] \quad (2.17)$$

and

$$\begin{aligned} f(\mathbf{p} + m \mathbf{v}_{II}) &= f_0(|\mathbf{p} + m \mathbf{v}_{II}|) [1 + \Phi(\mathbf{p} + m \mathbf{v}_{II})] \\ &\approx f_0(p) + \frac{\partial f_0(p)}{\partial p} \cdot m \mathbf{v}_{II} + f_0(p) \Phi(\mathbf{p}). \end{aligned} \quad (2.18)$$

Due linearization has been applied and

$$\frac{\partial f_0}{\partial p} = -f_0 \frac{p}{m k T_0}$$

should be noted. — This ends the comment which gives a direct insight into the origin of Equation (2.13).

3. Comparison with Conventional Approach

For a comparison of the boundary condition in the formulation of Eq. (2.7) with the conventional approach [6] which states a connection between the “outgoing” and the “incoming” distribution, a convenient formal notation is introduced. First, a half space integration element $d\Gamma$ is defined through

$$d\Gamma \equiv (1/\epsilon_0) P_+(c) c d\gamma, \quad \int d\Gamma = 1, \quad (3.1)$$

with

$$\epsilon_0 = \int P_+(c) c d\gamma = (k T_0 / 2 \pi m)^{1/2}.$$

The half space unity operator is denoted by

$$\begin{aligned} \mathbb{U}(\mathbf{p}, \mathbf{p}') &\equiv P_+(c) \delta(\mathbf{p}, \mathbf{p}') \frac{\epsilon_0 d^3 p'}{c' d\gamma'} P_+(c') \\ &= \mathbb{U}(\mathbf{p}', \mathbf{p}), \end{aligned} \quad (3.2)$$

and the operator \mathfrak{L} is introduced via*

$$\mathfrak{L}(\mathbf{p}, \mathbf{p}') \equiv \epsilon_0 \frac{1}{c} L(\mathbf{p}, \mathbf{p}') \frac{1}{c'} = \mathfrak{L}(\mathbf{p}', \mathbf{p}). \quad (3.3)$$

As a property of \mathbb{U} we note e.g.

$$\int \mathbb{U}(\mathbf{p}, \mathbf{p}'') \mathfrak{L}(\mathbf{p}'', \mathbf{p}') d\Gamma'' = \mathfrak{L}(\mathbf{p}, \mathbf{p}').$$

With the formal \mathfrak{L} -operation

$$(\mathfrak{L} \Phi_{I\text{II}})(\mathbf{p}) \equiv \int \mathfrak{L}(\mathbf{p}, \mathbf{p}') \Phi_{I\text{II}}(\mathbf{p}') d\Gamma' \quad (3.4)$$

the boundary condition (2.7) can then be rewritten as

$$\mathbb{U}(\Phi_{I\text{II}} - \Phi_{I\text{II}T}) = \mathfrak{L}(\Phi_{I\text{II}} + \Phi_{I\text{II}T}). \quad (3.5)$$

If the inverse of $\mathbb{U} + \mathfrak{L}$ is defined by

$$(\mathbb{U} + \mathfrak{L})^{-1}(\mathbb{U} + \mathfrak{L}) = (\mathbb{U} + \mathfrak{L})(\mathbb{U} + \mathfrak{L})^{-1} = \mathbb{U}$$

Eq. (3.5) can be solved for $\Phi_{I\text{II}T}$:

$$\mathbb{U} \Phi_{I\text{II}T} = \mathfrak{H} \Phi_{I\text{II}}, \quad (3.6)$$

where the operator \mathfrak{H} is given by

$$\begin{aligned} \mathfrak{H} &= (\mathbb{U} + \mathfrak{L})^{-1}(\mathbb{U} - \mathfrak{L}) \quad \text{or} \\ \mathfrak{L} &= (\mathbb{U} + \mathfrak{H})^{-1}(\mathbb{U} - \mathfrak{H}). \end{aligned} \quad (3.7)$$

The operator product is understood as, e.g.,

$$\begin{aligned} (\mathbb{U} \mathfrak{L})(\mathbf{p}, \mathbf{p}') &= \int \mathbb{U}(\mathbf{p}, \mathbf{p}'') \mathfrak{L}(\mathbf{p}'', \mathbf{p}') d\Gamma'' \\ &= (\mathfrak{L} \mathbb{U})(\mathbf{p}, \mathbf{p}'). \end{aligned}$$

According to Eqs. (3.2) and (3.3) the operators \mathbb{U} and \mathfrak{L} are symmetric, hence \mathfrak{H} is symmetric too:

$$\mathfrak{H}(\mathbf{p}, \mathbf{p}') = \mathfrak{H}(\mathbf{p}', \mathbf{p}). \quad (3.8)$$

In terms of the operator \mathfrak{L} , Eq. (2.11) is

$$\int \mathfrak{L}(\mathbf{p}, \mathbf{p}') d\Gamma' = 0,$$

or in formal notation

$$\mathfrak{L} 1 = 0. \quad (3.9)$$

Together with $\mathbb{U} 1 = \mathbb{U} P_+ = P_+$, this leads to

$$\mathfrak{H} 1 = P_+. \quad (3.10)$$

Finally, the positivity property of the operator \mathfrak{H} is investigated. The interfacial entropy production rate in terms of \mathfrak{L} is

$$\begin{aligned} \dot{S}_\sigma &= \int d\sigma \frac{P_0}{T_0} \epsilon_0 \iint d\Gamma d\Gamma' F_{I\text{II}}(\mathbf{p}) \\ &\quad \cdot \mathfrak{L}(\mathbf{p}, \mathbf{p}') F_{I\text{II}}(\mathbf{p}') d\Gamma'. \end{aligned} \quad (3.11)$$

* The definitions here are a little different from the corresponding ones in Ref. [1], Equation (5.12).

In order to obtain an expression in terms of \mathfrak{S} , we rewrite the integrand by use of definition (2.2) and of Eqs. (3.6) and (3.7)

$$\begin{aligned} F_{\text{I}\text{II}} \mathfrak{L} F'_{\text{I}\text{II}} &= \frac{1}{2} (\Phi_{\text{I}\text{II}} + \Phi_{\text{I}\text{II}\text{T}}) \mathfrak{L} (\Phi'_{\text{I}\text{II}} + \Phi'_{\text{I}\text{II}\text{T}}) \\ &= \frac{1}{2} \Phi_{\text{I}\text{II}} (\mathfrak{L} + \mathfrak{S}) \mathfrak{L} (\mathfrak{L} + \mathfrak{S}) \Phi'_{\text{I}\text{II}} \\ &= \frac{1}{2} \Phi_{\text{I}\text{II}} (\mathfrak{L} - \mathfrak{S}) (\mathfrak{L} + \mathfrak{S}) \Phi'_{\text{I}\text{II}}. \end{aligned}$$

So, the interfacial entropy production becomes

$$\begin{aligned} \dot{S}_\sigma &= \int_{\sigma_{\text{I}\text{II}}} d\sigma \frac{P_0}{T_0} \hat{e}_0 \cdot \frac{1}{2} \iint d\Gamma \Phi_{\text{I}\text{II}}(\mathbf{p}) \\ &\quad \cdot (\mathfrak{L} - \mathfrak{S}^2)(\mathbf{p}, \mathbf{p}') \Phi_{\text{I}\text{II}}(\mathbf{p}') d\Gamma'. \end{aligned} \quad (3.12)$$

Consequently, \mathfrak{L} and $\mathfrak{L} - \mathfrak{S}^2$ have to be positive operators.

The linear boundary condition (3.6) gives a relation between the distribution functions $\Phi_{\text{I}\text{II}}(t, \mathbf{x}, \mathbf{p}')$ and $\Phi_{\text{I}\text{II}\text{T}}(t, \mathbf{x}, \mathbf{p}) = \Phi_{\text{I}\text{II}}(t, \mathbf{x}, -\mathbf{p})$ in the momentum half spaces $c' > 0$, $c > 0$. It represents the linearized version of the conventional relation [6] between the distributions of incoming particles

$$(\mathbf{c}' - \mathbf{v}_{\text{II}}) \cdot \mathbf{n}_{\text{I}} > 0$$

and outgoing particles

$$(\mathbf{c} - \mathbf{v}_{\text{II}}) \cdot \mathbf{n}_{\text{I}} < 0.$$

In order to see more clearly the connection of our approach with the conventional formulation of boundary conditions, we rewrite Eq. (3.6) with the help of Eq. (3.10) in the form

$$\mathfrak{L}(1 + \Phi_{\text{I}\text{II}\text{T}}) = \mathfrak{S}(1 + \Phi_{\text{I}\text{II}}). \quad (3.13)$$

Now we take the motion-reversed form of this equation, recall (1.15), viz.

