Generalization of the Moment Method of Maxwell-Grad for Multi-Temperature Gas Mixtures and Plasmas

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A coupled system of balance equations is derived for the coefficients of orthogonal expansions of the velocity distribution functions. The orthogonal functions are not specified, but the initial functions must be local Maxwellians with different temperatures for different species of particles. Closed expressions for the matrix elements of the non-linearized Boltzmann operator are given, whose dominant terms are determined and compared.

1. Introduction

Tensorial velocity moments, i. e. polyadic products of the velocity vector averaged with the velocity distribution function as weight function, are meaningful physical quantities. Those up to the second order, viz. density, flow, and pressure, are directly measurable as well as energy flow, the trace of the third order moment. Therefore Maxwell[1] derived a coupled system of balance equations for these moments from the Boltzmann equation. With these balance equations transport coefficients and relaxation times could be calculated.

The balance equation for the n-th order moment contains the divergence of the $n+1$st order moment, contributing to the coupling among the balance equations. The closure of the system regarding this particular coupling is usually done by an approximative expression for a certain moment, which contains no higher order moments.

To calculate the collision integral of a balance equation the velocity distribution functions for the species of colliding particles must be known in general. Maxwell overcame this difficulty using the so called Maxwell interaction between the particles, the only type of interaction where the knowledge of the distribution functions is not required for the calculation of the collision moments. To avoid this restriction for the particle interaction Grad[2] expanded the velocity distribution function in an orthogonal series of tensorial Hermite functions. The coefficients are averages of tensorial Hermite polynomials and therefore linear combinations of the velocity moments. Thus the collision moments become infinite series of moments with calculable coefficients, causing complicated coupling between the balance equations for non-Maxwellian interactions.

To close the system of balance equations with regard to this coupling Grad[2] proposed an a priori cutoff of the orthogonal expansion. This heuristic procedure has to be justified ad hoc. In the present paper we avoid this cutoff. Instead of this we develop a method to compare the order of magnitude of the infinite sequence of coupling coefficients (Chapter 4). This allows their neglection according to a prescribed accuracy.

Instead of Grad's tensorial Hermite functions other systems of orthogonal functions have been used: products of three ordinary Hermite functions with the cartesian velocity components as arguments[3] and Burnett functions, viz. products of spherical harmonics with generalized Laguerre functions[4]. In Chapter 2 of the present paper we develop a general formalism without specification of the orthogonal system used for the expansion of the distribution functions. In contrast to previous treatments we assume different kinetic temperatures for the different species of particles. This is particularly important for plasmas. Due to the large mass ratio between electrons and heavy particles (ions and neutrals) their energy exchange is much slower than the mutual exchange between the electrons themselves and between the heavier particles. Therefore very often different temperatures are maintained for the different species of particles and must be taken into account in all expressions describing the behaviour of these plasmas.

The collision operator is not linearized. For all of its elements closed expressions are calculated using transformation theory (Chapter 2 and 3). Trans-

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formation coefficients depending on the choice of orthogonal functions are given in the appendix. Instead of the Ω-integrals introduced by Chapman and Cowling [5] and extensively used by Hirschfelder, Curtiss and Bird [6], we prefer linear combinations of them, the transport collision frequencies introduced by Suchy and Rawer [7]. Their advantages are discussed in Chapter 4.

2. General Formalism

2.1. Derivation of a System of Balance Equations

The kinetic equation for the velocity distribution function $f(i) = f(\boldsymbol{x}_i, \mathbf{c}_i; t)$ for particles of species i can be written as

$$D(i)\,[f(i)] = \sum_j B(i,j)\,[f(i), f(j)]\,. \qquad (2.1)$$

The operator

$$D(i) \equiv \frac{\partial}{\partial t} + \mathbf{c}_i \cdot \frac{\partial}{\partial \boldsymbol{x}_i} + \dot{\mathbf{c}}_i \cdot \frac{\partial}{\partial \mathbf{c}_i}$$

acts as total derivation. $B(i,j)$ describes binary interactions between particles of species i and j. The particular Boltzmann form

$$B(i,j)\,[f(i), f(j)] = \int \mathrm{d}^3 c_j \int \mathrm{d}\Omega'\, \sigma_{ij}\, g\, [f(i')f(j') - f(i)f(j)] \qquad (2.2)$$

is bilinear in the two functions $f(i)$ and $f(j)$; primed and unprimed arguments distinguish variables before and after the collision, the differential cross section σ_{ij} depends on the relative velocity

$$\boldsymbol{g} := \mathbf{c}_j - \mathbf{c}_i\,. \qquad (2.3)$$

To introduce a generalized moment-method we represent the distribution functions f as elements of a linear space spanned by a basis system $\{\varphi_\lambda\}$:

$$f(\boldsymbol{x}_i, \mathbf{c}_i; t) = a^\lambda(\boldsymbol{x}_i, t)\, \varphi_\lambda(\boldsymbol{x}_i, \mathbf{c}_i; t)\,, \qquad (2.4\,\mathrm{a})$$

abbreviated as

$$f(i) = a_i^\lambda\, \varphi_\lambda(i)\,. \qquad (2.4\,\mathrm{b})$$

The basis functions $\varphi_\lambda(\boldsymbol{x}_i, t; \mathbf{c}_i)$ are to be considered as functions of the variable $\mathbf{c}_i$ with $\boldsymbol{x}_i, t$ as parameters which only appear in a normalization speed and a reference velocity, e.g. $\sqrt{K_\mathrm{B} T_i(\boldsymbol{x}_i, t)/m_i}$ and $\mathbf{c}_{i0}(\boldsymbol{x}_i, t)$, cf. Equation (2.8 a). The convention is used to sum over all indices appearing once and only once as a superscript and a subscript. As we restrict ourselves in the explicit calculations to elastic collisions, we let λ denote a triple of indices and define an inner product by

$$\langle \varphi \,|\, \psi \rangle := \int \mathrm{d}^3 c\, \varphi(\mathbf{c})\, \psi(\mathbf{c})\,. \qquad (2.5)$$

This enables the construction of a dual basis system requiring

$$\langle \varphi^{\lambda'}(i) \,|\, \varphi_\lambda(i) \rangle = \int \mathrm{d}^3 c_i\, \varphi^{\lambda'}(i)\, \varphi_\lambda(i) = \delta_\lambda{}^{\lambda'}. \qquad (2.6)$$

Hence the expansion coefficients in (2.4), the "generalized moments", are inner products:

$$a_i^\lambda = \langle \varphi^\lambda(i) \,|\, f(i) \rangle = \int \mathrm{d}^3 c_i\, \varphi^\lambda(i)\, f(i)\,. \qquad (2.7)$$

To treat deviations from thermodynamic equilibrium the basis system $\{\varphi_\lambda(i)\}$ is chosen such that $\varphi_0(i)$ is proportional to the local Maxwellian:

$$\varphi_0(i) := \left(2\pi \frac{K_\mathrm{B} T_i}{m_i}\right)^{-3/2} \exp\left\{-\frac{1}{2}\frac{m_i}{K_\mathrm{B} T_i}(\mathbf{c}_i - \mathbf{c}_{i0})^2\right\} \qquad (2.8\,\mathrm{a})$$

with an arbitrary reference velocity $\mathbf{c}_{i0}$. Condition (2.6) for the dual basis then yields

$$\varphi^0(i) = 1\,. \qquad (2.8\,\mathrm{b})$$

Starting with $\varphi_0(i)$ as a "weight function" we have two possibilities to construct the basis system: threedimensional Hermite-functions [2, 3] and Burnett-functions [8]. Both systems can be represented in tensorial or scalar notation; a special choice, used in the following calculations, is discussed in the Appendix A1 together with some of the related generalized moments a_i^λ. In both cases the order of a_i^λ, $\varphi_\lambda(i)$ and $\varphi^\lambda(i)$ is given by the highest power of $|\mathbf{c}_i - \mathbf{c}_{i0}|$ in the polynomial $\varphi^\lambda(i)$. For simplicity the following convention shall be used: a small greek letter denotes a triple of indices if used as an index but it is the order of the moment if used in algebraic expressions, e. g. inequalities or powers. Thus all such expressions are valid for both types of basis systems according to the transformation matrices, given in the Appendix A2.

