The kinetic theory of partially ionized reactive gas mixtures II

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Abstract

We investigate the kinetic theory of partially ionized reactive gas mixtures in strong magnetic fields following Giovangigli *et al* (2003 *Physica* A **327** 313–48). A new tensor basis is introduced for expanding the perturbed distribution functions associated with the viscous tensor. New symmetry properties of transport coefficients are established as well as simplified bracket expressions. A variational framework is introduced for a direct evaluation of the thermal conductivity and the thermal diffusion ratios. The transport linear systems corresponding to the usual Sonine/Wang–Chang Uhlenbeck polynomial expansions are evaluated. The behavior of transport coefficients and transport fluxes for vanishing magnetic fields is investigated using series expansions. Practical implementation of iterative algorithms for solving the resulting complex symmetric constrained singular linear systems is discussed as well as various approximations of the transport coefficients.

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List of symbols

A	heat–mass transport matrices
$\boldsymbol{B}$	magnetic field
$\boldsymbol{C}_i$	peculiar velocity of the ith species
$\boldsymbol{d}_i$	diffusion driving force of the ith species
$\mathcal{D}_{ij}$	binary diffusion coefficients
D_{ij}	multicomponent diffusion coefficients
e_i	charge of the ith species
$\boldsymbol{E}$	electric field
$\mathcal{E}$	internal energy per unit volume
f_i	distribution function of the ith species

i	$i^2 = -1$
m_i	molecular mass of the ith species
n_i	number density of the ith species
p	pressure
$\boldsymbol{q}$	heat flux
R	rotation matrices
T	absolute temperature
$\boldsymbol{v}$	velocity of the mixture
$\boldsymbol{V}_i$	diffusion velocity of the ith species
X_i	mole fractions of the ith species
Y_i	mass fractions of the ith species
z_i	charge per unit mass of the ith species
Re	real part
Im	imaginary part
α	generic solution of the TLS
β	generic right hand side of the TLS
δ	Kronecker symbol
ϕ_i	perturbed distribution of the ith species
ϕ^{abrk}	generic expansion polynomials
φ_i	auxiliary perturbed distribution functions
Ψ	right hand sides of integral equations
κ	volume viscosity
η	viscosities
λ	thermal conductivities
$\widehat{\lambda}$	partial thermal conductivities
μ	generic transport coefficients
$\boldsymbol{\Pi}$	viscous tensor
σ_i	electrical conductivity of the ith species
ρ_i	mass density of the ith species
θ_i	thermal diffusion coefficient of the ith species
Ω	collision integrals
χ_i	thermal diffusion ratio of the ith species
$\parallel$	parallel superscript
$\perp$	perpendicular superscript
$\odot$	transverse superscript
B	imaginary part of TLS superscript

1. Introduction

Ionized magnetized reactive gas mixtures have many practical applications such as laboratory plasmas, high-speed gas flows, lean flame stabilization or atmospheric phenomena [1–7]. Application of the Chapman–Enskog theory to partially ionized mixtures of monatomic gases in the presence of electric and magnetic fields has been discussed in particular by Chapman and Cowling [3] and Ferziger and Kaper [6] in a regime where there is only one temperature in the mixture, assuming that the electric field is not intense [6, 7]. The proper collision operator to be used is then the Boltzmann collision operator with shielded potentials [6]. Mixtures of monatomic gases that are not at thermodynamic equilibrium with multitemperature transport arising from small electron/ion mass ratio asymptotics have also been investigated by Chmieleski and Ferziger [8], and in the fully ionized case by Braginsky using the Landau

equation [1, 9]. Multitemperature models also naturally arise with strong electric fields—which are out of the scope of the present paper—in particular in swarm physics [10]. Higher order evaluations of transport coefficients have been performed by Kaneko and coworkers for binary neutral mixtures in uniform magnetic fields in a simplified steady kinetic framework [11, 12]. Convergence properties of the Chapman–Enskog expansion for transport coefficients of magnetized argon plasmas have been investigated by Bruno and coworkers [2, 13, 14]. The degree of anisotropy of various transport coefficients introduced by the magnetic field has been studied in terms of the electron Hall parameter. Bruno and coworkers have established in particular the important influence of the Ramsauer minimum in the electron–argon cross sections on the transport coefficients of magnetized argon plasmas [2, 14].

In a recent paper [15], the authors have investigated the kinetic theory of partially ionized magnetized polyatomic reactive gas mixtures. The macroscopic equations in the zeroth-order and first-order regimes, together with expressions for the transport fluxes and the transport coefficients, have been obtained. New bracket expressions have been established for the perpendicular and transverse diffusion, thermal diffusion and partial thermal conductivity coefficients as well as for the shear viscosity coefficients. A new definition of the thermal conductivity and of the thermal diffusion ratios—consistent with the zero magnetic fields limit—has also been introduced. Positivity properties of multicomponent diffusion matrices have been investigated and the mathematical structure of the transport linear systems has also been addressed.

We further investigate in this paper the kinetic theory of partially ionized reactive gas mixtures in the strong magnetic field regime. A new tensor basis is first introduced for expanding the anisotropic perturbed species distribution functions associated with the viscous tensor which has better properties than the *linearly dependent* generating family previously used [6, 15]. This new basis is constituted of five independent traceless symmetric tensors constructed with the particle velocity vector and the magnetic field pseudovector. These five tensors are orthogonal to collisional invariants and the derivation of the corresponding linearized integral equations and transport linear systems is clarified.

New simplified bracket expressions for diffusion, thermal diffusion and partial thermal conductivity coefficients are also obtained from which we deduce new symmetry properties of these transport coefficients. These symmetry properties result from clever manipulations of the real and imaginary parts of Boltzmann linearized complex integral equations. As a consequence, we also simplify the positivity properties of the resulting multicomponent diffusion matrices and heat–mass transport matrices parallel, perpendicular and transverse to the magnetic field.

Generalizing previous work on non-ionized species [16] we further introduce a variational framework for a direct evaluation of the thermal conductivities and the thermal diffusion ratios without the intermediate evaluation of the partial thermal conductivities and the thermal diffusion coefficients. The resulting transport linear systems are of reduced size which is interesting from a computational point of view.

All transport linear systems corresponding to the first usual Sonine/Wang–Chang Uhlenbeck polynomial expansions are evaluated, making use of previous work on neutral species mixtures [17]. The mathematical structure of the transport linear systems is discussed as well as the evaluation of the corresponding transport coefficients parallel, perpendicular and transverse to the magnetic field. The convergence of the successive approximations in the Chapman–Enskog expansion of the transport coefficients is still known to converge more slowly in plasmas than in neutral mixtures [1, 2, 10].

Since the size of the transport linear systems can be relatively large and since the transport coefficients have to be evaluated at each computational cell in space and time, transport

properties evaluation may become computationally expensive, especially for multidimensional numerical simulations. In this regard, the use of iterative techniques has been shown to be an interesting and appealing alternative [17–19]. We discuss practical implementation of iterative techniques for solving the resulting complex symmetric constrained singular transport linear systems. The accuracy of various approximated transport coefficients is investigated and numerical tests are performed for weakly ionized air at 10 000 K.

The behavior of all transport coefficients and of anisotropic transport fluxes for vanishing magnetic fields is finally investigated using series expansions in terms of the intensity of the magnetic field. These series expansions show that, for vanishing magnetic field, the mass and heat fluxes as well as the viscous tensor behave smoothly. Onsager reciprocal relations are also more closely investigated for anisotropic transport fluxes in particular for the viscous tensor.

In section 2, we summarize the kinetic framework and in section 3 we present the new tensor expansion associated with the viscous tensor. In section 4 we investigate new symmetry properties of the bracket expressions and in section 5 we discuss the variational framework for a direct evaluation of the thermal conductivity and the thermal diffusion ratios. The dependence on the magnetic field is studied in section 6 and the Onsager reciprocal relations are finally investigated in section 7.

2. Theoretical framework

2.1. Generalized Boltzmann equation

We consider a dilute reactive gas mixture composed of n^s chemical species having internal degrees of freedom. The Boltzmann equations for polyatomic gas mixtures are written in a semi-classical framework with degeneracy averaged collision cross sections [20] and the chemical source terms is taken from [21–24].

The state of the mixture is described by the species distribution functions denoted by $f_i(t, \boldsymbol{x}, \boldsymbol{c}_i, \text{I})$, where i is the index of the species, t is the time, $\boldsymbol{x}$ is the three-dimensional spatial coordinate, $\boldsymbol{c}_i$ is the velocity and I is the index for the internal energy state of the ith species. We denote by $\mathcal{S}$ the species indexing set $\mathcal{S} = \{1, \ldots, n^s\}$, by m_i, e_i, and $z_i = e_i/m_i$ the molecular mass, charge, and charge per unit mass of the ith species, and finally by $\mathcal{E}_{i\text{I}}$ the internal energy of the ith species in the Ith state. For a family of functions ξ_i, $i \in \mathcal{S}$, we will use the compact notation $\xi = (\xi_i)_{i \in \mathcal{S}}$.

The family of species distribution functions $f = (f_i)_{i \in \mathcal{S}}$ is the solution of the generalized Boltzmann equations

$$\widetilde{\mathcal{D}}_i(f_i) + \frac{1}{\epsilon^{\mathsf{b}}}\widehat{\mathcal{D}}_i(f_i) = \frac{1}{\epsilon}\mathcal{S}_i(f) + \epsilon^{\mathsf{a}}\mathcal{C}_i(f), \qquad i \in \mathcal{S}, \tag{1}$$

where $\widetilde{\mathcal{D}}_i$ is the streaming operator $\widetilde{\mathcal{D}}_i(f_i) = \partial_t f_i + \boldsymbol{c}_i \cdot \partial_{\boldsymbol{x}} f_i + \widetilde{\boldsymbol{b}}_i \cdot \partial_{\boldsymbol{c}_i} f_i$ associated with the reduced force $\widetilde{\boldsymbol{b}}_i = \boldsymbol{g} + z_i(\boldsymbol{E} + \boldsymbol{v} \wedge \boldsymbol{B})$, where $\boldsymbol{g}$ is a species independent external force, $\boldsymbol{E}$ is the electric field, $\boldsymbol{B}$ is the magnetic field and $\widehat{\mathcal{D}}_i(f_i) = z_i((\boldsymbol{c}_i - \boldsymbol{v}) \wedge \boldsymbol{B}) \cdot \partial_{\boldsymbol{c}_i} f_i$. The reactive source term $\mathcal{C}_i(f)$ and the nonreactive source term $\mathcal{S}_i(f)$ are described in [20–25] and are both compatible with the *H*-theorem [23]. In these equations, ϵ is the usual formal parameter associated with the Enskog expansion, and a and b are nonnegative integers which depend on the regime under consideration. In this paper, we only consider the strong magnetic field regime $\mathsf{b} = 1$ and the Maxwellian reaction regime $\mathsf{a} = 1$ and we refer to [15, 23, 25] for more details on other regimes.

The scalar collisional invariants of the nonreactive collision operator $\mathcal{S}$ form a vector space spanned by ψ^l, $l \in \{1, \ldots, n^s + 4\}$, with $\psi^l = (\delta_{li})_{i \in \mathcal{S}}$, for $l \in \mathcal{S}$, $\psi^l = (m_i c_{iv})_{i \in \mathcal{S}}$,

for $l = n^s + \nu$, $\nu = 1, 2, 3$, and $\psi^l = \left(\frac{1}{2} m_i \boldsymbol{c}_i \cdot \boldsymbol{c}_i + \mathcal{E}_{i\mathrm{I}}\right)_{i \in \mathcal{S}}$, for $l = n^s + 4$, where $c_{i\nu}$ is the component of $\boldsymbol{c}_i$ in the νth spatial coordinate. For two families $\xi = (\xi_i)_{i \in \mathcal{S}}$ and $\zeta = (\zeta_i)_{i \in \mathcal{S}}$, we define the scalar product by

$$\langle\!\langle \xi, \zeta \rangle\!\rangle = \sum_{i,\mathrm{I}} \int \xi_i \odot \overline{\zeta}_i \, \mathrm{d}\boldsymbol{c}_i,$$

where $\xi_i \odot \overline{\zeta}_i$ denotes the maximum contracted product between the tensor ξ_i and the complex conjugate tensor $\overline{\zeta}_i$. The scalar product is defined for families of complex tensors as such quantities naturally arise in the solution of Boltzmann linearized equations in the presence of magnetic fields.

An approximate solution to the Boltzmann equations (1) is obtained by using the Enskog expansion

$$f_i = f_i^0(1 + \epsilon\phi_i + \mathcal{O}(\epsilon^2)), \qquad i \in \mathcal{S}, \tag{2}$$

where f^0 yields the same local macroscopic properties as f

$$\langle\!\langle f^0, \psi^l \rangle\!\rangle = \langle\!\langle f, \psi^l \rangle\!\rangle, \qquad l \in \{1, \ldots, n^s + 4\}. \tag{3}$$

The family of zeroth-order species distribution functions $f^0 = \left(f_i^0\right)_{i \in \mathcal{S}}$ is shown to be given by generalized Maxwellian distributions [6, 15]

$$f_i^0 = \frac{n_i}{\beta_{i\mathrm{I}} Q_i} \exp\left(-\frac{m_i}{2k_\mathrm{B}T} \boldsymbol{C}_i \cdot \boldsymbol{C}_i - \frac{\mathcal{E}_{i\mathrm{I}}}{k_\mathrm{B}T}\right), \qquad i \in \mathcal{S}, \tag{4}$$

where n_i is the number density of the ith species, k_B is the Boltzmann constant, $\boldsymbol{C}_i = \boldsymbol{c}_i - \boldsymbol{v}$ is the relative velocity of the ith species, T is the temperature, Q_i is the full partition function per unit volume of the ith species $Q_i = Q_i^{\mathrm{int}} Q_i^{\mathrm{tr}}$ with $Q_i^{\mathrm{int}} = \sum_\mathrm{I} \alpha_{i\mathrm{I}} \exp\left(-\frac{\mathcal{E}_{i\mathrm{I}}}{k_\mathrm{B}T}\right)$ and $Q_i^{\mathrm{tr}} = \left(\frac{2\pi m_i k_\mathrm{B}T}{\mathrm{h}_\mathrm{P}^2}\right)^{3/2}$, $\alpha_{i\mathrm{I}}$ is the degeneracy of the ith species in the Ith state, h_P is the Planck constant and $\beta_{i\mathrm{I}} = \mathrm{h}_\mathrm{P}^3 / \alpha_{i\mathrm{I}} m_i^3$.

The macroscopic conservation equations at zeroth order are obtained by taking the scalar product of Boltzmann equations by collisional invariants and by only keeping the zeroth-order terms $\langle\!\langle \widetilde{\mathcal{D}}(f^0), \psi^l \rangle\!\rangle + \langle\!\langle \widehat{\mathcal{D}}(f^0\phi), \psi^l \rangle\!\rangle = 0, l \in \{1, \ldots, n^s + 4\}$, where $\widetilde{\mathcal{D}}(f^0) = \left(\widetilde{\mathcal{D}}_i(f_i^0)\right)_{i \in \mathcal{S}}$ and $\widehat{\mathcal{D}}(f^0\phi) = \left(\widehat{\mathcal{D}}_i(f_i^0\phi_i)\right)_{i \in \mathcal{S}}$. These zeroth-order equations, together with Maxwell's equations, yield the magnetogasdynamic equations [3, 6, 15].

2.2. Linearized Boltzmann equations

The linearized Boltzmann operator, $\boldsymbol{\mathcal{F}}^{\boldsymbol{\mathcal{S}}} = \left(\mathcal{F}_i^{\boldsymbol{\mathcal{S}}}\right)_{i \in \mathcal{S}}$, can be written as

$$\mathcal{F}_i^{\boldsymbol{\mathcal{S}}}(\phi) = \sum_{j \in \mathcal{S}} \sum_{\mathrm{I}'\mathrm{JJ}'} \int f_j^0(\phi_i + \phi_j - \phi_i' - \phi_j') \mathrm{W}_{ij}^{\mathrm{IJI}'\mathrm{J}'} \, \mathrm{d}\boldsymbol{c}_j \, \mathrm{d}\boldsymbol{c}_i' \, \mathrm{d}\boldsymbol{c}_j', \qquad i \in \mathcal{S}, \tag{5}$$

where $\phi = (\phi_i)_{i \in \mathcal{S}}$ and $\mathrm{W}_{ij}^{\mathrm{IJI}'\mathrm{J}'}$ is the transition probability between colliding molecules [21, 22, 25]. An important property is that the linearized Boltzmann operator is isotropic, i.e., it converts a tensor constructed from $(\boldsymbol{c}_i)_{i \in \mathcal{S}}$ into another tensor of the same type as in the monatomic case [6]. The bracket operator is defined by $[\![\xi, \zeta]\!] = \langle\!\langle f^0\xi, \boldsymbol{\mathcal{F}}^{\boldsymbol{\mathcal{S}}}(\zeta) \rangle\!\rangle$, where $\xi = (\xi_i)_{i \in \mathcal{S}}, \zeta = (\zeta_i)_{i \in \mathcal{S}}$, and ξ_i and ζ_i depend on $\boldsymbol{c}_i$ and I. This bracket operator is Hermitian $[\![\xi, \zeta]\!] = \overline{[\![\zeta, \xi]\!]}$, positive semi-definite $[\![\xi, \xi]\!] \geqslant 0$, and its kernel is spanned by the collisional invariants, that is, $[\![\xi, \xi]\!] = 0$ implies that ξ is a (tensorial) collisional invariant, so that all its tensorial components are scalar collisional invariants [3, 6, 15, 26].

The first-order integro-differential equations governing $\phi = (\phi_i)_{i \in \mathcal{S}}$ are easily obtained from (1) and written as $\mathcal{F}_i^{\boldsymbol{\mathcal{S}}}(\phi) = -z_i(\boldsymbol{C}_i \wedge \boldsymbol{B}) \cdot \partial_{\boldsymbol{c}_i}\phi_i - \widetilde{\mathcal{D}}_i(\log f_i^0), i \in \mathcal{S}$, with the scalar

constraints $\langle\langle f^0\phi, \psi^l \rangle\rangle = 0, l \in \{1, \ldots, n^s + 4\}$. By linearity and isotropy of the linearized Boltzmann operator $\mathcal{F}^\mathcal{S}$, the solution $\phi = (\phi_i)_{i\in\mathcal{S}}$ is expanded in the form

$$\phi_i = -\phi_i^\eta : \partial_x v - \frac{1}{3}\phi_i^\kappa \, \partial_x \cdot v - \sum_{j\in\mathcal{S}} \phi_i^{D_j} \cdot (\partial_x p_j - \rho_j \widetilde{b}_j) - \phi_i^{\widehat{\lambda}} \cdot \partial_x\left(\frac{1}{k_B T}\right). \qquad (6)$$

After some algebra, the tensorial functionals ϕ^μ, for $\mu \in \{\eta, \kappa, (D_j)_{j\in\mathcal{S}}, \widehat{\lambda}\}$, are shown to satisfy the integro-dif-fe-ren-tial equations

$$\mathcal{F}_i^\mathcal{S}(\phi^\mu) + z_i(C_i \wedge B) \cdot \partial_{c_i}\phi_i^\mu + \sum_{j,J} \frac{m_i e_j}{\rho k_B T} C_i \cdot \int f_j^0 C_j \wedge B\phi_j^\mu \, \mathrm{d}c_j = \Psi_i^\mu, \qquad i \in \mathcal{S}, \ (7)$$

and the scalar constraints

$$\langle\langle f^0\phi^\mu, \psi^l \rangle\rangle = 0, \qquad l \in \{1, \ldots, n^s + 4\}, \qquad (8)$$

where $\Psi_i^\eta = \frac{m_i}{k_B T}(C_i \otimes C_i - \frac{1}{3}C_i \cdot C_i I)$, $\Psi_i^\kappa = \frac{2c^{\mathrm{int}}}{c_v k_B T}\left(\frac{1}{2}m_i C_i \cdot C_i - \frac{3}{2}k_B T\right) + \frac{2c_v^{\mathrm{tr}}}{c_v k_B T}(\overline{\mathcal{E}_i} - \mathcal{E}_{iI})$, $\Psi_i^{D_j} = \frac{1}{p_i}\left(\delta_{ij} - \frac{\rho_i}{\rho}\right)C_i$, $\Psi_i^{\widehat{\lambda}} = \left(\frac{5}{2}k_B T - \frac{1}{2}m_i C_i \cdot C_i + \overline{\mathcal{E}_i} - \mathcal{E}_{iI}\right)C_i$, for $i \in \mathcal{S}$, where c_v^{tr} is the translational heat capacity per molecule at constant volume, c^{int} is the internal heat capacity per molecule of the mixture, $c_v = c_v^{\mathrm{tr}} + c^{\mathrm{int}}$ is the heat capacity at constant volume per molecule of the mixture, $\overline{\mathcal{E}_i} = \sum_I \alpha_{iI}\mathcal{E}_{iI} \exp\left(-\frac{\mathcal{E}_{iI}}{k_B T}\right)/Q_i^{\mathrm{int}}$ is the averaged internal energy per molecule of the ith species and p_i is the partial pressure of the ith species.

2.3. First-order conservation equations

The macroscopic conservation equations at first order are obtained by taking the scalar product of Boltzmann equations with collisional invariants and by keeping the zeroth- and first-order terms $\langle\langle \widetilde{\mathcal{D}}(f^0 + f^0\phi), \psi^l \rangle\rangle + \langle\langle \widehat{\mathcal{D}}(f^0\phi), \psi^l \rangle\rangle = \langle\langle \mathcal{C}(f^0), \psi^l \rangle\rangle, l \in \{1, \ldots, n^s + 4\}$, where we have defined $\mathcal{C}(f^0) = (\mathcal{C}_i(f^0))_{i\in\mathcal{S}}$. Note that the terms $\langle\langle \widetilde{\mathcal{D}}(f^0\phi^{(2)}), \psi^l \rangle\rangle$ associated with second-order currents have been neglected [4, 15].