$$1 + \Phi_{\text{I}\text{II}} = f/f_{\text{II}},$$

and get in detail

$$\begin{aligned} P_+(-c) \frac{f}{f_{\text{II}}} & \quad (3.14) \\ &= \int P_+(-c) \cdot \mathfrak{S}(-\mathbf{p}, \mathbf{p}') P_+(c') c' \frac{f'}{f_{\text{II}}} \frac{1}{\hat{e}_0} d\gamma'. \end{aligned}$$

This relation is quite similar to the usual form of the boundary condition which connects the distribution f for incoming and outgoing particles [6]:

$$\begin{aligned} P_+(-\tilde{c})(-\tilde{c}) f(t, \mathbf{x}, \mathbf{p}) & \quad (3.15) \\ &= \int R(\tilde{\mathbf{p}}' \rightarrow \tilde{\mathbf{p}}) P_+(\tilde{c}') \tilde{c}' f(t, \mathbf{x}, \mathbf{p}') d^3p'; \end{aligned}$$

$\tilde{\mathbf{c}} = \tilde{\mathbf{p}}/m \equiv \mathbf{c} - \mathbf{v}_{\text{II}}$ is the particle velocity with respect to the wall. Starting from Eq. (3.15) one arrives at (3.14) in the following way: First, Eq. (3.15)

is divided by $-\tilde{c}f_{\text{II}}$, then, in the spirit of our linear theory, \tilde{c} , $\tilde{\mathbf{p}}$ are replaced by c , \mathbf{p} . As an intermediate result we note

$$\begin{aligned} P_+(-c) \frac{f}{f_{\text{II}}} &= \int \hat{e}_0 P_+(-c) \frac{R(\mathbf{p}' \rightarrow \mathbf{p})}{(-c) f_{\text{II}}/n_{\text{II}}} \\ &\quad \cdot P_+(c') c' \frac{f'}{f_{\text{II}}} \frac{1}{\hat{e}_0} \frac{f_{\text{II}}}{n_{\text{II}}} d^3p'. \end{aligned}$$

In a linear boundary condition, the integration element $(f'_{\text{II}}/n_{\text{II}}) d^3p'$ has to be replaced by $(f'_0/n_0) \cdot d^3p' \equiv d\gamma'$, and the operator $R/(f_{\text{II}}/n_{\text{II}})$ has to be taken for the equilibrium values $\mathbf{v}_{\text{II}} = 0$, $T_{\text{II}} = T_0$, etc. Comparison with Eq. (3.14) then gives the relation

$$\mathfrak{S}(-\mathbf{p}, \mathbf{p}') = \hat{e}_0 P_+(-c) \left(\frac{R(\mathbf{p}' \rightarrow \mathbf{p})}{(-c) f_{\text{II}}/n_{\text{II}}} \right)_{eq} P_+(c'). \quad (3.16)$$

As a transition probability which connects positive distribution functions, the function $R(\mathbf{p}' \rightarrow \mathbf{p})$ has to be non-negative for all arguments with $c' > 0$, $c < 0$:

$$R(\mathbf{p}' \rightarrow \mathbf{p}) \geq 0. \quad (3.17)$$

Together with particle conservation [6] (the equivalent of Eqs. (2.9), (3.10)),

$$\int R(\mathbf{p}' \rightarrow \mathbf{p}) P_+(-c) d^3p = P_+(c'), \quad (3.18)$$

and with the “detailed balance” relation [6, 10] (the counterpart of Eq. (3.8))

$$\begin{aligned} P_+(c') c' f_{\text{II}}(\mathbf{p}') R(\mathbf{p}' \rightarrow \mathbf{p}) P_+(-c) & \quad (3.19) \\ &= P_+(-c) (-c) f_{\text{II}}(\mathbf{p}) R(-\mathbf{p} \rightarrow -\mathbf{p}') P_+(c'), \end{aligned}$$

the positivity statement (3.17) is sufficient to establish [6, 11] the positivity of the interfacial entropy production \dot{S}_σ from Equation (1.14). Finally, we note that, as a consequence of Eqs. (3.16) and (3.17), the function $\mathfrak{S}(\mathbf{p}, \mathbf{p}')$ has to be non-negative,

$$\mathfrak{S}(\mathbf{p}, \mathbf{p}') \geq 0, \quad (3.20)$$

for all arguments with $c > 0$, $c' > 0$.

4. Boundary Conditions for Moments

The distribution function Φ is a solution of the linearized Boltzmann equation

$$\frac{\partial}{\partial t} \Phi + \mathbf{c} \cdot \nabla \Phi + \omega(\Phi) = 0 \quad (4.1)$$

with the boundary condition (2.13). In the moment method [7], the Boltzmann equation is replaced by

a set of transport-relaxation equations for the moments, dependent on t and \mathbf{x} only. The purpose of this section is the derivation of boundary conditions for these moments from the boundary condition (2.13) for Φ . In Ref. [1], the general method has been outlined already for arbitrary moments $a_i, i = 1, 2, \dots$; here the details of irreducible Cartesian tensors $a_{\mu_1 \dots \mu_l}^{(r)}$ are explicitly worked out for $0 \leq l \leq 3$. Or in other words: a reduction of the boundary conditions is now performed by making use of the rotational invariance about the local surface normal.

For the solution of Eq. (4.1) by the moment method [7], the distribution Φ is expanded as

$$\Phi(t, \mathbf{x}, \mathbf{p}) = \sum_{l \geq 0} \sum_{r \geq 0} a_{\mu_1 \dots \mu_l}^{(r)}(t, \mathbf{x}) \Phi_{\mu_1 \dots \mu_l}^{(r)}(\mathbf{p}), \quad (4.2)$$

where the $\Phi_{\mu_1 \dots \mu_l}^{(r)}$ are a complete set of symmetric traceless tensors constructed by the help of the dimensionless momentum vector

$$\mathbf{W} = \mathbf{p}/(2mkT_0)^{1/2} \quad (4.3)$$

in the way

$$\Phi_{\mu_1 \dots \mu_l}^{(r)} = \left[\frac{r!(2l+1)!! \frac{1}{2} \sqrt{\pi}}{l! \Gamma(l+r+\frac{3}{2})} \right]^{1/2} S_{l+\frac{3}{2}}^{(r)}(W^2) \overline{W_{\mu_1 \dots \mu_l}}. \quad (4.4)$$

Here, $S_{l+\frac{3}{2}}^{(r)}$ is a Sonine-polynomial of degree r in W^2 , and the numerical factor is chosen such that the tensors are normalized [7] according to

$$\int \Phi_{\mu_1 \dots \mu_l}^{(r)} \Phi_{\mu'_1 \dots \mu'_l}^{(r')} d\gamma = \delta_{rr'} \delta_{ll'} \Delta_{\mu_1 \dots \mu_l, \mu'_1 \dots \mu'_l}^{(l)}. \quad (4.5)$$

The irreducible isotropic tensor $\Delta^{(l)}$ is chosen such that

$$\Delta_{\mu_1 \dots \mu_l, \mu_1 \dots \mu_l}^{(l)} = 2l + 1$$

applies. With the normalization (4.5), the expansion coefficients $a_{\mu_1 \dots \mu_l}^{(r)}(t, \mathbf{x})$ are moments of the distribution function:

$$a_{\mu_1 \dots \mu_l}^{(r)}(t, \mathbf{x}) = \int \Phi_{\mu_1 \dots \mu_l}^{(r)}(\mathbf{p}) \Phi(t, \mathbf{x}, \mathbf{p}) d\gamma. \quad (4.6)$$

By taking moments of the linearized Boltzmann equation (4.1), a set of coupled linear first order differential equations for the $a_{\mu_1 \dots \mu_l}^{(r)}(t, \mathbf{x})$ is obtained, the transport-relaxation equations [7]. The boundary conditions for the moments which are needed for the solution of these differential equations are derived from the boundary condition (2.7) or (2.13) for Φ , first for a general expansion con-

taining tensors up to rank 3 ($0 \leq l \leq 3$), then for the special set used in [8].

If \mathbf{W} is replaced by $-\mathbf{W}$, the tensor $\Phi_{\mu_1 \dots \mu_l}^{(r)}$ changes by a factor $(-1)^l$. Consequently, according to Eq. (2.2), the surface force F_{II} occurring on the right hand side of Eq. (2.7) contains only tensors with even l , i.e. here with $l=0$ and $l=2$. The surface flux J_{II} on the left hand side, apart from a factor c , contains only tensors with odd l , i.e. here $l=1$ and $l=3$. For the derivation of boundary conditions, Eq. (2.7) is multiplied by one of the even-in- l tensors and integrated (de facto over the half space $c > 0$):

$$\begin{aligned} \int d\gamma \Phi_{\mu_1 \dots \mu_l}^{(r)} J_{\text{II}} \\ = \iint d\gamma \Phi_{\mu_1 \dots \mu_l}^{(r)} L(\mathbf{p}, \mathbf{p}') F'_{\text{II}} d\gamma' \end{aligned} \quad (4.7)$$

with $l = 0, 2$.

