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Some solutions (linear in the spatial variables) and generalized Chapman–Enskog functions basic to the linearized Boltzmann equations for a binary mixture of rigid spheres

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Abstract. A Legendre expansion of the (matrix) scattering kernel relevant to the (vector-valued) linearized Boltzmann equation for a binary mixture of rigid spheres is used to define twelve solutions that are linear in the spatial variables $\{x, y, z\}$. The twelve (asymptotic) solutions are expressed in terms of three vector-valued functions $\boldsymbol{A}^{(1)}(c)$, $\boldsymbol{A}^{(2)}(c)$, and $\boldsymbol{B}(c)$. These functions are generalizations of the Chapman–Enskog functions used to define asymptotic solutions and viscosity and heat conduction coefficients for the case of a single-species gas. To provide evidence that the three Chapman–Enskog vectors exist as solutions of the defining linear integral equations, numerical results developed in terms of expansions based on Hermite cubic splines and a collocation scheme are reported for two binary mixtures (Ne-Ar and He-Xe) with various molar concentrations.

Keywords. Rarefied gas dynamics, binary mixtures, rigid spheres.

1. Introduction

In a recent work, Garcia, Siewert and Williams [1] reported explicit forms of the collision operators required to establish the linearized (vector-valued) Boltzmann equation for a binary mixture of rigid spheres that are assumed to scatter isotropically in the center-of-mass system. In a subsequent work, Garcia and Siewert [2] used the GSW expressions [1] for the matrix scattering kernel to establish a basic flow condition and to confirm the validity of six exact solutions (corresponding to conservation of number, energy and momentum) of the relevant Boltzmann equation. In this work we use a Legendre expansion of the scattering kernel to define twelve additional (asymptotic) solutions that are linear in the spatial variables $\{x, y, z\}$, and to provide evidence that three required Chapman–Enskog (vector-valued) functions exist, numerical results for these functions are reported for two binary mixtures with various molar concentrations of each species.

To start this work, we write the coupled linearized Boltzmann equations for the considered binary mixture of rigid spheres in the form reported by Garcia,

Siewert and Williams [1], viz.

$$\boldsymbol{c}\cdot\nabla_r h_\alpha(\boldsymbol{r},\boldsymbol{c})+\varpi_\alpha(c)h_\alpha(\boldsymbol{r},\boldsymbol{c})=\sum_{\beta=1}^{2}\int \mathrm{e}^{-c'^2}K_{\alpha,\beta}(\boldsymbol{c}':\boldsymbol{c})h_\beta(\boldsymbol{r},\boldsymbol{c}')\mathrm{d}^3c',\quad \alpha=1,2, \tag{1}$$

where $\boldsymbol{r}$, with Cartesian coordinates $\{x,y,z\}$, is the spatial variable and $\boldsymbol{c}$, with coordinates $\{c_x,c_y,c_z\}$ and magnitude c, denotes the dimensionless velocity vector. In addition

$$K_{1,1}(\boldsymbol{c}':\boldsymbol{c})=4n_1\sigma_{1,1}\pi^{1/2}\mathcal{P}(\boldsymbol{c}':\boldsymbol{c})+n_2\sigma_{1,2}\pi^{1/2}\mathcal{F}_{1,2}(\boldsymbol{c}':\boldsymbol{c}), \tag{2}$$

$$K_{1,2}(\boldsymbol{c}':\boldsymbol{c})=4n_2\sigma_{1,2}\pi^{1/2}\mathcal{G}_{1,2}(\boldsymbol{c}':\boldsymbol{c}), \tag{3}$$

$$K_{2,1}(\boldsymbol{c}':\boldsymbol{c})=4n_1\sigma_{2,1}\pi^{1/2}\mathcal{G}_{2,1}(\boldsymbol{c}':\boldsymbol{c}), \tag{4}$$

and

$$K_{2,2}(\boldsymbol{c}':\boldsymbol{c})=4n_2\sigma_{2,2}\pi^{1/2}\mathcal{P}(\boldsymbol{c}':\boldsymbol{c})+n_1\sigma_{2,1}\pi^{1/2}\mathcal{F}_{2,1}(\boldsymbol{c}':\boldsymbol{c}). \tag{5}$$

Here

$$\mathcal{P}(\boldsymbol{c}':\boldsymbol{c})=\frac{1}{\pi}\Big(\frac{2}{|\boldsymbol{c}'-\boldsymbol{c}|}\exp\Big\{\frac{|\boldsymbol{c}'\times\boldsymbol{c}|^2}{|\boldsymbol{c}'-\boldsymbol{c}|^2}\Big\}-|\boldsymbol{c}'-\boldsymbol{c}|\Big) \tag{6}$$

is the basic kernel for a single-species gas used by Pekeris [3],

$$\mathcal{F}_{\alpha,\beta}(\boldsymbol{c}':\boldsymbol{c})=\mathcal{F}(a_{\alpha,\beta};\boldsymbol{c}':\boldsymbol{c}), \tag{7}$$

and

$$\mathcal{G}_{\alpha,\beta}(\boldsymbol{c}':\boldsymbol{c})=\mathcal{G}(a_{\alpha,\beta};\boldsymbol{c}':\boldsymbol{c}), \tag{8}$$

where

$$a_{\alpha,\beta}=(m_\beta/m_\alpha)^{1/2}, \tag{9}$$

$$\mathcal{F}(a;\boldsymbol{c}':\boldsymbol{c})=\frac{(a+1/a)^2}{\pi a|\boldsymbol{c}'-\boldsymbol{c}|}\exp\Big\{a^2\frac{|\boldsymbol{c}'\times\boldsymbol{c}|^2}{|\boldsymbol{c}'-\boldsymbol{c}|^2}-\frac{(a-1/a)^2(c'^2+c^2)}{4}-\frac{(a^2-1/a^2)\boldsymbol{c}'\cdot\boldsymbol{c}}{2}\Big\}, \tag{10}$$

and

$$\mathcal{G}(a;\boldsymbol{c}':\boldsymbol{c})=\frac{1}{a\pi}\big|\boldsymbol{c}'-a\boldsymbol{c}\big|[J(a;\boldsymbol{c}':\boldsymbol{c})-1]. \tag{11}$$

In addition,

$$\varpi_\alpha(c)=\varpi_\alpha^{(1)}(c)+\varpi_\alpha^{(2)}(c), \tag{12}$$

with

$$\varpi_\alpha^{(\beta)}(c)=4\pi^{1/2}n_\beta\sigma_{\alpha,\beta}a_{\beta,\alpha}\nu(a_{\alpha,\beta}c) \tag{13}$$

and

$$\nu(c)=\frac{2c^2+1}{c}\int_0^c \mathrm{e}^{-x^2}\mathrm{d}x+\mathrm{e}^{-c^2}. \tag{14}$$

Since Eq. (1) is written in terms of a dimensionless velocity variable $\boldsymbol{c}$, we note that the basic velocity distribution functions are available from

$$f_\alpha(\boldsymbol{r},\boldsymbol{v}) = f_{\alpha,0}(v)[1 + h_\alpha(\boldsymbol{r},\lambda_\alpha^{1/2}\boldsymbol{v})], \tag{15}$$

where $\lambda_\alpha = m_\alpha/(2kT_0)$ and where

$$f_{\alpha,0}(v) = n_\alpha(\lambda_\alpha/\pi)^{3/2}\mathrm{e}^{-\lambda_\alpha v^2} \tag{16}$$

is the Maxwellian distribution for n_α particles of mass m_α in equilibrium at temperature T_0. Note that k is the Boltzmann constant. To complete our starting equations, we note from Ref. [2] that

$$J(a;\boldsymbol{c}':\boldsymbol{c}) = \frac{(a+1/a)^2}{2\Delta(a;\boldsymbol{c}':\boldsymbol{c})}\exp\Big\{\frac{-2C(a;\boldsymbol{c}':\boldsymbol{c})}{(a-1/a)^2}\Big\}\sinh\Big\{\frac{2\Delta(a;\boldsymbol{c}':\boldsymbol{c})}{(a-1/a)^2}\Big\}, \quad a \neq 1, \tag{17a}$$

and

$$J(a;\boldsymbol{c}':\boldsymbol{c}) = \frac{1}{|\boldsymbol{c}'-\boldsymbol{c}|^2}\exp\Big\{\frac{|\boldsymbol{c}'\times\boldsymbol{c}|^2}{|\boldsymbol{c}'-\boldsymbol{c}|^2}\Big\}, \quad a = 1, \tag{17b}$$

where, to write Eq. (17a), we have used the definitions [2]

$$\Delta(a;\boldsymbol{c}':\boldsymbol{c}) = \big\{C^2(a;\boldsymbol{c}':\boldsymbol{c}) + (a-1/a)^2|\boldsymbol{c}'\times\boldsymbol{c}|^2\big\}^{1/2} \tag{18}$$

and

$$C(a;\boldsymbol{c}':\boldsymbol{c}) = {c'}^2 + c^2 - (a+1/a)\boldsymbol{c}'\cdot\boldsymbol{c}. \tag{19}$$

Finally, and to be clear, we note that we use $\sigma_{\alpha,\beta}$ to denote the differential-scattering cross section, which for the case of rigid-sphere scattering that is isotropic in the center-of-mass system we write, after consultation with Chapman and Cowling [4], as

$$\sigma_{\alpha,\beta} = \frac{1}{4}\Big(\frac{d_\alpha + d_\beta}{2}\Big)^2, \tag{20}$$

where d_1 and d_2 are the atomic diameters of the two types of gas particles.