Inserting the expansion (2.4) into the kinetic Eq. (2.1) yields

$$D(i)\,[\varphi_\lambda(i)\, a_i^\lambda] = \sum_j B(i,j)\,[\varphi_\lambda(i)\, a_i^\lambda, \varphi_\mu(j)\, a_j^\mu]\,. \qquad (2.9)$$

If we assume the operator $B(i,j)$ to be bilinear – as in the Boltzmann form (2.2) –, multiplication with $\varphi^{\lambda'}(i)$ and integration over $\mathrm{d}^3 c_i$ yields a system of coupled equations:

$$D_\lambda^{\lambda'}(i)\, a_i^\lambda = \sum_j B_{\lambda\mu}^{\lambda'}(i,j)\, a_i^\lambda\, a_j^\mu\,. \qquad (2.10)$$

This is a system of "balance-equations" for the generalized moments. The choice (2.8) of the basis functions yields for $\lambda' = 0$ the mass balance or continuity equation, for $\lambda' = 1$ the momentum balance or equation of motion, etc. The coefficients

$$D_{\lambda}^{\lambda'}(i) := \langle \varphi^{\lambda'}(i) \,|\, D(i)\,[\varphi_{\lambda}(i)] \rangle \tag{2.11}$$

and

$$B_{\lambda\mu}^{\lambda'}(i,j) := \langle \varphi^{\lambda'}(i) \,|\, B(i,j)\,[\varphi_{\lambda}(i), \varphi_{\mu}(j)] \rangle \tag{2.12}$$

themselves are in general operators acting on the moments a_i^{λ}, a_j^{μ}. Expression (2.12), however, becomes multiplicative if the variation of the moments can be neglected in the temporal and spatial scale of the molecular interaction. Therefore in the case of the Boltzmann integral (2.2) the generalized moments may be drawn out of the integrations over $\mathrm{d}^3 c_i$, $\mathrm{d}^3 c_j$ yielding the collision elements

$$B_{\lambda\mu}^{\lambda'}(i,j) = \int \mathrm{d}^3 c_i \int \mathrm{d}^3 c_j \int \mathrm{d}\Omega' \, \sigma_{ij}\, g \times \varphi^{\lambda'}(i) \,\{\varphi_{\lambda}(i')\, \varphi_{\mu}(j') - \varphi_{\lambda}(i)\, \varphi_{\mu}(j)\}\,. \tag{2.13}$$

2.2. *Representation of the Collision Elements B*

The first step in the evaluation of (2.13) is the expansion of the product of two one-particle basis functions:

$$\varphi_{\lambda}(i)\, \varphi_{\mu}(j) = T_{\lambda\mu}^{\alpha\varkappa}\, \chi_{\alpha}(\mathbf{G})\, \Phi_{\varkappa}(\boldsymbol{g})\,, \tag{2.14 a}$$

$$\varphi^{\lambda'}(i)\, \varphi^{\mu'}(j) = T_{\alpha'\varkappa'}^{\lambda'\mu'}\, \chi^{\alpha'}(\mathbf{G})\, \Phi^{\varkappa'}(\boldsymbol{g})\,, \tag{2.14 b}$$

where in addition to the relative velocity $\boldsymbol{g} = \mathbf{c}_j - \mathbf{c}_i$, Eq. (2.3), the center-of-mass velocity

$$\mathbf{G} := \frac{m_i}{m_i + m_j}\, \mathbf{c}_i + \frac{m_j}{m_i + m_j}\, \mathbf{c}_j \tag{2.15}$$

is introduced. The functions Φ and χ are dual in the sense of the definitions (2.5) and (2.6):

$$\int \mathrm{d}^3 G\, \chi^{\alpha'}(\mathbf{G})\, \chi_{\alpha}(\mathbf{G}) = \delta_{\alpha}^{\alpha'} \tag{2.16 a}$$

as well as

$$\int \mathrm{d}^3 g\, \Phi^{\varkappa'}(\boldsymbol{g})\, \Phi_{\varkappa}(\boldsymbol{g}) = \delta_{\varkappa}^{\varkappa'}\,. \tag{2.16 b}$$

Because of the definitions (2.3) for $\boldsymbol{g}$ and (2.15) for $\mathbf{G}$ we have

$$\mathrm{d}^3 c_i\, \mathrm{d}^3 c_j = \mathrm{d}^3 g\, \mathrm{d}^3 G\,. \tag{2.17}$$

Thus we may uniquely define an inner product for two-particle functions $\xi(i,j)$ and $\eta(i,j)$:

$$\langle \xi \,|\, \eta \rangle := \int \mathrm{d}^3 c_i\, \mathrm{d}^3 c_j\, \xi\, \eta = \int \mathrm{d}^3 G\, \mathrm{d}^3 g\, \xi\, \eta\,. \tag{2.18}$$

Hence the transformation coefficients of the expansions (2.14 a, b) are

$$T_{\lambda\mu}^{\alpha\varkappa} = \langle \chi^{\alpha}(\mathbf{G})\, \Phi^{\varkappa}(\boldsymbol{g}) \,|\, \varphi_{\lambda}(i)\, \varphi_{\mu}(j) \rangle \tag{2.19 a}$$

and

$$T_{\alpha'\varkappa'}^{\lambda'\mu'} = \langle \varphi^{\lambda'}(i)\, \varphi^{\mu'}(j) \,|\, \chi_{\alpha'}(\mathbf{G})\, \Phi_{\varkappa'}(\boldsymbol{g}) \rangle\,. \tag{2.19 b}$$

Using $\varphi^0 = 1$, Eq. (2.8 b), we insert the expansions (2.14 a, b) into the collision elements (2.13) and obtain

$$B_{\lambda\mu}^{\lambda'}(i,j) = T_{\alpha'\varkappa'}^{\lambda'0}\, \Psi_{\alpha\ \varkappa}^{\alpha'\varkappa'}\, T_{\lambda\mu}^{\alpha\varkappa} \tag{2.20 a}$$

with

$$\Psi_{\alpha'\varkappa'}^{\alpha'\varkappa'} := \int \mathrm{d}^3 g \int \mathrm{d}^3 G \int \mathrm{d}\Omega' \, \sigma_{ij}\, g \times \chi^{\alpha'}(\mathbf{G})\, \Phi^{\varkappa'}(\boldsymbol{g})\, \{\chi_{\alpha}(\mathbf{G}')\, \Phi_{\varkappa}(\boldsymbol{g}') - \chi_{\alpha}(\mathbf{G})\, \Phi_{\varkappa}(\boldsymbol{g})\}\,. \tag{2.20 b}$$

Thus we obtain a representation for the collision elements with the following features:

a) The transformation coefficients T, Eq. (2.19), merely depend on the choice of the base functions φ, χ and Φ. Their calculation is a purely mathematical problem.

b) The "collision matrices" Ψ, Eq. (2.20), depend on the properties of the particle interactions. Their calculation can be facilitated by simplifying assumptions about these interactions.

2.3. *Calculation of the Collision Matrices Ψ*

In this section we make the following assumptions regarding the interactions between the colliding particles: 1) conservation of total momentum, 2) isotropic intermolecular potential, 3) elastic collisions.

2.3.1. Conservation of Total Momentum

If the sum of the masses of the colliding particles is conserved, the center of mass velocity $\mathbf{G}$ is conserved, i. e. $\mathbf{G} = \mathbf{G}'$, yielding

$$\Psi_{\alpha'\varkappa'}^{\alpha'\varkappa'} = \delta_{\alpha}^{\alpha'}\, \Psi_{\varkappa}^{\varkappa'} \tag{2.21 a}$$

with the "reduced collision matrix"

$$\Psi_{\varkappa}^{\varkappa'} = \int \mathrm{d}^3 g \int \mathrm{d}\Omega' \, \sigma(\Omega', \boldsymbol{g})\, g \times \Phi^{\varkappa'}(\boldsymbol{g})\, \{\Phi_{\varkappa}(\boldsymbol{g}') - \Phi_{\varkappa}(\boldsymbol{g})\}\,, \tag{2.21 b}$$

where the particle species indices i and j are omitted. The Kronecker-δ represents the completeness of the basis functions $\chi_{\alpha}(\mathbf{G})$, Equation (2.14).