This is a complete set of boundary conditions for our moments. We shall come back to this assertion after Eq. (4.21).

The main algebraic problem with Eq. (4.7) occurs in context with the second rank tensors and with the disentangling of the equations into separate boundary conditions for scalars, tangential vectors and tangential second rank tensors. For the solution of this problem the irreducible second rank tensor $\Phi_{\mu\nu}^{(r)}$ is decomposed into three parts,

$$\begin{aligned} \Phi_{\mu\nu}^{(r)} = & \sqrt{\frac{3}{2}} P_{\mu\nu, \mu'\nu'}^{(0)} n_{\mu'} n_{\nu'} \varphi^{(2r)} \\ & + \sqrt{2} P_{\mu\nu, \mu'\nu'}^{(1)} n_{\mu'} \varphi_{\nu'}^{(2r)} \\ & + P_{\mu\nu, \mu'\nu'}^{(2)} \varphi_{\mu'\nu'}^{(2r)}, \end{aligned} \quad (4.8)$$

containing, respectively, a surface scalar

$$\begin{aligned} \varphi^{(2r)} & \equiv \sqrt{\frac{3}{2}} n_{\mu} n_{\nu} P_{\mu\nu, \mu'\nu'}^{(0)} \Phi_{\mu'\nu'}^{(r)} \\ & = \sqrt{\frac{3}{2}} n_{\mu} n_{\nu} \Phi_{\mu\nu}^{(r)}, \end{aligned} \quad (4.9a)$$

a tangential surface vector (2 components)

$$\begin{aligned} \varphi_{\mu}^{(2r)} & \equiv \sqrt{2} n_{\nu} P_{\mu\nu, \mu'\nu'}^{(1)} \Phi_{\mu'\nu'}^{(r)} \\ & = \sqrt{2} T_{\mu\mu'} \Phi_{\mu'\nu'}^{(r)} n_{\nu'}, \end{aligned} \quad (4.9b)$$

and a tangential symmetric traceless surface tensor (2 components)

$$\begin{aligned} \varphi_{\mu\nu}^{(2r)} & \equiv P_{\mu\nu, \mu'\nu'}^{(2)} \Phi_{\mu'\nu'}^{(r)} \\ & = T_{\mu\mu'} \Phi_{\mu'\nu'}^{(r)} T_{\nu\nu'} - \frac{1}{2} T_{\mu\nu} T_{\mu'\nu'} \Phi_{\mu'\nu'}^{(r)}. \end{aligned} \quad (4.9c)$$

The quantities $P_{\mu\nu, \mu'\nu'}^{(s)}$, $s=0, 1, 2$, are projection tensors* built up from the normal $\mathbf{n} \equiv \mathbf{n}_1$ and the

* These three projection tensors $\mathbf{P}^{(0)}$, $\mathbf{P}^{(1)}$, $\mathbf{P}^{(2)}$ are the symmetric traceless parts of $\mathcal{P}^{(0)}$, $\mathcal{P}^{(1)} + \mathcal{P}^{(-1)}$, and $\mathcal{P}^{(2)} + \mathcal{P}^{(-2)}$, respectively, where $\mathcal{P}^{(m)}$, $m=0, \pm 1, \pm 2$, are the five projection tensors used by Hess and Waldmann [12].

tensors

$$\overline{n_\mu n_\nu} = n_\mu n_\nu - \frac{1}{3} \delta_{\mu\nu}, \quad T_{\mu\nu} = \delta_{\mu\nu} - n_\mu n_\nu$$

in the following way:

$$\begin{aligned} P_{\mu\nu, \mu'\nu'}^{(0)} &= \frac{2}{3} \overline{n_\mu n_\nu n_{\mu'} n_{\nu'}}, \\ P_{\mu\nu, \mu'\nu'}^{(1)} &= \frac{1}{2} [n_\mu n_{\mu'} T_{\nu\nu'} + n_\mu n_{\nu'} T_{\nu\mu'} \\ &\quad + n_\nu n_{\mu'} T_{\mu\nu'} + n_\nu n_{\nu'} T_{\mu\mu'}], \\ P_{\mu\nu, \mu'\nu'}^{(2)} &= \frac{1}{2} [T_{\mu\mu'} T_{\nu\nu'} + T_{\mu\nu'} T_{\nu\mu'} - T_{\mu\nu} T_{\mu'\nu'}]. \end{aligned} \quad (4.10)$$

We note the properties

$$\begin{aligned} P_{\mu\nu, \lambda\kappa}^{(s)} P_{\lambda\kappa, \mu'\nu'}^{(s')} &= \delta_{ss'} P_{\mu\nu, \mu'\nu'}^{(s)}, \\ \sum_{s=0}^2 P_{\mu\nu, \mu'\nu'}^{(s)} &= \Delta_{\mu\nu, \mu'\nu'}^{(2)}, \\ P_{\mu\nu, \mu'\nu'}^{(s)} &= P_{\mu'\nu', \mu\nu}^{(s)}, \quad \Delta_{\mu\nu, \lambda\kappa}^{(2)} P_{\lambda\kappa, \mu'\nu'}^{(s)} = P_{\mu\nu, \mu'\nu'}^{(s)}. \end{aligned} \quad (4.11)$$

If we write

$$\Phi(r) \equiv \varphi^{(0r)}, \quad (4.9d)$$

the normalization (4.5) for the even-in- l tensors can be formulated in terms of the

$$\begin{aligned} \varphi_{\mu_1 \dots \mu_s}^{(lr)} \quad (l=0, 2; 0 \leq s \leq l) \quad \text{as} \\ \int \varphi_{\mu_1 \dots \mu_s}^{(lr)} \varphi_{\mu'_1 \dots \mu'_s}^{(l'r')} d\gamma \\ = \int P_+(c) \sqrt{2} \varphi_{\mu_1 \dots \mu_s}^{(lr)} \sqrt{2} \varphi_{\mu'_1 \dots \mu'_s}^{(l'r')} d\gamma \\ = \delta_{ss'} \delta_{ll'} \delta_{rr'} T_{\mu_1 \dots \mu_s, \mu'_1 \dots \mu'_s}^{(s)}, \end{aligned} \quad (4.12)$$

with the isotropic projectors into the tangential plane

$$\begin{aligned} T^{(0)} &= 1, \quad T_{\mu, \mu'}^{(1)} = T_{\mu\mu'}, \\ T_{\mu\nu, \mu'\nu'}^{(2)} &= P_{\mu\nu, \mu'\nu'}^{(2)}. \end{aligned} \quad (4.13)$$

In terms of the tensors $\varphi_{\mu_1 \dots \mu_s}^{(lr)}$, the surface force $F_{\text{I}\text{II}}$ from Eq. (2.2) is rewritten as

$$F_{\text{I}\text{II}} = P_+(c) \sqrt{2} \sum_{l=0, 2} \sum_{s=0}^l \sum_{r \geq 0} \varphi_{\mu_1 \dots \mu_s}^{(lr)} \varphi_{\mu'_1 \dots \mu'_s}^{(l'r')}, \quad (4.14)$$

where the “forces” $\varphi_{\mu_1 \dots \mu_s}^{(lr)}$ are given by

$$\begin{aligned} f^{(00)} &= (n - n_{\text{II}})/n_0, \\ f^{(01)} &= -\sqrt{\frac{3}{2}} (T - T_{\text{II}})/T_0. \end{aligned} \quad (4.15a)$$

and otherwise, in analogy to Eq. (4.6), by

$$\varphi_{\mu_1 \dots \mu_s}^{(lr)} = \int \varphi_{\mu_1 \dots \mu_s}^{(lr)} \Phi d\gamma. \quad (4.15b)$$

The Eqs. (4.15a, b) are summarized in the relation

$$\varphi_{\mu_1 \dots \mu_s}^{(lr)} = \int \sqrt{2} \varphi_{\mu_1 \dots \mu_s}^{(lr)} F_{\text{I}\text{II}} d\gamma, \quad (4.15c)$$

which follows from Eqs. (4.12), (4.14) and from the projector property

$$T_{\mu_1 \dots \mu_s, \mu'_1 \dots \mu'_s}^{(s)} \varphi_{\mu'_1 \dots \mu'_s}^{(l'r')} = \varphi_{\mu_1 \dots \mu_s}^{(lr)}.$$

For the derivation of Eq. (4.14) from Eqs. (2.2), (4.2), the tensor $a_{\mu\nu}^{(r)}$ has been decomposed into its

three parts $f^{(2r)}$, $f_{\mu}^{(2r)}$, $f_{\mu\nu}^{(2r)}$ in the same way as it has been done for $\Phi_{\mu\nu}^{(r)}$ in Equation (4.8).