2. Exact solutions

To be complete, we repeat here a listing of the exact solutions of Eq. (1) that were discussed in our previous work [2]. But first, we rewrite Eq. (1) as

$$\boldsymbol{c}\cdot\nabla_r\boldsymbol{H}(\boldsymbol{r},\boldsymbol{c}) + \boldsymbol{\Sigma}(c)\boldsymbol{H}(\boldsymbol{r},\boldsymbol{c}) = \int \mathrm{e}^{-c'^2}\boldsymbol{K}(\boldsymbol{c}':\boldsymbol{c})\boldsymbol{H}(\boldsymbol{r},\boldsymbol{c}')\mathrm{d}^3c', \tag{21}$$

where

$$\boldsymbol{H}(\boldsymbol{r},\boldsymbol{c}) = \begin{bmatrix} h_1(\boldsymbol{r},\boldsymbol{c}) \\ h_2(\boldsymbol{r},\boldsymbol{c}) \end{bmatrix} \tag{22}$$

and

$$\boldsymbol{K}(\boldsymbol{c}':\boldsymbol{c}) = \begin{bmatrix} K_{1,1}(\boldsymbol{c}':\boldsymbol{c}) & K_{1,2}(\boldsymbol{c}':\boldsymbol{c}) \\ K_{2,1}(\boldsymbol{c}':\boldsymbol{c}) & K_{2,2}(\boldsymbol{c}':\boldsymbol{c}) \end{bmatrix}. \tag{23}$$

Here the elements of the scattering matrix $\boldsymbol{K}(\boldsymbol{c}' : \boldsymbol{c})$ are given by Eqs. (2)–(5), and

$$\boldsymbol{\Sigma}(c) = \begin{bmatrix} \varpi_1(c) & 0 \\ 0 & \varpi_2(c) \end{bmatrix}. \tag{24}$$

In a recent work [5] in which the McCormack model [6] was used to describe a binary mixture of rigid spheres, six exact solutions related to the conservation of number, energy and momentum were reported (in our current notation) as

$$\boldsymbol{H}_1(\boldsymbol{r}, \boldsymbol{c}) = \boldsymbol{H}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \boldsymbol{H}_2(\boldsymbol{r}, \boldsymbol{c}) = \boldsymbol{H}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \tag{25a, b}$$

$$\boldsymbol{H}_3(\boldsymbol{r}, \boldsymbol{c}) = \boldsymbol{H}_3(c) = c^2 \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \boldsymbol{H}_4(\boldsymbol{r}, \boldsymbol{c}) = \boldsymbol{H}_4(\boldsymbol{c}) = c\mu \begin{bmatrix} 1 \\ a_{1,2} \end{bmatrix}, \tag{25c, d}$$

$$\boldsymbol{H}_5(\boldsymbol{r}, \boldsymbol{c}) = \boldsymbol{H}_5(\boldsymbol{c}) = c(1-\mu^2)^{1/2} \cos\phi \begin{bmatrix} 1 \\ a_{1,2} \end{bmatrix}, \tag{25e}$$

and

$$\boldsymbol{H}_6(\boldsymbol{r}, \boldsymbol{c}) = \boldsymbol{H}_6(\boldsymbol{c}) = c(1-\mu^2)^{1/2} \sin\phi \begin{bmatrix} 1 \\ a_{1,2} \end{bmatrix}. \tag{25f}$$

Here we use the spherical coordinates $\{c, \theta, \phi\}$, with $\mu = \cos\theta$, to define the dimensionless vector $\boldsymbol{c}$ so that $c_z = c\mu$, $c_x = c(1-\mu^2)^{1/2}\cos\phi$ and $c_y = c(1-\mu^2)^{1/2}\sin\phi$. As we have formally shown [2] that the six solutions listed as Eqs. (25) are valid also for the linearized Boltzmann equation considered in this work, we are ready now to discuss additional solutions.

3. A Legendre expansion and additional solutions

The exact solutions (collisional invariants) listed as Eqs. (25) are the results of the three conservation laws: number, energy and momentum. However, we have seen in regard to the linearized Boltzmann equation for a single-species gas [7] and for the McCormack model for binary mixtures [5] that we should expect also to find (asymptotic) solutions that are linear in the spatial variables. While, at this point, we are not able to define these solutions as explicitly as those given by Eqs. (25), we can compute these solutions. To start, we note that since the (matrix) kernel in Eq. (21) depends only on $\{c, c', \mu_0\}$, where $\boldsymbol{c}' \cdot \boldsymbol{c} = c'c\mu_0$, we can make use of a Legendre expansion and write

$$\boldsymbol{K}(\boldsymbol{c}' : \boldsymbol{c}) = \frac{1}{4\pi} \sum_{n=0}^{\infty} \sum_{m=0}^{n} (2n+1)(2-\delta_{0,m}) P_n^m(\mu') P_n^m(\mu) \boldsymbol{K}_n(c', c) \cos m(\phi' - \phi). \tag{26}$$

Here the *normalized* Legendre functions

$$P_n^m(\mu) = \left[\frac{(n-m)\,!}{(n+m)\,!}\right]^{1/2} (1-\mu^2)^{m/2} \frac{\mathrm{d}^m}{\mathrm{d}\mu^m} P_n(\mu), \quad n \geq m, \tag{27}$$

where $P_n(\mu)$ denotes one of Legendre polynomials, are such that

$$\int_{-1}^{1} P_n^m(\mu) P_{n'}^m(\mu) \mathrm{d}\mu = \Big(\frac{2}{2n+1}\Big)\delta_{n,n'}. \tag{28}$$

Given that we can write the scattering kernel as expressed in Eq. (26), we can use the solutions given by Eqs. (25) to conclude that

$$\Big\{\boldsymbol{\Sigma}(c) - \int_0^\infty \mathrm{e}^{-c'^2} \boldsymbol{K}_0(c',c) c'^2 \mathrm{d}c'\Big\} \left[\begin{array}{c} 1 \\ 0 \end{array}\right] = \boldsymbol{0}, \tag{29a}$$

$$\Big\{\boldsymbol{\Sigma}(c) - \int_0^\infty \mathrm{e}^{-c'^2} \boldsymbol{K}_0(c',c) c'^2 \mathrm{d}c'\Big\} \left[\begin{array}{c} 0 \\ 1 \end{array}\right] = \boldsymbol{0}, \tag{29b}$$

$$\Big\{c^2\boldsymbol{\Sigma}(c) - \int_0^\infty \mathrm{e}^{-c'^2} \boldsymbol{K}_0(c',c) c'^4 \mathrm{d}c'\Big\} \left[\begin{array}{c} 1 \\ 1 \end{array}\right] = \boldsymbol{0}, \tag{29c}$$

and

$$\Big\{c\boldsymbol{\Sigma}(c) - \int_0^\infty \mathrm{e}^{-c'^2} \boldsymbol{K}_1(c',c) c'^3 \mathrm{d}c'\Big\} \left[\begin{array}{c} 1 \\ a_{1,2} \end{array}\right] = \boldsymbol{0}. \tag{29d}$$

Now, to be more specific, we use the spatial variables $\{x, y, z\}$ to measure distances in the $\{\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}\}$ directions and rewrite Eq. (21) as

$$\Big\{c(1-\mu^2)^{1/2}\Big[\cos\phi\frac{\partial}{\partial x} + \sin\phi\frac{\partial}{\partial y}\Big] + c\mu\frac{\partial}{\partial z}\Big\}\boldsymbol{H}(\boldsymbol{r},\boldsymbol{c}) = \boldsymbol{\mathcal{L}}\{\boldsymbol{H}\}(\boldsymbol{r},\boldsymbol{c}), \tag{30}$$

where

$$\boldsymbol{\mathcal{L}}\{\boldsymbol{H}\}(\boldsymbol{r},\boldsymbol{c}) = -\boldsymbol{\Sigma}(c)\boldsymbol{H}(\boldsymbol{r},\boldsymbol{c}) + \int \mathrm{e}^{-c'^2} \boldsymbol{K}(\boldsymbol{c}' : \boldsymbol{c}) \boldsymbol{H}(\boldsymbol{r},\boldsymbol{c}') \mathrm{d}^3 c'. \tag{31}$$

Following a work [5] with the McCormack model, we seek additional solutions to Eq. (21) of the forms

$$\boldsymbol{H}_7(\boldsymbol{r},\boldsymbol{c}) = z\boldsymbol{\Phi}_1(c) - \mu\boldsymbol{F}^{(1)}(c) \tag{32a}$$

and

$$\boldsymbol{H}_8(\boldsymbol{r},\boldsymbol{c}) = z\boldsymbol{\Phi}_2(c) - \mu\boldsymbol{F}^{(2)}(c), \tag{32b}$$

where $\boldsymbol{\Phi}_1(c)$ and $\boldsymbol{\Phi}_2(c)$ are two (suitably chosen) linearly independent combinations of the solutions listed as Eqs. (25a,b,c) and where the vector-valued functions $\boldsymbol{F}^{(1)}(c)$ and $\boldsymbol{F}^{(2)}(c)$ are to be determined from the inhomogeneous integral equations

$$\boldsymbol{\Sigma}(c)\boldsymbol{F}^{(1)}(c) - \int_0^\infty \mathrm{e}^{-c'^2} \boldsymbol{K}_1(c',c) \boldsymbol{F}^{(1)}(c') c'^2 \mathrm{d}c' = c\boldsymbol{\Phi}_1(c) \tag{33a}$$

and

$$\boldsymbol{\Sigma}(c)\boldsymbol{F}^{(2)}(c) - \int_0^\infty \mathrm{e}^{-c'^2} \boldsymbol{K}_1(c',c) \boldsymbol{F}^{(2)}(c') c'^2 \mathrm{d}c' = c\boldsymbol{\Phi}_2(c). \tag{33b}$$

To establish a necessary solvability condition on the vector-valued functions $\boldsymbol{\Phi}_1(c)$ and $\boldsymbol{\Phi}_2(c)$, we first rewrite (in general terms) Eqs. (33) as

$$\boldsymbol{\Sigma}(c)\boldsymbol{F}(c) - \int_0^\infty \mathrm{e}^{-c'^2} \boldsymbol{K}_1(c', c)\boldsymbol{F}(c')c'^2 \mathrm{d}c' = \boldsymbol{R}(c). \tag{34}$$

We now let $c_\alpha = n_\alpha/(n_1 + n_2)$, multiply Eq. (34) by

$$\boldsymbol{\Pi}(c) = \left[\begin{array}{cc} c_1 & c_2 \end{array} \right] c^3 \mathrm{e}^{-c^2}, \tag{35}$$

and integrate over all c to find that $\boldsymbol{R}(c)$ must satisfy

$$\left[\begin{array}{cc} c_1 & c_2 \end{array} \right] \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{R}(c) c^3 \mathrm{d}c = 0. \tag{36}$$

In obtaining the condition listed as Eq. (36), we have used Eq. (29d) and the fact that, in general,

$$\boldsymbol{S}\boldsymbol{K}^T(\boldsymbol{c} : \boldsymbol{c}') = \boldsymbol{K}(\boldsymbol{c}' : \boldsymbol{c})\boldsymbol{S}, \tag{37}$$

where the superscript T denotes the transpose operation and where

$$\boldsymbol{S} = \left[\begin{array}{cc} c_2 & 0 \\ 0 & c_1 a_{1,2} \end{array} \right]. \tag{38}$$

Considering that the McCormack model for a binary mixture is a kinetic model which admits all of the exact solutions listed as Eqs. (25), we find it reasonable to speculate that the linear combinations $\boldsymbol{\Phi}_1(c)$ and $\boldsymbol{\Phi}_2(c)$ to be used in Eqs. (33) should be the same as those found [5] for the McCormack model, i.e.,

$$\boldsymbol{\Phi}_\alpha(c) = \boldsymbol{\Phi}_{\alpha,0} + (c^2 - 5/2)\boldsymbol{\Phi}_{\alpha,2}, \quad \alpha = 1, 2, \tag{39}$$

where

$$\boldsymbol{\Phi}_{1,0} = \left[\begin{array}{c} c_1 - 1 \\ c_1 \end{array} \right], \quad \boldsymbol{\Phi}_{1,2} = \left[\begin{array}{c} c_1 \\ c_1 \end{array} \right], \tag{40a, b}$$

$$\boldsymbol{\Phi}_{2,0} = \left[\begin{array}{c} c_2 \\ c_2 - 1 \end{array} \right], \quad \text{and} \quad \boldsymbol{\Phi}_{2,2} = \left[\begin{array}{c} c_2 \\ c_2 \end{array} \right]. \tag{40c, d}$$