2.3.2 Isotropic Intermolecular Potential

In this case the differential cross section σ merely depends on the relative speed g and the angle of deflection $x = \arccos \hat{\boldsymbol{g}} \cdot \hat{\boldsymbol{g}}'$. Thus the orthogonal expansion of σ with respect to Ω' is

$$\sigma(x, g) = \sigma^{\mathrm{L}}(g)\, P_{\mathrm{L}}(\cos x)\,, \tag{2.22}$$

where $P_{\mathrm{L}}(\cos x)$ are Legendre polynomials, hence

$$\sigma^{\mathrm{L}}(g) = \tfrac{1}{2}(2\,\mathrm{L}+1) \int_{-1}^{+1} \mathrm{d}\cos x\, \sigma(x, g) P_{\mathrm{L}}(\cos x)\,. \tag{2.23}$$

Factorising the functions $\Phi^{\varkappa'}$ and $\Phi_{\varkappa}$ as

$$\Phi_{\varkappa}(\boldsymbol{g}) \equiv \Phi_{qlm}(\boldsymbol{g}) = \Phi_{ql}(g)\, Y_{lm}(\hat{\boldsymbol{g}}) \tag{2.24 a}$$

and

$$\Phi^{\varkappa'}(\boldsymbol{g}) \equiv \Phi^{q'l'm'}(\boldsymbol{g}) = \Phi^{q'}_{l'}(g)\, Y^{m'}_{l'}(\hat{\boldsymbol{g}}) \tag{2.24 b}$$

with the spherical harmonics $Y_{lm}(\hat{\boldsymbol{g}})$ and their complex conjugates

$$Y^{m'}_{l'}(\hat{\boldsymbol{g}}) := Y^{*}_{l'm'}(\hat{\boldsymbol{g}})\,, \tag{2.24 c}$$

we have instead of Eq. (2.21 b):

$$\Psi^{q'l'm'}_{q\,l\,m} = \int_0^\infty g^3\,\mathrm{d}g \int \mathrm{d}\Omega \int \mathrm{d}\Omega'\, \sigma(x, g) \times \Phi^{q'}_{l'}(g)\, Y^{m'}_{l'}(\hat{\boldsymbol{g}}) \{\Phi_{ql}(g')\, Y_{lm}(\hat{\boldsymbol{g}}') - \Phi_{ql}(g)\, Y_{lm}(\hat{\boldsymbol{g}})\}\,. \tag{2.25}$$

We insert the expansion $\sigma = \sigma^{\mathrm{L}} P_{\mathrm{L}}$, Eq. (2.22), into (2.25) and replace the Legendre Polynomials P_{L} by the addition theorem for spherical harmonics:

$$\Psi^{q'l'm'}_{q\,l\,m} = \sum_{\mathrm{L}} \frac{4\pi}{2\,\mathrm{L}+1} \int_0^\infty g^3\,\mathrm{d}g \int \mathrm{d}\Omega \int \mathrm{d}\Omega'\, \sigma^{\mathrm{L}}(g) \times Y_{\mathrm{LM}}(\hat{\boldsymbol{g}})\, Y^{\mathrm{M}}_{\mathrm{L}}(\hat{\boldsymbol{g}}')\, \Phi^{q'}_{l'}(g)\, Y^{m'}_{l'}(\hat{\boldsymbol{g}}) \times \{\Phi_{ql}(g')\, Y_{lm}(\hat{\boldsymbol{g}}') - \Phi_{ql}(g)\, Y_{lm}(\hat{\boldsymbol{g}})\}\,. \tag{2.26}$$

Because of the orthogonality of the spherical harmonics, the integrations over the solid angles $\mathrm{d}\Omega$ and $\mathrm{d}\Omega'$ then yield

$$\Psi^{q'l'm'}_{q\,l\,m} = \delta^{m'}_{m}\, \delta^{l'}_{l}\, \Psi^{q'}_{ql} \tag{2.27 a}$$

with the "isotropic collision matrix"

$$\Psi^{q'}_{ql} := -4\pi \int_0^\infty g^3\,\mathrm{d}g\, \Phi_{l}{}^{q'}(g) \times \left\{\sigma^0(g)\, \Phi_{ql}(g') - \sigma^l(g) \cdot \frac{1}{2\,l+1}\, \Phi_{ql}(g)\right\}, \tag{2.27 b}$$

which has only three significant indices q, q' and l.

2.3.3. Elastic Collisions

As shown in Chapter 3, the functions $\Phi_{ql}(g)$, Eq. (2.24 a), and $\Phi^{q'}_{l'}(g)$, Eq. (2.24 b), explicitly depend on the normalized relative kinetic energy

$$\varepsilon := \frac{1}{2}\, g^2 \Big/ \left(\frac{K_{\mathrm{B}} T_i}{m_i} + \frac{K_{\mathrm{B}} T_j}{m_j}\right) = \frac{1}{2}\, \frac{m_i m_j}{m_i + m_j}\, \frac{g^2}{K_{\mathrm{B}} T_{ij}} \tag{2.28 a}$$

with

$$T_{ij} := \frac{m_j}{m_i + m_j}\, T_i + \frac{m_i}{m_i + m_j}\, T_j \tag{2.28 b}$$

in the following way:

$$\Phi_{ql}(g) = \left(\frac{K_{\mathrm{B}} T_i}{m_i} + \frac{K_{\mathrm{B}} T_j}{m_j}\right)^{-(q+3)/2} \cdot 2^{(l+1)/2} \cdot \frac{1}{\sqrt{2\pi}} \times \frac{1}{(q+l+1)!!}\, e^{-\varepsilon}\, \varepsilon^{l/2}\, L^{(l+1/2)}_{(q-l)/2}(\varepsilon) \tag{2.29 a}$$

and

$$\Phi^{q'}_{l'}(g) = \left(\frac{K_{\mathrm{B}} T_i}{m_i} + \frac{K_{\mathrm{B}} T_j}{m_j}\right)^{q'/2} \times 2^{(l'+1)/2}\, (q'-l')!!\, \varepsilon^{l'/2}\, L^{(l'+1/2)}_{(q'-l')/2}(\varepsilon)\,. \tag{2.29 b}$$

The polynomials $L^{(l+1/2)}_{(q-l)/2}$ are generalized Laguerre polynomials with half integer superscripts, so called Sonine polynomials. With

$$g^2\,\mathrm{d}g = \sqrt{2} \left(\frac{K_{\mathrm{B}} T_i}{m_i} + \frac{K_{\mathrm{B}} T_j}{m_j}\right)^{3/2} \sqrt{\varepsilon}\,\mathrm{d}\varepsilon \tag{2.30}$$

the expression (2.27 b) for the isotropic collision matrix becomes in the case of elastic collisions

$$\Psi^{q'}_{ql} = -\left(\frac{K_{\mathrm{B}} T_i}{m_i} + \frac{K_{\mathrm{B}} T_j}{m_j}\right)^{(q'-q)/2} \int_0^\infty \varepsilon^{l+1/2}\,\mathrm{d}\varepsilon \cdot 2^{l+3/2} \times \frac{1}{\sqrt{2\pi}}\, \frac{(q'-l)!!}{(q+l+1)!!}\, e^{-\varepsilon}\, L^{(l+1/2)}_{(q-l)/2}(\varepsilon) \times L^{(l+1/2)}_{(q'-l)/2}(\varepsilon)\, \nu^{(l)}(\varepsilon)\, \frac{m_j}{\varrho_j}\,. \tag{2.31}$$

For the "transfer collision frequencies" $\nu^{(l)}(\varepsilon)$ we have [cf. (2.23)]

$$\nu^{(l)}(\varepsilon) := \frac{\varrho_j}{m_j} \cdot g \cdot 4\pi \cdot \left(\sigma^0(g) - \frac{1}{2\,l+1}\, \sigma^l(g)\right) = \frac{\varrho_j}{m_j} \cdot g \cdot 2\pi \int \mathrm{d}\cos x\, \sigma(x, g) \{1 - P_l(\cos x)\} \tag{2.32}$$

with ϱ_j as the mass density of the j-th species.