In the boundary condition (4.7) the tensor $\Phi_{\mu_1 \dots \mu_s}^{(r)}$ is now replaced by its components $\varphi_{\mu_1 \dots \mu_s}^{(lr)}$. To this end it is convenient to define “fluxes” $j_{\mu_1 \dots \mu_s}^{(lr)}$ through

$$\begin{aligned} j_{\mu_1 \dots \mu_s}^{(lr)} &\equiv \int \sqrt{2} \varphi_{\mu_1 \dots \mu_s}^{(lr)} J_{\text{I}\text{II}} d\gamma \\ &= \int \varphi_{\mu_1 \dots \mu_s}^{(lr)} c(\Phi - \mathbf{p} \cdot \mathbf{v}_{\text{II}}/kT_0) d\gamma. \end{aligned} \quad (4.16)$$

In particular with $\varphi^{(00)} = 1$ and after Eq. (2.6) one has $j^{(00)} = 0$. With these definitions, Eq. (4.7) leads to the relation

$$\begin{aligned} j_{\mu_1 \dots \mu_s}^{(lr)} &= \sum_{l'=0, 2} \sum_{s'=0}^l \sum_{r' \geq 0} \iint d\gamma \sqrt{2} \varphi_{\mu_1 \dots \mu_s}^{(lr)} \\ &\quad \cdot L(\mathbf{p}, \mathbf{p}') \sqrt{2} \varphi_{\mu'_1 \dots \mu'_s}^{(l'r')} d\gamma' \varphi_{\mu'_1 \dots \mu'_s}^{(l'r')}. \end{aligned}$$

In the integral, the operator L is rotationally invariant about the normal, and the tensors $\varphi_{\dots}^{(\dots)}$ are irreducible in the tangential plane. Therefore, the L -matrix element is different from zero only for $s=s'$ and can be written as:

$$\begin{aligned} \iint d\gamma \sqrt{2} \varphi_{\mu_1 \dots \mu_s}^{(lr)} L(\mathbf{p}, \mathbf{p}') \sqrt{2} \varphi_{\mu'_1 \dots \mu'_s}^{(l'r')} d\gamma' \\ \equiv (\sqrt{2} \varphi_{\mu_1 \dots \mu_s}^{(lr)} | L | \sqrt{2} \varphi_{\mu'_1 \dots \mu'_s}^{(l'r')}) \\ = \delta_{ss'} L_s(l'r') T_{\mu_1 \dots \mu_s, \mu'_1 \dots \mu'_s}^{(s)}. \end{aligned} \quad (4.17)$$

The reduced matrix-element is given by

$$L_s(l'r') = \frac{1}{T_s} (\sqrt{2} \varphi_{\mu_1 \dots \mu_s}^{(lr)} | L | \sqrt{2} \varphi_{\mu'_1 \dots \mu'_s}^{(l'r')}), \quad (4.18)$$

where

$$\begin{aligned} T_s &\equiv T_{\mu_1 \dots \mu_s, \mu_1 \dots \mu_s}^{(s)}, \\ \text{i.e. } T_0 &= 1, \quad T_1 = T_2 = 2. \end{aligned}$$

The symmetry (2.10) of the L -operator entails the symmetry

$$L_s(l'r') = L_s(l'r'), \quad (4.19a)$$

and the property (2.11) leads to

$$L_s(0^0) = L_s(0^0_0) = 0. \quad (4.19b)$$

With Eq. (4.17), the boundary conditions for the moments read

$$j_{\mu_1 \dots \mu_s}^{(lr)} = \sum_{l'=0, 2} \sum_{r' \geq 0} L_s(l'r') f_{\mu_1 \dots \mu_s}^{(l'r')}, \quad l=0, 2. \quad (4.20)$$

These are three separate sets of boundary conditions for scalars ($s=0$), tangential vectors ($s=1$) and tangential symmetric traceless tensors of second rank ($s=2$). As a consequence of Eq. (4.19b), the condition $j^{(00)} = 0$ is fulfilled by the boundary condition (4.20), and, furthermore, the force $f^{(00)}$ does not contribute to the right hand side of Equation (4.20). We have now obtained the boundary

(matching) conditions which are needed for the solution of the transport-relaxation equations involving all the moments $a_{\mu_1 \dots \mu_l}^{(r)}$, $0 \leq l \leq 3$, chosen, together with the heat conduction, etc., equation for the solid or liquid wall. The forces and fluxes in Eqs. (4.20) are linear combinations of these moments such, that the forces $f^{(0r)}$, $f^{(2r)}$, $f_{\mu}^{(2r)}$, $f_{\mu\nu}^{(2r)}$, according to Eq. (4.15c) stem from the moments $a^{(r)}$ and $a_{\mu\nu}^{(r)}$, whereas, cf. Eq. (4.16), the fluxes $j^{(0r)}$, $j^{(2r)}$, $j_{\mu}^{(2r)}$, $j_{\mu\nu}^{(2r)}$ stem from the moments $a_{\mu}^{(r)}$ and $a_{\mu\nu\lambda}^{(r)}$.

Due to Eqs. (4.8) and (4.17), the matrix element of the operator L with two second rank tensors has the form

$$(\Phi_{\mu\nu}^{(r)} | L | \Phi_{\mu'\nu'}^{(r')}) = \frac{1}{2} \sum_{s=0}^2 L_s \left(\frac{2r}{2r'} \right) P_{\mu\nu, \mu'\nu'}^{(s)}.$$

Only if all three quantities

$$L_s \left(\frac{2r}{2r'} \right), \quad s = 0, 1, 2,$$

are equal to one reduced matrix element $L \left(\frac{2r}{2r'} \right)$ the result is an isotropic tensor, viz.

$$(\Phi_{\mu\nu}^{(r)} | L | \Phi_{\mu'\nu'}^{(r')}) = \frac{1}{2} L \left(\frac{2r}{2r'} \right) \Delta_{\mu\nu, \mu'\nu'}^{(2)}.$$

For $r = r' = 0$ and the special L -model of Eq. (5.12), three different values for the $L_s \left(\frac{20}{20} \right)$ are obtained, cf. Eqs. (5.14), (5.16) and (5.17).

Finally, let us look at the interfacial entropy production. By insertion of the expansion (4.14) into Eq. (2.1) and subsequent use of the definition (4.16), one finds

$$\dot{S}_{\sigma} = \int d\sigma \frac{P_0}{T_0} \sum_{l=0,2} \sum_{s=0}^l \sum_{r \geq 0} j_{\mu_1 \dots \mu_s}^{(lr)} f_{\mu_1 \dots \mu_s}^{(lr)}, \quad (4.21)$$

i.e. \dot{S}_{σ} is a scalar product of the fluxes $j_{\mu_1 \dots \mu_s}^{(lr)}$ with the forces $f_{\mu_1 \dots \mu_s}^{(lr)}$. This form of the entropy production leads, along the lines of the previous work [4, 2], indeed to boundary conditions of the type (4.20), which are equivalent to those of Equation (4.7). Therefore we think that our boundary conditions are a complete set. If e.g. one would form moments in analogy to Eq. (4.7), however by means of the expansion tensors for $l=1, 3$, one would destroy the canonical form of the entropy production (4.21), essential for the derivation of complete boundary conditions.

As an application of the general procedure described so far, the boundary conditions used in Ref. [8] shall be extracted from Eq. (4.20). To this end, the expansion (4.2) for Φ is approximated by the following tensors:

$$\Phi^{(0)}, \Phi^{(1)}, \Phi^{(2)}, \Phi_{\mu\nu}^{(1)} \quad \text{and} \quad \Phi_{\mu}^{(0)}, \Phi_{\mu}^{(1)}, \Phi_{\mu}^{(2)}, \Phi_{\mu\nu\lambda}^{(0)}. \quad (4.22)$$

Besides the even-in- l tensors listed in (4.22), all odd-in- l tensors contained in $c_{\mu} \Phi^{(r)}$ and in $c_{\mu} \Phi_{\nu\lambda}^{(0)}$ are considered. The scheme in Ref. [8] de facto was a little simpler: the third rank tensor $\Phi_{\mu\nu\lambda}^{(0)}$ had been omitted. According to Eqs. (4.9), (4.15), (4.16) the following tensors $\varphi_{\mu_1 \dots \mu_s}^{(lr)}$, forces $f_{\mu_1 \dots \mu_s}^{(lr)}$ and fluxes $j_{\mu_1 \dots \mu_s}^{(lr)}$ are connected with the list (4.22): one set of scalars which play no role in the boundary conditions