It is a simple matter to show that $c\boldsymbol{\Phi}_1(c)$ and $c\boldsymbol{\Phi}_2(c)$ both satisfy the solvability condition listed as Eq. (36). Continuing to follow Ref. [5], we look for additional solutions expressed as

$$\boldsymbol{H}_9(\boldsymbol{r}, \boldsymbol{c}) = z\boldsymbol{H}_5(\boldsymbol{c}) - \mu(1 - \mu^2)^{1/2} \cos\phi \boldsymbol{F}(c) \tag{41a}$$

and

$$\boldsymbol{H}_{10}(\boldsymbol{r}, \boldsymbol{c}) = z\boldsymbol{H}_6(\boldsymbol{c}) - \mu(1 - \mu^2)^{1/2} \sin\phi \boldsymbol{F}(c), \tag{41b}$$

where the vector-valued function $\boldsymbol{F}(c)$ is to be determined from the inhomogeneous integral equation

$$\boldsymbol{\Sigma}(c)\boldsymbol{F}(c) - \int_0^\infty \mathrm{e}^{-c'^2} \boldsymbol{K}_2(c', c)\boldsymbol{F}(c')c'^2 \mathrm{d}c' = c^2\boldsymbol{\Phi}, \tag{42}$$

where

$$\mathbf{\Phi} = \begin{bmatrix} 1 \\ a_{1,2} \end{bmatrix}. \tag{43}$$

The proposed solutions listed in Eqs. (32) and (41) are to be used when a given problem has variations in the z direction, but we can list proposed solutions relevant to variations in the other two directions, i.e.,

$$\boldsymbol{H}_{11}(\boldsymbol{r},\boldsymbol{c}) = x\mathbf{\Phi}_1(c) - (1-\mu^2)^{1/2}\cos\phi\boldsymbol{F}^{(1)}(c), \tag{44a}$$

$$\boldsymbol{H}_{12}(\boldsymbol{r},\boldsymbol{c}) = x\mathbf{\Phi}_2(c) - (1-\mu^2)^{1/2}\cos\phi\boldsymbol{F}^{(2)}(c), \tag{44b}$$

$$\boldsymbol{H}_{13}(\boldsymbol{r},\boldsymbol{c}) = x\boldsymbol{H}_4(c) - \mu(1-\mu^2)^{1/2}\cos\phi\boldsymbol{F}(c), \tag{44c}$$

$$\boldsymbol{H}_{14}(\boldsymbol{r},\boldsymbol{c}) = x\boldsymbol{H}_6(\boldsymbol{c}) - (1-\mu^2)\cos\phi\sin\phi\boldsymbol{F}(c), \tag{44d}$$

$$\boldsymbol{H}_{15}(\boldsymbol{r},\boldsymbol{c}) = y\mathbf{\Phi}_1(c) - (1-\mu^2)^{1/2}\sin\phi\boldsymbol{F}^{(1)}(c), \tag{45a}$$

$$\boldsymbol{H}_{16}(\boldsymbol{r},\boldsymbol{c}) = y\mathbf{\Phi}_2(c) - (1-\mu^2)^{1/2}\sin\phi\boldsymbol{F}^{(2)}(c), \tag{45b}$$

$$\boldsymbol{H}_{17}(\boldsymbol{r},\boldsymbol{c}) = y\boldsymbol{H}_4(c) - \mu(1-\mu^2)^{1/2}\sin\phi\boldsymbol{F}(c), \tag{45c}$$

and

$$\boldsymbol{H}_{18}(\boldsymbol{r},\boldsymbol{c}) = y\boldsymbol{H}_5(\boldsymbol{c}) - (1-\mu^2)\sin\phi\cos\phi\boldsymbol{F}(c). \tag{45d}$$

While we have listed in this section additional solutions to Eq. (21), it is clear that more work must be done to justify these results. In particular, in order that the solutions proposed in this section be valid, it should be shown that solutions to the integral equations defined by Eqs. (33), (39), and (40) and Eqs. (42) and (43) actually exist. This, of course, will be a difficult task; in fact, we not aware of any such proofs even for the one-gas case. However, as has been done [8–10] for the one-gas case, we can provide some numerical evidence that the equivalent integral equations defined in this work for mixtures can be solved. And so in subsequent sections of this paper, we use Hermite cubic splines and a collocation scheme to solve normalized versions of Eqs. (33), (39), and (40) and Eqs. (42) and (43).

Before we can develop numerical solutions of the relevant integral equations, we must be able to compute well the Legendre components $\boldsymbol{K}_n(c',c)$ for the special cases of $n = 1$ and $n = 2$. However to solve well more general problems based on the Boltzmann equation, we will require $\boldsymbol{K}_n(c',c)$ for additional values of n, say $n = 0, 1, 2, ..., 8$, for example. And so, noting that the velocity dependence of $\boldsymbol{K}(\boldsymbol{c}' : \boldsymbol{c})$ can be expressed in terms of c', c, and μ_0, where $\boldsymbol{c}' \cdot \boldsymbol{c} = c'c\mu_0$, we can write

$$\boldsymbol{K}_n(c',c) = \pi^{1/2}\begin{bmatrix} K_n^{(1,1)}(c',c) & K_n^{(1,2)}(c',c) \\ K_n^{(2,1)}(c',c) & K_n^{(2,2)}(c',c) \end{bmatrix}, \tag{46}$$

where

$$K_n^{(1,1)}(c',c) = 4n_1\sigma_{1,1}\mathcal{P}^{(n)}(c',c) + n_2\sigma_{1,2}\mathcal{F}^{(n)}(a_{1,2};c',c) \tag{47a}$$

$$K_n^{(1,2)}(c',c) = 4n_2\sigma_{1,2}\mathcal{G}^{(n)}(a_{1,2};c',c), \tag{47b}$$

$$K_n^{(2,1)}(c',c) = 4n_1\sigma_{2,1}\mathcal{G}^{(n)}(a_{2,1};c',c), \tag{47c}$$

and

$$K_n^{(2,2)}(c',c) = 4n_2\sigma_{2,2}\mathcal{P}^{(n)}(c',c) + n_1\sigma_{2,1}\mathcal{F}^{(n)}(a_{2,1};c',c). \tag{47d}$$

Here the Legendre moments can be written as

$$\mathcal{P}^{(n)}(c',c) = 2\pi\int_{-1}^{1}\mathcal{P}(c',c,\mu_0)P_n(\mu_0)\mathrm{d}\mu_0, \tag{48}$$

$$\mathcal{F}^{(n)}(a;c',c) = 2\pi\int_{-1}^{1}\mathcal{F}(a;c',c,\mu_0)P_n(\mu_0)\mathrm{d}\mu_0, \tag{49}$$

and

$$\mathcal{G}^{(n)}(a;c',c) = 2\pi\int_{-1}^{1}\mathcal{G}(a;c',c,\mu_0)P_n(\mu_0)\mathrm{d}\mu_0, \tag{50}$$

where

$$\mathcal{P}(c',c,\mu_0) = \frac{1}{\pi}\Big[\frac{2}{r(c',c,\mu_0)}\exp\Big\{\frac{{c'}^2c^2(1-\mu_0^2)}{r^2(c',c,\mu_0)}\Big\} - r(c',c,\mu_0)\Big], \tag{51}$$

$$\mathcal{F}(a;c',c,\mu_0) = \frac{(a+1/a)^2}{\pi a r(c',c,\mu_0)}\exp\Big\{\frac{a^2{c'}^2c^2(1-\mu_0^2)}{r^2(c',c,\mu_0)} - \frac{(a-1/a)^2({c'}^2+c^2)}{4} - \frac{(a^2-1/a^2)c'c\mu_0}{2}\Big\}, \tag{52}$$

and

$$\mathcal{G}(a;c',c,\mu_0) = \frac{r(c',ac,\mu_0)}{\pi a}\big[J(a;c',c,\mu_0)-1\big], \tag{53}$$

with

$$J(a;c',c,\mu_0) = \frac{(a+1/a)^2}{2\Delta(a;c',c,\mu_0)}\exp\Big\{-\frac{2C(a;c',c,\mu_0)}{(a-1/a)^2}\Big\}\sinh\Big\{\frac{2\Delta(a;c',c,\mu_0)}{(a-1/a)^2}\Big\}, \tag{54a}$$

for $a \neq 1$, or

$$J(a;c',c,\mu_0) = \frac{1}{r^2(c',c,\mu_0)}\exp\Big\{\frac{{c'}^2c^2(1-\mu_0^2)}{r^2(c',c,\mu_0)}\Big\}, \tag{54b}$$

for $a = 1$. Here

$$r(c',c,\mu_0) = ({c'}^2 + c^2 - 2c'c\mu_0)^{1/2}, \tag{55}$$

$$C(a;c',c,\mu_0) = {c'}^2 + c^2 - (a+1/a)c'c\mu_0, \tag{56}$$

and

$$\Delta(a;c',c,\mu_0) = \big[C^2(a;c',c,\mu_0) + (a-1/a)^2{c'}^2c^2(1-\mu_0^2)\big]^{1/2}. \tag{57}$$

Note that

$$J(a;c',c,\mu_0) = J(a;c,c',\mu_0), \tag{58a}$$

$$J(a;c',c,\mu_0) = J(1/a;c',c,\mu_0), \tag{58b}$$

$$\mathcal{P}^{(n)}(c,c') = \mathcal{P}^{(n)}(c',c), \tag{59}$$

$$\mathcal{F}^{(n)}(a;c,c') = \mathcal{F}^{(n)}(a;c',c), \tag{60}$$

and

$$\mathcal{G}^{(n)}(a;c',c) = (1/a)\mathcal{G}^{(n)}(1/a;c,c'). \tag{61}$$

We choose to introduce

$$\varepsilon_0 = (n_1+n_2)\pi^{1/2}\Big(\frac{n_1d_1+n_2d_2}{n_1+n_2}\Big)^2 \tag{62}$$

and write the Boltzmann equation in the form

$$\boldsymbol{c}\cdot\nabla_r\boldsymbol{H}(\boldsymbol{r},\boldsymbol{c}) + \varepsilon_0\boldsymbol{V}(c)\boldsymbol{H}(\boldsymbol{r},\boldsymbol{c}) = \varepsilon_0\int \mathrm{e}^{-c'^2}\boldsymbol{\mathcal{K}}(\boldsymbol{c}':\boldsymbol{c})\boldsymbol{H}(\boldsymbol{r},\boldsymbol{c}')\mathrm{d}^3c', \tag{63}$$

where

$$\boldsymbol{V}(c) = (1/\varepsilon_0)\boldsymbol{\Sigma}(c) \tag{64}$$

and

$$\boldsymbol{\mathcal{K}}(\boldsymbol{c}':\boldsymbol{c}) = (1/\varepsilon_0)\boldsymbol{K}(\boldsymbol{c}':\boldsymbol{c}). \tag{65}$$