The product of the two Sonine polynomials in (2.31) can be replaced by the expansion

$$L^{(l+1/2)}_{(q'-l)/2}(\varepsilon)\, L^{(l+1/2)}_{(q-l)/2}(\varepsilon) = \sum_s a^{sq'}_{q}(l)\, L^{(l+1/2)}_{s}(\varepsilon)\,, \tag{2.33}$$

which determines the coupling coefficients [9]:

$$a_q^{sq'}(l) = (-1)^{(q+q')/2-l+s} \cdot \binom{\frac{q+l+1}{2}}{\frac{q-l}{2}} \binom{s+l+1/2}{s}^{-1} \sum_K \binom{\frac{q-l}{2}}{\frac{q+q'}{2}-K-l} \times \binom{\frac{q'+l+1}{2}}{\frac{q-q'}{2}+\frac{K}{2}} \binom{\frac{q+q'}{2}-l-K}{s-K} . \qquad (2.34)$$

Because of Eq. (2.33) they should be symmetric with respect to q and q' and this can indeed be shown by re-organizing the factorials contained in the binomial coefficients of Equation (2.34). We insert the expansion (2.33) into the expression (2.31) for the isotropic collision matrix and obtain

$$\Psi_{ql}^{q'} = -\frac{m_j}{\varrho_j} \frac{1}{\sqrt{2}\,\pi} \left(\frac{K_{\rm B} T_i}{m_i} + \frac{K_{\rm B} T_j}{m_j} \right)^{(q'-q)/2} \cdot 2^{l+1} \times \frac{(q'-l)!!}{(q+l+1)!!} \sum_s (-1)^s a_q^{sq'}(l) \frac{(s+l+1/2)!}{s!} \nu^{(ls)} . \qquad (2.35)$$

The "transport collision frequencies" [7]

$$\nu^{(ls)} := (-1)^s \frac{s!}{(s+l+1/2)!} \times \int \mathrm{d}\varepsilon\, \varepsilon^{l+1/2} e^{-\varepsilon} L_s^{(l+1/2)}(\varepsilon)\, \nu^{(l)}(\varepsilon) \qquad (2.36\,\text{a})$$

are the coefficients in the orthogonal expansion

$$\nu^{(l)}(\varepsilon) = \sum_s (-1)^s \nu^{(ls)} L_s^{(l+1/2)}(\varepsilon) \qquad (2.36\,\text{b})$$

of the transfer collision frequencies $\nu^{(l)}(\varepsilon)$, Eq. (2.32), and thus form a null sequence with increasing s. For Maxwell interactions they are independent of ε; hence all transport collision frequencies $\nu^{(ls)}$, Eq. (2.36), vanish in this particular case for $s \geqq 1$.

2.4. Discussion of the Transformation Coefficients

In the case of momentum conservation we have $\Psi_{\alpha\varkappa}^{\alpha'\varkappa'} = \delta_\alpha^{\alpha'} \Psi_\varkappa^{\varkappa'}$, (2.21 a), and the product (2.20 a) for the collision elements B becomes

$$B_{\lambda\mu}^{\lambda'}(i,j) = T_{\alpha'\varkappa'}^{\lambda'0}\, \delta_\alpha^{\alpha'}\, T_{\lambda\mu}^{\alpha\varkappa}\, \Psi_\varkappa^{\varkappa'} =: \Delta_{\lambda\mu,\varkappa'}^{\lambda',\varkappa} \Psi_\varkappa^{\varkappa'} . \qquad (2.37)$$

The combined transformation coefficients Δ incorporate the "summation operator" $\delta_\alpha{}^{\alpha'}$, the expression for the completeness of the basis functions $\chi_\alpha(\mathbf{G})$. Because of the completeness of the $\Phi_\varkappa(\boldsymbol{g})$ we can write

$$\Delta_{\lambda\mu,\varkappa'}^{\lambda';\varkappa} = \int \mathrm{d}^3 g \int \mathrm{d}^3 g'\, \Phi^\varkappa(\boldsymbol{g}')\, J_{\lambda\mu}^{\lambda'}(\boldsymbol{g},\boldsymbol{g}')\, \Phi_{\varkappa'}(\boldsymbol{g}) \qquad (2.38)$$

with the functions

$$J_{\lambda\mu}^{\lambda'}(\boldsymbol{g},\boldsymbol{g}') := \int \mathrm{d}^3 G\, \varphi^{\lambda'}(i)\, \varphi_\lambda(i')\, \varphi_\mu(j') . \qquad (2.39)$$

For isotropic interaction potentials we have $\Psi_\varkappa^{\varkappa'} \equiv \delta_m^{m'} \delta_l^{l'} \Psi_{ql}^{q'}$, (2.27a), and therefore in this case we merely need the trace of the coefficients with respect to m and m' for $l' = l$.

2.5. Summary of the General Formalism

In Section 2.2 the collision elements $B_{\lambda\mu}^{\lambda'}(i,j)$ have been represented as a linear combination (2.20 a) of collision matrices $\Psi_{\alpha\varkappa}^{\alpha'\varkappa'}$, Eq. (2.20 b), and transformation coefficients $T_{\lambda\mu}^{\alpha\varkappa}$, Eq. (2.19 a), and $T_{\alpha'\varkappa'}^{\lambda'\mu'}$, Equation (2.19 b). While the transformation coefficients are purely mathematical expressions depending on the choice of the basis system $\{\varphi_\lambda(i)\}$, see Section 2.4, the collision matrices depend on the physical properties of the interaction of the colliding particles (Section 2.3).

The mass conservation allowed the introduction of combined transformation coefficients $\Delta_{\lambda\mu,\varkappa'}^{\lambda';\varkappa}$, Eq. (2.38), instead of the T coefficients and of reduced collision matrices $\Psi_\varkappa^{\varkappa'}$, Eq. (2.21 b), instead of the collision matrices $\Psi_{\alpha\varkappa}^{\alpha'\varkappa'}$ Equation (2.20 b).

In the following chapter the combined transformation coefficients Δ are evaluated with the aim to represent the collision elements $B_{\lambda\mu}^{\lambda'}(i,j)$ by the transport collision frequencies $\nu^{(ls)}$, Equation (2.36 a). The adventage of this representation is used in Chapter 4.

3. Calculation of the Collision Elements *B*

3.1. Evaluation of the Combined Transformation Coefficients

The first step is the calculation of the J-functions in the expression (2.38) for the combined transformation coefficients Δ. This will be done in the following way:

a) $J_{00}^0(\boldsymbol{g},\boldsymbol{g}')$ is obtained simply by integration.

b) $J_{\lambda\mu}^{\lambda'}(\boldsymbol{g},\boldsymbol{g}')$ is expanded by means of basis functions $\varphi_\sigma(\tilde{\boldsymbol{g}}')$, $\varphi^{\sigma'}(\tilde{\boldsymbol{g}})$, whose arguments $\tilde{\boldsymbol{g}}', \tilde{\boldsymbol{g}}$ are reduced relative velocities, Equation (3.4 b).

With local Maxwellians for φ_0, Eq. (2.8 a), and $\varphi^0 = 1$, Eq. (2.8 b), we have

$$\varphi^0(i)\, \varphi_0(i')\, \varphi_0(j') = \frac{1}{\sqrt{2\pi}^{\,6}} \sqrt{\frac{m_i}{K_{\rm B} T_i} \frac{m_j}{K_{\rm B} T_j}}^{\,3} \times \exp\left\{ -\frac{1}{2} \left(\frac{m_i}{K_{\rm B} T_i} \mathbf{C}_i'^2 + \frac{m_j}{K_{\rm B} T_j} \mathbf{C}_j'^2 \right) \right\} \qquad (3.1)$$

with the intrinsic velocities

$$\boldsymbol{C}_i := \boldsymbol{c}_i - \boldsymbol{c}_{i0}\,. \qquad (3.2)$$

These are related with the center of mass velocity $\boldsymbol{G}$, Eq. (2.15), and the relative velocity $\boldsymbol{g}$, Eq. (2.3), by

$$\boldsymbol{C}_i = \tilde{\boldsymbol{G}} - \frac{m_j}{m_i + m_j}\,\tilde{\boldsymbol{g}} \qquad (3.3\,\mathrm{a})$$

and

$$\boldsymbol{C}_j = \tilde{\boldsymbol{G}} + \frac{m_i}{m_i + m_j}\,\tilde{\boldsymbol{g}}\,, \qquad (3.3\,\mathrm{b})$$

where the reduced velocities

$$\tilde{\boldsymbol{G}} := \boldsymbol{G} - \left(\frac{m_i}{m_i + m_j}\,\boldsymbol{c}_{i0} + \frac{m_j}{m_i + m_j}\,\boldsymbol{c}_{j0}\right) \qquad (3.4\,\mathrm{a})$$

and

$$\tilde{\boldsymbol{g}} := \boldsymbol{g} - (\boldsymbol{c}_{j0} - \boldsymbol{c}_{i0}) \qquad (3.4\,\mathrm{b})$$

are introduced with arbitrary reference velocities $\boldsymbol{c}_{i0}$ and $\boldsymbol{c}_{j0}$. Substitution of the expressions (3.3 a, b) and (3.4 a, b) into the relation (3.1) and integration over $\mathrm{d}^3 G = \mathrm{d}^3 G'$ yields with (2.39)

$$J^0_{00}(\tilde{\boldsymbol{g}}, \tilde{\boldsymbol{g}}') = \left\{2\pi\left(\frac{K_\mathrm{B} T_i}{m_i} + \frac{K_\mathrm{B} T_j}{m_j}\right)\right\}^{-3/2} \times \exp\left\{-\frac{1}{2}\,\tilde{\boldsymbol{g}}'^2 \Big/ \left(\frac{K_\mathrm{B} T_i}{m_i} + \frac{K_\mathrm{B} T_j}{m_j}\right)\right\}. \qquad (3.5)$$