$$\varphi^{(00)} = 1, \quad f^{(00)} = (n - n_{II})/n_0, \quad j^{(00)} = 0,$$

three relevant sets of scalars,

$$\begin{aligned} \varphi^{(01)} &= -\sqrt{\frac{2}{3}} \left(W^2 - \frac{3}{2} \right), \quad \varphi^{(02)} = \sqrt{\frac{2}{15}} \left(\frac{15}{4} - 5W^2 + W^4 \right), \quad \varphi^{(20)} = \sqrt{3} \left((\mathbf{W} \cdot \mathbf{n})^2 - \frac{1}{3} W^2 \right), \\ f^{(01)} &= -\sqrt{\frac{3}{2}} \frac{T - T_{II}}{T_0}, \quad f^{(02)} = \sqrt{\frac{15}{8}} \frac{A}{T_0}, \quad f^{(20)} = \sqrt{\frac{3}{4}} \mathbf{n} \cdot \bar{\mathbf{P}} \cdot \mathbf{n} P_0^{-1}, \\ j^{(01)} &= -\sqrt{\frac{2}{3}} \frac{\mathbf{q} \cdot \mathbf{n}}{P_0}, \quad j^{(02)} = \sqrt{\frac{8}{15}} \frac{(\mathbf{A} + \mathbf{q}) \cdot \mathbf{n}}{P_0}, \quad j^{(20)} = \frac{3}{\sqrt{2}} c_0 a_{\mu\nu\lambda}^{(0)} n_{\mu} n_{\nu} n_{\lambda} + \frac{2}{5} \sqrt{\frac{4}{3}} \frac{\mathbf{q} \cdot \mathbf{n}}{P_0}; \end{aligned} \quad (4.23)$$

one set of tangential vectors

$$\begin{aligned} \varphi_{\mu}^{(20)} &= 2 W_{\mu} \tan \mathbf{W} \cdot \mathbf{n}, \quad f_{\mu}^{(20)} = (\bar{P}_{\mu\nu} n_{\nu}) \tan P_0^{-1}, \\ j_{\mu}^{(20)} &= [v_{\mu} - v_{II\mu} + \frac{2}{5} q_{\mu} P_0^{-1} + c_0 \sqrt{6} a_{\mu\nu\lambda}^{(0)} n_{\nu} n_{\lambda}] \tan; \end{aligned} \quad (4.24)$$

and one set of tangential symmetric traceless tensors of second rank

$$\begin{aligned} \varphi_{\mu\nu}^{(20)} &= \sqrt{2} [W_{\mu} \tan W_{\nu} \tan - \frac{1}{2} T_{\mu\nu} \mathbf{W} \tan \cdot \mathbf{W} \tan], \\ f_{\mu\nu}^{(20)} &= \frac{1}{\sqrt{2}} [T_{\mu\mu'} \bar{P}_{\mu'\nu'} T_{\nu\nu'} - \frac{1}{2} T_{\mu\nu} T_{\mu'\nu'} \bar{P}_{\mu'\nu'}] P_0^{-1}, \\ j_{\mu\nu}^{(20)} &= \sqrt{3} c_0 [T_{\mu\mu'} a_{\mu'\nu'\lambda}^{(0)} n_{\lambda} T_{\nu\nu'} - \frac{1}{2} T_{\mu\nu} T_{\mu'\nu'} a_{\mu'\nu'\lambda}^{(0)} n_{\lambda}]. \end{aligned} \quad (4.25)$$

Here, the abbreviation

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

has been used; the superscript "tan" denotes the tangential component of a vector, e.g.

$$W_\mu^{\text{tan}} = T_{\mu\nu} W_\nu = W_\mu - n_\mu n_\nu W_\nu.$$

The boundary conditions (4.20) for the fluxes and forces noted in Eqs. (4.23)–(4.25) contain three types of reduced matrix elements, cf. Eq. (4.18):

$$\begin{aligned} L_0(l_{r'}) &= 2(\varphi^{(lr)} | L | \varphi^{(l'r')}), \\ L_1(\frac{20}{20}) &= 4(W_\mu^{\text{tan}} \mathbf{W} \cdot \mathbf{n} | L | W_\mu^{\text{tan}} \mathbf{W} \cdot \mathbf{n}), \\ L_2(\frac{20}{20}) &= 2(W_\mu^{\text{tan}} W_\nu^{\text{tan}} | L | W_\mu^{\text{tan}} W_\nu^{\text{tan}}) \\ &\quad - (\mathbf{W}^{\text{tan}} \cdot \mathbf{W}^{\text{tan}} | L | \mathbf{W}^{\text{tan}} \cdot \mathbf{W}^{\text{tan}}). \end{aligned} \quad (4.26)$$

In Ref. [8], the third rank tensor $a_{\mu\nu\lambda}^{(0)}$ had been neglected completely. Consequently, in Ref. [8] the boundary condition for $j_{\mu\nu}^{(20)}$ does not occur, and in $j_u^{(20)}$ the term with $c_0 \sqrt{6} (a_{\mu\nu\lambda}^{(0)} n_\nu n_\lambda)^{\text{tan}}$ is missing.

For a comparison of the present scalar boundary conditions with those of Ref. [8], the fluxes

$$j^{(01)} \equiv j_q, \quad j^{(02)} \equiv j_A, \quad j^{(20)} \equiv j_a$$

are rearranged by a linear transformation

$$J_\alpha = \sum_{\alpha'} U_{\alpha\alpha'} j_{\alpha'}, \quad \alpha, \alpha' = q, A, a,$$

in such a way that the new fluxes J_α coincide, apart from constant factors, with those of Ref. [8]:

$$\begin{aligned} J_q &= \frac{\mathbf{q} \cdot \mathbf{n}}{P_0}, \quad J_A = \frac{\mathbf{A} \cdot \mathbf{n}}{P_0}, \\ J_a &= \frac{3}{2} \sqrt{\frac{3}{2}} c_0 a_{\mu\nu\lambda}^{(0)} n_\mu n_\nu n_\lambda. \end{aligned} \quad (4.27)$$

The new forces F_α are chosen in such a way that the interfacial entropy production \dot{S}_σ remains invariant under the transformation $U_{\alpha\alpha'}$,

$$\sum_\alpha f_\alpha j_\alpha = \sum_\alpha F_\alpha J_\alpha.$$

Hence, one has to take

$$F_\alpha = \sum_{\alpha'} f_{\alpha'} U_{\alpha'}^{-1},$$

or in detail

$$\begin{aligned} F_q &= [T - T_{\text{II}} + A + \frac{2}{5} T_0 P_0^{-1} \mathbf{n} \cdot \overline{\mathbf{P}} \cdot \mathbf{n}] T_0^{-1}, \\ F_A &= A T_0^{-1}, \quad F_a = \mathbf{n} \cdot \overline{\mathbf{P}} \cdot \mathbf{n} P_0^{-1}. \end{aligned} \quad (4.28)$$

In terms of the J_α , F_α , the boundary conditions read

$$\begin{aligned} J_\alpha &= \sum_{\alpha'} L_{\alpha\alpha'}^{(U)} F_{\alpha'}, \\ L_{\alpha\alpha'}^{(U)} &= \sum_\beta \sum_{\beta'} U_{\alpha\beta} L_{\beta\beta'} U_{\alpha'\beta'}, \end{aligned}$$

where the $L_{\beta\beta'}$ are the $L_0(l_{r'})$ renamed in an obvious way. Instead of the polynomials φ_α from Eq. (4.23), the polynomials ψ_α are introduced:

$$\psi_\alpha = \sum_{\alpha'} U_{\alpha\alpha'} \varphi_{\alpha'}.$$

Then the matrix elements can be written as

$$L_{\alpha\alpha'}^{(U)} = 2(\psi_\alpha | L | \psi_{\alpha'}),$$

in analogy to Equation (4.26). Explicitly one has

$$\begin{aligned} \psi_q &= W^2 - \frac{3}{2}, \quad \psi_A = \frac{1}{2} W^4 - \frac{7}{2} W^2 + \frac{27}{8}, \\ \psi_a &= \frac{3}{2} (\mathbf{W} \cdot \mathbf{n})^2 - \frac{9}{10} W^2 + \frac{3}{5} \end{aligned} \quad (4.29)$$

for the new polynomials.

The boundary conditions of Ref. [8] are obtained by putting $F_a = 0$ and by dropping the line for J_a . The dimensionless coefficients $C_{\alpha\alpha'}$ from Ref. [8] are, in the present notation, given by

$$C_{\alpha\alpha'} = \left(\frac{8}{15 c_0} \right) (\psi_\alpha | L | \psi_{\alpha'}). \quad (4.30)$$

In the most simple approximation for heat transfer problems, only one scalar boundary condition is considered [8]:

$$T - T_{\text{II}} = C_t \frac{4}{15} \frac{T_0}{P_0 c_0} \mathbf{q} \cdot \mathbf{n}.$$

Then the temperature-jump coefficient C_t is obtained from

$$\left(\frac{4 C_t}{15 c_0} \right)^{-1} = \frac{3}{2} L_0(\frac{01}{01}) = 2(W^2 | L | W^2). \quad (4.31)$$

Similarly, in flow problems frequently the vectorial boundary conditions are used in the truncated form

$$(\mathbf{v} - \mathbf{v}_{\text{II}})^{\text{tan}} = C_m \frac{c_0}{P_0} (\mathbf{n} \cdot \overline{\mathbf{P}})^{\text{tan}}.$$

Hence, the mechanical slip coefficient C_m is expressed as

$$\begin{aligned} C_m c_0 &= L_1(\frac{20}{20}) \\ &= 4(W_\mu^{\text{tan}} \mathbf{W} \cdot \mathbf{n} | L | W_\mu^{\text{tan}} \mathbf{W} \cdot \mathbf{n}). \end{aligned} \quad (4.32)$$

Numbers for these two "classical" slip coefficients will be given for the special L -model treated in the next section.