After some algebra, the species mass conservation equations, obtained for $l = 1, \ldots, n^s$, are in the form

$$\partial_t \rho_i + \partial_x \cdot (\rho_i v) + \partial_x \cdot (\rho_i V_i) = m_i \overline{\omega}_i^0, \qquad i \in \mathcal{S}, \qquad (9)$$

where $V_i = \frac{1}{n_i}\sum_I \int C_i f_i^0 \phi_i \, \mathrm{d}c_i$ is the diffusion velocities and $\overline{\omega}_i^0 = \sum_I \int \mathcal{C}_i(f^0) \, \mathrm{d}c_i$ the chemical source term of the ith species discussed in [25]. The momentum conservation equation, obtained from $l = n^s + 1, n^s + 2$, and $n^s + 3$, reads

$$\partial_t(\rho v) + \partial_x \cdot (\rho v \otimes v + p I) + \partial_x \cdot \Pi = \rho g + \mathcal{Q}(E + v \wedge B) + j \wedge B, \qquad (10)$$

where $\mathcal{Q} = \sum_{i\in\mathcal{S}} n_i e_i$ is the total charge per unit volume, $j = \sum_{i\in\mathcal{S}} n_i e_i V_i$ is the conduction current and $\Pi = \sum_{i,I} \int m_i C_i \otimes C_i f_i^0 \phi_i \, \mathrm{d}c_i$ is the viscous tensor. The energy conservation equation, obtained for $l = n^s + 4$, finally reads

$$\partial_t\left(\frac{1}{2}\rho v \cdot v + \mathcal{E}\right) + \partial_x \cdot \left(\left(\frac{1}{2}\rho v \cdot v + \mathcal{E} + p\right)v\right) + \partial_x \cdot (q + \Pi \cdot v)$$
$$= (\rho g + \mathcal{Q}(E + v \wedge B)) \cdot v + j \cdot E, \qquad (11)$$

where $q = \sum_{i,I} \int \left(\frac{1}{2}m_i C_i \cdot C_i + \mathcal{E}_{iI}\right)c_i f_i^0 \phi_i \, \mathrm{d}c_i$ is the heat flux vector.

3. The shear viscosities

3.1. A new expansion for ϕ^η

The solution $\phi^\eta = \left(\phi_i^\eta\right)_{i\in\mathcal{S}}$ of (7) and (8) with $\mu = \eta$ is such that ϕ_i^η is composed from all symmetric traceless second-order tensors created from the vector $\mathcal{C}_i = \sqrt{m_i/2k_B T}\,C_i$ and the

pseudovector $\boldsymbol{B}$ which form a space of dimension five [27]. In this paper, we introduce the new tensor expansion

$$\phi_i^\eta = \phi_i^{\eta(1)}\mathbf{T}_i^{(1)} + \phi_i^{\eta(2)}\mathbf{T}_i^{(2)} + \phi_i^{\eta(3)}\mathbf{T}_i^{(3)} + \phi_i^{\eta(4)}\mathbf{T}_i^{(4)} + \phi_i^{\eta(5)}\mathbf{T}_i^{(5)}, \tag{12}$$

where $\phi_i^{\eta(l)}$, $l = 1, \ldots, 5$, are scalar functions of $\mathcal{C}_i \cdot \mathcal{C}_i$, $(\mathcal{C}_i \cdot \boldsymbol{B})^2$ and $\boldsymbol{B} \cdot \boldsymbol{B}$, for $i \in \mathcal{S}$, in terms of the five *independent* tensors $\mathbf{T}_i^{(1)}, \ldots, \mathbf{T}_i^{(5)}$, defined by

$$\mathbf{T}_i^{(1)} = \mathcal{C}_i \otimes \mathcal{C}_i - \tfrac{1}{3}\mathcal{C}_i \cdot \mathcal{C}_i \boldsymbol{I},$$

$$\mathbf{T}_i^{(2)} = \tfrac{1}{2}[\mathcal{C}_i \otimes (\mathcal{C}_i \wedge \boldsymbol{B}) + (\mathcal{C}_i \wedge \boldsymbol{B}) \otimes \mathcal{C}_i],$$

$$\mathbf{T}_i^{(3)} = (\mathcal{C}_i \wedge \boldsymbol{B}) \otimes (\mathcal{C}_i \wedge \boldsymbol{B}) - \tfrac{1}{3}\mathcal{C}_i \cdot \mathcal{C}_i \boldsymbol{B} \cdot \boldsymbol{B}\boldsymbol{I} + (\mathcal{C}_i \cdot \boldsymbol{B})^2 \boldsymbol{B} \otimes \boldsymbol{B}/\boldsymbol{B} \cdot \boldsymbol{B},$$

$$\mathbf{T}_i^{(4)} = \tfrac{1}{2}\mathcal{C}_i \cdot \boldsymbol{B}[\mathcal{C}_i \otimes \boldsymbol{B} + \boldsymbol{B} \otimes \mathcal{C}_i] - (\mathcal{C}_i \cdot \boldsymbol{B})^2 \boldsymbol{B} \otimes \boldsymbol{B}/\boldsymbol{B} \cdot \boldsymbol{B},$$

$$\mathbf{T}_i^{(5)} = \tfrac{1}{2}\mathcal{C}_i \cdot \boldsymbol{B}[\boldsymbol{B} \otimes (\mathcal{C}_i \wedge \boldsymbol{B}) + (\mathcal{C}_i \wedge \boldsymbol{B}) \otimes \boldsymbol{B}].$$

The former *generating family* of six tensors $\mathbf{T}_i^{[1]}, \ldots, \mathbf{T}_i^{[6]}$ is related to the new *basis* by $\mathbf{T}_i^{[1]} = \mathbf{T}_i^{(1)}$, $\mathbf{T}_i^{[2]} = \mathbf{T}_i^{(2)}$, $\mathbf{T}_i^{[5]} = \mathbf{T}_i^{(5)}$, $\mathbf{T}_i^{[6]} = \frac{(\mathcal{C}_i \cdot \boldsymbol{B})^2 \boldsymbol{B} \cdot \boldsymbol{B}}{\mathcal{C}_i \cdot \mathcal{C}_i \boldsymbol{B} \cdot \boldsymbol{B} - 3(\mathcal{C}_i \cdot \boldsymbol{B})^2}\left(2\mathbf{T}_i^{(4)} - \mathbf{T}_i^{(3)} - \boldsymbol{B} \cdot \boldsymbol{B}\mathbf{T}_i^{(1)}\right)$, $\mathbf{T}_i^{[3]} = \mathbf{T}_i^{(3)} - \frac{1}{\boldsymbol{B} \cdot \boldsymbol{B}}\mathbf{T}_i^{[6]}$, $\mathbf{T}_i^{[4]} = \mathbf{T}_i^{(4)} + \frac{1}{\boldsymbol{B} \cdot \boldsymbol{B}}\mathbf{T}_i^{[6]}$. These six tensors are linearly dependent and the linear relation $\mathcal{C}_i \cdot \mathcal{C}_i \mathbf{T}_i^{[6]} + (\mathcal{C}_i \cdot \boldsymbol{B})^2\left[\mathbf{T}_i^{[3]} + \boldsymbol{B} \cdot \boldsymbol{B}\mathbf{T}_i^{[1]} - 2\mathbf{T}_i^{[4]}\right] = 0$ holds [6]. After some algebra, it is established that the former expansion $\phi_i^\eta = \sum_{l=1}^{6} \phi_i^{\eta[l]}\mathbf{T}_i^{[l]}$ and the new one are equally valid and that $\phi_i^{\eta(l)} = \phi_i^{\eta[l]}$, $i \in \mathcal{S}$, $l \in \{1, \ldots, 5\}$.

3.2. Properties of the new tensor basis

Substituting expansion (12) into equation (7) for $\mu = \eta$, using the isotropy of the Boltzmann linearized operator $\mathcal{F}^\mathcal{S}$, and equating the corresponding terms, yield five equations, each one involving one tensor $\mathbf{T}_i^{(l)}$ for $l = 1, \ldots, 5$. An important property of the new tensors, however, is that they are simple linear transformations of the tensor $\mathbf{T}_i^{(1)} = \mathcal{C}_i \otimes \mathcal{C}_i - \tfrac{1}{3}\mathcal{C}_i \cdot \mathcal{C}_i \boldsymbol{I}$ with coefficients *independent* of the particle velocities $\mathcal{C}_i$, $i \in \mathcal{S}$

$$\mathbf{T}_i^{(2)} = \frac{1}{2}\left(\mathbf{T}_i^{(1)}R(\boldsymbol{B}) - R(\boldsymbol{B})\mathbf{T}_i^{(1)}\right), \tag{13}$$

$$\mathbf{T}_i^{(3)} = -R(\boldsymbol{B})\mathbf{T}_i^{(1)}R(\boldsymbol{B}) + \frac{1}{\boldsymbol{B} \cdot \boldsymbol{B}}\boldsymbol{B} \otimes \boldsymbol{B}\mathbf{T}_i^{(1)}\boldsymbol{B} \otimes \boldsymbol{B}, \tag{14}$$

$$\mathbf{T}_i^{(4)} = \frac{1}{2}\left(\mathbf{T}_i^{(1)}\boldsymbol{B} \otimes \boldsymbol{B} + \boldsymbol{B} \otimes \boldsymbol{B}\mathbf{T}_i^{(1)}\right) - \frac{1}{\boldsymbol{B} \cdot \boldsymbol{B}}\boldsymbol{B} \otimes \boldsymbol{B}\mathbf{T}_i^{(1)}\boldsymbol{B} \otimes \boldsymbol{B}, \tag{15}$$

$$\mathbf{T}_i^{(5)} = \frac{1}{2}\left(\boldsymbol{B} \otimes \boldsymbol{B}\mathbf{T}_i^{(1)}R(\boldsymbol{B}) - R(\boldsymbol{B})\mathbf{T}_i^{(1)}\boldsymbol{B} \otimes \boldsymbol{B}\right), \tag{16}$$

where $\boldsymbol{B} \otimes \boldsymbol{B}$ denotes the tensor product of the magnetic field $\boldsymbol{B}$ with itself and $R(\boldsymbol{B})$ the rotation matrix associated with $\boldsymbol{B}$. For any vector $\mathbf{Z}$, the rotation matrix $R(\mathbf{Z})$ is defined by

$$R(\boldsymbol{Z}) = \begin{pmatrix} 0 & -Z_3 & Z_2 \\ Z_3 & 0 & -Z_1 \\ -Z_2 & Z_1 & 0 \end{pmatrix}.$$

Using these relations and the linear equations associated with each tensor $\mathbf{T}_i^{(l)}$ we naturally obtain five coupled equations between the family of tensors $\phi^{\eta(l)} = \left(\phi_i^{\eta(l)}\right)_{i \in \mathcal{S}}$ defined for $l = 1, \ldots, 5$, by

$$\phi_i^{\eta(l)} = \phi_i^{\eta(l)}\left(\mathcal{C}_i \otimes \mathcal{C}_i - \tfrac{1}{3}\mathcal{C}_i \cdot \mathcal{C}_i \boldsymbol{I}\right), \qquad i \in \mathcal{S}.$$

The resulting equations are in the form

$$\mathcal{F}_i^{\mathcal{S}}(\phi^{\eta(1)}) - z_i B^2 \phi_i^{\eta(2)} = \mathbf{\Psi}_i^{\eta}, \qquad i \in \mathcal{S}, \tag{17}$$

$$\mathcal{F}_i^{\mathcal{S}}(\phi^{\eta(2)}) + 2z_i\left(\phi_i^{\eta(1)} - B^2 \phi_i^{\eta(3)}\right) = 0, \qquad i \in \mathcal{S}, \tag{18}$$

$$\mathcal{F}_i^{\mathcal{S}}(\phi^{\eta(3)}) + z_i \phi_i^{\eta(2)} = 0, \qquad i \in \mathcal{S}, \tag{19}$$

$$\mathcal{F}_i^{\mathcal{S}}(\phi^{\eta(4)}) + z_i\left(\phi_i^{\eta(2)} - B^2 \phi_i^{\eta(5)}\right) = 0, \qquad i \in \mathcal{S}, \tag{20}$$

$$\mathcal{F}_i^{\mathcal{S}}(\phi^{\eta(5)}) + z_i\left(2\phi_i^{\eta(3)} + \phi_i^{\eta(4)}\right) = 0, \qquad i \in \mathcal{S}, \tag{21}$$

and the derivation of (17)–(21) is clear and direct at variance with the case of the former generating family where the derivation of similar equations was somewhat obscure mainly because of the dependence on particle velocities of the proportionality coefficients between $\mathbf{T}_i^{[3]}$, $\mathbf{T}_i^{[4]}$, $\mathbf{T}_i^{[6]}$ and $\mathbf{T}_i^{[1]}$. Upon introducing the usual auxiliary complex quantities

$$\varphi_i^{\eta(1)} = \phi_i^{\eta(1)} + B^2 \phi_i^{\eta(3)},$$
$$\varphi_i^{\eta(2)} = \phi_i^{\eta(1)} + \mathrm{i}B \phi_i^{\eta(2)} - B^2 \phi_i^{(3)},$$
$$\varphi_i^{\eta(3)} = \phi_i^{\eta(1)} + \tfrac{1}{2}\mathrm{i}B \phi_i^{\eta(2)} + \tfrac{1}{2}B^2 \phi_i^{\eta(4)} + \tfrac{1}{2}\mathrm{i}B^3 \phi_i^{\eta(5)},$$

where $\mathrm{i}^2 = -1$, we recover the integral equations

$$\mathcal{F}^{\mathcal{S}}(\varphi^{\eta(1)}) = \mathbf{\Psi}^{\eta}, \quad (\mathcal{F}^{\mathcal{S}} + 2\mathrm{i}B\mathcal{F}^{z,m})(\varphi^{\eta(2)}) = \mathbf{\Psi}^{\eta}, \quad (\mathcal{F}^{\mathcal{S}} + \mathrm{i}B\mathcal{F}^{z,m})(\varphi^{\eta(3)}) = \mathbf{\Psi}^{\eta}, \tag{22}$$

and the scalar constraints are *automatically* satisfied. Note that this was *not* the case for the former tensor expansion since $\mathbf{T}_i^{[3]}$, $\mathbf{T}_i^{[4]}$, and $\mathbf{T}_i^{[6]}$ are not orthogonal to collisional invariant and the constraint $\boldsymbol{B} \cdot \boldsymbol{B} \phi_i^{\eta[6]} = \phi_i^{\eta[3]} - \phi_i^{\eta[4]}$ was needed among the former expansion coefficients. The operator $\mathcal{F}^{z,m} = \left(\mathcal{F}_i^{z,m}\right)_{i \in \mathcal{S}}$ is defined for $\mathbf{u} = (\mathbf{u}_i)_{i \in \mathcal{S}}$ by $\mathcal{F}_i^{z,m}(\mathbf{u}) = z_i \mathbf{u}_i$, $i \in \mathcal{S}$, where $\mathbf{u}_i$ is the product of $\mathcal{C}_i \otimes \mathcal{C}_i - \frac{1}{3}\mathcal{C}_i \cdot \mathcal{C}_i \boldsymbol{I}$ by a complex scalar function of $\boldsymbol{C}_i \cdot \boldsymbol{C}_i$, $(\boldsymbol{C}_i \cdot \boldsymbol{B})^2$ and $\boldsymbol{B} \cdot \boldsymbol{B}$. These systems are shown to be well posed [15] and imply that the scalar function $\varphi_i^{\eta(\mathrm{l})}$ such that $\varphi_i^{\eta(\mathrm{l})} = \varphi_i^{\eta(\mathrm{l})}\left(\mathcal{C}_i \otimes \mathcal{C}_i - \frac{1}{3}\mathcal{C}_i \cdot \mathcal{C}_i \boldsymbol{I}\right)$ only depends on $\boldsymbol{C}_i \cdot \boldsymbol{C}_i$ and $\boldsymbol{B} \cdot \boldsymbol{B}$, for $\mathrm{l} \in \{1, 2, 3\}$ [6].

3.3. Expressions of the viscous stress tensor Π

From the relation $\mathbf{\Pi} = k_{\mathrm{B}}T \langle\!\langle \mathbf{\Psi}^{\eta}, f^0 \phi \rangle\!\rangle + \frac{1}{3}k_{\mathrm{B}}T \langle\!\langle \mathbf{\Psi}^{\kappa}, f^0 \phi \rangle\!\rangle \boldsymbol{I}$ and the expansion of ϕ it is obtained that

$$-\mathbf{\Pi} = \kappa(\partial_x \cdot v)\boldsymbol{I} + \eta_1 \mathbf{S} + \eta_2(R(\mathcal{B})\mathbf{S} - \mathbf{S}R(\mathcal{B})) + \eta_3(\mathcal{B}^t \mathbf{S}\mathcal{B}\mathcal{B} \otimes \mathcal{B} - R(\mathcal{B})\mathbf{S}R(\mathcal{B}))$$
$$+ \eta_4(\mathbf{S}\mathcal{B} \otimes \mathcal{B} + \mathcal{B} \otimes \mathcal{B}\mathbf{S} - 2\mathcal{B}^t \mathbf{S}\mathcal{B}\mathcal{B} \otimes \mathcal{B}) + \eta_5(\mathcal{B} \otimes \mathcal{B}\mathbf{S}R(\mathcal{B}) - R(\mathcal{B})\mathbf{S}\mathcal{B} \otimes \mathcal{B}), \tag{23}$$

where $\mathbf{S} = \partial_x v + \partial_x v^t - \frac{2}{3}(\partial_x \cdot v)\boldsymbol{I}$, $\kappa = \frac{1}{9}k_{\mathrm{B}}T[\![\phi^{\kappa}, \phi^{\kappa}]\!]$ and the five shear viscosities $\eta_1, \ldots, \eta_5$ are given by

$$\eta_1 = \tfrac{1}{20}k_{\mathrm{B}}T([\![\varphi^{\eta(1)}, \varphi^{\eta(1)}]\!] + [\![\varphi^{\eta(2)}, \varphi^{\eta(2)}]\!]), \tag{24}$$

$$\eta_2 = -\tfrac{1}{10}k_{\mathrm{B}}T(\!(\varphi^{\eta(2)}, \varphi^{\eta(2)})\!) \tag{25}$$

$$\eta_3 = \tfrac{1}{20}k_{\mathrm{B}}T([\![\varphi^{\eta(1)}, \varphi^{\eta(1)}]\!] - [\![\varphi^{\eta(2)}, \varphi^{\eta(2)}]\!]), \tag{26}$$

$$\eta_4 = \tfrac{1}{10}k_{\mathrm{B}}T([\![\varphi^{\eta(3)}, \varphi^{\eta(3)}]\!] - \tfrac{1}{2}[\![\varphi^{\eta(1)}, \varphi^{\eta(1)}]\!] - \tfrac{1}{2}[\![\varphi^{\eta(2)}, \varphi^{\eta(2)}]\!]), \tag{27}$$

$$\eta_5 = \tfrac{1}{10} k_{\mathrm{B}} T ((\!(\boldsymbol{\varphi}^{\eta(2)}, \boldsymbol{\varphi}^{\eta(2)})\!) - (\!(\boldsymbol{\varphi}^{\eta(3)}, \boldsymbol{\varphi}^{\eta(3)})\!)), \tag{28}$$

where we have defined the scalar product

$$(\!(\xi, \zeta)\!) = \sum_{k,K} z_k B \int f_k^0 \xi_k \odot \overline{\zeta}_k \, \mathrm{d}\boldsymbol{c}_k. \tag{29}$$

The new tensor basis finally yields identical integral equations and bracket expressions for the five shear viscosities but in a clear and straightforward way. After some algebra, denoting by $\mathrm{Re}(z)$ and $\mathrm{Im}(z)$ the real and imaginary part of a complex quantity $z = \mathrm{Re}(z) + \mathrm{i}\,\mathrm{Im}(z)$, it is further obtained that

$$\eta_1 = \tfrac{1}{20} k_{\mathrm{B}} T (\langle\!\langle f^0 \boldsymbol{\varphi}^{\eta(1)}, \boldsymbol{\Psi}^\eta \rangle\!\rangle + \mathrm{Re}(\langle\!\langle f^0 \boldsymbol{\varphi}^{\eta(2)}, \boldsymbol{\Psi}^\eta \rangle\!\rangle)), \tag{30}$$

$$\eta_2 = \tfrac{1}{20} k_{\mathrm{B}} T \, \mathrm{Im}(\langle\!\langle f^0 \boldsymbol{\varphi}^{\eta(2)}, \boldsymbol{\Psi}^\eta \rangle\!\rangle), \tag{31}$$

$$\eta_3 = \tfrac{1}{20} k_{\mathrm{B}} T (\langle\!\langle f^0 \boldsymbol{\varphi}^{\eta(1)}, \boldsymbol{\Psi}^\eta \rangle\!\rangle - \mathrm{Re}(\langle\!\langle f^0 \boldsymbol{\varphi}^{\eta(2)}, \boldsymbol{\Psi}^\eta \rangle\!\rangle)), \tag{32}$$

$$\eta_4 = \tfrac{1}{20} k_{\mathrm{B}} T (2\,\mathrm{Re}(\langle\!\langle f^0 \boldsymbol{\varphi}^{\eta(3)}, \boldsymbol{\Psi}^\eta \rangle\!\rangle) - \langle\!\langle f^0 \boldsymbol{\varphi}^{\eta(1)}, \boldsymbol{\Psi}^\eta \rangle\!\rangle - \mathrm{Re}(\langle\!\langle f^0 \boldsymbol{\varphi}^{\eta(2)}, \boldsymbol{\Psi}^\eta \rangle\!\rangle)), \tag{33}$$

$$\eta_5 = \tfrac{1}{20} k_{\mathrm{B}} T (2\,\mathrm{Im}(\langle\!\langle f^0 \boldsymbol{\varphi}^{\eta(3)}, \boldsymbol{\Psi}^\eta \rangle\!\rangle) - \mathrm{Im}(\langle\!\langle f^0 \boldsymbol{\varphi}^{\eta(2)}, \boldsymbol{\Psi}^\eta \rangle\!\rangle)). \tag{34}$$

These new linear relations between the viscosity coefficients and the solutions of the linearized Boltzmann equations will be used to evaluate the shear viscosities from Galerkin approximate solutions. Finally note that the volume viscosity is not influenced by the magnetic field and its evaluation is already discussed in [15, 17].