This function has the mathematical form of a local Maxwellian $\varphi_0(i')$, Eq. (2.8 a), if we replace $K_\mathrm{B} T_i/m_i$ and $\boldsymbol{C}_i'$ by $K_\mathrm{B} T_i/m_i + K_\mathrm{B} T_j/m_j$ and $\tilde{\boldsymbol{g}}'$ resp. Therefore it is useful to introduce basis functions $\varphi_\sigma(\tilde{\boldsymbol{g}}')$ and $\varphi^{\sigma'}(\tilde{\boldsymbol{g}})$ in the same way as the one-particle basis functions $\varphi_\lambda(i')$ and $\varphi^{\lambda'}(i)$, besides of the substitution just mentioned. Thus we expand the J-functions as follows:

$$J^{\lambda'}_{\lambda\mu}(\tilde{\boldsymbol{g}}, \tilde{\boldsymbol{g}}') = \Gamma^{\lambda',\,\sigma}_{\lambda\mu,\,\sigma'}\,\varphi^{\sigma'}(\tilde{\boldsymbol{g}})\,\varphi_\sigma(\tilde{\boldsymbol{g}}')\,. \qquad (3.6)$$

The calculation of the expansion coefficients Γ has been done using algebraic relations of the basis functions to derive recurrence relations for the J-functions with the following result [10]:

$$\Gamma^{\lambda',\,\sigma}_{\lambda\mu,\,\sigma'} = \left\{\frac{K_B(T_j - T_i)}{m_i + m_j}\right\}^{\frac{1}{2}(\lambda' - \lambda - \mu + \sigma - \sigma')} \gamma^{\lambda',\,\sigma}_{\lambda\mu,\,\sigma'}\left(\frac{m_j}{m_i + m_j}\right). \qquad (3.7)$$

It should be recalled that small greek letters as indices represent index triples, but denote the order of a (generalized) moment or basis function if used in algebraic expressions like powers, inequalities etc. (cf. Section 2.1).

The coefficients γ, depending merely on the mass ratio $m_j/(m_i + m_j)$ and not on the temperatures T_i, T_j, are given in the Appendix (A 3). Their algebraic form depends on the special choice of the basis functions φ. Inserting the expansion (3.6) for $J^{\lambda'}_{\lambda\mu}$ into the expression (2.38) for the combined transformation coefficients $\varDelta$ we can write

$$\varDelta^{\lambda',\,\varkappa}_{\lambda\mu,\,\varkappa'} = T^{\varkappa}_{\sigma}\,\Gamma^{\lambda',\,\sigma}_{\lambda\mu,\,\sigma'}\,T^{\sigma'}_{\varkappa'} \qquad (3.8)$$

with the "transformation matrices"

$$T_\sigma{}^{\varkappa} := \int \mathrm{d}^3\tilde{\boldsymbol{g}}\;\Phi^{\varkappa}(\tilde{\boldsymbol{g}})\,\varphi_\sigma(\tilde{\boldsymbol{g}}) \qquad (3.9\,\mathrm{a})$$

and

$$T^{\sigma'}_{\varkappa'} := \int \mathrm{d}^3\tilde{\boldsymbol{g}}\;\varphi^{\sigma'}(\tilde{\boldsymbol{g}})\,\Phi_{\varkappa'}(\tilde{\boldsymbol{g}})\,, \qquad (3.9\,\mathrm{b})$$

which are given in the Appendix (A 2) in connection with the discussion of special basis systems.

3.2. *Final Expression for the Collision Elements B*

Combining the expression (3.8) for the combined transformation coefficients $\varDelta$ with the expression (2.35) for the isotropic collision matrices Ψ and requiring the same reference velocity for all species of particles [cf. (3.4)] we obtain in the case of elastic collisions from Eq. (2.37)

$$B^{\lambda'}_{\lambda\mu}(i,j) = \left(\frac{K_\mathrm{B} T_i}{m_i} + \frac{K_\mathrm{B} T_j}{m_j}\right)^{\frac{1}{2}[\lambda' - (\lambda + \mu)]} \times \sum_r \tau^{\frac{1}{2}[\lambda' - (\lambda + \mu)] + r} \sum_{l,s} \frac{m_j}{\varrho_j}\,\nu^{(ls)}\,F^{\lambda'}_{\lambda\mu}\left(l, r, s; \frac{m_j}{m_i + m_j}\right). \qquad (3.10)$$

The ranges of r, l, s are [11]

$$1 \leqq l \leqq \min\left[\lambda', \tfrac{1}{2}(\lambda + \mu + \lambda')\right] \qquad (3.11)$$

$$\tfrac{1}{2}(\lambda + \mu - \lambda') \leqq r \leqq \tfrac{1}{2}(\lambda + \mu + \lambda') - l \qquad (3.12)$$

$$|r| \leqq s \leqq \tfrac{1}{2}(\lambda + \mu + \lambda') - l\,. \qquad (3.13)$$

The parameter

$$\tau := \frac{K_\mathrm{B}(T_j - T_i)}{m_i + m_j} \Big/ \left(\frac{K_\mathrm{B} T_i}{m_i} + \frac{K_\mathrm{B} T_j}{m_j}\right) \qquad (3.14)$$

is a measure for the difference of the temperatures of different particle species i and j. It was intentionally normalized to

$$|\tau| < 1\,.$$

Thus increasing powers of τ form a null sequence, a property used in Chapter 4. For the mass dependent coefficients F in the expression (3.10) we have

$$F^{\lambda'}_{\lambda\mu}\left(l, r, s; \frac{m_j}{m_i + m_j}\right) = -\sum_{q - q' = 2r} T^{qlm}_{\sigma}\,T^{\sigma'}_{q'lm}\,\gamma^{\lambda',\,\sigma}_{\lambda\mu,\,\sigma'}\left(\frac{m_j}{m_i + m_j}\right) a^{sq'}_{q}(l)\left(-\frac{1}{2}\right)^s \frac{(q' - l)\,!!\,[2(s + l) + 1]\,!!}{(q + l + 1)\,!!\;s\,!} \qquad (3.16)$$

where the two sums over q and q' are to be taken over all values of q and q' with $q-q'=2r$. More detailed expressions for T and γ require the choice of the basis functions. They are given in the Appendix A1, A2.

4. Discussion of the Order of Magnitude of the Collision Elements B

To compare different collision elements we employ the two null sequences introduced in (2.36) and (3.14), (3.15) resp.

a) The null sequence of the transport collision frequencies $\nu^{(ls)}$, Eq. (2.36), with increasing s. As an example: In the case of Maxwell interaction all $\nu^{(ls)}$ vanish for $s \geqq 1$.

b) The null sequence of increasing powers of the normalized temperature difference τ, Equation (3.14). For equal temperatures of all particle species we have $\tau=0$, so only the terms with τ^0 do not vanish.