4. The generalized Chapman–Enskog functions

Having introduced ε_0 to normalize the considered Boltzmann equation, we now seek to solve Eqs. (33) and (42) rewritten as

$$\boldsymbol{V}(c)\boldsymbol{A}^{(1)}(c) - \int_0^\infty \mathrm{e}^{-c'^2}\boldsymbol{\mathcal{K}}_1(c',c)\boldsymbol{A}^{(1)}(c')c'^2\mathrm{d}c' = c\boldsymbol{\Phi}_1(c), \quad c\in[0,\infty), \tag{66a}$$

and

$$\boldsymbol{V}(c)\boldsymbol{A}^{(2)}(c) - \int_0^\infty \mathrm{e}^{-c'^2}\boldsymbol{\mathcal{K}}_1(c',c)\boldsymbol{A}^{(2)}(c')c'^2\mathrm{d}c' = c\boldsymbol{\Phi}_2(c), \quad c\in[0,\infty), \tag{66b}$$

and

$$\boldsymbol{V}(c)\boldsymbol{B}(c) - \int_0^\infty \mathrm{e}^{-c'^2}\boldsymbol{\mathcal{K}}_2(c',c)\boldsymbol{B}(c')c'^2\mathrm{d}c' = c^2\boldsymbol{\Phi}, \quad c\in[0,\infty), \tag{67}$$

where Eqs. (39), (40) and (43) are to be used. Here

$$\boldsymbol{A}^{(1)}(c) = \varepsilon_0\boldsymbol{F}^{(1)}(c), \quad \boldsymbol{A}^{(2)}(c) = \varepsilon_0\boldsymbol{F}^{(2)}(c), \quad \text{and} \quad \boldsymbol{B}(c) = \varepsilon_0\boldsymbol{F}(c). \tag{68a, b, c}$$

To be complete, we note that we have introduced $\boldsymbol{V}(c) = (1/\varepsilon_0)\boldsymbol{\Sigma}(c)$ and $\boldsymbol{\mathcal{K}}_n(c',c) = (1/\varepsilon_0)\boldsymbol{K}_n(c',c)$, so that

$$\boldsymbol{V}(c) = \begin{bmatrix} v_1(c) & 0 \\ 0 & v_2(c) \end{bmatrix}, \tag{69}$$

where now

$$v_1(c) = p_1\nu(c) + g_2a_{2,1}\nu(a_{1,2}c) \tag{70a}$$

and

$$v_2(c) = p_2\nu(c) + g_1 a_{1,2}\nu(a_{2,1}c), \tag{70b}$$

with

$$p_\alpha = c_\alpha\Big(\frac{nd_\alpha}{n_1d_1 + n_2d_2}\Big)^2, \quad \alpha = 1, 2, \tag{71a}$$

$$g_\alpha = c_\alpha\Big(\frac{nd_{\rm avg}}{n_1d_1 + n_2d_2}\Big)^2, \quad \alpha = 1, 2, \tag{71b}$$

$$n = n_1 + n_2, \quad \text{and} \quad d_{\rm avg} = (d_1 + d_2)/2. \tag{72a, b}$$

In addition,

$$\boldsymbol{\mathcal{K}}_n(c', c) = \left[\begin{array}{cc} \mathcal{K}_n^{(1,1)}(c', c) & \mathcal{K}_n^{(1,2)}(c', c) \\ \mathcal{K}_n^{(2,1)}(c', c) & \mathcal{K}_n^{(2,2)}(c', c) \end{array}\right], \tag{73}$$

where

$$\mathcal{K}_n^{(1,1)}(c', c) = p_1\mathcal{P}^{(n)}(c', c) + (g_2/4)\mathcal{F}^{(n)}(a_{1,2}; c', c), \tag{74a}$$

$$\mathcal{K}_n^{(1,2)}(c', c) = g_2\mathcal{G}^{(n)}(a_{1,2}; c', c), \tag{74b}$$

$$\mathcal{K}_n^{(2,1)}(c', c) = g_1\mathcal{G}^{(n)}(a_{2,1}; c', c), \tag{74c}$$

and

$$\mathcal{K}_n^{(2,2)}(c', c) = p_2\mathcal{P}^{(n)}(c', c) + (g_1/4)\mathcal{F}^{(n)}(a_{2,1}; c', c). \tag{74d}$$

It can be seen from Eq. (29d) and Eqs. (68a,b) that

$$\boldsymbol{A}_h(c) = \lambda c\left[\begin{array}{c} 1 \\ a_{1,2} \end{array}\right], \tag{75}$$

for any value of λ, is a solution of the homogeneous versions of Eqs. (66), so we intend to add $\boldsymbol{A}_h(c)$ to any solution we find of Eq. (66a) or (66b) and then determine the constants λ_1 and λ_2 so that our final solutions will satisfy the normalization conditions

$$\left[\begin{array}{cc} c_1 & c_2 \end{array}\right]\int_0^\infty \mathrm{e}^{-c^2}\boldsymbol{A}^{(\alpha)}(c)c^3\mathrm{d}c = 0, \quad \alpha = 1, 2. \tag{76}$$

5. Hermite cubic splines and numerical results

Before we develop our numerical solutions of the generalized Chapman–Enskog integral equations listed as Eqs. (66), (67), and (76), we must be able to compute well the Legendre components, as defined by Eqs. (46)–(57), of the scattering matrix. As this part of our work is especially important in regard to numerical work, and since these components eventually will be used to solve a collection of basic problems defined in terms of the linearized Boltzmann equation for a mixture of rigid spheres, we devote Appendix A of this work to a discussion of the various algorithms we have used to obtain our working subroutines for these components.

Considering that we have good subroutines available to compute the Legendre components of the scattering matrix, we now proceed to generalize (to the case of mixtures) the spline solutions of the Chapman–Enskog integral equations for the one-gas case reported in Ref. [9]. The Hermite cubic spline functions we use in this work are taken from Schultz [11]. To be specific and to define the notation we use, we list these splines here. First of all, we consider there to be $M+1$ knots ζ_α defined on the interval [0,1] by

$$\zeta_\alpha = (\alpha/M)^m, \quad \alpha = 0, 1, ..., M. \tag{77}$$

In this work we use the quadratic distribution ($m = 2$). And so to approximate a function, say $Y(x)$, for $x \in [0, 1]$, in terms of the spline functions we write

$$Y(x) = \sum_{\alpha=0}^{K} a_\alpha \mathcal{F}_\alpha(x), \tag{78}$$

where the a_α are constants and where $K = 2M + 1$. We note that there are two spline functions $\mathcal{F}_\alpha(x)$ associated with each knot and that the spline functions are defined differently for even or odd values of α. And so we write

$$\mathcal{F}_{2\beta}(x) = \Phi_\beta(x) \quad \text{and} \quad \mathcal{F}_{2\beta+1}(x) = \Psi_\beta(x) \tag{79a, b}$$

for $\beta = 0, 1, ..., M$. Making use of the definitions

$$p_\alpha(x) = \frac{x - \zeta_{\alpha-1}}{\zeta_\alpha - \zeta_{\alpha-1}} \tag{80a}$$

and

$$g_\alpha(x) = \frac{\zeta_{\alpha+1} - x}{\zeta_{\alpha+1} - \zeta_\alpha} \tag{80b}$$

and considering that the spline functions are zero unless otherwise defined, we can write the Φ functions as

$$\Phi_0(x) = g_0^2(x)\big[3 - 2g_0(x)\big], \quad x \in [\zeta_0, \zeta_1], \tag{81a}$$

$$\Phi_\alpha(x) = \begin{cases} p_\alpha^2(x)\big[3 - 2p_\alpha(x)\big], & x \in [\zeta_{\alpha-1}, \zeta_\alpha], \\ g_\alpha^2(x)\big[3 - 2g_\alpha(x)\big], & x \in [\zeta_\alpha, \zeta_{\alpha+1}], \end{cases} \tag{81b}$$

for $\alpha = 1, 2, ..., M - 1$, and

$$\Phi_M(x) = p_M^2(x)\big[3 - 2p_M(x)\big], \quad x \in [\zeta_{M-1}, \zeta_M]. \tag{81c}$$

In a similar way we can write the Ψ functions as

$$\Psi_0(x) = x g_0^2(x), \quad x \in [\zeta_0, \zeta_1], \tag{82a}$$

$$\Psi_\alpha(x) = \begin{cases} (x - \zeta_\alpha) p_\alpha^2(x), & x \in [\zeta_{\alpha-1}, \zeta_\alpha], \\ (x - \zeta_\alpha) g_\alpha^2(x), & x \in [\zeta_\alpha, \zeta_{\alpha+1}], \end{cases} \tag{82b}$$

for $\alpha = 1, 2, ..., M - 1$, and

$$\Psi_M(x) = (x - \zeta_M) p_M^2(x), \quad x \in [\zeta_{M-1}, \zeta_M]. \tag{82c}$$

Having defined the spline functions we use, we are ready to proceed with our calculations. To make use of the interval [0,1], we introduce the variables

$$u(c) = \mathrm{e}^{-c} \quad \text{and} \quad u'(c') = \mathrm{e}^{-c'} \tag{83a, b}$$

and rewrite our (general) problem defined by Eqs. (66) and (67) as

$$\boldsymbol{V}(-\ln u)\boldsymbol{F}(-\ln u) - \int_0^1 \boldsymbol{\mathcal{K}}(-\ln u', -\ln u)\boldsymbol{F}(-\ln u')J(u')\mathrm{d}u' = \boldsymbol{R}(-\ln u), \quad u \in [0,1], \tag{84}$$

where

$$J(u) = (1/u)(\ln u)^2 \mathrm{e}^{-(\ln u)^2}. \tag{85}$$

In order to apply this formulation both to Eqs. (66) and to Eq. (67), we have omitted a subscript n on the kernel function in Eq. (84); clearly $\boldsymbol{F(c)}$ can refer to $\boldsymbol{A}^{(1)}(c)$, $\boldsymbol{A}^{(2)}(c)$ or $\boldsymbol{B}(c)$, as $\boldsymbol{R}(c)$ refers to $c\boldsymbol{\Phi}_1(c)$, $c\boldsymbol{\Phi}_2(c)$ or $c^2\boldsymbol{\Phi}$. Continuing to follow Ref. [9], we now introduce the spline representation

$$\boldsymbol{F}(-\ln u) = \sum_{\alpha=0}^{K} \boldsymbol{A}_\alpha \mathcal{F}_\alpha(u) \tag{86}$$

into Eq. (84) to obtain

$$\sum_{\alpha=0}^{K} [\boldsymbol{V}(-\ln u)\mathcal{F}_\alpha(u) - \boldsymbol{U}_\alpha(u) - \boldsymbol{V}_\alpha(u)]\boldsymbol{A}_\alpha = \boldsymbol{R}(-\ln u), \tag{87}$$

where

$$\boldsymbol{U}_\alpha(u) = \int_0^u \boldsymbol{\mathcal{K}}(-\ln u', -\ln u)J(u')\mathcal{F}_\alpha(u')\mathrm{d}u' \tag{88a}$$

and

$$\boldsymbol{V}_\alpha(u) = \int_u^1 \boldsymbol{\mathcal{K}}(-\ln u', -\ln u)J(u')\mathcal{F}_\alpha(u')\mathrm{d}u'. \tag{88b}$$