3.4. Expansion polynomials

The integral equations (22) are typically solved by a (Hermitian) Galerkin procedure where the perturbed distribution functions are expanded into polynomials. We will use the traditional basis polynomials ϕ^{a0cdk} defined by

$$\phi^{a0cdk}(\boldsymbol{c}_k, \kappa) = \left(S_{a+\frac{1}{2}}^c (\boldsymbol{w}_k \cdot \boldsymbol{w}_k) W_k^d (\epsilon_{k\kappa}) \overline{\otimes^a \boldsymbol{w}_k} \, \delta_{ki} \right)_{i \in \mathcal{S}},$$

where $\boldsymbol{w}_k = \sqrt{m_k / 2 k_{\mathrm{B}} T} (\boldsymbol{c}_k - \boldsymbol{v})$ is the reduced relative velocity of the molecules of the kth species and $\epsilon_{k\kappa} = \mathcal{E}_{k\mathrm{I}} / k_{\mathrm{B}} T$ is the reduced internal energy of the kth species in the κth state. In addition, a, c, and d are integers, $S_{a+1/2}^c$ is the Laguerre and Sonine polynomial of order c with parameter $a + 1/2$, W_k^d is the Wang–Chang and Uhlenbeck polynomial of order d for the kth species, and $\overline{\otimes^a \boldsymbol{w}_k}$ is a tensor of rank a with respect to the three-dimensional space, given by $\overline{\otimes^0 \boldsymbol{w}_k} = 1$, $\overline{\otimes^1 \boldsymbol{w}_k} = \boldsymbol{w}_k$ and $\overline{\otimes^2 \boldsymbol{w}_k} = \boldsymbol{w}_k \otimes \boldsymbol{w}_k - \tfrac{1}{3} \boldsymbol{w}_k \cdot \boldsymbol{w}_k \boldsymbol{I}$ [17, 20, 28]. In the notation ϕ^{abcdk}, the first index a thus refers to the tensorial rank with respect to $\mathbb{R}^3$, the second index $b = 0$ refers to the absence of polarization effects [17], the third index c refers to the Laguerre and Sonine polynomial, the fourth index d refers to the Wang–Chang and Uhlenbeck polynomial and the last index k refers to the species. These functions have important orthogonality properties [20, 28] and various properties of the Laguerre and Sonine polynomials, Wang–Chang and Uhlenbeck polynomials, and functions ϕ^{a0cdk} are summarized in [6, 17, 28]. We will also frequently use the notation introduced in [17] to write the transport linear systems obtained from Galerkin procedures.

3.5. Transport linear systems associated with the shear viscosities

The traceless matrix integral equations associated with the shear viscosities are in the form $(\mathcal{F}^{\mathcal{S}} + (2\delta_{2\mathsf{l}} + \delta_{3\mathsf{l}})\mathrm{i}B\mathcal{F}^{z,m})(\varphi^{\eta(\mathsf{l})}) = \Psi^{\eta}$, with $\mathsf{l} \in \{1, 2, 3\}$, where $\Psi^{\eta} = 2\sum_{k \in \mathcal{S}} \phi^{2000k}$, and $\phi^{2000k} = \left(\left(\boldsymbol{w}_k \otimes \boldsymbol{w}_k - \frac{1}{3}\boldsymbol{w}_k \cdot \boldsymbol{w}_k \boldsymbol{I}\right)\delta_{ki}\right)_{i \in \mathcal{S}}$ [17]. By isotropy, the variational approximation space $\mathcal{A}^{\eta}$ to be considered in the first place is the space spanned by ϕ^{2000k}, $k \in \mathcal{S}$ [3, 6, 17, 20]. The simulations by Bruno and coworkers have shown that the corresponding coefficients are sufficiently accurate so that higher order expansions of $\varphi^{\eta(\mathsf{l})}$, $\mathsf{l} \in \{1, 2, 3\}$ are not required [2, 14]. A (Hermitian) Galerkin approach is used by requiring the difference between the approximated $(\mathcal{F}^{\mathcal{S}} + (2\delta_{2\mathsf{l}} + \delta_{3\mathsf{l}})\mathrm{i}B\mathcal{F}^{z,m})(\varphi^{\eta(\mathsf{l})})$ and Ψ^{η} to be orthogonal to the approximation space.

For convenience $\varphi^{\eta(\mathsf{l})}$ is taken in the form

$$\varphi^{\eta(\mathsf{l})} = (2/p) \sum_{k \in \mathcal{S}} \alpha_k^{\eta(\mathsf{l})} \phi^{2000k}, \qquad \mathsf{l} \in \{1, 2, 3\}.$$

The matrix associated with the variational procedure is denoted by H and is rescaled such that $H_{kl} = (2/5np)[\![\phi^{2000k}, \phi^{2000l}]\!]$, $k, l \in \mathcal{S}$, where n denotes the mixture number density. We also rescale the right-hand side vector $\beta_k^{\eta} = (1/5n)\langle\!\langle f^0 \phi^{2000k}, \Psi^{\eta}\rangle\!\rangle$, $k \in \mathcal{S}$. We then have $H \in \mathbb{R}^{n,n}$, $\beta^{\eta} \in \mathbb{R}^n$, and the linear system for $\alpha^{\eta(1)} \in \mathbb{R}^n$ and $\alpha^{\eta(2)}, \alpha^{\eta(3)} \in \mathbb{C}^n$ are in the form

$$H\alpha^{\eta(1)} = \beta^{\eta}, \qquad (H + 2\mathrm{i}H^B)\alpha^{\eta(2)} = \beta^{\eta}, \qquad (H + \mathrm{i}H^B)\alpha^{\eta(3)} = \beta^{\eta}. \tag{35}$$

The coefficients of the matrix H are given by [17]

$$H_{kk} = \sum_{\substack{l \in \mathcal{S} \\ l \neq k}} \frac{16}{5k_{\mathrm{B}}T} \frac{X_k X_l m_l^2}{(m_k + m_l)^2}\left[\frac{10}{3}\frac{m_k}{m_l}\Omega_{kl}^{(1,1)} + \Omega_{kl}^{(2,2)}\right] + \frac{8}{5k_{\mathrm{B}}T}X_k^2\Omega_{kk}^{(2,2)}, \qquad k \in \mathcal{S}, \tag{36}$$

$$H_{kl} = \frac{16}{5k_{\mathrm{B}}T} \frac{X_k X_l m_k m_l}{(m_k + m_l)^2}\left[-\frac{10}{3}\Omega_{kl}^{(1,1)} + \Omega_{kl}^{(2,2)}\right], \qquad k, l \in \mathcal{S}, \qquad k \neq l, \tag{37}$$

where $\Omega_{kl}^{(i,j)}$ are the classical collision integrals [3, 6, 28] and H^B is the diagonal matrix $H_{kl}^B = \delta_{kl}BX_k z_k/p$, $k, l \in \mathcal{S}$. The right-hand side member β^{η} is given by $\beta_k^{\eta} = X_k$ where X_k is the mole fraction of the kth species.

The matrix H is symmetric positive definite [17] and from (30)–(34) the shear viscosities are finally given by the scalar products

$$\eta_1 = \tfrac{1}{2}\langle\alpha^{\eta(1)}, \beta^{\eta}\rangle + \tfrac{1}{2}\mathrm{Re}(\langle\alpha^{\eta(2)}, \beta^{\eta}\rangle), \tag{38}$$

$$\eta_2 = \tfrac{1}{2}\mathrm{Im}(\langle\alpha^{\eta(2)}, \beta^{\eta}\rangle), \tag{39}$$

$$\eta_3 = \tfrac{1}{2}\langle\alpha^{\eta(1)}, \beta^{\eta}\rangle - \tfrac{1}{2}\mathrm{Re}(\langle\alpha^{\eta(2)}, \beta^{\eta}\rangle), \tag{40}$$

$$\eta_4 = \mathrm{Re}(\langle\alpha^{\eta(3)}, \beta^{\eta}\rangle) - \tfrac{1}{2}\langle\alpha^{\eta(1)}, \beta^{\eta}\rangle - \tfrac{1}{2}\mathrm{Re}(\langle\alpha^{\eta(2)}, \beta^{\eta}\rangle), \tag{41}$$

$$\eta_5 = \mathrm{Im}(\langle\alpha^{\eta(3)}, \beta^{\eta}\rangle) - \tfrac{1}{2}\mathrm{Im}(\langle\alpha^{\eta(2)}, \beta^{\eta}\rangle), \tag{42}$$

where we have denoted by $\langle x, y\rangle = \sum_{k \in \mathcal{S}} x_k \overline{y}_k$ the Hermitian scalar product.

In the situation of non-ionized and nonmagnetized mixtures, it has been shown that one step of the conjugate gradient algorithm—preconditioned by the diagonal—already yields excellent accuracy for the shear viscosity [17, 18], much better than the Wilke formula. In the situation of ionized magnetized mixtures, however, it is not possible anymore to use *strictly speaking* a conjugate gradient technique since in general there does not exist short

recurrence iterative algorithms which simultaneously corresponds to a global minimization of some error norm over the corresponding Krylov subspaces spanned by the successive residual error vectors [29]. Nevertheless, it is possible to introduce *orthogonal error* techniques which guarantee that the successive residual error vectors are orthogonal [30–32]. These techniques are especially suited to the linear systems arising from the Galerkin procedure since it has been shown that—with a proper formulation—such systems are symmetric complex with a positive semi-definite real part and for such systems orthogonal error algorithms are proved to be convergent [15, 32]. The transport linear systems can also be solved in their complex form which is convenient and benefits from interesting numerical properties [31].

Numerical test have been conducted with weakly ionized air at temperature 10 000 K and pressure $p = 1$ atm with collision integrals taken from [33] and thermodynamic properties taken from [34]. The species associated with ionized air are the $n^s = 11$ species N_2, O_2, NO, N, O, N_2^+, O_2^+, NO^+, N^+, O^+ and E^-. The choice of a particular temperature or pressure for weakly ionized air is not significant since convergence properties would essentially be similar at other temperatures or pressures. The numerical tests have first shown that the transport linear systems for ionized mixtures are usually more difficult to solve than that for neutral species because of the greater disparity between collision integrals. Nevertheless, the simulations have indicated that orthogonal error methods preconditioned by the diagonal yield efficient algorithms that converge in a few iterates whatever be the intensity of the magnetic field. Relative errors of the order of 10^{-3} are typically obtained within three iterations. As already shown by Bruno and coworkers for ionized argon, the extra viscosities η_j, $j = 2, 3, 4, 5$ are generally much smaller than η_1 even for large values of the electron Hall parameter [2].

4. Mass and heat transport coefficients

4.1. Equations associated with $\phi^{\widehat{\lambda}}$

The solution $\phi^{\widehat{\lambda}} = \left(\phi_i^{\widehat{\lambda}}\right)_{i \in \mathcal{S}}$ of (7) and (8) with $\mu = \widehat{\lambda}$ is in the form

$$\phi_i^{\widehat{\lambda}} = \phi_i^{\widehat{\lambda}(1)} C_i + \phi_i^{\widehat{\lambda}(2)} C_i \wedge B + \phi_i^{\widehat{\lambda}(3)} C_i \cdot BB,$$

where $\phi_i^{\widehat{\lambda}(1)}$, $\phi_i^{\widehat{\lambda}(2)}$ and $\phi_i^{\widehat{\lambda}(3)}$ are scalar functions of $C_i \cdot C_i$, $(C_i \cdot B)^2$ and $B \cdot B$. Substituting this expansion into the integro-differential equations associated with $\phi^{\widehat{\lambda}}$ and using isotropy first yield three scalar coupled integral equations. Further simplification is then obtained if, for each species i, instead of three real quantities $\phi_i^{\widehat{\lambda}(1)}$, $\phi_i^{\widehat{\lambda}(2)}$ and $\phi_i^{\widehat{\lambda}(3)}$, one real and one complex unknowns are introduced

$$\varphi_i^{\widehat{\lambda}(1)} = \phi_i^{\widehat{\lambda}(1)} + B^2 \phi_i^{\widehat{\lambda}(3)}, \qquad \varphi_i^{\widehat{\lambda}(2)} = \phi_i^{\widehat{\lambda}(1)} + iB \phi_i^{\widehat{\lambda}(2)}, \qquad i \in \mathcal{S}.$$

Upon defining $\boldsymbol{\varphi}^{\widehat{\lambda}(1)} = \left(\varphi_i^{\widehat{\lambda}(1)} C_i\right)_{i \in \mathcal{S}}$, $\boldsymbol{\varphi}^{\widehat{\lambda}(2)} = \left(\varphi_i^{\widehat{\lambda}(2)} C_i\right)_{i \in \mathcal{S}}$, and introducing the operator $\boldsymbol{\mathcal{F}}^{z,v} = \left(\boldsymbol{\mathcal{F}}_i^{z,v}\right)_{i \in \mathcal{S}}$ defined for $\mathbf{u} = (\mathbf{u}_i)_{i \in \mathcal{S}}$ by

$$\boldsymbol{\mathcal{F}}_i^{z,v}(\mathbf{u}) = -m_i C_i \sum_{j, J} \frac{e_j}{3 \rho k_B T} \int f_j^0 \mathbf{u}_j \cdot C_j \, \mathrm{d}C_j + z_i \mathbf{u}_i, \qquad i \in \mathcal{S},$$

where $\mathbf{u}_i$ is the product of C_i by a complex scalar function of $C_i \cdot C_i$, $(C_i \cdot B)^2$ and $B \cdot B$, it is easily shown that

$$\boldsymbol{\mathcal{F}}^{\mathcal{S}}(\boldsymbol{\varphi}^{\widehat{\lambda}(1)}) = \boldsymbol{\Psi}^{\widehat{\lambda}}, \qquad (\boldsymbol{\mathcal{F}}^{\mathcal{S}} + iB \boldsymbol{\mathcal{F}}^{z,v})(\boldsymbol{\varphi}^{\widehat{\lambda}(2)}) = \boldsymbol{\Psi}^{\widehat{\lambda}}. \tag{43}$$

Furthermore, the constraint equations (8) are easily rewritten in the form

$$\langle\!\langle f^0 \boldsymbol{\varphi}^{\widehat{\lambda}(1)}, \psi^l \rangle\!\rangle = 0, \qquad \langle\!\langle f^0 \boldsymbol{\varphi}^{\widehat{\lambda}(2)}, \psi^l \rangle\!\rangle = 0, \qquad l \in \{1, \ldots, n^s + 4\}. \tag{44}$$

The structure of the first integral equation in (43) is classical and the structure of the second equation is similar in a complex framework [15]. From the isotropy of the operator $\mathcal{F}^{\mathcal{S}}$ the functions $\varphi^{\widehat{\lambda}(1)}$ and $\varphi^{\widehat{\lambda}(2)}$ cannot be functions of $(\boldsymbol{C} \cdot \boldsymbol{B})^2$ [6].

We define the unitary vector $\mathcal{B}$ by $\mathcal{B} = \boldsymbol{B}/B$ and, for any vector $\mathbf{X}$, we introduce the associated vectors

$$\mathbf{X}^{\|} = (\mathbf{X} \cdot \mathcal{B})\mathcal{B}, \qquad \mathbf{X}^{\perp} = \mathbf{X} - \mathbf{X}^{\|}, \qquad \mathbf{X}^{\odot} = \mathcal{B} \wedge \mathbf{X}.$$

The vectors $\mathbf{X}^{\|}$, $\mathbf{X}^{\perp}$ and $\mathbf{X}^{\odot}$ are mutually orthogonal and obtained from $\mathbf{X}$ by applying the linear operators $\mathsf{M}^{\|} = \mathcal{B} \otimes \mathcal{B}$, $\mathsf{M}^{\perp} = \boldsymbol{I} - \mathcal{B} \otimes \mathcal{B}$ and $\mathsf{M}^{\odot} = \boldsymbol{R}(\mathcal{B})$. It is then straightforward to obtain that

$$\phi_i^{\widehat{\lambda}} = \big(\varphi_i^{\widehat{\lambda}(1)} \mathcal{B} \otimes \mathcal{B} + \operatorname{Re}\big(\varphi_i^{\widehat{\lambda}(2)}\big)(\boldsymbol{I} - \mathcal{B} \otimes \mathcal{B}) - \operatorname{Im}\big(\varphi_i^{\widehat{\lambda}(2)}\big)\boldsymbol{R}(\mathcal{B})\big)\boldsymbol{C}_i, \qquad (45)$$

or equivalently that $\phi_i^{\widehat{\lambda}} = \operatorname{Re}\big(\varphi_i^{\widehat{\lambda}(1)}\boldsymbol{C}_i^{\|} + \varphi_i^{\widehat{\lambda}(2)}\big(\boldsymbol{C}_i^{\perp} + \mathrm{i}\boldsymbol{C}_i^{\odot}\big)\big)$, where $\operatorname{Re}(z)$ and $\operatorname{Im}(z)$ denote the real and imaginary part of a complex quantity $z = \operatorname{Re}(z) + \mathrm{i}\operatorname{Im}(z)$.

4.2. Equations associated with ϕ^{D_j}

The above development can be followed through for the solution ϕ^{D_j} of (7) and (8) with $\mu = D_j$ as well. More specifically, the perturbed distribution function $\phi^{D_j} = \big(\phi_i^{D_j}\big)_{i \in \mathcal{S}}$ is expanded in the form

$$\phi_i^{D_j} = \phi_i^{D_j(1)}\boldsymbol{C}_i + \phi_i^{D_j(2)}\boldsymbol{C}_i \wedge \boldsymbol{B} + \phi_i^{D_j(3)}\boldsymbol{C}_i \cdot \boldsymbol{B}\boldsymbol{B},$$

and defining $\varphi_i^{D_j(1)} = \phi_i^{D_j(1)} + B^2\phi_i^{D_j(3)}$, $\varphi_i^{D_j(2)} = \phi_i^{D_j(1)} + \mathrm{i}B\phi_i^{D_j(2)}$, $i, j \in \mathcal{S}$, and $\boldsymbol{\varphi}^{D_j(1)} = (\varphi_i^{D_j(1)}\boldsymbol{C}_i)_{i \in \mathcal{S}}$, $\boldsymbol{\varphi}^{D_j(2)} = (\varphi_i^{D_j(2)}\boldsymbol{C}_i)_{i \in \mathcal{S}}$, $j \in \mathcal{S}$, we obtain for all $j \in \mathcal{S}$

$$\mathcal{F}^{\mathcal{S}}(\boldsymbol{\varphi}^{D_j(1)}) = \boldsymbol{\Psi}^{D_j}, \qquad (\mathcal{F}^{\mathcal{S}} + \mathrm{i}B\mathcal{F}^{z,v})(\boldsymbol{\varphi}^{D_j(2)}) = \boldsymbol{\Psi}^{D_j}, \qquad (46)$$

$$\langle\!\langle f^0\boldsymbol{\varphi}^{D_j(1)}, \psi^l \rangle\!\rangle = 0, \qquad \langle\!\langle f^0\boldsymbol{\varphi}^{D_j(2)}, \psi^l \rangle\!\rangle = 0, \qquad l \in \{1, \ldots, n^s + 4\}. \qquad (47)$$

We can also write that

$$\phi_i^{D_j} = \big(\varphi_i^{D_j(1)}\mathcal{B} \otimes \mathcal{B} + \operatorname{Re}\big(\varphi_i^{D_j(2)}\big)(\boldsymbol{I} - \mathcal{B} \otimes \mathcal{B}) - \operatorname{Im}\big(\varphi_i^{D_j(2)}\big)\boldsymbol{R}(\mathcal{B})\big)\boldsymbol{C}_i, \qquad (48)$$

or equivalently that $\phi_i^{D_j} = \operatorname{Re}\big(\varphi_i^{D_j(1)}\boldsymbol{C}_i^{\|} + \varphi_i^{D_j(2)}\big(\boldsymbol{C}_i^{\perp} + \mathrm{i}\boldsymbol{C}_i^{\odot}\big)\big)$.