In conclusion of this section we shall once more derive the formulae (4.31) and (4.32) for the temperature jump and the mechanical slip, renouncing generality, in a most direct and simple way.

The distribution in a heat-conducting gas is

$$\Phi \approx \left(\varepsilon - \frac{3}{2} \right) \frac{T - T_0}{T_0} + \frac{2}{5} \left(\varepsilon - \frac{5}{2} \right) \frac{p_\mu q_\mu}{k T_0 P_0}. \quad (4.33)$$

This distribution is assumed to be valid as far as the wall, so that T in the following means the gas temperature at the wall. The dimensionless particle energy is denoted by $\varepsilon = W^2 = p^2/2mkT_0$; \mathbf{q} is the heat flux. The corresponding interfacial force-flux pair is

$$\begin{aligned} F_{\text{I}\Pi} &= \frac{1}{\sqrt{2}} P_+ \left(\Phi + \Phi_{\text{T}} - 2\varepsilon \frac{T_{\text{II}} - T_0}{T_0} + \text{const} \right) \\ &= \frac{1}{\sqrt{2}} P_+ \left(2\varepsilon \frac{T - T_{\text{II}}}{T_0} + \text{const} \right), \end{aligned} \quad (4.34)$$

$$\begin{aligned} J_{\text{I}\Pi} &= \frac{1}{\sqrt{2}} P_+ c (\Phi - \Phi_{\text{T}}) \\ &= \frac{1}{\sqrt{2}} P_+ c \cdot \frac{4}{5} \left(\varepsilon - \frac{5}{2} \right) \frac{p_\mu q_\mu}{k T_0 P_0}. \end{aligned} \quad (4.35)$$

Insertion into Eq. (2.1) gives for the interfacial entropy production per unit area

$$\begin{aligned} \frac{d\dot{S}}{d\sigma} &= \frac{2}{5} \int \left(\varepsilon - \frac{5}{2} \right) \varepsilon \frac{c_\nu p_\mu}{k T_0} d\gamma n_\nu q_\mu \frac{T - T_{\text{II}}}{T_0^2} \\ &= \frac{2}{5} \left(\frac{5}{2} \cdot \frac{7}{2} - \frac{5}{2} \cdot \frac{5}{2} \right) \delta_{\mu\nu} n_\nu q_\mu \frac{T - T_{\text{II}}}{T_0^2} \\ &= \frac{1}{T_0} \mathbf{n} \cdot \mathbf{q} \frac{T - T_{\text{II}}}{T_0}, \end{aligned} \quad (4.36)$$

where \mathbf{n} is the outer unit normal of the gas. Expression (4.36) shows that for the truncated distribution (4.33) one scalar boundary condition has to be aimed for. The full boundary condition

$$J_{\text{I}\Pi}(\mathbf{p}) = \int L(\mathbf{p}, \mathbf{p}') F_{\text{I}\Pi}(\mathbf{p}') d\gamma' \quad (4.37)$$

originally is in this case

$$\begin{aligned} P_+ c \cdot \frac{4}{5} \left(\varepsilon - \frac{5}{2} \right) \frac{p_\mu q_\mu}{k T_0 P_0} \\ \approx \int L(\mathbf{p}, \mathbf{p}') \cdot 2\varepsilon' \frac{T - T_{\text{II}}}{T_0} d\gamma'. \end{aligned} \quad (4.38)$$

With only two available parameters, \mathbf{q} and $T - T_{\text{II}}$, it can only be fulfilled "on the average". The "averaging" shall be performed in such a way that on the right side a diagonal L -matrix element appears. This means that Eq. (4.38) has to be mul-

tiplied by ε and integrated over $d\gamma$. On the left side the same integral as in (4.36) comes

$$\begin{aligned} \frac{4}{5} \int d\gamma P_+ \varepsilon \left(\varepsilon - \frac{5}{2} \right) \frac{c p_\mu}{k T_0} \\ = \frac{2}{5} \int d\gamma \varepsilon \left(\varepsilon - \frac{5}{2} \right) \frac{c_\nu p_\mu}{k T_0} n_\nu = n_\mu. \end{aligned}$$

Thus, the result of the averaging is the simple temperature jump condition

$$\mathbf{n} \cdot \mathbf{q} / P_0 = 2 \iint d\gamma \varepsilon L(\mathbf{p}, \mathbf{p}') \varepsilon' d\gamma' \frac{T - T_{\text{II}}}{T_0}. \quad (4.39)$$

This is equivalent to Eq. (4.31). It has already been found in [3], Eq. (7.9), and, as a scalar relation, is in accordance with the interfacial entropy production (4.36).

The distribution in a streaming gas with friction is

$$\Phi \approx \frac{p_\mu v_\mu}{k T_0} + \frac{1}{2} \frac{\overline{c_\mu p_\nu} \overline{P_{\mu\nu}}}{k T_0 P_0}, \quad (4.40)$$

which again is assumed to be valid as far as the wall, so that in the following \mathbf{v} means the gas velocity at the wall. The (irreducible) friction pressure tensor is denoted by $\overline{P_{\mu\nu}}$. The interfacial force-flux pair now is

$$F_{\text{I}\Pi} = \frac{1}{\sqrt{2}} P_+ \frac{\overline{c_\mu p_\nu} \overline{P_{\mu\nu}}}{k T_0 P_0}, \quad (4.41)$$

$$J_{\text{I}\Pi} = \frac{1}{\sqrt{2}} P_+ c \cdot \frac{2 p_\mu \tan}{k T_0} v_{\mu \text{I}\Pi}^{\tan}, \quad (4.42)$$

where

$$\mathbf{v}_{\text{I}\Pi} = \mathbf{v} - \mathbf{v}_{\text{II}} = \mathbf{v}_{\text{I}\Pi}^{\tan}$$

means the gas velocity relative and tangential to the wall with velocity \mathbf{v}_{II} . The component normal to the wall of this relative velocity vanishes. Insertion into Eq. (2.1) and use of the formula

$$\begin{aligned} \int d\gamma c_\mu p_\nu c_{\mu'} p_{\nu'} / (k T_0)^2 \\ = \delta_{\mu\nu} \delta_{\mu'\nu'} + \delta_{\mu\mu'} \delta_{\nu\nu'} + \delta_{\mu\nu'} \delta_{\nu\mu'} \end{aligned} \quad (4.43)$$

at once gives the interfacial entropy production

$$\frac{d\dot{S}}{d\sigma} = \frac{1}{T_0} \mathbf{v}_{\text{I}\Pi}^{\tan} \cdot \mathbf{k}_{\text{I}\Pi}^{\tan}, \quad (4.44)$$

with the friction force per unit area

$$\mathbf{k}_{\mu \text{I}\Pi} = n_\nu \overline{P_{\nu\mu}}. \quad (4.45)$$

Expression (4.44) shows that for the truncated distribution (4.40) a tangential vector boundary con-

dition is required. The full boundary condition (4.37), in terms of the force-flux pair (4.41) and (4.42), originally is

$$\frac{2}{kT_0} P_+ c p_{\nu}^{\tan} v_{\nu \text{ I II}}^{\tan} \approx \int L(\mathbf{p}, \mathbf{p}') \frac{1}{kT_0} c'_{\mu'} p'_{\nu'} d\gamma' \overline{\frac{P_{\mu' \nu'}}{P_0}}. \quad (4.46)$$

Again, this can be fulfilled only on the average which again shall be performed in such a way that finally a diagonal L -matrix element appears. For this aim, we multiply (4.46) by

$$\frac{1}{kT_0} c p_{\mu}^{\tan}$$

and integrate. Writing

$$p_{\mu}^{\tan} = T_{\mu\mu'} p_{\mu'}$$

with

$$T_{\mu\mu'} = \delta_{\mu\mu'} - n_{\mu} n_{\mu'}, \quad n_{\mu} T_{\mu\mu'} = 0, \quad (4.47)$$

the projection tensor into the tangential (wall) plane, we obtain on the left side, by use of (4.43),

$$\begin{aligned} & \frac{1}{(kT_0)^2} \int d\gamma c p_{\mu}^{\tan} c p_{\nu}^{\tan} \\ &= n_{\mu'} T_{\mu\mu'} n_{\nu'} T_{\nu\nu'} \int d\gamma c_{\mu'} p_{\mu''} c_{\nu'} p_{\nu''} / (kT_0)^2 \\ &= T_{\mu\nu}. \end{aligned} \quad (4.48)$$