At this point we use a collocation technique to obtain from Eq. (87) a system of linear algebraic equations we can solve to find the (vector) constants $\{\boldsymbol{A}_\alpha\}$ required to complete the (approximate) solution listed as Eq. (86). To be specific, we evaluate Eq. (87) at the collocation points

$$u_\alpha = (\alpha/K)^m, \quad \alpha = 0, 1, ..., K, \tag{89}$$

(again with $m = 2$) and solve the resulting system to find the constants $\{\boldsymbol{A}_\alpha\}$. This algorithm thus establishes our first (approximate) solution which we call our "standard" solution, and which we label $\boldsymbol{F}_a(-\ln u)$. A second "postprocessed" solution $\boldsymbol{F}_b(-\ln u)$ can be found by using $\boldsymbol{F}_a(-\ln u)$ in the integral term in Eq. (84) and solving the resulting equation to find

$$\boldsymbol{F}_b(-\ln u) = \boldsymbol{V}^{-1}(-\ln u)\Big\{\boldsymbol{R}(-\ln u) + \sum_{\alpha=0}^{K} \big[\boldsymbol{U}_\alpha(u) + \boldsymbol{V}_\alpha(u)\big]\boldsymbol{A}_\alpha\Big\}. \tag{90}$$

We note that some comments (useful here for the case of mixtures) relevant to the numerical evaluation of the one-gas versions of $\boldsymbol{U}_\alpha(u)$ and $\boldsymbol{V}_\alpha(u)$ can be found in Ref. [9].

At this point we can report some numerical results for two specific cases: the first is a mixture of Ne and Ar atoms, while the second is a mixture of He and Xe atoms. For the sake of our computations we consider that the data

$$m_2 = 39.948 \quad m_1 = 20.183 \quad d_2/d_1 = 1.406 \quad \text{(Ne-Ar mixture)}$$

and

$$m_2 = 131.30 \quad m_1 = 4.0026 \quad d_2/d_1 = 2.226 \quad \text{(He-Xe mixture)}$$

are exact. We tabulate our results for these two cases in terms of the molar concentration defined (in terms of the first particle) as

$$c_1 = \frac{n_1/n_2}{1 + n_1/n_2}. \tag{91}$$

We note that the generalized Chapman–Enskog (vector-valued) functions $\boldsymbol{A}^{(1)}(c)$, $\boldsymbol{A}^{(2)}(c)$ and $\boldsymbol{B}(c)$, as defined, depend only on three ratios: n_1/n_2, d_1/d_2 and m_1/m_2. We list in Tables 1–3 selected values of the three (vector-valued) generalized Chapman–Enskog functions for the Ne-Ar mixture for three values of the concentration parameter: $c_1 = 0.1, 0.5, 0.9$. Results for the He-Xe mixture are given in Tables 4–6. To establish some confidence in the accuracy of our results, we first generated a set of results using $M = 320$ and a quadrature based on four Gauss points per subinterval to evaluate the integrals in Eqs. (88a,b). We then increased M to 640 and the number of Gauss points per subinterval to eight to obtain a second set of results in which the first seven significant figures of the post-processed results agreed perfectly with those of the first set of results, for all cases. Moreover, we have observed that in our second set of results the first seven figures of the standard and postprocessed results were the same for all cases studied.

In addition to computing the basic functions $\boldsymbol{A}^{(1)}(c)$, $\boldsymbol{A}^{(2)}(c)$, and $\boldsymbol{B}(c)$, we have evaluated some basic integrals of the functions. First of all, we generalize the notation used in Ref. [9] and introduce the definitions

$$\varepsilon_{p,\alpha} = \frac{16}{15\pi^{1/2}} \int_0^\infty \mathrm{e}^{-c^2} B_\alpha(c) c^4 \mathrm{d}c, \quad \alpha = 1, 2, \tag{92}$$

where $B_1(c)$ and $B_2(c)$ are the two elements of $\boldsymbol{B}(c)$. We choose to report both $\varepsilon_{p,1}$ and $\varepsilon_{p,2}$ so that various definitions of the viscosity can be accommodated. For example, we note that Takata, Yasuda, Aoki and Shibata [12] have reported (graphically) a quantity denoted by $\hat{\mu}$ that is related to the viscosity. We find we can obtain the results reported for $\hat{\mu}$ in Ref. [12] from the expression

$$\hat{\mu} = 2(2)^{1/2} \Big(\frac{d_1}{c_1 d_1 + c_2 d_2} \Big)^2 (c_1 \varepsilon_{p,1} + c_2 \varepsilon_{p,2}). \tag{93}$$

In Table 7 we report, for the two considered mixtures, $\varepsilon_{p,1}$ and $\varepsilon_{p,2}$ as functions of the concentration c_1. In regard to the three ways to obtain the one-gas limit

Table 1. The generalized Chapman–Enskog functions for the Ne-Ar mixture for the case $c_1 = 0.1$

c	$A_1^{(1)}(c)$	$A_2^{(1)}(c)$	$A_1^{(2)}(c)$	$A_2^{(2)}(c)$	$B_1(c)$	$B_2(c)$
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.1	–1.245503(–1)	–1.409118(–2)	–1.738694(–1)	–1.924604(–1)	8.948039(–3)	8.420111(–3)
0.2	–2.454715(–1)	–2.749876(–2)	–3.389238(–1)	–3.786977(–1)	3.545276(–2)	3.353171(–2)
0.3	–3.595333(–1)	–3.956072(–2)	–4.869640(–1)	–5.526839(–1)	7.855316(–2)	7.490027(–2)
0.4	–4.641940(–1)	–4.965572(–2)	–6.108743(–1)	–7.087589(–1)	1.368178(–1)	1.318384(–1)
0.5	–5.577233(–1)	–5.721760(–2)	–7.048582(–1)	–8.417624(–1)	2.085412(–1)	2.034548(–1)
1.0	–8.436373(–1)	–4.178085(–2)	–6.059229(–1)	–1.021675	7.100345(–1)	7.433387(–1)
1.5	–8.648387(–1)	8.661882(–2)	5.679476(–1)	–1.730976(–1)	1.339594	1.488148
2.0	–6.840484(–1)	3.431839(–1)	2.865881	1.839379	2.019132	2.338906
2.5	–3.367670(–1)	7.332641(–1)	6.300654	5.060461	2.717517	3.240245
3.0	1.595875(–1)	1.259082	1.087826(1)	9.507213	3.421611	4.163716
3.5	7.960557(–1)	1.921764	1.660196(1)	1.518787(1)	4.125616	5.094889
4.0	1.567748	2.721960	2.347361(1)	2.210719(1)	4.826999	6.026471
4.5	2.471868	3.660075	3.149430(1)	3.026820(1)	5.524760	6.954864
5.0	3.506761	4.736372	4.066470(1)	3.967297(1)	6.218626	7.878411

Table 2. The generalized Chapman–Enskog functions for the Ne-Ar mixture for the case $c_1 = 0.5$

c	$A_1^{(1)}(c)$	$A_2^{(1)}(c)$	$A_1^{(2)}(c)$	$A_2^{(2)}(c)$	$B_1(c)$	$B_2(c)$
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.1	–1.759689(–1)	–5.641100(–2)	–8.340683(–2)	–1.157864(–1)	7.690682(–3)	7.288256(–3)
0.2	–3.459208(–1)	–1.100222(–1)	–1.628603(–1)	–2.286262(–1)	3.053225(–2)	2.905193(–2)
0.3	–5.042490(–1)	–1.581027(–1)	–2.346130(–1)	–3.356472(–1)	6.786436(–2)	6.499422(–2)
0.4	–6.460811(–1)	–1.980533(–1)	–2.952902(–1)	–4.341181(–1)	1.186811(–1)	1.146411(–1)
0.5	–7.674636(–1)	–2.274563(–1)	–3.419917(–1)	–5.215038(–1)	1.817459(–1)	1.773693(–1)
1.0	–9.903001(–1)	–1.474921(–1)	–2.977210(–1)	–7.205150(–1)	6.346182(–1)	6.592924(–1)
1.5	–5.149137(–1)	4.312002(–1)	2.982508(–1)	–3.999013(–1)	1.221164	1.345306
2.0	6.481473(–1)	1.596114	1.491435	5.255536(–1)	1.865655	2.151078
2.5	2.476767	3.384604	3.296620	2.088339	2.534725	3.023796
3.0	4.957299	5.814195	5.720655	4.301663	3.213507	3.933287
3.5	8.081924	8.894227	8.767374	7.171799	3.895101	4.862534
4.0	1.184601(1)	1.263020(1)	1.243911(1)	1.070222(1)	4.576255	5.801829
4.5	1.624667(1)	1.702560(1)	1.673735(1)	1.489508(1)	5.255462	6.745558
5.0	2.128209(1)	2.208271(1)	2.166309(1)	1.975182(1)	5.932088	7.690450

Table 3. The generalized Chapman–Enskog functions for the Ne-Ar mixture for the case $c_1 = 0.9$

c	$A_1^{(1)}(c)$	$A_2^{(1)}(c)$	$A_1^{(2)}(c)$	$A_2^{(2)}(c)$	$B_1(c)$	$B_2(c)$
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.1	–2.095077(–1)	–8.014456(–2)	–1.436240(–2)	–6.149881(–2)	6.486759(–3)	6.248353(–3)
0.2	–4.118904(–1)	–1.561522(–1)	–2.810636(–2)	–1.223455(–1)	2.581069(–2)	2.493178(–2)
0.3	–6.003073(–1)	–2.239562(–1)	–4.063264(–2)	–1.819019(–1)	5.757558(–2)	5.586826(–2)
0.4	–7.684454(–1)	–2.796246(–1)	–5.137809(–2)	–2.395562(–1)	1.011612(–1)	9.876387(–2)
0.5	–9.106937(–1)	–3.194169(–1)	–5.982829(–2)	–2.947342(–1)	1.557752(–1)	1.532257(–1)
1.0	–1.092038	–1.670828(–1)	–5.364365(–2)	–5.168369(–1)	5.615379(–1)	5.805261(–1)
1.5	–1.912675(–1)	7.921714(–1)	5.624104(–2)	–6.198911(–1)	1.109914	1.211018
2.0	1.892417	2.747218	2.853847(–1)	–5.839802(–1)	1.727389	1.976274
2.5	5.182043	5.796402	6.401853(–1)	–4.033457(–1)	2.375998	2.826901
3.0	9.683136	9.992629	1.123772	–7.743484(–2)	3.037333	3.731066
3.5	1.539739(1)	1.536659(1)	1.737945	3.929136(–1)	3.702490	4.668925
4.0	2.232549(1)	2.193748(1)	2.483844	1.006699	4.367176	5.628092
4.5	3.046779(1)	2.971803(1)	3.362236	1.763062	5.029391	6.600728
5.0	3.982447(1)	3.871706(1)	4.373658	2.661323	5.688295	7.581783