4.3. New symmetry properties of the mass transport coefficients

Substituting the expansion (6) into the identity $\boldsymbol{V}_i = k_{\mathrm{B}}T \langle\!\langle \boldsymbol{\Psi}^{D_i}, f^0\phi \rangle\!\rangle$, only the terms in ϕ^{D_j}, $j \in \mathcal{S}$, and $\phi^{\widehat{\lambda}}$, yield non-null contributions. Expanding ϕ^{D_j}, $j \in \mathcal{S}$, and $\phi^{\widehat{\lambda}}$, with (45) and (48), using isotropy and denoting by $\boldsymbol{d}_j = (\partial_x p_j - \rho_j \widetilde{\boldsymbol{b}}_j)/p$ the unconstrained diffusion driving force for the jth species, we obtain

$$\boldsymbol{V}_i = -\sum_{j \in \mathcal{S}} \big(D_{ij}^{\|}\boldsymbol{d}_j^{\|} + D_{ij}^{\perp}\boldsymbol{d}_j^{\perp} + D_{ij}^{\odot}\boldsymbol{d}_j^{\odot}\big)$$

$$- \big(\theta_i^{\|}(\partial_x \log T)^{\|} + \theta_i^{\perp}(\partial_x \log T)^{\perp} + \theta_i^{\odot}(\partial_x \log T)^{\odot}\big), \qquad (49)$$

where $D_{ij}^{\|} = (pk_{\mathrm{B}}T/3)\langle\!\langle f^0\boldsymbol{\varphi}^{D_j(1)}, \boldsymbol{\Psi}^{D_i} \rangle\!\rangle$, $D_{ij}^{\perp} + \mathrm{i}D_{ij}^{\odot} = (pk_{\mathrm{B}}T/3)\langle\!\langle f^0\boldsymbol{\varphi}^{D_j(2)}, \boldsymbol{\Psi}^{D_i} \rangle\!\rangle$ and $\theta_i^{\|} = -(1/3)\langle\!\langle f^0\boldsymbol{\varphi}^{\widehat{\lambda}(1)}, \boldsymbol{\Psi}^{D_i} \rangle\!\rangle$, $\theta_i^{\perp} + \mathrm{i}\theta_i^{\odot} = -(1/3)\langle\!\langle f^0\boldsymbol{\varphi}^{\widehat{\lambda}(2)}, \boldsymbol{\Psi}^{D_i} \rangle\!\rangle$. These coefficients are easily rewritten in the symmetrized form

$$D_{ij}^{\|} = \tfrac{1}{3}pk_{\mathrm{B}}T[\![\boldsymbol{\varphi}^{D_i(1)}, \boldsymbol{\varphi}^{D_j(1)}]\!], \qquad (50)$$

$$D_{ij}^\perp + \mathrm{i}D_{ij}^\odot = \tfrac{1}{3}pk_\mathrm{B}T([\![\varphi^{D_i(2)}, \varphi^{D_j(2)}]\!] - \mathrm{i}(\!(\varphi^{D_i(2)}, \varphi^{D_j(2)})\!)), \tag{51}$$

$$\theta_i^\parallel = -\tfrac{1}{3}[\![\varphi^{D_i(1)}, \varphi^{\widehat{\lambda}(1)}]\!], \tag{52}$$

$$\theta_i^\perp + \mathrm{i}\theta_i^\odot = -\tfrac{1}{3}([\![\varphi^{D_i(2)}, \varphi^{\widehat{\lambda}(2)}]\!] - \mathrm{i}(\!(\varphi^{D_i(2)}, \varphi^{\widehat{\lambda}(2)})\!)). \tag{53}$$

Note the negative sign in front of the bracket $(\!(\cdot, \cdot)\!)$ contributions of $D_{ij}^\perp + \mathrm{i}D_{ij}^\odot$ and $\theta_i^\perp + \mathrm{i}\theta_i^\odot$ overlooked in expressions (5.11) and (5.13) of [15].

The new symmetry properties of the perpendicular and transverse transport coefficients, which are established in appendix A, can then be written as

$$D_{ij}^\perp = \tfrac{1}{3}pk_\mathrm{B}T[\![\varphi^{D_i(2)}, \varphi^{D_j(2)}]\!] = \tfrac{1}{3}pk_\mathrm{B}T\,\mathrm{Re}[\![\varphi^{D_i(2)}, \varphi^{D_j(2)}]\!], \tag{54}$$

$$D_{ij}^\odot = -\tfrac{1}{3}pk_\mathrm{B}T(\!(\varphi^{D_i(2)}, \varphi^{D_j(2)})\!) = -\tfrac{1}{3}pk_\mathrm{B}T\,\mathrm{Re}(\!(\varphi^{D_i(2)}, \varphi^{D_j(2)})\!), \tag{55}$$

$$\theta_i^\perp = -\tfrac{1}{3}[\![\varphi^{D_i(2)}, \varphi^{\widehat{\lambda}(2)}]\!] = -\tfrac{1}{3}\,\mathrm{Re}[\![\varphi^{D_i(2)}, \varphi^{\widehat{\lambda}(2)}]\!], \tag{56}$$

$$\theta_i^\odot = \tfrac{1}{3}(\!(\varphi^{D_i(2)}, \varphi^{\widehat{\lambda}(2)})\!) = \tfrac{1}{3}\,\mathrm{Re}(\!(\varphi^{D_i(2)}, \varphi^{\widehat{\lambda}(2)})\!), \tag{57}$$

where Re and Im denote the real and the imaginary parts.

These new symmetry relations (54)–(57) imply in particular that $D_{ij}^\perp = D_{ji}^\perp$, $D_{ij}^\odot = D_{ji}^\odot$, $\theta_i^\perp = -\tfrac{1}{3}[\![\varphi^{\widehat{\lambda}(2)}, \varphi^{D_i(2)}]\!]$ and $\theta_i^\odot = \tfrac{1}{3}(\!(\varphi^{\widehat{\lambda}(2)}, \varphi^{D_i(2)})\!)$. Moreover, proceeding essentially as in [17], one can establish that the nullspace of the real matrices $D^\parallel$ and $D^\perp$ is spanned by Y in $\mathbb{R}^{n^s}$, where $Y = (Y_1, \ldots, Y_{n^s})^t$ and Y_k is the mass fraction of the kth species, and that their range is the (Euclidean) orthogonal complement of Y in $\mathbb{R}^{n^s}$, and similarly that the nullspace of the complex matrix $D^\perp + \mathrm{i}D^\odot$ is spanned by Y in $\mathbb{C}^{n^s}$ and that its range is the (Hermitian) orthogonal complement of Y in $\mathbb{C}^{n^s}$. In addition, the thermal diffusion coefficients satisfy the constraints $\langle\theta^\parallel, Y\rangle = \langle\theta^\perp, Y\rangle = \langle\theta^\odot, Y\rangle = 0$. Finally, the usual constrained diffusion driving forces $\widetilde{d}_i = d_i - Y_i \sum_{j\in\mathcal{S}} d_j$ can equivalently be used to formulate the mass fluxes thanks to the properties of transport coefficients.

4.4. New symmetry properties of the heat transport coefficients

From the relation $q = -\langle\!\langle\Psi^{\widehat{\lambda}}, f^0\phi\rangle\!\rangle + \sum_{i\in\mathcal{S}} \left(\tfrac{5}{2}k_\mathrm{B}T + \overline{\mathcal{E}_i}\right)n_i V_i$ and the expansion of ϕ we obtain

$$\begin{aligned}
q = -(\widehat{\lambda}^\parallel(\partial_x T)^\parallel + \widehat{\lambda}^\perp(\partial_x T)^\perp + \widehat{\lambda}^\odot(\partial_x T)^\odot) \\
- p\sum_{i\in\mathcal{S}} \left(\theta_i^\parallel d_i^\parallel + \theta_i^\perp d_i^\perp + \theta_i^\odot d_i^\odot\right) + \sum_{i\in\mathcal{S}} \left(\frac{5}{2}k_\mathrm{B}T + \overline{\mathcal{E}_i}\right)n_i V_i,
\end{aligned} \tag{58}$$

where $\widehat{\lambda}^\parallel = (1/3k_\mathrm{B}T^2)\langle\!\langle f^0\varphi^{\widehat{\lambda}(1)}, \Psi^{\widehat{\lambda}}\rangle\!\rangle$ and $\widehat{\lambda}^\perp + \mathrm{i}\widehat{\lambda}^\odot = (1/3k_\mathrm{B}T^2)\langle\!\langle f^0\varphi^{\widehat{\lambda}(2)}, \Psi^{\widehat{\lambda}}\rangle\!\rangle$. These coefficients are easily rewritten in the symmetri-zed form

$$\widehat{\lambda}^\parallel = \frac{1}{3k_\mathrm{B}T^2}[\![\varphi^{\widehat{\lambda}(1)}, \varphi^{\widehat{\lambda}(1)}]\!], \tag{59}$$

$$\widehat{\lambda}^\perp + \mathrm{i}\widehat{\lambda}^\odot = \frac{1}{3k_\mathrm{B}T^2}([\![\varphi^{\widehat{\lambda}(2)}, \varphi^{\widehat{\lambda}(2)}]\!] - \mathrm{i}(\!(\varphi^{\widehat{\lambda}(2)}, \varphi^{\widehat{\lambda}(2)})\!)). \tag{60}$$

The thermal diffusion coefficients involved in the expansion of $\langle\!\langle\Psi^{\widehat{\lambda}}, f^0\phi\rangle\!\rangle$ are first written in the form $\widehat{\theta}_i^\parallel = -(1/3)\langle\!\langle f^0\varphi^{D_i(1)}, \Psi^{\widehat{\lambda}}\rangle\!\rangle$ and $\widehat{\theta}_i^\perp + \mathrm{i}\widehat{\theta}_i^\odot = -(1/3)\langle\!\langle f^0\varphi^{D_i(2)}, \Psi^{\widehat{\lambda}}\rangle\!\rangle$, but upon

writing these coefficients in a symmetric form $\widehat{\theta}_i^{\parallel} = -\frac{1}{3}[\![\varphi^{\widehat{\lambda}(1)}, \varphi^{D_i(1)}]\!]$, and $\widehat{\theta}_i^{\perp} + i\widehat{\theta}_i^{\odot} = -\frac{1}{3}([\![\varphi^{\widehat{\lambda}(2)}, \varphi^{D_i(2)}]\!] - i((\varphi^{\widehat{\lambda}(2)}, \varphi^{D_i(2)})))$, we obtain from (52) and (53) that $\widehat{\theta}_i^{\parallel} = \theta_i^{\parallel}, \widehat{\theta}_i^{\perp} = \theta_i^{\perp}$, and $\widehat{\theta}_i^{\odot} = \theta_i^{\odot}, i \in \mathcal{S}$. The new symmetry properties of perpendicular and transverse transport coefficients, established in appendix A, then read

$$\widehat{\lambda}^{\perp} = \frac{1}{3k_B T^2}[\![\varphi^{\widehat{\lambda}(2)}, \varphi^{\widehat{\lambda}(2)}]\!] = \frac{1}{3k_B T^2}\operatorname{Re}[\![\varphi^{\widehat{\lambda}(2)}, \varphi^{\widehat{\lambda}(2)}]\!], \tag{61}$$

$$\widehat{\lambda}^{\odot} = -\frac{1}{3k_B T^2}((\varphi^{\widehat{\lambda}(2)}, \varphi^{\widehat{\lambda}(2)})) = -\frac{1}{3k_B T^2}\operatorname{Re}((\varphi^{\widehat{\lambda}(2)}, \varphi^{\widehat{\lambda}(2)})). \tag{62}$$

As a consequence, the heat–mass transport matrices

$$A^{\parallel} = \begin{pmatrix} \frac{T}{p}\widehat{\lambda}^{\parallel} & \theta^{\parallel t} \\ \theta^{\parallel} & D^{\parallel} \end{pmatrix}, \qquad A^{\perp} = \begin{pmatrix} \frac{T}{p}\widehat{\lambda}^{\perp} & \theta^{\perp t} \\ \theta^{\perp} & D^{\perp} \end{pmatrix}, \qquad A^{\odot} = \begin{pmatrix} \frac{T}{p}\widehat{\lambda}^{\odot} & \theta^{\odot t} \\ \theta^{\odot} & D^{\odot} \end{pmatrix}$$

are real symmetric, $A^{\parallel}$ and $A^{\perp}$ are positive semi-definite, and their nullspace is spanned by $(0, Y_1, \ldots, Y_{n^s})^t$ where Y_k is the mass fraction of the kth species.

4.5. Entropy production due to heat and mass transfer

By using the new symmetry properties of transport coefficient, it is now much easier to establish that the entropy production term associated with the heat flux and the diffusion velocities $\Upsilon_v = -\left(q - \sum_{i \in \mathcal{S}} \rho_i h_i V_i\right) \cdot \frac{\partial_x T}{T^2} - \sum_{i \in \mathcal{S}} \frac{p}{T} V_i \cdot d_i$ is nonnegative [15]. By using the expressions of V_i and q, and the new symmetry properties we can indeed write

$$\Upsilon_v = \frac{1}{T^2}\widehat{\lambda}^{\parallel}(\partial_x T)^{\parallel} \cdot (\partial_x T)^{\parallel} + 2\frac{p}{T^2}\sum_{i \in \mathcal{S}}\theta_i^{\parallel}d_i^{\parallel} \cdot (\partial_x T)^{\parallel} + \frac{p}{T}\sum_{i,j \in \mathcal{S}}D_{ij}^{\parallel}d_j^{\parallel} \cdot d_i^{\parallel}$$

$$+ \frac{1}{T^2}\widehat{\lambda}^{\perp}(\partial_x T)^{\perp} \cdot (\partial_x T)^{\perp} + 2\frac{p}{T^2}\sum_{i \in \mathcal{S}}\theta_i^{\perp}d_i^{\perp} \cdot (\partial_x T)^{\perp} + \frac{p}{T}\sum_{i,j \in \mathcal{S}}D_{ij}^{\perp}d_j^{\perp} \cdot d_i^{\perp},$$

so that $\Upsilon_v = (p/T)(\langle A^{\parallel}x^{\parallel}, x^{\parallel}\rangle + \langle A^{\perp}x^{\perp}, x^{\perp}\rangle)$ with $x_0^{\parallel} = (\partial_x \log T)^{\parallel}, x_i^{\parallel} = (d_i)^{\parallel}, x_0^{\perp} = (\partial_x \log T)^{\perp}$, and $x_i^{\perp} = (d_i)^{\perp}$. Note in particular that the terms $\sum_{i \in \mathcal{S}}\theta_i^{\odot}d_i^{\odot} \cdot (\partial_x T)^{\perp} + \sum_{i \in \mathcal{S}}\theta_i^{\odot}(\partial_x T)^{\odot} \cdot d_i^{\perp}$ and $\sum_{i,j \in \mathcal{S}}D_{ij}^{\odot}d_i^{\perp} \cdot d_j^{\odot}$ appearing in the expression of Υ_v in [15] all vanish since $\widehat{\theta} = \theta$, $D^{\odot}$ is symmetric, and $x^{\odot} \cdot y^{\perp} + x^{\perp} \cdot y^{\odot} = 0$ for any vectors x and y. The term $\sum_{i,j \in \mathcal{S}}D_{ij}^{\odot}d_i^{\perp} \cdot d_j^{\odot}$ was erroneously typed $\sum_{i,j \in \mathcal{S}}D_{ij}^{\odot}d_i^{\perp} \cdot d_j^{\perp}$ in [15].

4.6. First-order transport linear systems associated with D

The vector integral equations associated with multicomponent diffusion coefficients are in the form $(\mathcal{F}^{\mathcal{S}} + \delta_{2l}iB\mathcal{F}^{z,v})(\varphi^{D_j(l)}) = \Psi^{D_j}$, with $l \in \{1, 2\}$, $j \in \mathcal{S}$, and

$$\Psi^{D_j} = \sum_{k \in \mathcal{S}}\sqrt{2/m_k k_B T}(\delta_{jk} - Y_k)/n_k\phi^{1000k},$$

where $\phi^{1000k} = (w_k\delta_{ki})_{i \in \mathcal{S}}$ [17]. By isotropy, the variational approximation space $\mathcal{A}_{[00]}^D$ to be considered in the first place is the space spanned by $\phi^{1000k}, k \in \mathcal{S}$, and we will denote by $\varphi_{[00]}^{D_j(l)}$ the corresponding approximation using the notation from [17].

For convenience, $\varphi_{[00]}^{D_j(l)}$ is taken in the form

$$\varphi_{[00]}^{D_j(l)} = \frac{\sqrt{2}}{p\sqrt{k_B T}}\sum_{k \in \mathcal{S}}\sqrt{m_k}\alpha_{[00]k}^{00D_j(l)}\phi^{1000k}, \qquad l \in \{1, 2\}, \qquad j \in \mathcal{S}.$$

The matrix associated with the variational procedure is denoted by $\Delta_{[00]}$ and is rescaled such that $\Delta_{[00]kl} = (2\sqrt{m_k m_l}/3p)[\![\phi^{1000k}, \phi^{1000l}]\!]$, $k, l \in \mathcal{S}$. We also rescale the right-hand side $\beta_{[00]k}^{00D_j} = (\sqrt{2m_k k_B T}/3)\langle\!\langle f^0\phi^{1000k}, \Psi^{D_j}\rangle\!\rangle$, $k \in \mathcal{S}$. We then have $\Delta_{[00]}, \Delta_{[00]}^{B} \in \mathbb{R}^{n^s, n^s}$, $\beta_{[00]}^{D_j}$, $\alpha_{[00]}^{D_j(1)} \in \mathbb{R}^{n^s}, \alpha_{[00]}^{D_j(2)} \in \mathbb{C}^{n^s}$, and the linear systems for $\alpha_{[00]}^{D_j(1)} = \left(\alpha_{[00]k}^{00D_j(1)}\right)_{k\in\mathcal{S}}$ and $\alpha_{[00]}^{D_j(2)} = \left(\alpha_{[00]k}^{00D_j(2)}\right)_{k\in\mathcal{S}}$ are in the form

$$\begin{cases} \Delta_{[00]}\alpha_{[00]}^{D_j(1)} = \beta_{[00]}^{D_j}, \\ \langle\alpha_{[00]}^{D_j(1)}, Y\rangle = 0, \end{cases} \qquad \begin{cases} \left(\Delta_{[00]} + i\Delta_{[00]}^{B}\right)\alpha_{[00]}^{D_j(2)} = \beta_{[00]}^{D_j}, \\ \langle\alpha_{[00]}^{D_j(2)}, Y\rangle = 0. \end{cases} \tag{63}$$

The coefficients of the matrix $\Delta_{[00]}$ are given by

$$\Delta_{[00]kk} = \sum_{\substack{l\in\mathcal{S} \\ l\neq k}} \frac{X_k X_l}{\mathcal{D}_{kl}}, \quad k \in \mathcal{S}, \qquad \Delta_{[00]kl} = -\frac{X_k X_l}{\mathcal{D}_{kl}}, \qquad k, l \in \mathcal{S}, \quad k \neq l,$$

where $\mathcal{D}_{kl}$ is the binary diffusion coefficient of the species pair (k, l), and the right-hand side vectors $\beta_{[00]}^{D_j} = \left(\beta_{[00]k}^{00D_j}\right)_{k\in\mathcal{S}}$ are given by

$$\beta_{[00]k}^{00D_j} = \delta_{jk} - Y_k, \qquad k, j \in \mathcal{S}.$$

The constraint vector is $Y = (Y_1, \ldots, Y_{n^s})^t$ where Y_k is the mass fraction of the kth species and we have denoted by $\langle x, y\rangle = \sum_{k\in\mathcal{S}} x_k \overline{y}_k$ the Hermitian scalar product. The binary diffusion coefficient $\mathcal{D}_{kl}$ can also be written as $\mathcal{D}_{kl} = 3k_B T/16nm_{kl}\Omega_{kl}^{(1,1)}$ where $m_{kl} = m_k m_l/(m_k + m_l)$ is the reduced mass of the species pair (k, l). Moreover, we have $\Delta_{[00]}^{B} = (\mathbb{I} - Y \otimes U)\mathfrak{D}^{B}(\mathbb{I} - U \otimes Y)$ where $\mathfrak{D}^{B}$ is the diagonal matrix $\mathfrak{D}_{kl}^{B} = \delta_{kl}n_k e_k B/p$ and $U = (1, \ldots, 1)^t \in \mathbb{R}^{n^s}$.

The real matrix $\Delta_{[00]}$ is symmetric positive semi-definite, $N(\Delta_{[00]}) = \mathbb{R}U$, $R(\Delta_{[00]}) = U^\perp$ in $\mathbb{R}^{n^s}$ [17], whereas the complex matrix $\Delta_{[00]} + i\Delta_{[00]}^{B}$ is such that $N\left(\Delta_{[00]} + i\Delta_{[00]}^{B}\right) = \mathbb{C}U$, $R\left(\Delta_{[00]} + i\Delta_{[00]}^{B}\right) = U^\perp$ in $\mathbb{C}^{n^s}$, where the nullspace and range of a matrix A are denoted by $N(A)$ and $R(A)$, respectively. The resulting approximated diffusion coefficients are denoted by $D_{[00]}^\parallel, D_{[00]}^\perp, D_{[00]}^\odot$, and are given by

$$D_{[00]ij}^\parallel = \langle\alpha_{[00]}^{D_j(1)}, \beta_{[00]}^{D_i}\rangle = \alpha_{[00]i}^{00D_j(1)} = \alpha_{[00]j}^{00D_i(1)}, \tag{64}$$

$$D_{[00]ij}^\perp + iD_{[00]ij}^\odot = \langle\alpha_{[00]}^{D_j(2)}, \beta_{[00]}^{D_i}\rangle = \alpha_{[00]i}^{00D_j(2)} = \alpha_{[00]j}^{00D_i(2)}. \tag{65}$$

In addition, for all $a > 0$, we have $D_{[00]}^\parallel = (\Delta_{[00]} + aY \otimes Y)^{-1} - (1/a)U \otimes U$ and also $D_{[00]}^\perp + iD_{[00]}^\odot = \left(\Delta_{[00]} + i\Delta_{[00]}^{B} + aY \otimes Y\right)^{-1} - (1/a)U \otimes U$.

Projected standard iterative techniques as well as projected generalized conjugate gradient methods can be used to solve the constrained singular systems associated with the first-order diffusion coefficients (63). Iterative techniques for the real transport linear system associated with the real matrix $D_{[00]}^\parallel$ are similar to that of non-ionized mixtures which have been investigated comprehensively [17, 35]. We only discuss in the following the evaluation by iterative techniques of the complex matrix $D_{[00]}^\perp + iD_{[00]}^\odot$.