On the right side, the third rank tensor appears

$$L_{\mu; \mu' \nu'} = \frac{1}{(kT_0)^2} \cdot \int d\gamma c p_{\mu}^{\tan} L(\mathbf{p}, \mathbf{p}') c'_{\mu'} p'_{\nu'} d\gamma', \quad (4.49)$$

symmetric in μ' , ν' and of the dimension of a velocity. Because \mathbf{n} is the only vector available to construct this tensor, it must have the shape

$$L_{\mu; \mu' \nu'} = A n_{\mu} \delta_{\mu' \nu'} + B (\delta_{\mu\mu'} n_{\nu'} + \delta_{\mu\nu'} n_{\mu'}) + C n_{\mu} n_{\mu'} n_{\nu'}.$$

But from $n_{\mu} p_{\mu}^{\tan} = 0$ follows that

$$n_{\mu} L_{\mu; \mu' \nu'} = 0,$$

which leads to $A = 0$, $C = -2B$. Hence, with the abbreviation $2B = L_{\text{red}}$, the tensor assumes the form

$$L_{\mu; \mu' \nu'} = L_{\text{red}} \cdot \frac{1}{2} (T_{\mu\mu'} n_{\nu'} + T_{\mu\nu'} n_{\mu'}). \quad (4.50)$$

The reduced matrix element L_{red} is obtained by multiplication with $n_{\nu'}$

$$L_{\mu; \mu' \nu'} n_{\nu'} = L_{\text{red}} \cdot \frac{1}{2} T_{\mu\mu'},$$

followed by the contraction $\mu = \mu'$ ($T_{\mu\mu} = 2$):

$$L_{\text{red}} = L_{\mu; \mu \nu'} n_{\nu'} \quad (4.51)$$

$$= \frac{1}{(kT_0)^2} \int d\gamma c p_{\mu}^{\tan} L(\mathbf{p}, \mathbf{p}') c' p_{\mu'}^{\tan} d\gamma',$$

because

$$p_{\mu}^{\tan} p_{\mu'} = p_{\mu}^{\tan} p_{\mu'}^{\tan}.$$

This now is indeed a diagonal matrix element. Combining the results (4.48) for the left side and (4.49) resp. (4.50) for the right side yields the slip boundary condition

$$v_{\mu \text{ I II}}^{\tan} = L_{\mu; \mu \nu'} \frac{\overline{P_{\mu' \nu'}}}{P_0} = L_{\text{red}} \frac{k_{\mu \text{ I II}}^{\tan}}{P_0}. \quad (4.52)$$

This is equivalent to Eq. (4.32) and, as a tangential vector relation, it is in accordance with the interfacial entropy production (4.44).

The accordance in both cases with the entropy expressions which had been freed from all redundant surface variables, guarantees a unique existing solution [4], [2] of the transport-relaxation equations for the moments occurring in Eqs. (4.33) and (4.40), i.e. for T , \mathbf{q} and \mathbf{v} , \mathbf{P} respectively. — This ends the most direct and simple consideration of these two cases, temperature jump and mechanical slip.

5. A Model for the Interfacial Kernel

To construct such a model it is most appropriate to begin with the transition operator R defined in Equation (3.15). It is sufficient to consider a wall at rest ($\mathbf{v}_{\text{II}} = 0$). Our ansatz ist

$$\begin{aligned} R(\mathbf{p}' \rightarrow \mathbf{p}) &= P_+ (-c) \left\{ \beta (1 - \alpha) \delta(\mathbf{p}, -\mathbf{p}') \right. \\ &\quad + (1 - \beta) (1 - \alpha) \delta(\mathbf{p}, \mathbf{p}' - 2\mathbf{n} \mathbf{n} \cdot \mathbf{p}') \\ &\quad \left. + \alpha \frac{(-c)}{\hat{c}_{\text{II}}} \frac{f_{\text{II}}(\mathbf{p})}{n_{\text{II}}} \right\} P_+(c'). \end{aligned} \quad (5.1)$$

Obviously, the “detailed balance” relation (3.19) is fulfilled. Particle conservation (3.18) is guaranteed by the choice

$$\begin{aligned} \hat{c}_{\text{II}} &= \int P_+ (-c) (-c) \frac{f_{\text{II}}(\mathbf{p})}{n_{\text{II}}} d^3p \\ &= (kT_{\text{II}}/2\pi m)^{1/2}. \end{aligned} \quad (5.2a)$$

Since R has to be positive, cf. Eq. (3.17), the two parameters α , β have to be positive and smaller than unity:

$$0 \leq \alpha \leq 1, \quad 0 \leq \beta \leq 1. \quad (5.3)$$

If the density n_{II} is chosen as

$$n_{II} = \frac{1}{\hat{c}_{II}} \int P_+(c') c' f(t, \mathbf{x}, \mathbf{p}') d^3 p'. \quad (5.2b)$$

the distribution function of the particles leaving the wall is expressed, via Eq. (3.15), by the "incoming" distribution in the following way:

$$\begin{aligned} P_+(-c) f(t, \mathbf{x}, \mathbf{p}) \\ = P_+(-c) \{ \beta(1 - \alpha) f(t, \mathbf{x}, -\mathbf{p}) \\ + (1 - \beta)(1 - \alpha) f(t, \mathbf{x}, \mathbf{p} - 2\mathbf{n}\mathbf{n} \cdot \mathbf{p}) \\ + \alpha f_{II}(\mathbf{p}) \}. \end{aligned} \quad (5.4)$$

This equation gives us a feeling for the two parameters α and β : the fraction α of the outgoing particles is thermalized, whereas the fraction $(1 - \beta)(1 - \alpha)$ is reflected specularly and the remaining particles, namely the fraction $\beta(1 - \alpha)$, are reflected in backward direction. To our knowledge, the back scattering term is considered here for the first time. Notice that complete accommodation is characterized by $\alpha = 1$ and any allowed value for β .

Now, we want to relate the parameters α , β to the usual definition of an accommodation coefficient $\alpha[\varphi]$ for a function $\varphi(\mathbf{p})$. Cercignani's definition is [6]

$$\begin{aligned} \alpha[\varphi] &= \left\{ \int P_+(c) c f \varphi d^3 p \right. \\ &\quad \left. - \int P_+(-c) (-c) f_{II} \varphi d^3 p \right\} \\ &= \int P_+(c) c f \varphi d^3 p - \int P_+(-c) (-c) f \varphi d^3 p. \end{aligned} \quad (5.5)$$

Complete accommodation, i.e.

$$P_+(-c) f = P_+(-c) f_{II},$$

is expressed by $\alpha[\varphi] = 1$. The accommodation coefficient in our model is obtained by insertion of $P_+(-c) f$ from Eq. (5.4) into Equation (5.5). After a short calculation one gets

$$\alpha[\varphi_{\text{even}}] = \alpha, \quad (5.6)$$

$$\alpha[\varphi_{\text{odd}}] = 1 - (1 - \alpha)(2\beta - 1) \equiv \alpha_{\text{odd}}. \quad (5.7)$$

So, the parameter α in the ansatz (5.1) for R is identical with the accommodation coefficient for functions which are even in the momentum \mathbf{p} and in the tangential momentum \mathbf{p}^{tan} ; examples for φ_{even} are the tensors $\varphi^{(01)}$, $\varphi^{(02)}$, $\varphi^{(20)}$, $\varphi_{\mu\nu}^{(20)}$ from Eqs. (4.23) and (4.25). The combination α_{odd} is the accommodation coefficient for functions which are even in \mathbf{p} and odd in \mathbf{p}^{tan} ; an example for φ_{odd} is the vector $\varphi_{\mu}^{(20)}$ from Eq. (4.24). Due to the restrictions (5.3) for α and β , the coefficient α_{odd} obeys the inequality

$$\alpha \leq \alpha_{\text{odd}} \leq 2 - \alpha. \quad (5.8)$$

If one puts $\beta = 0$, as usual, α_{odd} is given by

$$\alpha_{\text{odd}} = 2 - \alpha,$$

with

$$1 \leq \alpha_{\text{odd}} \leq 2.$$

For the R -model (5.1), the corresponding \mathfrak{H} -operator is obtained from Eq. (3.16) by the transformation $\mathbf{p} \rightarrow -\mathbf{p}$:

$$\begin{aligned} \mathfrak{H}(\mathbf{p}, \mathbf{p}') &= P_+(c) \left\{ \beta(1 - \alpha) \delta(\mathbf{p}, \mathbf{p}') \frac{\hat{c}_0 d^3 p'}{c' d\gamma'} \right. \\ &\quad \left. + (1 - \beta)(1 - \alpha) \delta(\mathbf{p}, -\mathbf{p}' + 2\mathbf{n}\mathbf{n} \cdot \mathbf{p}') \frac{\hat{c}_0 d^3 p'}{c' d\gamma'} + \alpha \right\} P_+(c'). \end{aligned} \quad (5.9)$$