In the following we approximate a collision element B, Eq. (3.10), by its dominant terms. Using **a** we replace the summation over s in Eq. (3.10) by taking only the lowest value $|r|$ of s according to Eq. (3.13):

$$B^{\lambda'}_{\lambda\mu}(i,j) \approx \left(\frac{K_{\mathrm{B}} T_i}{m_i}+\frac{K_{\mathrm{B}} T_j}{m_j}\right)^{\frac{1}{2}[\lambda'-(\lambda+\mu)]} \sum_r \tau^{\frac{1}{2}[\lambda'-(\lambda+\mu)]+r} \sum_l \frac{m_j}{\varrho_j}\, \nu^{(l|r|)}\, F^{\lambda'}_{\lambda\mu}\left(l, r, |r|; \frac{m_j}{m_i+m_j}\right). \tag{4.1}$$

The range of the r-summation is still given by Eq. (3.12). Now we replace the r-summation in Eq. (4.1) by taking into account only the r-index with the lowest absolute value. To do this we have to distinguish between two cases:

1) $\lambda+\mu \geqq \lambda'$: According to Eq. (3.12) we substitute the sum over r by taking the lowest r-value

$$r=|r|=\tfrac{1}{2}(\lambda+\mu-\lambda') \tag{4.2}$$

in the expression (4.1) and obtain

$$B^{\lambda'}_{\lambda\mu}(i,j) \approx \left(\frac{K_{\mathrm{B}} T_i}{m_i}+\frac{K_{\mathrm{B}} T_j}{m_j}\right)^{\frac{1}{2}[\lambda'-(\lambda+\mu)]} \tau^0 \sum_l \frac{m_j}{\varrho_j}\, \nu^{[l\frac{1}{2}(\lambda+\mu-\lambda')]}\, F^{\lambda'}_{\lambda\mu}\left(l, \frac{\lambda+\mu-\lambda'}{2}, \frac{\lambda+\mu-\lambda'}{2}; \frac{m_j}{m_i+m_j}\right). \tag{4.3}$$

2) $\lambda+\mu \leqq \lambda'$: According to Eq. (3.12) the summation over r begins at negative values and we have

$$|r| \geqq 0. \tag{4.4}$$

We insert $r=0$ in expression (4.1) and obtain

$$B^{\lambda'}_{\lambda\mu} \approx \left(\frac{K_{\mathrm{B}} T_i}{m_i}+\frac{K_{\mathrm{B}} T_j}{m_j}\right)^{\frac{1}{2}[\lambda'-(\lambda+\mu)]} \tau^{\frac{1}{2}[\lambda'-(\lambda+\mu)]} \sum_l \frac{m_j}{\varrho_j}\, \nu^{(l0)}\, F^{\lambda'}_{\lambda\mu}\left(l, 0, 0; \frac{m_j}{m_i+m_j}\right). \tag{4.5}$$

For equal temperatures $T_i=T_j$, i. e. $\tau=0$, the sum over r in the expression (3.10) for B is restricted to the minimum r-value $\frac{1}{2}(\lambda+\mu-\lambda')$. In this case the dominant terms of B are

$$B^{\lambda'}_{\lambda\mu}(i,j) \approx \left(\frac{K_{\mathrm{B}} T_i}{m_i}+\frac{K_{\mathrm{B}} T_j}{m_j}\right)^{\frac{1}{2}[\lambda'-(\lambda+\mu)]} \sum_l \frac{m_j}{\varrho_j}\, \nu^{[l|\frac{1}{2}(\lambda+\mu-\lambda')|]}\, F^{\lambda'}_{\lambda\mu}\left(l, \frac{\lambda+\mu-\lambda'}{2}, \left|\frac{\lambda+\mu-\lambda'}{2}\right|; \frac{m_j}{m_i+m_j}\right) \tag{4.6}$$

for all combinations of λ', λ and μ.

The dominant terms (4.3), (4.5) and (4.6) of the collision elements B, Eq. (3.10), are illustrated in the Figs. 1 and 2. There all factors of the products of powers of τ with transport collision frequencies $\nu^{(ls)}$ in the approximations (4.3), (4.5) and (4.6) are omitted as well as the summation over l. Figure 1 is taken from the expressions (4.3) and (4.5) for multi temperature gas mixtures or plasmas with $T_i \neq T_j$, i. e. $\tau \neq 0$. Figure 2 illustrates the relation (4.6) for gas mixtures and plasmas with equal temperatures for the species of particles i and j, $T_i=T_j$, i. e. $\tau=0$.

The transition from Fig. 1 to Fig. 2 is trivial for the above-diagonal elements with $\lambda+\mu>\lambda'$. For the subdiagonal elements with $\lambda+\mu<\lambda'$, however, we have to apply two different procedures, selecting the dominant terms in the exact expression (3.10) for the collision elements B. So we obtain different dominant terms in Eq. (3.10) for different $(\tau \neq 0)$ and equal $(\tau=0)$ temperatures respectively. If the absolute value of the temperature difference decreases continuously then other terms in Eq. (3.10) raise to the same order of magnitude as those represented in the approximation (4.5). For vanishing temperature differences only the terms given in the expression (4.6) remain as the dominant ones. This gives an explanation for the contrast between the subdiagonal elements in Figures 1 and 2.

$\lambda+\mu$ λ'	0	1	2	3	4	5
0	0	0	0	0	0	0
1	0	$\nu^{(l0)}\,\tau^0$	0	$\nu^{(l1)}\,\tau^0$	0	$\nu^{(l2)}\,\tau^0$
2	$\nu^{(l0)}\,\tau^1$	0	$\nu^{(l0)}\,\tau^0$	0	$\nu^{(l1)}\,\tau^0$	0
3	0	$\nu^{(l0)}\,\tau^1$	0	$\nu^{(l0)}\,\tau^0$	0	$\nu^{(l1)}\,\tau^0$
4	$\nu^{(l0)}\,\tau^2$	0	$\nu^{(l0)}\,\tau^1$	0	$\nu^{(l0)}\,\tau^0$	0
5	0	$\nu^{(l0)}\,\tau^2$	0	$\nu^{(l0)}\,\tau^1$	0	$\nu^{(l0)}\,\tau^0$

Fig. 1. Products of transport collision frequencies $\nu^{(ls)}$ (2.36) with powers of normalized temperature differences τ (3.14) in the dominant terms of the collision elements $B_{\lambda\mu}^{\lambda'}$ (3.10) for plasmas with different temperatures for the species of particles.

$\lambda+\mu$ λ'	0	1	2	3	4	5
0	0	0	0	0	0	0
1	0	$\nu^{(l0)}$	0	$\nu^{(l1)}$	0	$\nu^{(l2)}$
2	0	0	$\nu^{(l0)}$	0	$\nu^{(l1)}$	0
3	0	$\nu^{(l1)}$	0	$\nu^{(l0)}$	0	$\nu^{(l1)}$
4	0	0	$\nu^{(l1)}$	0	$\nu^{(l0)}$	0
5	0	$\nu^{(l2)}$	0	$\nu^{(l1)}$	0	$\nu^{(l0)}$

Fig. 2. Transport collision frequencies $\nu^{(ls)}$ (2.36) in the dominant terms of the collision elements $B_{\lambda\mu}^{\lambda'}$ (3.10) for plasmas with equal temperatures for all species of particles.

Comparing for equal temperatures the absolute values of the dominant terms illustrated in Fig. 2 we observe values of the same order in the diagonal and a symmetric decrease with increasing distance from the diagonal. This is caused by the decrease of the absolute value of the transport collision frequencies $\nu^{(ls)}$, Eq. (2.36), with increasing s. The shape of the (symmetric) decrease of the off-diagonal terms depends on the molecular interaction. For the Maxwell interaction the transfer collision frequencies $\nu^{(l)}(\varepsilon)$, Eq. (2.32), are independent of the energy, hence all transport collision frequencies $\nu^{(ls)}$, Eq. (2.36), vanish for $s \geqq 1$. Thus in this particular case only the diagonal terms in Fig. 2 remain, while all off-diagonal terms vanish. This statement is true not only approximately in the sense of the dominant terms but exactly [cf. Eqs. (3.10), (3.12), (3.13)]. The more the intermolecular force deviates from the Maxwell interaction the less steep becomes the shape of the decrease. For long range interactions, e. g. (screened or cut off) Coulomb interaction, the descent is rather weak.

Comparing the absolute values of the dominant terms for different temperatures, illustrated in Fig. 1, we observe a decreasing order of magnitude with increasing distance from the diagonal, too, which is, however, not symmetric. For the super-diagonal terms the decrease is caused by the same reason as in the case of equal temperatures, Figure 2. For the subdiagonal terms the absolute value of the powers of τ [$|\tau| < 1$, cf. Eq. (3.15)] decreases with increasing distance from the diagonal, as the exponent increases. This descent is steep for small temperature differences and becomes less pronounced for increasing absolute value of τ. In contrast to the case of equal temperatures, Fig. 1 shows that only the descent of the super-diagonal terms depends on the deviation of the intermolecular force from the Maxwell interaction as discussed above.