When only the diffusion velocities are required—and not the diffusion coefficients—a complex form of the Stefan–Maxwell equations can be solved by using orthogonal error algorithms [30, 32]. In the absence of the Soret effect, these generalized complex Stefan–Maxwell equations are in the form

$$-\left(\Delta_{[00]} + i\Delta_{[00]}^{B}\right)(V^\perp - iV^\odot) = d^\perp - id^\odot - Y\sum_{l\in\mathcal{S}}\left(d_l^\perp - id_l^\odot\right), \tag{66}$$

where $\boldsymbol{V}^{\diamond} = \left(\boldsymbol{V}_1^{\diamond}, \ldots, \boldsymbol{V}_{n^s}^{\diamond}\right)^t$, $\boldsymbol{d}^{\diamond} = \left(\boldsymbol{d}_1^{\diamond}, \ldots, \boldsymbol{d}_{n^s}^{\diamond}\right)^t$, $\diamond \in \{\|, \perp, \odot\}$ and $Y = (Y_1, \ldots, Y_{n^s})^t$. The proper modification of the complex Stefan–Maxwell equations in the presence of the Soret effect are discussed in section 5. The vectors $\boldsymbol{d}_i^{\diamond}$, $\diamond \in \{\|, \perp, \odot\}$, are the unconstrained diffusion driving forces and $\widetilde{\boldsymbol{d}}_i^{\diamond} = \boldsymbol{d}_i^{\diamond} - Y_i \sum_{j \in \mathcal{S}} \boldsymbol{d}_j^{\diamond}$ are the corresponding constrained diffusion driving forces which sum up to zero. Only the diffusion velocities are required when an explicit time marching technique is used to compute a multicomponent flow for instance.

On the other hand, when the diffusion coefficients are to be evaluated, as is typically the case if an implicit time marching method is used, it is first possible to use a direct inversion method by forming $D_{[00]}^{\perp} + \mathrm{i}D_{[00]}^{\odot} = (\Delta_{[00]} + \mathrm{i}\Delta_{[00]}^{B} + aY \otimes Y)^{-1} - (1/a)U \otimes U$ where $a > 0$. The $(n^s)^2$ coefficients are then evaluated within $\mathcal{O}((n^s)^3)$ operations. It is nevertheless possible to evaluate approximate coefficients within $\mathcal{O}((n^s)^2)$ operations by using standard iterative techniques. More specifically, in order to solve iteratively $\left(\Delta_{[00]} + \mathrm{i}\Delta_{[00]}^{B}\right)\left(D_{[00]}^{\perp} + \mathrm{i}D_{[00]}^{\odot}\right) = \mathbb{I} - Y \otimes U$ with the constraint $(D_{[00]}^{\perp} + \mathrm{i}D_{[00]}^{\odot})Y = 0$, we introduce the splitting $\Delta_{[00]} + \mathrm{i}\Delta_{[00]}^{B} = M - Z$ where $M = \mathcal{D} + \mathrm{i}\Delta_{[00]}^{B}$ and $\mathcal{D}$ is a diagonal matrix such that $\mathcal{D}_{kk} = \Delta_{[00]kk}/(1 - Y_k)$. Denoting by T the iteration matrix $T = M^{-1}Z$, we then have the convergent asymptotic expansion

$$D_{[00]}^{\perp} + \mathrm{i}D_{[00]}^{\odot} = \sum_{j=0}^{\infty} (PT)^j P M^{-1} P^t,$$

where $P = \mathbb{P} - U \otimes Y$ denotes the projector matrix onto $Y^{\perp}$ parallel to U. This expansion can be shown to be convergent with a spectral radius of the product $PT = PM^{-1}Z$ strictly lower than unity, and this spectral radius is always lower in the magnetized case than in the unmagnetized case where the matrix $\Delta_{[00]}^{B}$ vanishes [32]. Various approximations can then be obtained by truncating this convergent series [32]. The first approximation $\left(D_{[00]}^{\perp} + \mathrm{i}D_{[00]}^{\odot}\right)^{[1]}$ generalizes the Hirschfelder–Curtiss approximation with a mass corrector [25, 35, 36] to the magnetized case

$$\left(D_{[00]}^{\perp} + \mathrm{i}D_{[00]}^{\odot}\right)^{[1]} = \mathcal{M} + \frac{\mathcal{M}\mathcal{D}U \otimes \mathcal{M}\mathcal{D}U}{\langle \mathcal{D}U - \mathcal{D}\mathcal{M}\mathcal{D}U, U \rangle}, \tag{67}$$

where $\mathcal{M} = (\mathcal{D} + \mathrm{i}\mathcal{D}^B)^{-1} - (\mathcal{D} + \mathrm{i}\mathcal{D}^B)^{-1}Y \otimes (\mathcal{D} + \mathrm{i}\mathcal{D}^B)^{-1}Y/\langle(\mathcal{D} + \mathrm{i}\mathcal{D}^B)^{-1}Y, Y\rangle$. The second-order approximation can be written as

$$\left(D_{[00]}^{\perp} + \mathrm{i}D_{[00]}^{\odot}\right)^{[2]} = \left(D_{[00]}^{\perp} + \mathrm{i}D_{[00]}^{\odot}\right)^{[1]} + \left(D_{[00]}^{\perp} + \mathrm{i}D_{[00]}^{\odot}\right)^{[1]}\left(\mathcal{D} - \Delta_{[00]}\right)\left(D_{[00]}^{\perp} + \mathrm{i}D_{[00]}^{\odot}\right)^{[1]}, \tag{68}$$

and yields a more accurate approximation still within $O((n^s)^2)$ operations. The interest of these algorithms is that they perform well whatever be the intensity of the magnetic field since the complete matrix $\mathrm{i}\Delta_{[00]}^{B}$ has been taken into account in the splitting matrix $M = \mathcal{D} + \mathrm{i}\Delta_{[00]}^{B}$. They do not perform well, however, independently of the ionization degree and convergence rates deteriorate as ionization levels increase as investigated by Garcia Muñoz [37] in the unmagnetized case.

The numerical tests conducted with weakly ionized air at temperature 10 000 K have shown that the second iterate is generally within one percent of the exact corresponding first-order matrix $D_{[00]}^{\perp} + \mathrm{i}D_{[00]}^{\odot}$ for usual matrix norms provided the ionization level is below 10^{-2}. When the ionization level increases, it becomes more and more difficult to evaluate the diffusion coefficients matrices by using standard iterative techniques and in this situation, we recommend either generalized conjugate gradient methods or direct methods.

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Remark. Taking into account the electron/heavy particles coefficients in the splitting matrix $M = \mathcal{D}' + \mathrm{i}\Delta^B_{[00]}$ with $\mathcal{D}'_{kl} = \mathcal{D}_{kl}$, if $k \neq n^s$ and $l \neq n^s$, and $\mathcal{D}'_{kl} = \Delta_{[00]kl}$ otherwise, assuming that the electron is the last species $k = n^s$, only slightly improves the convergence rates.

4.7. Higher order linear systems associated with D and electrical conductivities

Higher order approximations of the diffusion matrices, also accounting for the energy of the molecules, require to consider linear systems of size $2n^s + n^p$ where n^p denotes the number of polyatomic species of the mixture, that is, the number of species with at least two different internal energy states.

The corresponding variational approximation space $\mathcal{A}^D$ is the spanned by $\phi^{1000k}, k \in \mathcal{S}, \phi^{1010k}, k \in \mathcal{S}$, and $\phi^{1001k}, k \in \mathcal{P}$, where $\phi^{1010k} = \left(\left(\frac{5}{2} - \boldsymbol{w}_k \cdot \boldsymbol{w}_k\right)\boldsymbol{w}_k \delta_{ki}\right)_{i \in \mathcal{S}}, k \in \mathcal{S}, \phi^{1001k} = \left((\bar{\epsilon}_k - \epsilon_{kk})\boldsymbol{w}_k \delta_{ki}\right)_{i \in \mathcal{S}}, k \in \mathcal{P}, \mathcal{P}$ denotes the set of polyatomic species, and n^p the number of polyatomic species [17]. We will denote by φ^{D_j} the corresponding approximation and for convenience, $\varphi^{D_j(\mathsf{l})}$ is taken in the form

$$\varphi^{D_j(\mathsf{l})} = \frac{\sqrt{2}}{p\sqrt{k_{\mathrm{B}}T}} \left(\sum_{k \in \mathcal{S}} \sqrt{m_k}\left(\alpha_k^{00D_j(\mathsf{l})}\phi^{1000k} + \alpha_k^{10D_j(\mathsf{l})}\phi^{1010k}\right) + \sum_{k \in \mathcal{P}} \sqrt{m_k}\,\alpha_k^{01D_j(\mathsf{l})}\phi^{1001k}\right),$$

$$\mathsf{l} = 1, 2.$$

The matrix associated with the variational procedure is denoted by L and is rescaled such that $L_{kl} = (2\sqrt{m_k m_l}/3p)[\![\phi^{10rk}, \phi^{10sl}]\!], (r, k), (s, l) \in \{00\} \times \mathcal{S} \cup \{10\} \times \mathcal{S} \cup \{01\} \times \mathcal{P}$. We also rescale the right-hand side vector $\beta_k^{rD_j} = \sqrt{2m_k/k_{\mathrm{B}}T}/3p \langle\!\langle f^0\phi^{10rk}, \boldsymbol{\Psi}^{D_j}\rangle\!\rangle, (r, k) \in \{00\} \times \mathcal{S} \cup \{10\} \times \mathcal{S} \cup \{01\} \times \mathcal{P}$. We then have $L \in \mathbb{R}^{2n^s+n^p, 2n^s+n^p}, \beta^{D_j} \in \mathbb{R}^{2n^s+n^p}$, and the linear systems for $\alpha^{D_j(1)} \in \mathbb{R}^{2n^s+n^p}$ and $\alpha^{D_j(2)} \in \mathbb{C}^{2n^s+n^p}$ are in the form

$$\begin{cases} L\alpha^{D_j(1)} = \beta^{D_j}, \\ \langle\alpha^{D_j(1)}, \mathcal{Y}\rangle = 0, \end{cases} \qquad \begin{cases} (L + \mathrm{i}L^B)\alpha^{D_j(2)} = \beta^{D_j}, \\ \langle\alpha^{D_j(2)}, \mathcal{Y}\rangle = 0. \end{cases} \tag{69}$$

The coefficients of the matrix $L \in \mathbb{R}^{2n^s+n^p, 2n^s+n^p}$ are given in [17] and are summarized in section 5.3 and appendix C. The constraint vector $\mathcal{Y} \in \mathbb{R}^{2n^s+n^p}$ is given by $\mathcal{Y} = ((Y_k)_{k \in \mathcal{S}}, (0)_{k \in \mathcal{S}}, (0)_{k \in \mathcal{P}})^t$, and the vectors $\beta^{D_j} \in \mathbb{R}^{2n^s+n^p}$ are given by $\beta^{D_j} = \left(\beta^{D_j}_{[00]}, (0)_{k \in \mathcal{S}}, (0)_{k \in \mathcal{P}}\right)^t, j \in \mathcal{S}$. On the other hand, the matrix L^B is in the form $L^B = (\mathbb{I} - \mathcal{Y} \otimes \mathcal{U})\mathsf{L}^B(\mathbb{I} - \mathcal{U} \otimes \mathcal{Y})$ where L^B is the diagonal matrix $(\mathsf{L}^B)^{rs}_{kl} = \delta_{kl}\delta_{rs}n_k e_k B/p$, if $(r, k) \in \{00\} \times \mathcal{S}, (\mathsf{L}^B)^{rs}_{kl} = \delta_{kl}\delta_{rs}\frac{5}{2}n_k e_k B/p$, if $(r, k) \in \{10\} \times \mathcal{S}, (\mathsf{L}^B)^{rs}_{kl} = \delta_{kl}\delta_{rs}c_k^{\mathrm{int}}n_k e_k B/k_{\mathrm{B}}p$, if $(r, k) \in \{01\} \times \mathcal{P}$, and $\mathcal{U} = ((1)_{k \in \mathcal{S}}, (0)_{k \in \mathcal{S}}, (0)_{k \in \mathcal{P}})^t$. The matrix L is symmetric positive semi-definite [17] and the higher order coefficients are given by

$$D_{ij}^{\|} = \langle\alpha^{D_j(1)}, \beta^{D_i}\rangle = \alpha_i^{00D_j(1)} = \alpha_j^{00D_i(1)}, \tag{70}$$

$$D_{ij}^{\perp} + \mathrm{i}D_{ij}^{\odot} = \langle\alpha^{D_j(2)}, \beta^{D_i}\rangle = \alpha_i^{00D_j(2)} = \alpha_j^{00D_i(2)}. \tag{71}$$

Defining $\mathcal{V}^{\|} = -\sum_{j \in \mathcal{S}} \alpha^{D_j(1)}\boldsymbol{d}_j^{\|}$ and $\mathcal{V}^{\perp} - \mathrm{i}\mathcal{V}^{\odot} = -\sum_{j \in \mathcal{S}} \alpha^{D_j(2)}\left(\boldsymbol{d}_j^{\perp} - \mathrm{i}\boldsymbol{d}_j^{\odot}\right)$ the associated complex generalized Stefan–Maxwell equations are in the form

$$-(L + \mathrm{i}L^B)(\mathcal{V}^{\perp} - \mathrm{i}\mathcal{V}^{\odot}) = \sum_{j \in \mathcal{S}} \beta^{D_j}\left(\boldsymbol{d}_j^{\perp} - \mathrm{i}\boldsymbol{d}_j^{\odot}\right), \tag{72}$$

where $\mathcal{V}^{\diamond} = (\mathcal{V}^{00\diamond}, \mathcal{V}^{10\diamond}, \mathcal{V}^{01\diamond})^t$, and $\mathcal{V}^{00\diamond} = \boldsymbol{V}^{\diamond}, \diamond \in \{\|, \perp, \odot\}$. The modifications required in order to take into account thermal diffusion are discussed in section 5.
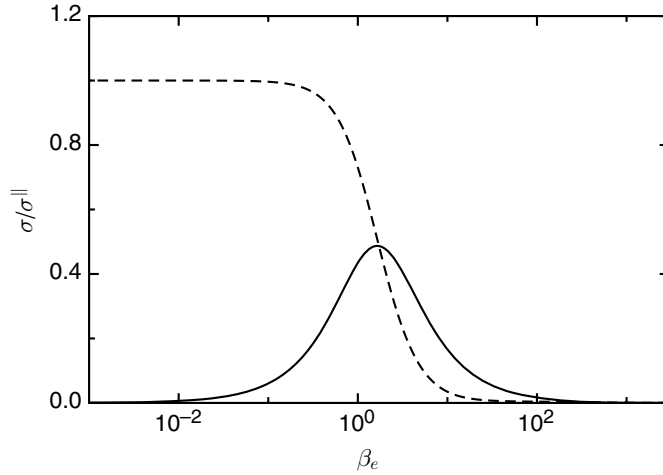
Figure 1. Electrical conductivity ratios $\sigma^{\perp}/\sigma^{\parallel}$– – – and $\sigma^{\odot}/\sigma^{\parallel}$—— for weakly ionized air at 10000 K as functions of the electron Hall parameter.

The same general strategy can be used to evaluate higher order diffusion mass fluxes as for first-order fluxes investigated in the preceding section. When only the diffusion velocities are required, an orthogonal error method can be used to solve the generalized Stefan–Maxwell equations. When the diffusion matrices are also required, either standard iterative algorithms or direct methods can be used to solve the corresponding transport linear systems. The same standard iterative algorithms can be used for instance by using splittings in the form $L + \mathrm{i}L^B = \mathcal{M} - \mathcal{Z}$ with $\mathcal{M} = \mathcal{D} + \mathrm{i}L^B$ where $\mathcal{D}$ is a diagonal matrix or a block diagonal matrix as described in [17]. Denoting by $\mathcal{T}$ the iteration matrix $\mathcal{T} = \mathcal{M}^{-1}\mathcal{Z}$, we then have the convergent asymptotic expansion

$$D^{\perp} + \mathrm{i}D^{\odot} = \Pi \left(\sum_{j=0}^{\infty} (\mathcal{PT})^{j}\mathcal{PM}^{-1}\mathcal{P}^{t} \right) \Pi^{t},$$

where $\mathcal{P} = \mathbb{I} - \mathcal{U} \otimes \mathcal{Y}$ denotes the projector matrix onto $\mathcal{Y}^{\perp}$ parallel to $\mathcal{U}$ where $\mathcal{U}$ is defined by $\mathcal{U} = (U, (0)_{k \in \mathcal{S}}, (0)_{k \in \mathcal{P}})^{t}$ and $\Pi \in \mathbb{R}^{n^{s}, 2n^{s} + n^{p}}$ is the rectangular matrix $\Pi = [\mathbb{I}, 0, 0]$. This expansion can be shown to be convergent with a spectral radius of the product $\mathcal{PT} = \mathcal{PM}^{-1}\mathcal{Z}$ strictly lower than unity. The second-order iterate $(D^{\perp} + \mathrm{i}D^{\odot})^{[2]}$ is a good trade off between precision and computational costs.

The higher order effects usually have a minor impact on the diffusion matrix of neutral species mixtures [17]. They have a more important impact, however, on ionized mixtures. Our numerical test for high temperature air have shown that the relative error in matrix norms $\|D^{\parallel} - D^{\parallel}_{[00]}\| / \|D^{\parallel}\|$, $\|D^{\perp} - D^{\perp}_{[00]}\| / \|D^{\perp}\|$, and $\|D^{\odot} - D^{\odot}_{[00]}\| / \|D^{\parallel}\|$, can be large for ionization rates above 10^{-2} and remain below 10^{-2} only when the ionization rate is below 10^{-3}. The same is true for $\|D^{\odot} - D^{\odot}_{[00]}\| / \|D^{\odot}\|$, unless B is small but then both $D^{\odot}$ and $D^{\odot}_{[00]}$ are small. Above the ionization level 10^{-3}, it is recommended to use the higher order approximations diffusion matrices D and to use generalized conjugate gradient or direct methods.

Higher order effects due to the energy of the molecules are always important, however, in order to evaluate the electrical conductivities, even for weakly ionized mixtures [1, 2, 6, 14].
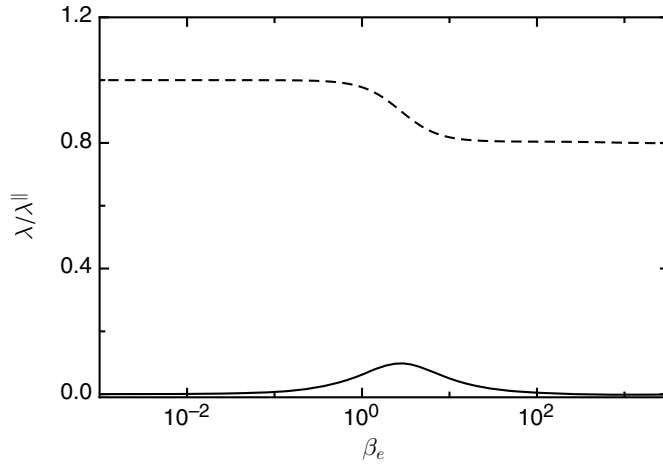
Figure 2. Thermal conductivity ratios $\lambda^{\perp}/\lambda^{\parallel}$– – – and $\lambda^{\odot}/\lambda^{\parallel}$—— for weakly ionized air at 10 000 K as functions of the electron Hall parameter.

The electrical conductivities $\sigma^{\parallel}$, $\sigma^{\perp}$, and $\sigma^{\odot}$ are defined by

$$p\sigma^{\parallel} = \sum_{i,j\in\mathcal{S}} D^{\parallel}_{ij} n_i e_i n_j e_j, \qquad p\sigma^{\perp} = \sum_{i,j\in\mathcal{S}} D^{\perp}_{ij} n_i e_i n_j e_j, \qquad p\sigma^{\odot} = \sum_{i,j\in\mathcal{S}} D^{\odot}_{ij} n_i e_i n_j e_j,$$

and since the species charge e_i, $i \in \mathcal{S}$, can be of different sign, cancellation of significant digits may arise so that using only the first-order diffusion coefficients may lead to large errors in the conductivities, as shown in particular by Bruno and coworkers in the monatomic approximation [1, 2, 14]. In the numerical simulations by Bruno and coworkers, the errors are even amplified because of the Ramsauer minimum in the electron–argon collision cross sections [2, 14]. We have evaluated the second-order electrical conductivities for air in the weakly ionized state $X_{N_2} = X_{O_2} = X_{NO} = X_N = X_O = 0.198$, $X_{N_2^+} = X_{O_2^+} = X_{NO^+} = X_{N^+} = X_{O^+} = 0.001$, $X_{E^-} = 0.005$, at temperature 10 000 K and pressure $p = 1$ atm. The corresponding parallel electrical conductivity is $\sigma^{\parallel} = 1108$ AV^{-1} m^{-1} and the ratios $\sigma^{\perp}/\sigma^{\parallel}$ and $\sigma^{\odot}/\sigma^{\parallel}$ are plotted in figure 1 as functions of the electron Hall parameter β_e. The electron Hall parameter is defined by $\beta_e = \omega_e \tau_e$ where ω_e denotes the electron Larmor frequency $\omega_e = eB/m_e$ and τ_e the Coulomb mean collision time $\tau_e = 3m_e/16\rho_e \Omega^{(1,1)}_{e,ion}$ [14].