For $d\gamma$, Eq. (1.23) is recalled. The symmetry requirement (3.8) and the particle conservation (3.10) are of course fulfilled. For the calculation of \mathfrak{Q} from Eq. (3.7), it is convenient to express our \mathfrak{H} in terms of three projection operators $\mathfrak{P}^{(m)}$, $m = 0, \pm 1$:

$$\begin{aligned} \mathfrak{P}^{(0)}(\mathbf{p}, \mathbf{p}') &= P_+(c) P_+(c'), \\ \mathfrak{P}^{(1)}(\mathbf{p}, \mathbf{p}') &= P_+(c) P_+(c') \left\{ \frac{1}{2} [\delta(\mathbf{p}, \mathbf{p}') + \delta(\mathbf{p}, -\mathbf{p}' + 2\mathbf{n}\mathbf{n} \cdot \mathbf{p}')] \frac{\hat{c}_0 d^3 p'}{c' d\gamma'} - 1 \right\}, \\ \mathfrak{P}^{(-1)}(\mathbf{p}, \mathbf{p}') &= P_+(c) P_+(c') \frac{1}{2} [\delta(\mathbf{p}, \mathbf{p}') - \delta(\mathbf{p}, -\mathbf{p}' + 2\mathbf{n}\mathbf{n} \cdot \mathbf{p}')] \frac{\hat{c}_0 d^3 p'}{c' d\gamma'}. \end{aligned}$$

They have the properties

$$\begin{aligned} \mathfrak{P}^{(m)} \mathfrak{P}^{(m')} &= \delta_{mm'} \mathfrak{P}^{(m)}, \quad m, m' = 0, \pm 1; \\ \sum_{m=-1}^{+1} \mathfrak{P}^{(m)} &= \mathbb{1}. \end{aligned}$$

This gives for \mathfrak{P} the expression

$$\mathfrak{P} = (1 - \alpha) \mathfrak{P}^{(1)} + (1 - \alpha_{\text{odd}}) \mathfrak{P}^{(-1)} + \mathfrak{P}^{(0)}, \quad (5.10)$$

and for \mathfrak{Q} follows immediately from (3.7)

$$\mathfrak{Q} = \frac{\alpha}{2 - \alpha} \mathfrak{P}^{(1)} + \frac{\alpha_{\text{odd}}}{2 - \alpha_{\text{odd}}} \mathfrak{P}^{(-1)}. \quad (5.11)$$

If the operator \mathfrak{Q} is applied to a function $\varphi(\mathbf{p})$, the result is

$$\begin{aligned} \mathfrak{Q}\varphi = P_+(c) & \left\{ \frac{\alpha}{2 - \alpha} \left[\frac{1}{2} \varphi(\mathbf{p}) + \frac{1}{2} \varphi(-\mathbf{p} + 2\mathbf{n}\mathbf{n} \cdot \mathbf{p}) - \int \varphi' d\Gamma' \right] \right. \\ & \left. + \frac{\alpha_{\text{odd}}}{2 - \alpha_{\text{odd}}} \left[\frac{1}{2} \varphi(\mathbf{p}) - \frac{1}{2} \varphi(-\mathbf{p} + 2\mathbf{n}\mathbf{n} \cdot \mathbf{p}) \right] \right\}. \end{aligned} \quad (5.11a)$$

In other words: all functions

$$P_+(c) [\varphi_{\text{even}} - \int \varphi'_{\text{even}} d\Gamma'], \quad \varphi_{\text{even}} \neq 1,$$

are eigenfunctions of \mathfrak{Q} with the same eigenvalue $\alpha/(2 - \alpha)$, and all functions $P_+(c)\varphi_{\text{odd}}$ are eigenfunctions with the eigenvalue $\alpha_{\text{odd}}/(2 - \alpha_{\text{odd}})$.

If we insert the expressions for the projectors $\mathfrak{P}^{(\pm 1)}$ into Eq. (5.11) and use Eq. (3.3), we get the explicit form

$$\begin{aligned} L(\mathbf{p}, \mathbf{p}') = \frac{\alpha}{2 - \alpha} P_+(c) c & \left\{ \frac{1}{2} [\delta(\mathbf{p}, \mathbf{p}') + \delta(\mathbf{p}, -\mathbf{p}' + 2\mathbf{n}\mathbf{n} \cdot \mathbf{p}')] \frac{d^3 p'}{c' d\gamma'} - \frac{1}{\hat{c}_0} \right\} c' P_+(c') \\ & + \frac{\alpha_{\text{odd}}}{2 - \alpha_{\text{odd}}} P_+(c) c \frac{1}{2} [\delta(\mathbf{p}, \mathbf{p}') - \delta(\mathbf{p}, -\mathbf{p}' + 2\mathbf{n}\mathbf{n} \cdot \mathbf{p}')] \frac{d^3 p'}{c' d\gamma'} c' P_+(c') \end{aligned} \quad (5.12)$$

for the interfacial kernel as it occurs in the boundary condition (2.7). With complete accommodation, $\alpha = \alpha_{\text{odd}} = 1$, this is the kernel already given in [1].

By help of Eq. (5.12) and of the formula

$$\int P_+ c (\mathbf{W} \cdot \mathbf{n})^N W^{2M} d\gamma = \frac{\hat{c}_0}{1 + N/2} \Gamma(2 + M + N/2); \quad M, N = 0, 1, 2, \dots, \quad (5.13)$$

the special matrix elements $L_s(l'r')$, defined in Eqs. (4.26) and (3.23), can now be calculated. In this way, the matrix

$$L_0(l'r') = \hat{c}_0 \frac{2\alpha}{2 - \alpha} \begin{pmatrix} \frac{4}{3} & -\frac{4}{3\sqrt{5}} & -\frac{1}{3}\sqrt{2} \\ -\frac{4}{3\sqrt{5}} & \frac{28}{15} & \frac{1}{3}\sqrt{\frac{2}{5}} \\ -\frac{1}{3}\sqrt{2} & \frac{1}{3}\sqrt{\frac{2}{5}} & \frac{5}{3} \end{pmatrix} \quad (5.14)$$

is obtained, where the rows and columns have to be labelled by (lr) , $(l'r') = (01), (02), (20)$. The equivalent matrix $C_{\lambda\lambda'}$ from Eq. (4.30) has the following form:

$$(C_{\lambda\lambda'}) = \frac{4}{15} \sqrt{\frac{2}{\pi}} \frac{\alpha}{2 - \alpha} \begin{pmatrix} 2 & -1 & -\frac{3}{10} \\ -1 & \frac{7}{2} & \frac{3}{20} \\ -\frac{3}{10} & \frac{3}{20} & \frac{117}{100} \end{pmatrix}; \quad (5.15)$$

here, the labels are $\lambda, \lambda' = q, A, a$. In the same way, the matrix elements are obtained:

$$L_1 \binom{20}{20} = 4 \hat{c}_0 \frac{\alpha_{\text{odd}}}{2 - \alpha_{\text{odd}}}, \quad (5.16)$$

$$L_2 \binom{20}{20} = 2 \hat{c}_0 \frac{\alpha}{2 - \alpha}. \quad (5.17)$$

Hence, the two coefficients C_t and C_m from Eqs. (4.31), (4.32) have the values

$$\frac{15}{4C_t} = 2 \sqrt{\frac{2}{\pi}} \frac{\alpha}{2 - \alpha}, \quad (5.18)$$

$$\begin{aligned} C_m &= 2 \sqrt{\frac{2}{\pi}} \frac{\alpha_{\text{odd}}}{2 - \alpha_{\text{odd}}} \\ &= 2 \sqrt{\frac{2}{\pi}} \frac{2 - \alpha - 2\beta(1 - \alpha)}{\alpha + 2\beta(1 - \alpha)}. \end{aligned} \quad (5.19)$$

The temperature-jump coefficient $C_t(\alpha)$, due to $\alpha \leq 1$, is always larger than $C_t(1)$,

$$C_t \geq \frac{15}{8} \sqrt{\frac{\pi}{2}} \approx 2.35.$$

The mechanical slip coefficient $C_m(\alpha, \beta)$ may have any positive value, depending on the numbers for α and β . In particular, we note

$$C_m(1, \beta) = C_m(\alpha, \tfrac{1}{2}) = 2 \sqrt{\frac{2}{\pi}} \approx 1.60,$$

$$C_m(\alpha, 0) = 2 \sqrt{\frac{2}{\pi}} \frac{2-\alpha}{\alpha} \geq 2 \sqrt{\frac{2}{\pi}},$$

$$C_m(\alpha, 1) = 2 \sqrt{\frac{2}{\pi}} \frac{\alpha}{2-\alpha} \leq 2 \sqrt{\frac{2}{\pi}}.$$

From the thermal force experienced by aerosol particles in argon, the data $C_t = 3.67$ and $C_m = 1.91$ have been determined [13]. These empirical values are reproduced by the parameters $\alpha = 0.78$, $\beta = 0.30$, i.e. $\alpha_{\text{odd}} = 1.09$, in our present model. These numbers seem to be quite reasonable.

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