Table 4. The generalized Chapman–Enskog functions for the He-Xe mixture for the case $c_1 = 0.1$

c	$A_1^{(1)}(c)$	$A_2^{(1)}(c)$	$A_1^{(2)}(c)$	$A_2^{(2)}(c)$	$B_1(c)$	$B_2(c)$
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.1	–4.528458(–1)	–1.187778(–2)	–5.154299(–1)	–1.849159(–1)	3.050749(–2)	3.378962(–2)
0.2	–7.687664(–1)	–2.309942(–2)	–8.641389(–1)	–3.639528(–1)	1.068797(–1)	1.345907(–1)
0.3	–9.486460(–1)	–3.302752(–2)	–1.040844	–5.313999(–1)	2.053841(–1)	3.007407(–1)
0.4	–1.044172	–4.106022(–2)	–1.102297	–6.818646(–1)	3.129096(–1)	5.295988(–1)
0.5	–1.093319	–4.664444(–2)	–1.091581	–8.103913(–1)	4.244460(–1)	8.177201(–1)
1.0	–1.102820	–2.263895(–2)	–4.899014(–1)	–9.877519(–1)	1.009060	2.996638
1.5	–9.819640(–1)	1.127405(–1)	7.126621(–1)	–1.671010(–1)	1.627307	6.012572
2.0	–7.900737(–1)	3.754622(–1)	2.446645	1.794837	2.276993	9.460218
2.5	–5.358228(–1)	7.711461(–1)	4.704925	4.948713	2.956657	1.311015(1)
3.0	–2.213670(–1)	1.302075	7.488581	9.315364	3.664323	1.684482(1)
3.5	1.527374(–1)	1.969399	1.080050(1)	1.490554(1)	4.397634	2.060532(1)
4.0	5.864443(–1)	2.773788	1.464389(1)	2.172571(1)	5.154014	2.436247(1)
4.5	1.079887	3.715662	1.902182(1)	2.978014(1)	5.930801	2.810232(1)
5.0	1.633258	4.795294	2.393703(1)	3.907175(1)	6.725367	3.181886(1)

Table 5. The generalized Chapman–Enskog functions for the He-Xe mixture for the case $c_1 = 0.5$

c	$A_1^{(1)}(c)$	$A_2^{(1)}(c)$	$A_1^{(2)}(c)$	$A_2^{(2)}(c)$	$B_1(c)$	$B_2(c)$
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.1	–3.666527(–1)	–2.411582(–2)	–1.395504(–1)	–9.455371(–2)	1.527023(–2)	2.786601(–2)
0.2	–6.761292(–1)	–4.610639(–2)	–2.554125(–1)	–1.869939(–1)	5.814503(–2)	1.111796(–1)
0.3	–9.076047(–1)	–6.387823(–2)	–3.377280(–1)	–2.752388(–1)	1.219944(–1)	2.490995(–1)
0.4	–1.067756	–7.539954(–2)	–3.875273(–1)	–3.572676(–1)	2.002270(–1)	4.402630(–1)
0.5	–1.170425	–7.872648(–2)	–4.091575(–1)	–4.311473(–1)	2.880717(–1)	6.828407(–1)
1.0	–1.152116	8.720255(–2)	–2.099672(–1)	–6.189792(–1)	7.973243(–1)	2.579754
1.5	–6.117239(–1)	6.768451(–1)	3.669525(–1)	–3.853634(–1)	1.359373	5.352794
2.0	2.909380(–1)	1.794980	1.259438	3.740377(–1)	1.950200	8.671471
2.5	1.512257	3.498007	2.450002	1.715519	2.564073	1.230070(1)
3.0	3.036575	5.817395	3.932736	3.670642	3.198823	1.609584(1)
3.5	4.857510	8.772162	5.705724	6.258626	3.853043	1.997289(1)
4.0	6.972430	1.237459(1)	7.768667	9.492016	4.525390	2.388402(1)
4.5	9.380410	1.663295(1)	1.012197(1)	1.337937(1)	5.214438	2.780230(1)
5.0	1.208135(1)	2.155296(1)	1.276633(1)	1.792669(1)	5.918679	3.171282(1)

from our formulation of the mixture problem, we note that

$$\varepsilon_{p,1} = \varepsilon_p, \quad c_2 = 0, \tag{94a}$$

$$\varepsilon_{p,2}/a_{1,2} = \varepsilon_p, \quad c_1 = 0, \tag{94b}$$

and

$$\varepsilon_{p,1} = \varepsilon_{p,2} = \varepsilon_p, \quad m_1/m_2 = 1, \quad d_1/d_2 = 1, \tag{94c}$$

where [9]

$$\varepsilon_p = 0.449027806\ldots . \tag{95}$$

Now, since we have two (vector-valued) functions $\boldsymbol{A}^{(1)}(c)$ and $\boldsymbol{A}^{(2)}(c)$, we report four basic integrals defined as

$$\varepsilon_{t,\alpha}^{(1)} = \frac{16}{15\pi^{1/2}} \int_0^\infty \mathrm{e}^{-c^2} A_\alpha^{(1)}(c) c^5 \mathrm{d}c, \quad \alpha = 1, 2, \tag{96a}$$

and

$$\varepsilon_{t,\alpha}^{(2)} = \frac{16}{15\pi^{1/2}} \int_0^\infty \mathrm{e}^{-c^2} A_\alpha^{(2)}(c) c^5 \mathrm{d}c, \quad \alpha = 1, 2, \tag{96b}$$

where $A_1^{(\beta)}(c)$ and $A_2^{(\beta)}(c)$ are the two elements of $\boldsymbol{A}^{(\beta)}(c)$, $\beta = 1, 2$. In Tables 8 and 9 we report, for the two considered mixtures, $\varepsilon_{t,1}^{(\beta)}$ and $\varepsilon_{t,2}^{(\beta)}$, $\beta = 1, 2$, as functions of the concentration c_1. Here the one-gas limits yield

$$\varepsilon_{t,1}^{(1)} = \varepsilon_t, \quad c_2 = 0, \tag{97a}$$

Table 6. The generalized Chapman–Enskog functions for the He-Xe mixture for the case $c_1 = 0.9$

c	$A_1^{(1)}(c)$	$A_2^{(1)}(c)$	$A_1^{(2)}(c)$	$A_2^{(2)}(c)$	$B_1(c)$	$B_2(c)$
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.1	–2.492079(–1)	7.231057(–2)	–1.109094(–2)	–6.637109(–2)	7.397869(–3)	2.506036(–2)
0.2	–4.844589(–1)	1.469693(–1)	–2.145935(–2)	–1.324771(–1)	2.936495(–2)	1.001712(–1)
0.3	–6.951110(–1)	2.263161(–1)	–3.044550(–2)	–1.980537(–1)	6.515651(–2)	2.251231(–1)
0.4	–8.743694(–1)	3.126738(–1)	–3.749127(–2)	–2.628388(–1)	1.135534(–1)	3.995709(–1)
0.5	–1.018120	4.083412(–1)	–4.214811(–2)	–3.265728(–1)	1.731147(–1)	6.230394(–1)
1.0	–1.147449	1.104203	–2.003078(–2)	–6.206827(–1)	5.922252(–1)	2.451043
1.5	–2.833403(–1)	2.352999	8.834649(–2)	–8.523629(–1)	1.128489	5.375200
2.0	1.521086	4.385376	2.861135(–1)	–9.955717(–1)	1.717866	9.250880
2.5	4.214463	7.394764	5.725844(–1)	–1.028471	2.333036	1.392669(1)
3.0	7.762440	1.154041(1)	9.468240(–1)	–9.330848(–1)	2.962572	1.926161(1)
3.5	1.214272(1)	1.695198(1)	1.408147	–6.947818(–1)	3.601714	2.513209(1)
4.0	1.734043(1)	2.373421(1)	1.956096	–3.017563(–1)	4.248524	3.143345(1)
4.5	2.334532(1)	3.197105(1)	2.590367	2.554409(–1)	4.902269	3.807875(1)
5.0	3.015013(1)	4.172934(1)	3.310768	9.843135(–1)	5.562708	4.499667(1)

$$\varepsilon_{t,2}^{(2)} = \varepsilon_t, \quad c_1 = 0, \tag{97b}$$

$$\varepsilon_{t,1}^{(1)} + \varepsilon_{t,1}^{(2)} = \varepsilon_t, \quad m_1/m_2 = 1, \quad d_1/d_2 = 1, \tag{97c}$$

and

$$\varepsilon_{t,2}^{(1)} + \varepsilon_{t,2}^{(2)} = \varepsilon_t, \quad m_1/m_2 = 1, \quad d_1/d_2 = 1, \tag{97d}$$

where [9]

$$\varepsilon_t = 0.679630049\ldots . \tag{98}$$

Finally, we note that the results reported in Tables 7–9 were obtained using the standard solutions generated with $M = 640$ in Eqs. (92) and (96) and four Gauss points per subinterval to perform the required integrations.