Remark. In order to improve the accuracy of the electrical conductivities, a natural possibility is to compute the higher order diffusion coefficients D and then the corresponding electrical conductivities. A second possibility, however, is to use the first-order diffusion coefficients $D_{[00]}$ in the species equations—when they are sufficiently accurate—and to only evaluate the solutions $\zeta^{(1)}$ and $\zeta^{(2)}$ of the linear systems

$$\begin{cases} L\zeta^{(1)} = \sum_{j\in\mathcal{S}} n_j e_j \beta^{D_j}, \\ \langle \zeta^{(1)}, \mathcal{Y} \rangle = 0, \end{cases} \qquad \begin{cases} (L + iL^B)\zeta^{(2)} = \sum_{j\in\mathcal{S}} n_j e_j \beta^{D_j}, \\ \langle \zeta^{(2)}, \mathcal{Y} \rangle = 0. \end{cases} \tag{73}$$

Once the vectors $\zeta^{(1)}$ and $\zeta^{(2)}$ are evaluated, the electrical conductivities are then obtained from $p\sigma^{\parallel} = \sum_{j\in\mathcal{S}} n_j e_j \zeta^{(1)}_j$ and $p(\sigma^{\perp} + i\sigma^{\odot}) = \sum_{j\in\mathcal{S}} n_j e_j \zeta^{(2)}_j$. The systems (73) can be solved by using an orthogonal error algorithm which converge within a few iterations independent of the magnetic field.

4.8. Transport linear systems associated with $\widehat{\lambda}$ and θ

The vector integral equations associated with the partial thermal conductivity are in the form $(\mathcal{F}^{\mathcal{S}} + \delta_{2l}\mathrm{i}B\mathcal{F}^{z,v})(\varphi^{\widehat{\lambda}(l)}) = \Psi^{\widehat{\lambda}}$, with $l = 1, 2$, and

$$\Psi^{\widehat{\lambda}} = \sum_{k\in\mathcal{S}} \sqrt{2(k_{\mathrm{B}}T)^3/m_k}\,\phi^{1010k} + \sum_{k\in\mathcal{P}} \sqrt{2(k_{\mathrm{B}}T)^3/m_k}\,\phi^{1001k}.$$

The variational approximation space $\mathcal{A}^{\widehat{\lambda}}$ to be considered in the first place is the space spanned by $\phi^{1000k}, k \in \mathcal{S}, \phi^{1010k}, k \in \mathcal{S}$, and $\phi^{1001k}, k \in \mathcal{P}$, and we will denote by $\varphi^{\widehat{\lambda}(l)}$ the corresponding approximation. For convenience, $\varphi^{\widehat{\lambda}(l)}$ is taken in the form

$$\varphi^{\widehat{\lambda}(l)} = \sqrt{2k_{\mathrm{B}}T}\left(\sum_{k\in\mathcal{S}} \sqrt{m_k}\big(\alpha_k^{00\widehat{\lambda}(l)}\phi^{1000k} + \alpha_k^{10\widehat{\lambda}(l)}\phi^{1010k}\big) + \sum_{k\in\mathcal{P}} \sqrt{m_k}\alpha_k^{01\widehat{\lambda}(l)}\phi^{1001k}\right), l = 1, 2.$$

The matrix associated with the variational procedure is denoted by L and is rescaled such that $L_{kl} = (2\sqrt{m_k m_l}/3p)[\![\phi^{10rk}, \phi^{10sl}]\!], (r, k), (s, l) \in \{00\}\times\mathcal{S}\cup\{10\}\times\mathcal{S}\cup\{01\}\times\mathcal{P}$. We also rescale the right-hand side vectors $\beta_k^{r\widehat{\lambda}} = \sqrt{2m_k/k_{\mathrm{B}}T}/3p\langle\!\langle f^0\phi^{10rk}, \Psi^{\widehat{\lambda}}\rangle\!\rangle, (r, k) \in \{00\}\times\mathcal{S}\cup\{10\}\times\mathcal{S}\cup\{01\}\times\mathcal{P}$. We then have $L \in \mathbb{R}^{2n^s+n^p, 2n^s+n^p}, \beta^{\widehat{\lambda}} \in \mathbb{R}^{2n^s+n^p}$, and the linear system for $\alpha^{\widehat{\lambda}(1)} \in \mathbb{R}^{2n^s+n^p}$ and $\alpha^{\widehat{\lambda}(2)} \in \mathbb{C}^{2n^s+n^p}$ are in the form

$$\begin{cases} L\alpha^{\widehat{\lambda}(1)} = \beta^{\widehat{\lambda}}, \\ \langle\alpha^{\widehat{\lambda}(1)}, \mathcal{Y}\rangle = 0, \end{cases} \qquad \begin{cases} (L + \mathrm{i}L^B)\alpha^{\widehat{\lambda}(2)} = \beta^{\widehat{\lambda}}, \\ \langle\alpha^{\widehat{\lambda}(2)}, \mathcal{Y}\rangle = 0. \end{cases}$$

The vector $\beta^{\widehat{\lambda}}$ is such that $\beta_k^{r\widehat{\lambda}} = 0, (r, k) \in \{00\}\times\mathcal{S}, \beta_k^{r\widehat{\lambda}} = \frac{5}{2}X_k, (r, k) \in \{10\}\times\mathcal{S}$, and $\beta_k^{r\widehat{\lambda}} = c_k^{\mathrm{int}}X_k/k_{\mathrm{B}}, (r, k) \in \{01\}\times\mathcal{P}$, where c_k^{int} is the internal heat capacity of the kth species per molecule. The partial thermal conductivities are given by the scalar products

$$\widehat{\lambda}^{\|} = \frac{p}{T}\langle\alpha^{\widehat{\lambda}(1)}, \beta^{\widehat{\lambda}}\rangle = \frac{p}{T}(\langle\alpha^{10\widehat{\lambda}(1)}, \beta^{10\widehat{\lambda}}\rangle + \langle\alpha^{01\widehat{\lambda}(1)}, \beta^{01\widehat{\lambda}}\rangle), \tag{74}$$

$$\widehat{\lambda}^{\perp} + \mathrm{i}\widehat{\lambda}^{\odot} = \frac{p}{T}\langle\alpha^{\widehat{\lambda}(2)}, \beta^{\widehat{\lambda}}\rangle = \frac{p}{T}(\langle\alpha^{10\widehat{\lambda}(2)}, \beta^{10\widehat{\lambda}}\rangle + \langle\alpha^{01\widehat{\lambda}(2)}, \beta^{01\widehat{\lambda}}\rangle), \tag{75}$$

and, the thermal diffusion coefficients are given by

$$\theta_i^{\|} = -\langle\alpha^{\widehat{\lambda}(1)}, \beta^{D_i}\rangle = -\alpha_i^{00\widehat{\lambda}(1)}, \qquad \theta_i^{\perp} + \mathrm{i}\theta_i^{\odot} = -\langle\alpha^{\widehat{\lambda}(2)}, \beta^{D_i}\rangle = -\alpha_i^{00\widehat{\lambda}(2)}. \tag{76}$$

Note, however, that it is computationally more interesting to directly evaluate the thermal conductivities $\lambda^{\|}, \lambda^{\perp}, \lambda^{\odot}$ and the thermal diffusion ratios $\chi^{\|}, \chi^{\perp}, \chi^{\odot}$ rather than the partial thermal conductivities $\widehat{\lambda}^{\|}, \widehat{\lambda}^{\perp}, \widehat{\lambda}^{\odot}$ and the thermal diffusion coefficients $\theta^{\|}, \theta^{\perp}, \theta^{\odot}$, as described in the following section.

5. Thermal conductivity and thermal diffusion ratios

We first present the usual definition of the thermal conductivities $\lambda^{\|}, \lambda^{\perp}, \lambda^{\odot}$ and the thermal diffusion ratios $\chi^{\|}, \chi^{\perp}, \chi^{\odot}$. We then introduce a variational framework allowing a direct evaluation of these coefficients without the intermediate evaluation of the partial thermal conductivities $\widehat{\lambda}^{\|}, \widehat{\lambda}^{\perp}, \widehat{\lambda}^{\odot}$ and the thermal diffusion coefficients $\theta^{\|}, \theta^{\perp}, \theta^{\odot}$.

5.1. First definition of the thermal conductivities and the thermal diffusion ratios

The thermal diffusion ratios $\chi^{\|} = \big(\chi_i^{\|}\big)_{i\in\mathcal{S}}, \chi^{\perp} = \big(\chi_i^{\perp}\big)_{i\in\mathcal{S}}$, and $\chi^{\odot} = \big(\chi_i^{\odot}\big)_{i\in\mathcal{S}}$ are defined from the linear systems [15]

$$\begin{cases} D^{\|}\chi^{\|} = \theta^{\|}, \\ \langle\chi^{\|}, U\rangle = 0, \end{cases} \qquad \begin{cases} (D^{\perp} + \mathrm{i}D^{\odot})(\chi^{\perp} + \mathrm{i}\chi^{\odot}) = \theta^{\perp} + \mathrm{i}\theta^{\odot}, \\ \langle\chi^{\perp} + \mathrm{i}\chi^{\odot}, U\rangle = 0, \end{cases} \tag{77}$$

where U is the vector of length n^s with unit components $U = (1, \ldots, 1)^t$. Thanks to the symmetry of $D^{\parallel}$, $D^{\perp}$ and $D^{\odot}$, transposing these systems yield that the thermal diffusion ratios coincide with the modified thermal diffusion ratios $\widehat{\chi}^{\parallel} = \chi^{\parallel}$, $\widehat{\chi}^{\perp} = \chi^{\perp}$ and $\widehat{\chi}^{\odot} = \chi^{\odot}$ also introduced in [15]. We next define the thermal conductivities from [15]

$$\lambda^{\parallel} = \widehat{\lambda}^{\parallel} - (p/T) \sum_{i,j \in \mathcal{S}} D_{ji}^{\parallel} \chi_j^{\parallel} \chi_i^{\parallel},$$

$$\lambda^{\perp} + \mathrm{i}\lambda^{\odot} = \widehat{\lambda}^{\perp} + \mathrm{i}\widehat{\lambda}^{\odot} - (p/T) \sum_{i,j \in \mathcal{S}} \left(D_{ji}^{\perp} + \mathrm{i}D_{ji}^{\odot} \right) \left(\chi_j^{\perp} + \mathrm{i}\chi_j^{\odot} \right) \left(\chi_i^{\perp} + \mathrm{i}\chi_i^{\odot} \right).$$

The diffusion velocities and the heat flux can then be written as

$$V_i = - \sum_{j \in \mathcal{S}} D_{ij}^{\parallel} \left(d_j^{\parallel} + \chi_j^{\parallel} (\partial_x \log T)^{\parallel} \right)$$

$$- \sum_{j \in \mathcal{S}} D_{ij}^{\perp} \left(d_j^{\perp} + \chi_j^{\perp} (\partial_x \log T)^{\perp} + \chi_j^{\odot} (\partial_x \log T)^{\odot} \right)$$

$$- \sum_{j \in \mathcal{S}} D_{ij}^{\odot} \left(d_j^{\odot} + \chi_j^{\perp} (\partial_x \log T)^{\odot} - \chi_j^{\odot} (\partial_x \log T)^{\perp} \right), \tag{78}$$

$$q = - \left(\lambda^{\parallel} (\partial_x T)^{\parallel} + \lambda^{\perp} (\partial_x T)^{\perp} + \lambda^{\odot} (\partial_x T)^{\odot} \right)$$

$$+ p \sum_{i \in \mathcal{S}} \left(\chi_i^{\parallel} V_i^{\parallel} + \chi_i^{\perp} V_i^{\perp} + \chi_i^{\odot} V_i^{\odot} \right) + \sum_{i \in \mathcal{S}} \left(\frac{5}{2} k_{\mathrm{B}} T + \overline{\mathcal{E}_i} \right) n_i V_i. \tag{79}$$

5.2. A variational framework for λ and χ

A variational framework for a direct evaluation of the thermal conductivity and the thermal diffusion ratios in a non-ionized gas has been introduced in [16, 17]. This framework can readily be used for the transport properties parallel to the magnetic field $\lambda^{\parallel}$ and $\chi^{\parallel}$. In this paper, we generalize this framework to the complex magnetized case for the perpendicular and transverse components $\lambda^{\perp} + \mathrm{i}\lambda^{\odot}$ and $\chi^{\perp} + \mathrm{i}\chi^{\odot}$. To this aim, we define

$$\varphi^{\lambda(1)} = \varphi^{\widehat{\lambda}(1)} + p k_{\mathrm{B}} T \sum_{j \in \mathcal{S}} \chi_j^{\parallel} \varphi^{D_j(1)}, \qquad \varphi^{\lambda(2)} = \varphi^{\widehat{\lambda}(2)} + p k_{\mathrm{B}} T \sum_{j \in \mathcal{S}} \left(\chi_j^{\perp} + \mathrm{i}\chi_j^{\odot} \right) \varphi^{D_j(2)},$$
$$\tag{80}$$

$$\Psi_{\parallel}^{\lambda} = \Psi^{\widehat{\lambda}} + p k_{\mathrm{B}} T \sum_{j \in \mathcal{S}} \chi_j^{\parallel} \Psi^{D_j}, \qquad \Psi_{\perp \odot}^{\lambda} = \Psi^{\widehat{\lambda}} + p k_{\mathrm{B}} T \sum_{j \in \mathcal{S}} \left(\chi_j^{\perp} + \mathrm{i}\chi_j^{\odot} \right) \Psi^{D_j}, \tag{81}$$

and it is easily shown that

$$\mathcal{F}^{\mathcal{S}}(\varphi^{\lambda(1)}) = \Psi_{\parallel}^{\lambda}, \qquad (\mathcal{F}^{\mathcal{S}} + \mathrm{i}B\mathcal{F}^{z,v})(\varphi^{\lambda(2)}) = \Psi_{\perp \odot}^{\lambda}, \tag{82}$$

$$\langle\!\langle f^0 \varphi^{\lambda(1)}, \psi^l \rangle\!\rangle = 0, \qquad \langle\!\langle f^0 \varphi^{\lambda(2)}, \psi^l \rangle\!\rangle = 0, \qquad l \in \{1, \ldots, n^s + 4\}. \tag{83}$$

From the definition of thermal diffusion ratios, it is then straightforward to check that $\langle\!\langle f^0 \varphi^{\lambda(1)}, \Psi^{D_j} \rangle\!\rangle = 0$ and $\langle\!\langle f^0 \varphi^{\lambda(2)}, \Psi^{D_j} \rangle\!\rangle = 0$ for $j \in \mathcal{S}$. However, the basis function ϕ^{1000j} is a linear combination of Ψ^{D_j} and of the vector collisional invariant $(m_k C_k)_{k \in \mathcal{S}} = \left((m_k (c_k - v)) \right)_{k \in \mathcal{S}}$ in such a way that $\langle\!\langle f^0 \varphi^{\lambda(1)}, \phi^{1000j} \rangle\!\rangle = 0$ and $\langle\!\langle f^0 \varphi^{\lambda(2)}, \phi^{1000j} \rangle\!\rangle = 0$ for $j \in \mathcal{S}$. One may thus use a Galerkin variational approximation space orthogonal to ϕ^{1000j}, $j \in \mathcal{S}$, in order to solve (82) and (83). It is important to observe then that for any basis function ϕ^{10rk} orthogonal to ϕ^{1000j}, $j \in \mathcal{S}$, we have the relations $\langle\!\langle f^0 \Psi_{\parallel}^{\lambda}, \phi^{10rk} \rangle\!\rangle = \langle\!\langle f^0 \Psi^{\widehat{\lambda}}, \phi^{10rk} \rangle\!\rangle$

and $\langle\!\langle f^0\Psi^\lambda_{\perp\odot}, \phi^{10rk}\rangle\!\rangle = \langle\!\langle f^0\Psi^{\widehat{\lambda}}, \phi^{10rk}\rangle\!\rangle$ so that the transport linear systems associated with a Galerkin approximation of (82) and (83) can readily be evaluated even though the thermal diffusion ratios are unknown. These orthogonality properties also imply that

$$\lambda^\| = \frac{1}{3k_BT^2}\langle\!\langle f^0\varphi^{\lambda(1)}, \Psi^\lambda_\|\rangle\!\rangle = \frac{1}{3k_BT^2}\langle\!\langle f^0\varphi^{\lambda(1)}, \Psi^{\widehat{\lambda}}\rangle\!\rangle,$$

$$\lambda^\perp + i\lambda^\odot = \frac{1}{3k_BT^2}\langle\!\langle f^0\varphi^{\lambda(2)}, \Psi^\lambda_{\perp\odot}\rangle\!\rangle = \frac{1}{3k_BT^2}\langle\!\langle f^0\varphi^{\lambda(2)}, \Psi^{\widehat{\lambda}}\rangle\!\rangle,$$

$$\chi^\|_k = \frac{m_k}{3pk_BT}\langle\!\langle f^0\Psi^\lambda_\|, \mathcal{C}_k\rangle\!\rangle, \quad \chi^\perp_k + i\chi^\odot_k = \frac{m_k}{3pk_BT}\langle\!\langle f^0\Psi^\lambda_{\perp\odot}, \mathcal{C}_k\rangle\!\rangle,$$

where $\mathcal{C}_k = (C_k\delta_{ik})_{i\in\mathcal{S}}$, so that

$$\lambda^\| = \frac{1}{3k_BT^2}[\![\varphi^{\lambda(1)}, \varphi^{\lambda(1)}]\!], \qquad \lambda^\perp + i\lambda^\odot = \frac{1}{3k_BT^2}([\![\varphi^{\lambda(2)}, \varphi^{\lambda(2)}]\!] - i(\!(\varphi^{\lambda(2)}, \varphi^{\lambda(2)})\!)), \tag{84}$$

$$\chi^\|_k = \frac{m_k}{3pk_BT}[\![\varphi^{\lambda(1)}, \mathcal{C}_k]\!], \qquad \chi^\perp_k + i\chi^\odot_k = \frac{m_k}{3pk_BT}[\![\varphi^{\lambda(2)}, \mathcal{C}_k]\!]. \tag{85}$$

5.3. Transport linear systems associated with λ, χ

The vector integral equations associated with the thermal conductivity and the thermal diffusion ratios coefficients are in the form $(\mathcal{F}^{\mathcal{S}} + \delta_{2l}iB\mathcal{F}^{z,v})(\varphi^{\lambda(l)}) = \Psi^{\lambda(l)}$, with $l = 1, 2$. Since we already know that $\varphi^{\lambda(l)}, l = 1, 2$, are orthogonal to $\phi^{1000k}, k \in \mathcal{S}$, the variational approximation space $\mathcal{A}^\lambda$ to be considered in the first place is the space spanned by $\phi^{1010k}, k \in \mathcal{S}$, and $\phi^{1001k}, k \in \mathcal{P}$. For convenience, $\varphi^{\lambda(l)}$ is taken in the form

$$\varphi^{\lambda(l)} = \sqrt{2k_BT}\left(\sum_{k\in\mathcal{S}}\sqrt{m_k}\alpha^{10\lambda(l)}_k\phi^{1010k} + \sum_{k\in\mathcal{P}}\sqrt{m_k}\alpha^{01\lambda(l)}_k\phi^{1001k}\right), \qquad l = 1, 2.$$

The matrix associated with the variational procedure is denoted by Λ and is rescaled such that $\Lambda^{rs}_{kl} = (2\sqrt{m_km_l}/3p)[\![\phi^{10rk}, \phi^{10sl}]\!], (r, k), (s, l) \in \{10\} \times \mathcal{S} \cup \{01\} \times \mathcal{P}$. It is then important to observe that $\beta^{r\lambda}_k = \sqrt{2m_k/k_BT}/3p\langle\!\langle f^0\phi^{10rk}, \Psi^{\widehat{\lambda}}\rangle\!\rangle$, so that $\beta^{r\lambda}_k = \beta^{r\widehat{\lambda}}_k$ for $(r, k) \in \{10\} \times \mathcal{S} \cup \{01\} \times \mathcal{P}$. We then have $\Lambda \in \mathbb{R}^{n^s+n^p, n^s+n^p}$, $\beta^\lambda \in \mathbb{R}^{n^s+n^p}$, and the linear systems for $\alpha^{\lambda(1)} \in \mathbb{R}^{n^s+n^p}$ and $\alpha^{\lambda(2)} \in \mathbb{C}^{n^s+n^p}$ are in the form

$$\Lambda\alpha^{\lambda(1)} = \beta^\lambda, \qquad (\Lambda + i\Lambda^B)\alpha^{\lambda(2)} = \beta^\lambda,$$

where Λ^B is diagonal and given by $(\Lambda^B)^{rs}_{kl} = \delta_{kl}\delta_{rs}\frac{5}{2}n_ke_kB/p$, for $(r, k) \in \{10\} \times \mathcal{S}$ and $(\Lambda^B)^{rs}_{kl} = \delta_{kl}\delta_{rs}c^{int}_kn_ke_kB/k_Bp$, for $(r, k) \in \{01\} \times \mathcal{P}$.

The matrix Λ is symmetric positive definite [17] and the thermal conductivities are given by the following scalar products:

$$\lambda^\| = \frac{p}{T}\langle\alpha^{\lambda(1)}, \beta^\lambda\rangle = \frac{p}{T}(\langle\alpha^{10\lambda(1)}, \beta^{10\lambda}\rangle + \langle\alpha^{01\lambda(1)}, \beta^{01\lambda}\rangle), \tag{86}$$

$$\lambda^\perp + i\lambda^\odot = \frac{p}{T}\langle\alpha^{\lambda(2)}, \beta^\lambda\rangle = \frac{p}{T}(\langle\alpha^{10\lambda(2)}, \beta^{10\lambda}\rangle + \langle\alpha^{01\lambda(2)}, \beta^{01\lambda}\rangle), \tag{87}$$

and the thermal diffusion ratios by

$$\chi^\| = L^{00\lambda}\alpha^{\widehat{\lambda}(1)}, \qquad \chi^\perp + i\chi^\odot = L^{00\lambda}\alpha^{00\widehat{\lambda}(2)}_i, \tag{88}$$

where $L^{00\lambda}$ is the upper right block of L of size $n^s \times (n^s + n^p)$ in such a way that the matrix L has the bloc decomposition

$$L = \begin{pmatrix} L^{0000} & L^{00\lambda} \\ L^{\lambda 00} & L^{\lambda\lambda} \end{pmatrix} = \begin{pmatrix} \Delta_{[00]} & L^{00\lambda} \\ L^{\lambda 00} & \Lambda \end{pmatrix}. \tag{89}$$

The matrix $L^{00\lambda}$ can be written as $L^{00\lambda} = (L^{0010}, L^{0001})$ and the coefficients of Λ, L^{0010} and L^{0001} are given in appendix C.