5. Concluding Remarks

For small deviations from thermodynamic equilibrium the initial term $a_i^0\,\varphi_0(i)$ in the orthogonal expansion (2.4) of the velocity distribution function f is the essential one if $\varphi_0(i)$ is taken proportional to the local Maxwellian (2.8). Therefore the condition

$$|a_{i,j}^{\lambda}| \ll |a_{i,j}^{0}| \quad \text{for } \lambda \geqq 1 \qquad (5.1)$$

is used to linearize the right-hand side of the system (2.10), which is equivalent to the kinetic Equation (2.1). Then the matrix elements of the linearized collision operator consist of $B_{\lambda 0}^{\lambda'} a_j^0$ and $B_{0\mu}^{\lambda'} a_i^0$. Therefore Figs. 1 and 2 directly illustrate these matrix elements. For the calculation of transport coefficients this infinite matrix must be inverted. In general this can be done only approximately. For the evaluation of an efficient approximation procedure it is necessary to know the order of magnitude of the different matrix elements. They have been discussed at the end of Chapter 4.

Although expressions for the matrix elements of the linearized collision operator can be taken from our general expression (3.10) for the non-linearized collision elements it is more advantageous to calculate them directly using Burnett functions as basis system of orthogonal function. These are products of spherical harmonics and generalized Laguerre polynomials with half-integer superscripts (Sonine polynomials). These Burnett functions allow certain short cuts in the calculation of the transformation coefficients corresponding to Equation (2.19). The results will be presented in a forthcoming paper.

Appendix

A 1. Hermite Functions and Some Related Moments

The basis functions $\varphi_\lambda(\boldsymbol{C}_i)$ are determined to

$$\begin{aligned}\varphi_\lambda(\boldsymbol{C}_i) &\equiv \varphi_{\lambda_1\lambda_2\lambda_3}(\boldsymbol{C}_i)\\ &=: \left(2\pi\frac{K_B T_i}{m_i}\right)^{-3/2}\exp\left\{-\frac{1}{2}\boldsymbol{C}_i^2\frac{m_i}{K_B T_i}\right\}\\ &\quad\times \mathrm{He}_{\lambda_1}\left(C_i^1\sqrt{\frac{m_i}{K_B T_i}}\right)\mathrm{He}_{\lambda_2}\left(C_i^2\sqrt{\frac{m_i}{K_B T_i}}\right)\\ &\quad\times \mathrm{He}_{\lambda_3}\left(C_i^3\sqrt{\frac{m_i}{K_B T_i}}\right),\end{aligned} \tag{A 1}$$

where C_i^1, C_i^2, C_i^3 are the cartesian components of the intrinsic velocity $\boldsymbol{C}_i$, Equation (3.2). Because of the orthogonality relation for the Hermite-polynomials, defined by

$$\mathrm{He}_n(x) := e^{x^2/2}\left(-\frac{\mathrm{d}}{\mathrm{d}x}\right)^n e^{-x^2/2} \tag{A 2}$$

we obtain

$$\begin{aligned}\varphi^\lambda(\boldsymbol{C}_i) &\equiv \varphi^{\lambda_1\lambda_2\lambda_3}(\boldsymbol{C}_i) := \frac{1}{\lambda_1!\,\lambda_2!\,\lambda_3!}\\ &\quad\times \mathrm{He}_{\lambda_1}\left(C_i^1\sqrt{\frac{m_i}{K_B T_i}}\right)\mathrm{He}_{\lambda_2}\left(C_i^2\sqrt{\frac{m_i}{K_B T_i}}\right)\\ &\quad\times \mathrm{He}_{\lambda_3}\left(C_i^3\sqrt{\frac{m_i}{K_B T_i}}\right).\end{aligned} \tag{A 3}$$

The order of the basis functions,

$$\lambda := \lambda_1 + \lambda_2 + \lambda_3\,, \tag{A 4}$$

denotes the tensorial order of the related generalized moments (cf. Section 2.1). Some of the moments

$$a_i^\lambda \equiv a_i^{\lambda_1\lambda_2\lambda_3} = \langle \varphi^\lambda(i) \,|\, f(i)\rangle \tag{A 5}$$

and their connection with physical properties are given in the following equations. If we assume the distribution function $f(i)$ to be normalized to

$$\langle 1 \,|\, f(i)\rangle = \varrho_i\,, \tag{A 6}$$

where ϱ_i is the mass density, we immediately have for $\lambda = 0$

$$a_i^{000} = \varrho_i\,. \tag{A 7}$$

For $\lambda = 1$ we obtain

$$\begin{pmatrix} a_i^{100} \\ a_i^{010} \\ a_i^{001}\end{pmatrix} = \begin{pmatrix} J_i^1 \\ J_i^2 \\ J_i^3\end{pmatrix} = \boldsymbol{J}_i := \langle \boldsymbol{C}_i \,|\, f(i)\rangle \tag{A 8}$$

with the diffusion flux $\boldsymbol{J}_i$. The tensorial pressure, defined as

$$\mathbf{p}_i := \langle \boldsymbol{C}_i\boldsymbol{C}_i \,|\, f(i)\rangle\,, \tag{A 9}$$

becomes with Eq. (A 3):

$$\mathbf{p}_i = \begin{pmatrix} 2a_i^{200} + \frac{K_B T_i}{m_i}a_i^{000}, & a_i^{110}, & a_i^{101} \\ a_i^{110}, & 2a_i^{020} + \frac{K_B T_i}{m_i}a_i^{000}, & a_i^{011} \\ a_i^{101}, & a_i^{011}, & 2a_i^{002} + \frac{K_B T_i}{m_i}a_i^{000}\end{pmatrix} \tag{A 10}$$

The scalar pressure is determined to

$$\begin{aligned} p_i &= \tfrac{1}{3}\,\mathrm{trace}\,\mathbf{p}_i \\ &= \tfrac{2}{3}\,(a_i^{200} + a_i^{020} + a_i^{002}) + \frac{K_B T_i}{m_i}a_i^{000}\,.\end{aligned} \tag{A 11}$$

Inserting the ideal gas equation

$$p_i = \varrho_i\frac{K_B T_i}{m_i} \tag{A 12}$$

into Eq. (A 11) yields

$$a_i^{200} + a_i^{020} + a_i^{002} = 0\,. \tag{A 13}$$

So we obtain in the case $\lambda = 2$ the traceless stress tensor:

$$\mathbf{p}_i^{\circ} = \begin{pmatrix} 2a_i^{200} & a_i^{110} & a_i^{101} \\ a_i^{110} & 2a_i^{020} & a_i^{011} \\ a_i^{101} & a_i^{011} & 2a_i^{002}\end{pmatrix}. \tag{A 14}$$

To close this discussion we shall give an expression for the heat flux vector, which belongs to the generalized moments in the case $\lambda = 3$. If we define

$$\mathbf{Q}_i := \left\langle \boldsymbol{C}_i\left(\boldsymbol{C}_i^2 - \frac{5}{2}\frac{K_B T_i}{m_i}\right) \middle|\, f(i)\right\rangle, \tag{A 15}$$

we obtain

$$\mathbf{Q}_i = \begin{pmatrix} 3a_i^{300} + a_i^{120} + a_i^{102} \\ a_i^{210} + 3a_i^{030} + a_i^{012} \\ a_i^{201} + a_i^{021} + 3a_i^{003}\end{pmatrix}. \tag{A 16}$$

A 2. Transformation between φ and Φ

At first we express a product of three Hermite-polynomials, as it appears in the basis functions φ, in terms of spherical harmonics $Y_{lm}(\vartheta, \psi)$ [12]. The argument is assumed to be a dimensionless vector $\boldsymbol{x}$ with the cartesian components $x^1 = r \sin\vartheta \cos\psi$, $x^2 = r \sin\vartheta \sin\psi$ and $x^3 = r \cos\vartheta$. The result can be written down in the form [13]

$$\mathrm{He}_{\varkappa_1}(x^1)\,\mathrm{He}_{\varkappa_2}(x^2)\,\mathrm{He}_{\varkappa_3}(x^3) = \sum_{l,m} \begin{bmatrix} l\,m \\ \varkappa_1\,\varkappa_2\,\varkappa_3 \end{bmatrix} F_\varkappa{}^l(r)\, Y_{lm}(\vartheta, \psi) \qquad \text{(A 17)}$$

with $\quad \varkappa = \varkappa_1 + \varkappa_2 + \varkappa_3$ and $0 \leqq \varkappa - l$ even.