6. Concluding remarks

In this work we have listed some solutions to an exact and explicit formulation of the (vector) linearized Boltzmann equation relevant to a binary mixture of rigid spheres that scatter isotropically in the center-of-mass system. The solutions (collisional invariants) reported in Ref. [2] and listed as Eqs. (25) are consequences of the conservation of number, energy, and momentum. We have also reported twelve additional solutions listed in Eqs. (32), (41), (44), and (45). These twelve solutions are linear in the spatial variables $\{x, y, z\}$ and are defined in terms of three vector-valued functions $\boldsymbol{F}^{(1)}(c)$, $\boldsymbol{F}^{(2)}(c)$ and $\boldsymbol{F}(c)$ that are solutions of the

Table 7. Values of $\varepsilon_{p,1}$ and $\varepsilon_{p,2}$

	Ne-Ar mixture		He-Xe mixture	
c_1	$\varepsilon_{p,1}$	$\varepsilon_{p,2}$	$\varepsilon_{p,1}$	$\varepsilon_{p,2}$
0.0	5.595420(–1)	6.317248(–1)	6.872939(–1)	2.571784
0.1	5.476674(–1)	6.176388(–1)	6.591318(–1)	2.496050
0.2	5.359138(–1)	6.036851(–1)	6.313460(–1)	2.424505
0.3	5.242967(–1)	5.898802(–1)	6.040327(–1)	2.358467
0.4	5.128351(–1)	5.762439(–1)	5.773241(–1)	2.299872
0.5	5.015515(–1)	5.627999(–1)	5.514060(–1)	2.251684
0.6	4.904734(–1)	5.495769(–1)	5.265471(–1)	2.218677
0.7	4.796344(–1)	5.366103(–1)	5.031460(–1)	2.209062
0.8	4.690763(–1)	5.239439(–1)	4.818064(–1)	2.238244
0.9	4.588517(–1)	5.116331(–1)	4.634256(–1)	2.338849
1.0	4.490278(–1)	4.997484(–1)	4.490278(–1)	2.593733

Table 8. Values of $\varepsilon_{t,1}^{(1)}$ and $\varepsilon_{t,2}^{(1)}$

	Ne-Ar mixture		He-Xe mixture	
c_1	$\varepsilon_{t,1}^{(1)}$	$\varepsilon_{t,2}^{(1)}$	$\varepsilon_{t,1}^{(1)}$	$\varepsilon_{t,2}^{(1)}$
0.0	–5.786993(–1)	0.0	–6.550719(–1)	0.0
0.1	–4.434017(–1)	1.308477(–1)	–5.382464(–1)	1.476024(–1)
0.2	–3.115692(–1)	2.576567(–1)	–4.266660(–1)	2.926300(–1)
0.3	–1.828680(–1)	3.808994(–1)	–3.196957(–1)	4.376882(–1)
0.4	–5.689983(–2)	5.011247(–1)	–2.163624(–1)	5.868217(–1)
0.5	6.681834(–2)	6.189829(–1)	–1.150978(–1)	7.466435(–1)
0.6	1.888842(–1)	7.352621(–1)	–1.320706(–2)	9.287041(–1)
0.7	3.100523(–1)	8.509388(–1)	9.434715(–2)	1.155004
0.8	4.312964(–1)	9.672537(–1)	2.181351(–1)	1.472751
0.9	5.539050(–1)	1.085827	3.844456(–1)	2.002584
1.0	6.796300(–1)	1.208839	6.796300(–1)	3.154640

integral equations listed as Eqs. (33) and (42). We consider these vector-valued functions, when multiplied by ε_0 as shown in Eqs. (68), to be generalizations of the Chapman–Enskog functions $A(c)$ and $B(c)$ that are very important in constructing rigorous asymptotic solutions [7], and for defining the viscosity and heat conduction coefficients [13,14] for a single-species gas of rigid spheres.

We believe that the solutions reported in this work are especially important if we wish to obtain the correct asymptotic behavior when solving basic problems for binary gas mixtures. While we have not given rigorous proof that solutions to Eqs. (33) and (42) exist (we are not aware of such proofs even for the one-gas case),

Table 9. Values of $\varepsilon_{t,1}^{(2)}$ and $\varepsilon_{t,2}^{(2)}$

	Ne-Ar mixture		He-Xe mixture	
c_1	$\varepsilon_{t,1}^{(2)}$	$\varepsilon_{t,2}^{(2)}$	$\varepsilon_{t,1}^{(2)}$	$\varepsilon_{t,2}^{(2)}$
0.0	1.173076	6.796300(–1)	1.005103	6.796300(–1)
0.1	1.038931	5.485715(–1)	8.839454(–1)	5.378480(–1)
0.2	9.092710(–1)	4.229940(–1)	7.693810(–1)	4.036160(–1)
0.3	7.839021(–1)	3.025904(–1)	6.612577(–1)	2.762283(–1)
0.4	6.625987(–1)	1.870182(–1)	5.593440(–1)	1.546015(–1)
0.5	5.450951(–1)	7.588717(–2)	4.632709(–1)	3.699208(–2)
0.6	4.310712(–1)	–3.125726(–2)	3.724127(–1)	–7.958390(–2)
0.7	3.201319(–1)	–1.349592(–1)	2.856177(–1)	–2.006686(–1)
0.8	2.117775(–1)	–2.358885(–1)	2.005164(–1)	–3.377880(–1)
0.9	1.053576(–1)	–3.348957(–1)	1.113681(–1)	–5.192500(–1)
1.0	0.0	–4.330988(–1)	0.0	–8.362999(–1)

we have provided numerical evidence that these equations can be solved with a good accuracy. We believe the numerical results listed in Tables 1–8 are valid to all figures given, and so our use of the Hermite cubic splines and a collocation scheme can be considered a good computational method for solving the considered integral equations. While there does not seem to be any numerical tabulation of the Chapman–Enskog (vector-valued) functions we have reported here, Takata, Yasuda, Aoki and Shibata [12] have reported (in graphical form) various transport coefficients that are related to integral moments of these (and other) functions. In order to increase confidence in our results, we (asked and) received from Aoki [15] some explicit numerical results upon which Figure 1 of Ref. [12] is based. For several values of X^A, as defined in Ref. [12], we found 6–8 figures of agreement for $\hat{\mu}$ as defined (in this work) by Eq. (93).

Finally, we believe that here, as well as in Ref. [2], we have demonstrated that the GSW form [1] of the scattering (matrix) kernel is especially useful for studies based on the linearized Boltzmann equation for a mixture of rigid spheres that scatter isotropically in the center-of-mass system.

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Appendix A. Algorithms for computing some basic Legendre moments

As shown by Eqs. (46) and (47) of Section 3, the Legendre components $\boldsymbol{K}_n(c',c)$ of the scattering matrix for a binary mixture of rigid sphere gases can be expressed in terms of the basic Legendre moments

$$\mathcal{P}^{(n)}(c',c) = 2\pi \int_{-1}^{1} \mathcal{P}(c',c,\mu_0) P_n(\mu_0) \mathrm{d}\mu_0, \tag{A.1a}$$

$$\mathcal{F}^{(n)}(a;c',c) = 2\pi \int_{-1}^{1} \mathcal{F}(a;c',c,\mu_0) P_n(\mu_0) \mathrm{d}\mu_0, \tag{A.1b}$$

and

$$\mathcal{G}^{(n)}(a;c',c) = 2\pi \int_{-1}^{1} \mathcal{G}(a;c',c,\mu_0) P_n(\mu_0) \mathrm{d}\mu_0, \tag{A.1c}$$

where

$$\mathcal{P}(c',c,\mu_0) = \frac{1}{\pi}\Big[\frac{2}{r(c',c,\mu_0)} \exp\Big\{\frac{{c'}^2 c^2 (1-\mu_0^2)}{r^2(c',c,\mu_0)}\Big\} - r(c',c,\mu_0)\Big], \tag{A.2a}$$

$$\mathcal{F}(a;c',c,\mu_0) = \frac{(a+1/a)^2}{\pi a r(c',c,\mu_0)} \exp\Big\{\frac{a^2 {c'}^2 c^2 (1-\mu_0^2)}{r^2(c',c,\mu_0)} - \frac{(a-1/a)^2({c'}^2+c^2)}{4} - \frac{(a^2-1/a^2)c'c\mu_0}{2}\Big\}, \tag{A.2b}$$

and

$$\mathcal{G}(a;c',c,\mu_0) = \frac{r(c',ac,\mu_0)}{\pi a}\big[J(a;c',c,\mu_0) - 1\big], \tag{A.2c}$$

with

$$J(a;c',c,\mu_0) = \frac{(a+1/a)^2}{2\Delta(a;c',c,\mu_0)} \exp\Big\{-\frac{2C(a;c',c,\mu_0)}{(a-1/a)^2}\Big\} \sinh\Big\{\frac{2\Delta(a;c',c,\mu_0)}{(a-1/a)^2}\Big\}, \tag{A.3a}$$

for $a \neq 1$, or

$$J(a;c',c,\mu_0) = \frac{1}{r^2(c',c,\mu_0)} \exp\Big\{\frac{{c'}^2 c^2 (1-\mu_0^2)}{r^2(c',c,\mu_0)}\Big\}, \tag{A.3b}$$

for $a = 1$. In these equations,

$$r(c',c,\mu_0) = ({c'}^2 + c^2 - 2c'c\mu_0)^{1/2}, \tag{A.4}$$

$$C(a;c',c,\mu_0) = {c'}^2 + c^2 - (a+1/a)c'c\mu_0, \tag{A.5}$$

and

$$\Delta(a;c',c,\mu_0) = \big[C^2(a;c',c,\mu_0) + (a-1/a)^2 {c'}^2 c^2 (1-\mu_0^2)\big]^{1/2}. \tag{A.6}$$

As mentioned in Section 3, the Legendre moments expressed by Eqs. (A.1) are required in this work only for $n = 1$ and $n = 2$. However, since in our continuing work on binary gas mixtures we intend to investigate and develop solutions for several basic problems formulated in terms of Eq. (63), using an expansion of the form of Eq. (26) for the kernel $\boldsymbol{\mathcal{K}}(\boldsymbol{c}' : \boldsymbol{c}) = (1/\varepsilon_0)\boldsymbol{K}(\boldsymbol{c}' : \boldsymbol{c})$, and since we have seen in previous works [16–20] on single-gas problems that a truncation at $n = 8$ in the single-gas version of Eq. (26) is usually sufficient, we discuss in this Appendix our algorithms for computing

$$\widehat{\mathcal{P}}^{(n)}(c', c) = \mathrm{e}^{-c'^2}\mathcal{P}^{(n)}(c', c), \tag{A.7a}$$

$$\widehat{\mathcal{F}}^{(n)}(a; c', c) = \mathrm{e}^{-c'^2}\mathcal{F}^{(n)}(a; c', c), \tag{A.7b}$$

and

$$\widehat{\mathcal{G}}^{(n)}(a; c', c) = \mathrm{e}^{-c'^2}\mathcal{G}^{(n)}(a; c', c) \tag{A.7c}$$

for $n = 0, 1, \ldots, 8$, $a \in (0, \infty)$, $c' \in [0, \infty)$, and $c \in [0, \infty)$. We note that, for convenience, we have included the factor $\exp\{-c'^2\}$ in the definitions of the moments to be computed, as this factor appears in the integrands of Eqs. (66) and (67) and, as we will see, it can be combined with the exponentials in the expressions for $\mathcal{P}(c', c, \mu_0)$, $\mathcal{F}(a; c', c, \mu_0)$, and $\mathcal{G}(a; c', c, \mu_0)$ to avoid exponentials with positive arguments and, consequently, to eliminate the risk of overflows in the calculation. Before starting the discussion of our algorithms for computing the moments defined by Eqs. (A.7), we note that we find it convenient to exclude the cases $c' = 0$ and/or $c = 0$ from our general presentation. These special cases will be treated at the end of this Appendix.