From the expression of the matricides L, Λ, or $L^{00\lambda}$, we note that, in addition to the classical $\Omega_{kl}^{(i,j)}$ integrals, many collision integrals associated with internal energy exchanges are required for the evaluation of transport properties of polyatomic species mixtures. These collision integrals are discussed in particular in [13, 17, 28] as well as some typical approximations like those of Mason and Monchick in terms of relaxation times. In order to solve the transport linear systems associated with the thermal conductivity we recommend a few step of an orthogonal error method preconditioned by the diagonal matrix $\mathrm{diag}(\Lambda) + i\Lambda^B$ [17, 18]. The thermal diffusion ratios are then readily evaluated from (88).

In the numerical simulations for air at 10 000 K, the relaxation times for internal energy of the polyatomic neutral molecules have been estimated as described in [17] whereas the rotational relaxation times for internal energy of the polyatomic ionized molecules have been approximated as the relaxation time of the corresponding neutral molecules [39]. The numerical simulations with weakly ionized air have shown that three iterations are generally required in order to evaluate the thermal diffusion ratios with a good accuracy, whereas two iterates are generally sufficient for the thermal conductivities. The thermal conductivities have been evaluated for air in the weakly ionized state $X_{N_2} = X_{O_2} = X_{NO} = X_N = X_O = 0.198$, $X_{N_2^+} = X_{O_2^+} = X_{NO^+} = X_{N^+} = X_{O^+} = 0.001$, $X_{E^-} = 0.005$, at temperature 10 000 K and pressure $p = 1$ atm. The parallel thermal conductivity is then $\lambda^{\parallel} = 0.658$ Wm^{-1} K^{-1} and the corresponding ratios $\lambda^{\perp}/\lambda^{\parallel}$ and $\lambda^{\odot}/\lambda^{\parallel}$ are plotted in figure 2 as functions of the electron Hall parameter β_e

5.4. Stefan–Maxwell equations with the Soret effect

Stefan–Maxwell equations associated with the real vector $\mathcal{V}^{\parallel}$ whose n^s first components are the diffusion velocities parallel to the magnetic field $\boldsymbol{V}^{\parallel} = \mathcal{V}^{00\parallel} = \Pi\mathcal{V}^{\parallel}$ are similar to that of non-ionized mixtures already investigated in [17, 35]. We thus only discuss in the following the generalized Stefan–Maxwell equations associated with the complex vector $\mathcal{V}^{\perp} - i\mathcal{V}^{\odot}$ defined by

$$\mathcal{V}^{\perp} - i\mathcal{V}^{\odot} = -\sum_{j \in \mathcal{S}} \alpha^{D_j(2)} \big((\boldsymbol{d}_j^{\perp} - i\boldsymbol{d}_j^{\odot}) + (\chi_j^{\perp} + i\chi_j^{\odot})((\partial_x \log T)^{\perp} - i(\partial_x \log T)^{\odot}) \big),$$

whose n^s first components are the diffusion velocities perpendicular and transverse to the magnetic field $\boldsymbol{V}^{\perp} - i\boldsymbol{V}^{\odot} = \mathcal{V}^{00\perp} - i\mathcal{V}^{00\odot} = \Pi(\mathcal{V}^{\perp} - i\mathcal{V}^{\odot})$.

The Stefan–Maxwell equations in the presence of the Soret effect are more conveniently written in terms of thermal diffusion ratios [3, 6, 20, 25]. Multiplying the transport linear system (69) for $\alpha^{D_j(2)}$ by the vector $\boldsymbol{d}_j^{\perp} - \boldsymbol{d}_j^{\odot} + (\chi_j^{\perp} + i\chi_j^{\odot})((\partial_x \log T)^{\perp} - i(\partial_x \log T)^{\odot})$ and summing over $j \in \mathcal{S}$ we obtain the proper generalization to the complex framework of the Stefan–Maxwell equations with the Soret effect

$$-(L + iL^B)(\mathcal{V}^{\perp} - i\mathcal{V}^{\odot}) = \sum_{j \in \mathcal{S}} \beta^{D_j} \big((\boldsymbol{d}_j^{\perp} - i\boldsymbol{d}_j^{\odot}) + (\chi_j^{\perp} + i\chi_j^{\odot})((\partial_x \log T)^{\perp} - i(\partial_x \log T)^{\odot}) \big).$$

$$\tag{90}$$

Upon introducing the Schur complement

$$\Delta + \mathrm{i}\Delta^B = \Delta_{[00]} + \mathrm{i}\Delta_{[00]}^B - L^{00\lambda}(\Lambda + \mathrm{i}\Lambda^B)^{-1}L^{\lambda 00},$$

the Stefan–Maxwell equations can also be rewritten in the form

$$-(\Delta + \mathrm{i}\Delta^B)(\boldsymbol{V}^\perp - \mathrm{i}\boldsymbol{V}^\odot) = \widetilde{\boldsymbol{d}}^\perp - \mathrm{i}\widetilde{\boldsymbol{d}}^\odot + (\chi^\perp + \mathrm{i}\chi^\odot)((\partial_x \log T)^\perp - \mathrm{i}(\partial_x \log T)^\odot), \qquad (91)$$

where $\widetilde{\boldsymbol{d}}^\perp - \mathrm{i}\widetilde{\boldsymbol{d}}^\odot = \sum_{j\in\mathcal{S}} \beta^{00D_j}\big(d_j^\perp - \mathrm{i}d_j^\odot\big) = \boldsymbol{d}^\perp - \mathrm{i}\boldsymbol{d}^\odot - Y\sum_{j\in\mathcal{S}}\big(d_j^\perp - \mathrm{i}d_j^\odot\big)$ are the constrained diffusion driving forces. These equations may be approximated by using the matrix $\Delta_{[00]} + \mathrm{i}\Delta_{[00]}^B$ instead of $\Delta + \mathrm{i}\Delta^B$, depending on the accuracy of the first-order diffusion matrices. Projected standard iterative techniques as well as projected generalized conjugate gradient methods can be used to solve the Stefan–Maxwell equations with or without the Soret effect and magnetic field effects [17, 19, 32].

6. Dependence of transport coefficients on the magnetic field

From a theoretical and computational point of view, it is important to investigate the behavior of transport coefficients and transport fluxes for vanishing magnetic fields. In this section we establish the proper structural properties of the transport coefficients which guarantee that all transport fluxes behave smoothly as $\boldsymbol{B}$ goes to zero.

6.1. Heat and mass transport coefficients

The operators $\mathcal{F}^\mathcal{S}$ and $\mathcal{F}^{z,v}$ do not depend on the magnetic field $\boldsymbol{B}$ so that the functions $\varphi_i^{\widehat{\lambda}(1)}, i\in\mathcal{S}$, and $\varphi_i^{D_j(1)}, i,j\in\mathcal{S}$, are independent of $\boldsymbol{B}$. On the other hand, in order to investigate the dependence on the magnetic field $\boldsymbol{B}$ of the perpendicular and transverse transport coefficients we expand the functions $\varphi^{\widehat{\lambda}(2)}$, and $\varphi^{D_j(2)}, j\in\mathcal{S}$, in series of the intensity of the magnetic field $B = \|\boldsymbol{B}\|$. More specifically, we write

$$\varphi_i^{\widehat{\lambda}(2)} = \sum_{n\in\mathbb{N}}(\mathrm{i}B)^n\varphi_{i,n}^{\widehat{\lambda}}, \qquad \varphi_i^{D_j(2)} = \sum_{n\in\mathbb{N}}(\mathrm{i}B)^n\varphi_{i,n}^{D_j}, \qquad i,j\in\mathcal{S}, \qquad (92)$$

where the functions $\varphi_{\cdot,n}^{\widehat{\lambda}} = \big(\varphi_{i,n}^{\widehat{\lambda}}\big)_{i\in\mathcal{S}}, \varphi_{\cdot,n}^{D_j} = \big(\varphi_{i,n}^{D_j}\big)_{i\in\mathcal{S}}, j\in\mathcal{S}, n\in\mathbb{N}$, do not depend on the magnetic field and satisfy the integro-differential equations $\mathcal{F}^\mathcal{S}\big(\varphi_{\cdot,0}^{\widehat{\lambda}}\big) = \Psi^{\widehat{\lambda}}, \mathcal{F}^\mathcal{S}\big(\varphi_{\cdot,n+1}^{\widehat{\lambda}}\big) = -\mathcal{F}^{z,v}\big(\varphi_{\cdot,n}^{\widehat{\lambda}}\big)$, for $n\geqslant 0$, and $\mathcal{F}^\mathcal{S}\big(\varphi_{\cdot,0}^{D_j}\big) = \mathfrak{g}^{D_j}, \mathcal{F}^\mathcal{S}\big(\varphi_{\cdot,n+1}^{D_j}\big) = -\mathcal{F}^{z,v}\big(\varphi_{\cdot,n}^{D_j}\big)$, for $n\geqslant 0, j\in\mathcal{S}$, and the scalar constraints $\big\langle\!\big\langle f^0\varphi_{\cdot,n}^{\widehat{\lambda}}, \psi^l\big\rangle\!\big\rangle = 0, \big\langle\!\big\langle f^0\varphi_{\cdot,n}^{D_j}, \psi^l\big\rangle\!\big\rangle = 0, n\geqslant 0, l\in\{0,\ldots,n^s+4\}$. These equations yield existence and uniqueness for $\varphi_{i,n}^{\widehat{\lambda}}, \varphi_{i,n}^{D_j}, i,j\in\mathcal{S}, n\in\mathbb{N}$. From the well posedness of the integral operator, the radius of convergence of these series is nonzero and we also remark that $\varphi_{i,0}^{\widehat{\lambda}} = \varphi_i^{\widehat{\lambda}(1)}$ and $\varphi_{i,0}^{D_j} = \varphi_i^{D_j(1)}, i,j\in\mathcal{S}$. From these series expansions, we can then expand the transport coefficients $D_{ij}^\|, D_{ij}^\perp$ and $D_{ij}^\odot, i,j\in\mathcal{S}$, in the form

$$D_{ij}^\| = \mathsf{a}_{ij}^0, \qquad D_{ij}^\perp = \sum_{l\geqslant 0} B^{2l}\mathsf{a}_{ij}^{2l}, \qquad D_{ij}^\odot = \sum_{l\geqslant 0} B^{2l+1}\mathsf{a}_{ij}^{2l+1}. \qquad (93)$$

The coefficients $\mathsf{a}_{ij}^l, i,j\in\mathcal{S}, l\geqslant 0$, do not depend on B and are given by

$$\mathsf{a}_{ij}^l = (-1)^{[\frac{l}{2}]}\frac{1}{3}pk_\mathrm{B}T\left(\sum_{n+m=l}(-1)^m[\![\varphi_{\cdot,n}^{D_i}, \varphi_{\cdot,m}^{D_j}]\!] - \sum_{n+m=l-1}(-1)^m\big(\!\big(\varphi_{\cdot,n}^{D_i}, \varphi_{\cdot,m}^{D_j}\big)\!\big)'\right),$$

where $(\!(\xi, \zeta)\!)'$ is the rescaled bracket defined by $B(\!(\xi, \zeta)\!)' = (\!(\xi, \zeta)\!)$. We then deduce the existence of regular functions denoted by $\psi_{D_{ij}}^\perp, \psi_{D_{ij}}^\odot, i,j\in\mathcal{S}$, so that

$$D_{ij}^\perp - D_{ij}^\| = B^2\psi_{D_{ij}}^\perp(B^2), \qquad D_{ij}^\odot = B\psi_{D_{ij}}^\odot(B^2). \qquad (94)$$

The above expansion can be followed through for all the transport coefficients but we omit the details for the sake of simplicity. We thus deduce that for any vector transport coefficient μ, the parallel component $\mu^{\parallel}$ is independent of B, whereas $\mu^{\perp} - \mu^{\parallel} = B^2 \psi_{\mu}^{\perp}(B^2)$ and $\mu^{\odot} = B \psi_{\mu}^{\odot}(B^2)$, where the functions $\psi_{\mu}^{\perp}$ and $\psi_{\mu}^{\odot}$ are smooth.

On the other hand, upon introducing the tensorial transport coefficients $\boldsymbol{D}_{ij}, i, j \in \mathcal{S}, \boldsymbol{\theta}_i, i \in \mathcal{S}$, and $\widehat{\boldsymbol{\lambda}}$ defined by

$$\boldsymbol{D}_{ij} = D_{ij}^{\parallel} \mathbf{M}^{\parallel} + D_{ij}^{\perp} \mathbf{M}^{\perp} + D_{ij}^{\odot} \mathbf{M}^{\odot},$$

$$\boldsymbol{\theta}_i = \theta_i^{\parallel} \mathbf{M}^{\parallel} + \theta_i^{\perp} \mathbf{M}^{\perp} + \theta_i^{\odot} \mathbf{M}^{\odot},$$

$$\widehat{\boldsymbol{\lambda}} = \widehat{\lambda}^{\parallel} \mathbf{M}^{\parallel} + \widehat{\lambda}^{\perp} \mathbf{M}^{\perp} + \widehat{\lambda}^{\odot} \mathbf{M}^{\odot},$$

where $\mathbf{M}^{\parallel} = \mathcal{B} \otimes \mathcal{B}, \mathbf{M}^{\perp} = \boldsymbol{I} - \mathcal{B} \otimes \mathcal{B}$, and $\mathbf{M}^{\odot} = \boldsymbol{R}(\mathcal{B})$, we obtain a compact formulation for diffusion velocities and heat flux

$$\boldsymbol{V}_i = -\sum_{j \in \mathcal{S}} \boldsymbol{D}_{ij} \boldsymbol{d}_j - \boldsymbol{\theta}_i \partial_x \log T, \tag{95}$$

$$\boldsymbol{q} = -\widehat{\boldsymbol{\lambda}} \partial_x T - p \sum_{i \in \mathcal{S}} \boldsymbol{\theta}_i \boldsymbol{d}_i + \sum_{i \in \mathcal{S}} \left(\frac{5}{2} k_B T + \overline{\mathcal{E}_i} \right) n_i \boldsymbol{V}_i. \tag{96}$$

However, for any set of coefficients $\mu^{\parallel}, \mu^{\perp}$, and $\mu^{\odot}$, such that $\mu^{\parallel}$ is independent of $B, \mu^{\perp} - \mu^{\parallel} = B^2 \psi_{\mu}^{\perp}(B^2)$ and $\mu^{\odot} = B \psi_{\mu}^{\odot}(B^2)$, where the functions $\psi_{\mu}^{\perp}$ and $\psi_{\mu}^{\odot}$ are smooth, we directly obtain that the tensorial coefficient $\mu^{\parallel} \mathbf{M}^{\parallel} + \mu^{\perp} \mathbf{M}^{\perp} + \mu^{\odot} \mathbf{M}^{\odot}$ can be written as

$$\mu^{\parallel} \mathbf{M}^{\parallel} + \mu^{\perp} \mathbf{M}^{\perp} + \mu^{\odot} \mathbf{M}^{\odot} = \mu^{\parallel} \boldsymbol{I} + \psi_{\mu}^{\perp}(B^2)(B^2 \mathbb{I} - \boldsymbol{B} \otimes \boldsymbol{B}) + \psi_{\mu}^{\odot}(B^2) \boldsymbol{R}(\boldsymbol{B}),$$

since $\boldsymbol{B} = B \mathcal{B}$ so that $\mu^{\parallel} \mathbf{M}^{\parallel} + \mu^{\perp} \mathbf{M}^{\perp} + \mu^{\odot} \mathbf{M}^{\odot}$ is smooth for any $\boldsymbol{B}$ and converges toward $\mu^{\parallel} \boldsymbol{I}$ as $\boldsymbol{B} \to 0$. As a consequence, the heat and mass diffusion fluxes are *smooth* functions of the magnetic field and we obtain in the limit case $\boldsymbol{B} \to 0$ the same contributions as with a zero magnetic field.

6.2. Momentum transport coefficients

We first note that the volume viscosity κ does not depend on the magnetic field. Similarly, since the operators $\mathcal{F}^{\mathcal{S}}$ and $\mathcal{F}^{z,m}$ do not depend on $\boldsymbol{B}$, the function $\varphi_i^{\eta[1]}$ does not depend on the magnetic field. On the other hand, in order to study the dependence on the magnetic field of the shear viscosities, we expand the functions $\varphi^{\eta[2]}$ and $\varphi^{\eta[3]}$ in the form

$$\varphi_i^{\eta[2]} = \sum_{n \geqslant 0} (2iB)^n \varphi_{i,n}^{\eta}, \qquad \varphi_i^{\eta[3]} = \sum_{n \geqslant 0} (iB)^n \varphi_{i,n}^{\eta}, \tag{97}$$

where the expansion coefficients $\varphi_{.,n}^{\eta} = \left(\varphi_{i,n}^{\eta} \right)_{i \in \mathcal{S}}, n \geqslant 0$, do not depend on the magnetic field B and satisfy the integro-differential equations $\mathcal{F}^{\mathcal{S}} \left(\varphi_{.,0}^{\eta} \right) = \Psi^{\eta}, \mathcal{F}^{\mathcal{S}} \left(\varphi_{.,n+1}^{\eta} \right) = -\mathcal{F}^{z,m} \left(\varphi_{.,n}^{\eta} \right), n \geqslant 0, \left\langle\!\left\langle f^0 \varphi_{.,n}^{\eta}, \psi^l \right\rangle\!\right\rangle = 0, l \in \{0, \ldots, n^s + 4\}$. Defining $\mathsf{a}^l = \frac{1}{20} k_B T \sum_{n+m=2l} (-1)^{m+l} [\![\varphi_{.,n}^{\eta}, \varphi_{.,m}^{\eta}]\!]$, and $\mathsf{b}^l = \frac{1}{20} k_B T \sum_{n+m=2l} (-1)^{m+l} \left(\left(\varphi_{.,n}^{\eta}, \varphi_{.,m}^{\eta} \right) \right)'$, it is easily established that

$$\eta_1 = \eta_1(0) + \sum_{l>0} 2^{2l} B^{2l} \mathsf{a}^l, \qquad \eta_2 = -\sum_{l \geqslant 0} 2^{2l} B^{2l+1} \mathsf{b}^l, \qquad \eta_3 = -\sum_{l>0} 2^{2l} B^{2l} \mathsf{a}^l, \tag{98}$$

$$\eta_4 = -\sum_{l>0} (2^{2l} - 2) B^{2l} \mathsf{a}^l, \qquad \eta_5 = -\sum_{l>0} (2^{2l+1} - 2) B^{2l+1} \mathsf{b}^l. \tag{99}$$

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As a consequence, there exist smooth functions $\zeta_1, \zeta_2, \zeta_3, \zeta_4, \zeta_5, \zeta_6$, of B^2 such that

$$\eta_1 = \zeta_1(B^2), \qquad \eta_2 = B\zeta_2(B^2), \qquad \eta_3 = B^2\zeta_3(B^2), \qquad \eta_4 = B^2\zeta_4(B^2), \qquad (100)$$

$$\eta_5 = B^3\zeta_5(B^2), \qquad 2\eta_4 - \eta_3 = B^4\zeta_6(B^2). \tag{101}$$

Note in particular the relation $2\eta_4 - \eta_3 = B^4\varphi_6(B^2)$ which is not straightforward to devise intuitively. It is then possible to rewrite the viscous tensor as a smooth function of the magnetic field in the form

$$-\mathbf{\Pi} = \kappa(\partial_x \cdot v)\mathbf{I} + \zeta_1(B^2)\mathbf{S} + \zeta_2(B^2)\big(R(B)\mathbf{S} - \mathbf{S}R(B)\big) - \zeta_3(B^2)R(B)\mathbf{S}R(B)$$
$$- \zeta_6(B^2)B^t\mathbf{S}BB \otimes B + \zeta_4(B^2)(\mathbf{S}B \otimes B + B \otimes B\mathbf{S})$$
$$+ \zeta_5(B^2)(B \otimes B\mathbf{S}R(B) - R(B)\mathbf{S}B \otimes B),$$

using $B = B\mathcal{B}$ so that $\mathbf{\Pi}$ is a smooth function of B. Hence we obtain in the limit case the same contribution as with a zero magnetic field for the viscous stress tensor since $\zeta_1(0) = \eta_1(0) = \frac{1}{10}k_B T [\![\varphi^{\eta(1)}, \varphi^{\eta(1)}]\!]$.

7. Onsager reciprocal relations

Onsager relations are symmetry properties which must hold between the transport coefficients. These constraints express the invariance of phenomena by time reversal transformation. In the framework of the kinetic theory of gases, these symmetry properties can directly be deduced from the symmetry properties of the linearized collision operator [1, 6, 25, 40].

Using the tensorial relations (95) and (96), Onsager reciprocal relations require that

$$D_{ij}(-B) = D_{ji}(B)^t, \qquad \theta_i(-B) = \theta_i(B)^t, \qquad \widehat{\lambda}(-B) = \widehat{\lambda}(B)^t,$$

and these equalities are easily established since the matrices $\mathbf{M}^\|$ and $\mathbf{M}^\perp$ are symmetric, the matrix $\mathbf{M}^\odot$ is antisymmetric, the matrices $\mathbf{M}^\|$ and $\mathbf{M}^\perp$ are even functions of B the matrix $\mathbf{M}^\odot$ is an odd function of B, the transport coefficients $D_{ij}^\|, D_{ij}^\perp, D_{ij}^\odot, i, j \in \mathcal{S}, \theta_i^\|, \theta_i^\perp, \theta_i^\odot, i \in \mathcal{S}, \widehat{\lambda}^\|, \widehat{\lambda}^\perp, \widehat{\lambda}^\odot$ are even functions of B because they only depend on the norm B of the magnetic field, and the transport coefficients satisfy $D_{ij}^\| = D_{ji}^\|, D_{ij}^\perp = D_{ji}^\perp, D_{ij}^\odot = D_{ji}^\odot, i, j \in \mathcal{S}$, as a result of (50), (54) and (55).