The coefficients $\begin{bmatrix} l\,m \\ \varkappa_1\,\varkappa_2\,\varkappa_3 \end{bmatrix}$ can be normalized to

$$\begin{bmatrix} l\,0 \\ 0\,0\,\varkappa \end{bmatrix} = 1\,. \qquad \text{(A 18)}$$

This yields

$$F_\varkappa{}^l(r) = \sqrt{4\pi\cdot(2l+1)}\,(-1)^{(\varkappa-l)/2}\,\frac{\varkappa!}{(\varkappa+l+1)!!} \times r^l\, L^{(l'+1/2)}_{(\varkappa-l)/2}\left(\tfrac{1}{2} r^2\right) \qquad \text{(A 19)}$$

with generalized Laguerre-polynomials with half-integer superscript (Sonine-polynomials)

$$L^{(l+1/2)}_{(\varkappa-l)/2}\left(\frac{1}{2} r^2\right) := \sum_{K=0}^{(\varkappa-l)/2} \frac{1}{K!}\left(-\frac{1}{2} r^2\right)^K \begin{pmatrix} (\varkappa+l+1)/2 \\ K+l+\frac{1}{2} \end{pmatrix}. \qquad \text{(A 20)}$$

The bracket-coefficients are given by [14]

$$\begin{aligned} \begin{bmatrix} l\,m \\ \varkappa_1\,\varkappa_2\,\varkappa_3 \end{bmatrix} &= (-1)^m \sqrt{\frac{(l+m)!}{(l-m)!}}\; 2^{-(\varkappa_1+\varkappa_2)}\,(-i)^{\varkappa_2} \\ &\times \frac{(\varkappa+l+1)!!\,(\varkappa-l)!!}{\varkappa!} \sum_\mu (-1)^\mu \begin{pmatrix} \varkappa_2 \\ \mu \end{pmatrix} \qquad \text{(A 21)} \\ &\times \begin{pmatrix} \varkappa_1 \\ \frac{1}{2}(\varkappa_1+\varkappa_2-m)-\mu \end{pmatrix} \sum_\tau (-1)^\tau \begin{pmatrix} \frac{1}{2}(\varkappa_1+\varkappa_2-m) \\ \tau \end{pmatrix} \\ &\times \frac{(\varkappa_3+2\tau)!}{(\varkappa_3+2\tau+l+m+1)!!\,(\varkappa_3+2\tau-l+m)!!}\,. \end{aligned}$$

Inserting the expansion (A 17) and the functions (A 19) into the definition (A 1) of the basis functions φ we obtain:

$$\begin{aligned} \varphi_{\varkappa_1\varkappa_2\varkappa_3}(\boldsymbol{g}) &= \sqrt{\frac{K_B T_i}{m_i} + \frac{K_B T_j}{m_j}}^{\,-(\varkappa+3)} \cdot \frac{1}{\sqrt{2\pi}^3} \\ &\times \sum_{l,m} \begin{bmatrix} l\,m \\ \varkappa_1\,\varkappa_2\,\varkappa_3 \end{bmatrix} \left(\boldsymbol{g}^2 \Big/ \left(\frac{K_B T_i}{m_i} + \frac{K_B T_j}{m_j}\right)\right)^{l/2} \\ &\times \sqrt{4\pi(2l+1)}\,(-1)^{(\varkappa-l)/2}\,\frac{\varkappa!}{(\varkappa+l+1)!!} \\ &\times L^{(l+1/2)}_{(\varkappa-l)/2}\left(\frac{\boldsymbol{g}^2}{2\left(\frac{K_B T_i}{m_i} + \frac{K_B T_j}{m_j}\right)}\right) \qquad \text{(A 22)} \\ &\times \exp\left\{-\frac{\boldsymbol{g}^2}{2\left(\frac{K_B T_i}{m_i} + \frac{K_B T_j}{m_j}\right)}\right\} Y_{lm}(\hat{\boldsymbol{g}})\,. \end{aligned}$$

The dual basis functions become

$$\begin{aligned} \varphi^{\varkappa_1\varkappa_2\varkappa_3}(\boldsymbol{g}) &= \sqrt{\frac{K_B T_i}{m_i} + \frac{K_B T_j}{m_j}}^{\,\varkappa} \frac{1}{\varkappa_1!\,\varkappa_2!\,\varkappa_3!} \\ &\times \sum_{lm} \begin{bmatrix} l\,m \\ \varkappa_1\,\varkappa_2\,\varkappa_3 \end{bmatrix}^* Y^*_{lm}(\hat{\boldsymbol{g}}) \left(\frac{\boldsymbol{g}^2}{\frac{K_B T_i}{m_i} + \frac{K_B T_j}{m_j}}\right)^{l/2} \\ &\times \sqrt{4\pi(2l+1)}\,(-1)^{(\varkappa-l)/2}\,\frac{\varkappa!}{(\varkappa+l+1)!!} \\ &\times L^{(l+1/2)}_{(\varkappa-l)/2}\left(\frac{\boldsymbol{g}^2}{2\left(\frac{K_B T_i}{m_i} + \frac{K_B T_j}{m_j}\right)}\right). \qquad \text{(A 23)} \end{aligned}$$

We compare these equations with the definitions (2.24 a, b) and (2.29 a, b) for the basis functions Φ and obtain for the transformation matrices, defined by the Equation (3.9 a, b):

$$T^{qlm}_{\varkappa_1\varkappa_2\varkappa_3} = \delta_\varkappa{}^q\,\varkappa! \begin{bmatrix} l\,m \\ \varkappa_1\,\varkappa_2\,\varkappa_3 \end{bmatrix} \qquad \text{(A 24)}$$

and

$$T^{\varkappa_1\varkappa_2\varkappa_3}_{qlm} = \delta_q{}^\varkappa \frac{\varkappa!}{\varkappa_1!\,\varkappa_2!\,\varkappa_3!}\,\frac{2l+1}{(\varkappa+l+1)!\,(q-l)!!} \times \begin{bmatrix} l\,m \\ \varkappa_1\,\varkappa_2\,\varkappa_3 \end{bmatrix}^*. \qquad \text{(A 25)}$$

A 3. Results for the Coefficients γ

If we use the definitions (A 1) and (A 3) for the basis functions φ, we obtain [10] for the coefficients γ, Eq. (3.10):

$$\begin{aligned} \gamma^{\lambda',\sigma}_{\lambda\mu,\sigma'} &= (-1)^{\lambda+\sigma'} \left(\frac{m_j}{m_i+m_j}\right)^{\frac{1}{2}(\lambda'+\lambda+\mu-\sigma+\sigma')} \qquad \text{(A 26)} \\ &\times \prod_{n=1}^{3} \left\{ \frac{1}{\left(\frac{\lambda_n' - \lambda_n - \mu_n + \sigma_n - \sigma_n'}{2}\right)!} \sum_{t_n} \left(-\frac{m_i}{m_j}\right)^{t_n} \begin{pmatrix} \lambda_n \\ t_n \end{pmatrix} \right. \\ &\left. \times \begin{pmatrix} \frac{\lambda_n' + \mu_n - \lambda_n + \sigma_n - \sigma_n'}{2} \\ \frac{\lambda_n' + \mu_n + \lambda_n - \sigma_n - \sigma_n'}{2} - t_n \end{pmatrix} \right\}. \end{aligned}$$

This can be expressed in terms of the Jacobi polynomials

$$P_N^{(a;\,b)}(x) := 2^{-N} \sum_t \begin{pmatrix} N+a \\ t \end{pmatrix} \begin{pmatrix} N+b \\ N-t \end{pmatrix} \times (x-1)^{N-t}\,(x+1)^t \qquad \text{(A 27)}$$

in the form

$$\gamma^{\lambda',\sigma}_{\lambda\mu,\sigma'} = (-1)^{\lambda'-\lambda} \left(\frac{m_j}{m_i+m_j}\right)^{\sigma'} \qquad \text{(A 28)}$$

$$\times \prod_{n=1}^{3} \frac{1}{\left(\frac{\lambda_n' - \lambda_n - \mu_n + \sigma_n - \sigma_n'}{2}\right)!}\, P_{N_n}^{(a_n;\,b_n)}\left(1 - 2\frac{m_j}{m_i+m_j}\right)$$

with

$$N_n := \tfrac{1}{2}(\lambda_n' + \lambda_n + \mu_n - \sigma_n - \sigma_n') \,, \tag{A 29}$$

$$a_n := \lambda_n - N_n \,, \tag{A 30}$$

$$b_n := \sigma_n - \lambda_n \,. \tag{A 31}$$

σ_n and σ_n' must satisfy the following conditions:

$$0 \leqq \sigma_n' \leqq \lambda_n' \tag{A 32}$$

and

$$\max(0, \lambda_n + \mu_n - \lambda_n' + \sigma_n') \leqq \sigma_n \text{ (step 2)} \leqq \lambda_n' + \lambda_n + \mu_n - \sigma_n' \,. \tag{A 33}$$

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