In order to express Onsager relations for viscosity coefficients, we rewrite the three columns of the viscous stress tensor in the form

$$\mathbf{\Pi}_i = -\sum_{j=1}^3 \big(\kappa\mathbf{M}_{ij}^\kappa + \eta_1\mathbf{M}_{ij}^{\eta_1} + \eta_2\mathbf{M}_{ij}^{\eta_2} + \eta_3\mathbf{M}_{ij}^{\eta_3} + \eta_4\mathbf{M}_{ij}^{\eta_4} + \eta_5\mathbf{M}_{ij}^{\eta_5}\big)\partial_j v, \qquad i \in \{1, 2, 3\},$$

where $\mathbf{\Pi}_i$ is the ith column of $\mathbf{\Pi}$, $i \in \{1, 2, 3\}$ and the matrices $\mathbf{M}_{ij}^\kappa, \mathbf{M}_{ij}^{\eta_\alpha}, i, j \in \{1, 2, 3\}, \alpha \in \{1, 2, 3, 4, 5\}$, are defined by

$$\mathbf{M}_{ij}^\kappa = e_i \otimes e_j,$$
$$\mathbf{M}_{ij}^{\eta_1} = \delta_{ij}\mathbf{I} + e_j \otimes e_i - \tfrac{2}{3}e_i \otimes e_j,$$
$$\mathbf{M}_{ij}^{\eta_2} = 2\delta_{ij}R(\mathcal{B}) + R(e_i)R(\mathcal{B})R(e_j) + 2e_i{}^t R(\mathcal{B})e_j \mathbf{I},$$
$$\mathbf{M}_{ij}^{\eta_3} = 2\mathcal{B}_i\mathcal{B}_j\mathcal{B} \otimes \mathcal{B} - \tfrac{2}{3}e_i \otimes e_j + 2R(\mathcal{B})e_j \otimes e_i R(\mathcal{B}) - R(\mathcal{B})e_i \otimes e_j R(\mathcal{B}),$$
$$\mathbf{M}_{ij}^{\eta_4} = -4\mathcal{B}_i\mathcal{B}_j\mathcal{B} \otimes \mathcal{B} + \mathcal{B}_i\mathcal{B}_j\mathbf{I} + \delta_{ij}\mathcal{B} \otimes \mathcal{B} + \mathcal{B}_i e_j \otimes \mathcal{B} + \mathcal{B}_j\mathcal{B} \otimes e_i,$$
$$\mathbf{M}_{ij}^{\eta_5} = -2\mathcal{B}_i\mathcal{B}_j R(\mathcal{B}) - R(e_i)R(\mathcal{B})R(e_j) - 2e_i{}^t R(\mathcal{B})e_j\mathcal{B} \otimes \mathcal{B},$$

Table 1. Main transport linear systems.

Systems	Size	Constraints	Coefficients
$H\alpha^{\eta(1)} = \beta^{\eta}$	n^s	–	$\eta_1 + \mathrm{i}\eta_2 = \frac{1}{2}\langle \alpha^{\eta(1)} + \alpha^{\eta(2)}, \beta^{\eta}\rangle$
$(H + 2\mathrm{i}H^B)\alpha^{\eta(2)} = \beta^{\eta}$			$\eta_1 + \eta_3 = \langle \alpha^{\eta(1)}, \beta^{\eta}\rangle$
$(H + \mathrm{i}H^B)\alpha^{\eta(3)} = \beta^{\eta}$			$\eta_4 + \mathrm{i}\eta_5 + \eta_1 + \mathrm{i}\eta_2 = \langle \alpha^{\eta(3)}, \beta^{\eta}\rangle$
$L\alpha^{D_j(1)} = \beta^{D_j}$	$2n^s + n^p$	$\langle \alpha^{D_j(1)}, \mathcal{Y}\rangle = 0$	$D_{ij}^{\parallel} = \langle \alpha^{D_j(1)}, \beta^{D_i}\rangle$
$(L + \mathrm{i}L^B)\alpha^{D_j(2)} = \beta^{D_j}$		$\langle \alpha^{D_j(2)}, \mathcal{Y}\rangle = 0$	$D_{ij}^{\perp} + \mathrm{i}D_{ij}^{\odot} = \langle \alpha^{D_j(2)}, \beta^{D_i}\rangle$
$L\alpha^{\widehat{\lambda}(1)} = \beta^{\widehat{\lambda}}$	$2n^s + n^p$	$\langle \alpha^{\widehat{\lambda}(1)}, \mathcal{Y}\rangle = 0$	$\widehat{\lambda}^{\parallel} = (p/T)\langle \alpha^{\widehat{\lambda}(1)}, \beta^{\widehat{\lambda}}\rangle$
$(L + \mathrm{i}L^B)\alpha^{\widehat{\lambda}(2)} = \beta^{\widehat{\lambda}}$		$\langle \alpha^{\widehat{\lambda}(2)}, \mathcal{Y}\rangle = 0$	$\widehat{\lambda}^{\perp} + \mathrm{i}\widehat{\lambda}^{\odot} = (p/T)\langle \alpha^{\widehat{\lambda}(2)}, \beta^{\widehat{\lambda}}\rangle$
			$\theta_i^{\parallel} = -\langle \alpha^{\widehat{\lambda}(1)}, \beta^{D_i}\rangle$
			$\theta_i^{\perp} + \mathrm{i}\theta_i^{\odot} = -\langle \alpha^{\widehat{\lambda}(2)}, \beta^{D_i}\rangle$
$\Lambda\alpha^{\lambda(1)} = \beta^{\lambda}$	$n^s + n^p$	–	$\lambda^{\parallel} = (p/T)\langle \alpha^{\lambda(1)}, \beta^{\lambda}\rangle$
$(\Lambda + \mathrm{i}\Lambda^B)\alpha^{\lambda(2)} = \beta^{\lambda}$			$\lambda^{\perp} + \mathrm{i}\lambda^{\odot} = (p/T)\langle \alpha^{\lambda(2)}, \beta^{\lambda}\rangle$
			$\chi^{\parallel} = L^{00\lambda}\alpha^{\lambda(1)}$
			$\chi^{\perp} + \mathrm{i}\chi^{\odot} = L^{00\lambda}\alpha^{\lambda(2)}$

where (e_1, e_2, e_3) denotes the canonical basis. Onsager relations require that

$$\left(\kappa\mathbf{M}_{ij}^{\kappa} + \eta_1\mathbf{M}_{ij}^{\eta_1} + \eta_2\mathbf{M}_{ij}^{\eta_2} + \eta_3\mathbf{M}_{ij}^{\eta_3} + \eta_4\mathbf{M}_{ij}^{\eta_4} + \eta_5\mathbf{M}_{ij}^{\eta_5}\right)(-B)$$
$$= \left(\kappa\mathbf{M}_{ji}^{\kappa} + \eta_1\mathbf{M}_{ji}^{\eta_1} + \eta_2\mathbf{M}_{ji}^{\eta_2} + \eta_3\mathbf{M}_{ji}^{\eta_3} + \eta_4\mathbf{M}_{ji}^{\eta_4} + \eta_5\mathbf{M}_{ji}^{\eta_5}\right)^t(B), \qquad i, j \in \{1, 2, 3\},$$

but these equalities are easily established since the matrix $R(X)$ is antisymmetric for any vector X, the matrix $R(B)$ is an odd function of B, the viscosities $\kappa, \eta_{\alpha}, \alpha \in \{1, 2, 3, 4, 5\}$, are even functions of B because they only depend on the norm of the magnetic field.

8. Conclusion

We have investigated the properties of the species perturbed distribution functions and the corresponding integral equations associated with the transport coefficients. The main transport linear systems obtained for the transport coefficients are summarized in table 1. The numerical simulations for high temperature air have shown that iterative techniques constitute a good trade off between precision and computational costs. It is likely that this conclusion is valid for higher order approximations of the transport coefficients.

Acknowledgments

Appendix A. Proof of the symmetry properties

In order to establish (54) and (55) for instance, we note that

$$\mathrm{Im}[\![\varphi^{D_i(2)}, \varphi^{D_j(2)}]\!] = [\![\mathrm{Im}\,\varphi^{D_i(2)}, \mathrm{Re}\,\varphi^{D_j(2)}]\!] - [\![\mathrm{Re}\,\varphi^{D_i(2)}, \mathrm{Im}\,\varphi^{D_j(2)}]\!]. \qquad (A.1)$$

Table B1. Reduced transport linear systems.

Systems	Size	Constraints	Coefficients
$\Delta\alpha_{[00]}^{D_j(1)} = \beta_{[00]}^{D_j}$	n^s	$\langle\alpha_{[00]}^{D_j(1)}, Y\rangle = 0$	$D_{[00]ij}^{\parallel} = \langle\alpha_{[00]}^{D_j(1)}, \beta_{[00]}^{D_i}\rangle$
$(\Delta + \mathrm{i}\Delta^B)\alpha_{[00]}^{D_j(2)} = \beta_{[00]}^{D_j}$		$\langle\alpha_{[00]}^{D_j(2)}, Y\rangle = 0$	$D_{[00]ij}^{\perp} + \mathrm{i}D_{[00]ij}^{\odot} = \langle\alpha_{[00]}^{D_j(2)}, \beta_{[00]}^{D_i}\rangle$
$\Lambda_{[e]}\alpha_{[e]}^{\lambda(1)} = \beta_{[e]}^{\lambda}$	n^s	–	$\lambda_{[e]}^{\parallel} = (p/T)\langle\alpha_{[e]}^{\lambda(1)}, \beta_{[e]}^{\lambda}\rangle$
$(\Lambda_{[e]} + \mathrm{i}\Lambda_{[e]})\alpha_{[e]}^{\lambda(2)} = \beta_{[e]}^{\lambda}$			$\lambda_{[e]}^{\perp} + \mathrm{i}\lambda_{[e]}^{\odot} = (p/T)\langle\alpha_{[e]}^{\lambda(2)}, \beta_{[e]}^{\lambda}\rangle$

By using the imaginary part of the second equations in (46), however, we also obtain that $\mathcal{F}^{\mathcal{S}}(\mathrm{Im}\,\varphi^{D_i(2)}) = -B\mathcal{F}^{z,v}(\mathrm{Re}\,\varphi^{D_i(2)})$, thanks to $\mathrm{Im}\,\Psi^{D_j} = 0$. Since $\mathcal{F}^{\mathcal{S}}$ is self-adjoint we next have

$$[\![\mathrm{Im}\,\varphi^{D_i(2)}, \mathrm{Re}\,\varphi^{D_j(2)}]\!] = \langle\!\langle f^0\mathcal{F}^{\mathcal{S}}\,\mathrm{Im}\,\varphi^{D_i(2)}, \mathrm{Re}\,\varphi^{D_j(2)}\rangle\!\rangle = -\langle\!\langle f^0 B\mathcal{F}^{z,v}\,\mathrm{Re}\,\varphi^{D_i(2)}, \mathrm{Re}\,\varphi^{D_j(2)}\rangle\!\rangle,$$

$$[\![\mathrm{Re}\,\varphi^{D_i(2)}, \mathrm{Im}\,\varphi^{D_j(2)}]\!] = \langle\!\langle f^0\mathrm{Re}\,\varphi^{D_i(2)}, \mathcal{F}^{\mathcal{S}}\,\mathrm{Im}\,\varphi^{D_j(2)}\rangle\!\rangle = -\langle\!\langle f^0\,\mathrm{Re}\,\varphi^{D_i(2)}, B\mathcal{F}^{z,v}\,\mathrm{Re}\,\varphi^{D_j(2)}\rangle\!\rangle,$$

so that $[\![\mathrm{Im}\,\varphi^{D_i(2)}, \mathrm{Re}\,\varphi^{D_j(2)}]\!] = [\![\mathrm{Re}\,\varphi^{D_i(2)}, \mathrm{Im}\,\varphi^{D_j(2)}]\!] = -((\mathrm{Re}\,\varphi^{D_i(2)}, \mathrm{Re}\,\varphi^{D_j(2)}))$ since the integral operator $\mathcal{F}^{z,v}$ is self-adjoint over the functionals orthogonal to collisional invariants. It is similarly established that $\mathrm{Im}((\varphi^{D_i(2)}, \varphi^{D_j(2)})) = 0$ so that both quantities $[\![\varphi^{D_i(2)}, \varphi^{D_j(2)}]\!]$ and $((\varphi^{D_i(2)}, \varphi^{D_j(2)}))$ are real and (51) completes the proof of (54) and (55). The relations (56) and (57), and (61) and (62), are established in a similar way.

Appendix B. Reduced transport linear systems

Reduced transport linear systems are obtained by using variational approximation spaces of smaller dimensions. These coefficients are sometimes very good approximations of the higher order coefficients. We refer to [17] for a detailed discussion in the situation of neutral gases. We have already presented in section 4.6 the transport linear systems associated with the first-order transport coefficients.

For the thermal conductivity, it is also possible to use a reduced linear system associated with the total energy vector functionals ϕ^{10ek}, $k \in \mathcal{S}$, defined by $\phi^{10ek} = \phi^{1010k} + \phi^{1001k}$ if $k \in \mathcal{P}$, and $\phi^{10ek} = \phi^{1010k}$ for monatomic species $k \in \mathcal{S}\backslash\mathcal{P}$. The corresponding reduced linear systems of size n^s are associated with the matrices $\Lambda_{[e]}$ and $\Lambda_{[e]} + \mathrm{i}\Lambda_{[e]}^B$, where $\Lambda_{[e]}$ is explicited in [16, 17] and where $\Lambda_{[e]}^B$ is the diagonal matrix defined by $\Lambda_{[e]kk}^B = c_{pk}n_k e_k B/p$, $k \in \mathcal{S}$. The right-hand side vector $\beta_{[e]}^{\lambda} \in \mathbb{R}^{n^s}$ is given by $\beta_{[e]k}^{\lambda} = c_{pk}X_k/k_{\mathrm{B}}$. It is also possible to define the corresponding diffusion coefficients $D_{[e]}$, thermal diffusion coefficients $\theta_{[e]}$ and thermal diffusion ratios $\chi_{[e]}$ parallel, perpendicular and transverse to the magnetic field generalizing the situation of non-ionized mixtures [17] but the details are omitted. These reduced linear systems generally yield accurate results at lower computational costs. For weakly ionized air at high temperature we have found that the reduced thermal conductivities are usually within one percent of the more accurate conductivity whereas the thermal diffusion ratios are only accurate within ten percents. The transport linear systems associated with the first-order diffusion coefficients and the approximated thermal conductivity are summarized in table B1.

Appendix C. Coefficients of the matrices Λ, L^{0010} and L^{0001}

The coefficients of the matrix Λ are intricated expressions that can be written in the form [17]

$$\Lambda_{kk}^{1010} = \sum_{\substack{l \in \mathcal{S} \\ l \neq k}} \frac{X_k X_l}{\mathcal{D}_{kl}} \frac{m_k m_l}{(m_k + m_l)^2} \left[\frac{15}{2} \frac{m_k}{m_l} + \frac{25}{4} \frac{m_l}{m_k} - 3 \frac{m_l}{m_k} \bar{B}_{kl} + 4 \bar{A}_{kl} \right.$$

$$\left. + \frac{25}{12} \frac{\llbracket (\Delta \epsilon_{kl})^2 \rrbracket_{kl}}{\Omega_{kl}^{(1,1)}} \right] + \frac{X_k^2}{2\mathcal{D}_{kk}} \left[4 \bar{A}_{kk} + \frac{25}{12} \frac{\llbracket (\Delta \epsilon_{kk})^2 \rrbracket_{kk}}{\Omega_{kk}^{(1,1)}} \right], \qquad k \in \mathcal{S},$$

$$\Lambda_{kl}^{1010} = -\frac{X_k X_l}{\mathcal{D}_{kl}} \frac{m_k m_l}{(m_k + m_l)^2} \left[\frac{55}{4} - 3 \bar{B}_{kl} - 4 \bar{A}_{kl} - \frac{25}{12} \frac{\llbracket (\Delta \epsilon_{kl})^2 \rrbracket_{kl}}{\Omega_{kl}^{(1,1)}} \right], \qquad k, l \in \mathcal{S}, k \neq l,$$

$$\Lambda_{kk}^{1001} = -\sum_{\substack{l \in \mathcal{S} \\ l \neq k}} \frac{X_k X_l}{\mathcal{D}_{kl}} \frac{m_k}{m_k + m_l} \left[\frac{5}{4} \frac{\llbracket \Delta \epsilon_k \Delta \epsilon_{kl} \rrbracket_{kl}}{\Omega_{kl}^{(1,1)}} + \frac{5}{2} \frac{m_l}{m_k} \frac{\llbracket \epsilon_{kk}^0 (\gamma^2 - \gamma \gamma' \cos \chi) \rrbracket_{kl}}{\Omega_{kl}^{(1,1)}} \right.$$

$$\left. - \frac{m_l}{m_k} \frac{\llbracket \epsilon_{kk}^0 (\gamma^4 - \gamma \gamma'^3 \cos \chi) \rrbracket_{kl}}{\Omega_{kl}^{(1,1)}} \right] - \frac{5}{8} \frac{X_k^2}{\mathcal{D}_{kk}} \frac{\llbracket (\Delta \epsilon_{kk})^2 \rrbracket_{kk}}{\Omega_{kk}^{(1,1)}}, \qquad k \in \mathcal{P},$$

$$\Lambda_{kl}^{1001} = \frac{X_k X_l}{\mathcal{D}_{kl}} \frac{m_l}{m_k + m_l} \left[-\frac{5}{4} \frac{\llbracket \widetilde{\Delta} \epsilon_l \Delta \epsilon_{kl} \rrbracket_{kl}}{\Omega_{kl}^{(1,1)}} + \frac{5}{2} \frac{\llbracket \epsilon_{lL}^0 (\gamma^2 - \gamma \gamma' \cos \chi) \rrbracket_{kl}}{\Omega_{kl}^{(1,1)}} \right.$$

$$\left. - \frac{\llbracket \epsilon_{lL}^0 (\gamma^4 - \gamma \gamma'^3 \cos \chi) \rrbracket_{kl}}{\Omega_{kl}^{(1,1)}} \right], \qquad k \in \mathcal{S}, \quad l \in \mathcal{P}, \quad k \neq l,$$

$$\Lambda_{kk}^{0101} = \sum_{\substack{l \in \mathcal{S} \\ l \neq k}} X_k X_l \left[\frac{c_k^{\text{int}}}{k_B \mathcal{D}_{k \text{int}, l}} + \frac{3}{4} \frac{m_k}{m_l} \frac{\llbracket (\Delta \epsilon_k)^2 \rrbracket_{kl}}{\Omega_{kl}^{(1,1)} \mathcal{D}_{kl}} \right]$$

$$+ X_k^2 \left[\frac{c_k^{\text{int}}}{k_B \mathcal{D}_{k \text{int}, k}} + \frac{3}{8} \frac{\llbracket (\Delta \epsilon_{kk})^2 \rrbracket_{kk}}{\Omega_{kk}^{(1,1)} \mathcal{D}_{kk}} \right], \qquad k \in \mathcal{P},$$

$$\Lambda_{kl}^{0101} = -X_k X_l \left[\frac{\llbracket \epsilon_{kk}^0 (\epsilon_{lL}^0 \gamma^2 - \epsilon_{lL'}^0 \gamma \gamma' \cos \chi) \rrbracket_{kl}}{\Omega_{kl}^{(1,1)} \mathcal{D}_{kl}} - \frac{3}{4} \frac{\llbracket \Delta \epsilon_k \widetilde{\Delta} \epsilon_l \rrbracket_{kl}}{\Omega_{kl}^{(1,1)} \mathcal{D}_{kl}} \right], \qquad k, l \in \mathcal{P}, \quad k \neq l,$$

where $\llbracket \cdot \rrbracket_{kl}$ is an averaging operator associated with collisions between the species pair (k, l). The details of the corresponding collision integrals are omitted for brevity and we refer to [17] for more details. Finally, the blocks L^{0010} and L^{0001} are given by

$$L_{kk}^{0010} = -\sum_{\substack{l \in \mathcal{S} \\ l \neq k}} \frac{X_k X_l}{2 \mathcal{D}_{kl}} \frac{m_l}{m_k + m_l} (6 \bar{c}_{kl} - 5), \qquad k \in \mathcal{S},$$

$$L_{kl}^{0010} = \frac{X_k X_l}{2 \mathcal{D}_{kl}} \frac{m_k}{m_k + m_l} (6 \bar{c}_{kl} - 5), \qquad k, l \in \mathcal{S}, \quad k \neq l,$$

$$L_{kk}^{0001} = -\sum_{\substack{l \in \mathcal{S} \\ l \neq k}} X_k X_l \frac{\llbracket \epsilon_{kk}^0 (\gamma^2 - \gamma \gamma' \cos \chi) \rrbracket_{kl}}{\Omega_{kl}^{(1,1)} \mathcal{D}_{kl}}, \qquad k \in \mathcal{P},$$

$$L_{kl}^{0001} = X_k X_l \frac{\llbracket \epsilon_{lL}^0 (\gamma^2 - \gamma \gamma' \cos \chi) \rrbracket_{kl}}{\Omega_{kl}^{(1,1)} \mathcal{D}_{kl}}, \qquad k \in \mathcal{S}, \quad l \in \mathcal{P}, \quad k \neq l.$$

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