Beginning our general discussion with $\widehat{\mathcal{P}}^{(n)}(c', c)$, we consider, without loss of generality, that $c \geq c'$. Because $\mathcal{P}^{(n)}(c', c)$ is invariant by an interchange of the arguments c' and c, it is clear that once a good way of computing $\widehat{\mathcal{P}}^{(n)}(c', c)$ for $c > c'$ is established, we can get $\widehat{\mathcal{P}}^{(n)}(c', c)$ for $c < c'$ from

$$\widehat{\mathcal{P}}^{(n)}(c', c) = \mathrm{e}^{-(c'^2 - c^2)}\widehat{\mathcal{P}}^{(n)}(c, c'). \tag{A.8}$$

Our working formula for $\widehat{\mathcal{P}}^{(n)}(c', c)$, $c \geq c'$, follows directly from the work of Pekeris [3]. First of all, we write

$$\widehat{\mathcal{P}}^{(n)}(c', c) = \widehat{\mathcal{P}}_1^{(n)}(c', c) - \widehat{\mathcal{P}}_2^{(n)}(c', c), \tag{A.9}$$

where

$$\widehat{\mathcal{P}}_1^{(n)}(c', c) = 4\int_{-1}^{1} \frac{1}{r(c', c, \mu_0)} \exp\{-[c'(c\mu_0 - c')/r(c', c, \mu_0)]^2\} P_n(\mu_0)\mathrm{d}\mu_0 \tag{A.10a}$$

and

$$\widehat{\mathcal{P}}_2^{(n)}(c', c) = 2\mathrm{e}^{-c'^2}\int_{-1}^{1} r(c', c, \mu_0) P_n(\mu_0)\mathrm{d}\mu_0. \tag{A.10b}$$

The integral in Eq. (A.10a) can be rewritten in a convenient way for numerical integration if we change the variable of integration from μ_0 to $r(c', c, \mu_0)$ and use

the transformation

$$z = (1/2)\big[r(c', c, \mu_0) - (c^2 - {c'}^2)/r(c', c, \mu_0)\big]. \tag{A.11}$$

Doing this, we find

$$\widehat{\mathcal{P}}_1^{(n)}(c', c) = \frac{4}{c'c}\int_{-c'}^{c'} \Big(1 + z/\sqrt{z^2 + c^2 - {c'}^2}\Big)\, \mathrm{e}^{-z^2} \times P_n\Big[(c'c)^{-1}\Big({c'}^2 - z^2 - z\sqrt{z^2 + c^2 - {c'}^2}\Big)\Big]\, \mathrm{d}z, \quad c \geq c'. \tag{A.12}$$

Next, we note that we can perform the integral in Eq. (A.10b) analytically if we use the relation

$$(2n+1)P_n(x) = \frac{\mathrm{d}}{\mathrm{d}x}P_{n+1}(x) - \frac{\mathrm{d}}{\mathrm{d}x}P_{n-1}(x), \tag{A.13}$$

followed by integration by parts and use of the generating function

$$\big[1 - 2\tau x + \tau^2\big]^{-1/2} = \sum_{k=0}^{\infty} \tau^k P_k(x), \quad |\tau| \leq 1, \tag{A.14}$$

for $\tau = c'/c$, along with the orthogonality property of the Legendre polynomials. We find

$$\widehat{\mathcal{P}}_2^{(n)}(c', c) = \frac{4c'\mathrm{e}^{-{c'}^2}}{2n+1}\Big[\Big(\frac{1}{2n+3}\Big)\Big(\frac{c'}{c}\Big)^{n+1} - \Big(\frac{1}{2n-1}\Big)\Big(\frac{c'}{c}\Big)^{n-1}\Big], \quad c \geq c'. \tag{A.15}$$

Our algorithm for computing $\widehat{\mathcal{P}}^{(n)}(c', c)$, $c \geq c'$, is thus based on Eqs. (A.9), (A.12), and (A.15), and the use of a 100-point Gauss–Legendre quadrature set mapped linearly onto $[-c', c']$ to calculate the integral in Eq. (A.12).

In regard to $\widehat{\mathcal{F}}^{(n)}(a; c', c)$, we start with the defining equation for these moments,

$$\widehat{\mathcal{F}}^{(n)}(a; c', c) = 2\pi\mathrm{e}^{-{c'}^2}\int_{-1}^{1} \mathcal{F}(a; c', c, \mu_0)P_n(\mu_0)\mathrm{d}\mu_0, \tag{A.16}$$

where $\mathcal{F}(a; c', c, \mu_0)$ is given by Eq. (A.2b). We find, after some algebraic manipulations, that Eq. (A.16) can be expressed as

$$\widehat{\mathcal{F}}^{(n)}(a; c', c) = (2/a)(a + 1/a)^2 \int_{-1}^{1} \frac{1}{r(c', c, \mu_0)} \times \exp\Big\{-\Big[\frac{c'c\mu_0 - (1+a^2){c'}^2/2 - (1-a^2)c^2/2}{ar(c', c, \mu_0)}\Big]^2\Big\} P_n(\mu_0)\mathrm{d}\mu_0, \tag{A.17}$$

where $r(c', c, \mu_0)$ is given by Eq. (A.4). During an extensive numerical testing procedure that was carried out with Eq. (A.17), we have found that this equation works well, except when $c' \to 0$ or $c' \to c$. The difficulty with the limiting case $c' \to 0$ can be easily accommodated if we add and subtract the term

$$(1/c)\exp\big\{-(a - 1/a)^2c^2/4\big\}P_n(\mu_0)$$

to and from the integrand of Eq. (A.17). We note that the added term can be integrated analytically, while the subtracted one serves to make the contribution to be computed by numerical integration less important. We find

$$\widehat{\mathcal{F}}^{(n)}(a;c',c) = (2/a)(a+1/a)^2 \int_{-1}^{1} \Big[\frac{1}{r(c',c,\mu_0)} \times \exp\Big\{ -\Big[\frac{c'c\mu_0 - (1+a^2){c'}^2/2 - (1-a^2)c^2/2}{ar(c',c,\mu_0)}\Big]^2\Big\} - (1/c)\exp\big\{ -(a-1/a)^2c^2/4\big\}\Big] P_n(\mu_0)\mathrm{d}\mu_0 + S(a,c), \quad (A.18)$$

where

$$S(a,c) = \frac{4(a+1/a)^2}{ac}\exp\big\{ -(a-1/a)^2c^2/4\big\}. \quad (A.19)$$

Now, to treat the limiting case $c' \to c$, we consider (without loss of generality) $c \geq c'$ and change the variable of integration from μ_0 to $s = r(c',c,\mu_0)/a$ to find the alternative form

$$\widehat{\mathcal{F}}^{(n)}(a;c',c) = \frac{2(a+1/a)^2}{c'c} \int_{(c-c')/a}^{(c+c')/a} \exp\big\{ -(1/4)[s-(c^2-{c'}^2)/s]^2\big\} \times P_n\big[(2c'c)^{-1}({c'}^2+c^2-a^2s^2)\big]\mathrm{d}s, \quad c \geq c'. \quad (A.20)$$

As done above for Eq. (A.17), we can improve the accuracy that can be obtained from this expression by adding and subtracting the term

$$\exp\big\{ -(1/4)[s-(c^2-{c'}^2)/s]^2\big\} P_n\big[(2c'c)^{-1}({c'}^2+c^2)\big]$$

to and from the integrand of Eq. (A.20). We find

$$\widehat{\mathcal{F}}^{(n)}(a;c',c) = \frac{2(a+1/a)^2}{c'c} \int_{(c-c')/a}^{(c+c')/a} \exp\big\{ -(1/4)[s-(c^2-{c'}^2)/s]^2\big\} \times \big\{P_n\big[(2c'c)^{-1}({c'}^2+c^2-a^2s^2)\big] - P_n\big[(2c'c)^{-1}({c'}^2+c^2)\big]\big\}\mathrm{d}s + T^{(n)}(a;c',c), \quad c \geq c', \quad (A.21)$$

where

$$T^{(n)}(a;c',c) = \widehat{\mathcal{F}}^{(0)}(a;c',c) P_n\big[(2c'c)^{-1}({c'}^2+c^2)\big]. \quad (A.22)$$

Here

$$\widehat{\mathcal{F}}^{(0)}(a;c',c) = \pi^{1/2}\frac{(a+1/a)^2}{c'c}\Big(\mathrm{e}^{c^2-{c'}^2}\big\{\mathrm{erf}\big[(a+1/a)c/2-(a-1/a)c'/2\big] - \mathrm{erf}\big[(a+1/a)c/2+(a-1/a)c'/2\big]\big\} + \mathrm{erf}\big[(a-1/a)c/2-(a+1/a)c'/2\big] - \mathrm{erf}\big[(a-1/a)c/2+(a+1/a)c'/2\big]\Big), \quad c \geq c', \quad (A.23)$$

a result that can be deduced with the help of formula 7.4.33 of Ref. [21]. To avoid the difficulty for $c \to \infty$ that is caused by the exponential function with a positive argument in Eq (A.23), we can use Taylor series expansions for the first two error functions in that equation and formula 7.1.19 of Ref. [21] to rewrite Eq. (A.23) as

$$\widehat{\mathcal{F}}^{(0)}(a;c',c) = -\frac{4(a+1/a)^2}{c'c}\exp\{-[(a-1/a)^2c^2/4+c'^2]\}$$
$$\times \sum_{m=0}^{\infty}\Big(\frac{1}{2m+1}\Big)[(a-1/a)c'/2]^{2m+1}H_{2m}[(a+1/a)c/2]$$
$$+\pi^{1/2}\frac{(a+1/a)^2}{c'c}\Big(\mathrm{erf}\big[(a-1/a)c/2-(a+1/a)c'/2\big]$$
$$-\mathrm{erf}\big[(a-1/a)c/2+(a+1/a)c'/2\big]\Big), \quad c \geq c', \quad \text{(A.24)}$$

where $H_n(x)$, with

$$H_0(x) = 1, \quad H_1(x) = 2x, \qquad \text{(A.25a, b)}$$

and

$$(n+1)H_{n+1}(x) = 2xH_n(x) - 2H_{n-1}(x), \quad n \geq 1, \qquad \text{(A.25c)}$$

are *normalized* Hermite polynomials.

Summarizing our algorithm for computing the $\widehat{\mathcal{F}}^{(n)}(a;c',c)$ moments, we use Eq. (A.18) for $0 < c' \leq 0.9c$ and Eqs. (A.21)–(A.23) for $0.9c < c' \leq c$, except if $c-c' > 10$, in which case instead of Eq. (A.23) we use Eq. (A.24) with the summation truncated for 16-figure accuracy. When $c' > c$, we first compute $\widehat{\mathcal{F}}^{(n)}(a;c,c')$ using the algorithm just discussed, and then we take

$$\widehat{\mathcal{F}}^{(n)}(a;c',c) = \mathrm{e}^{-(c'^2-c^2)}\hat{\mathcal{F}}^{(n)}(a;c,c'), \qquad \text{(A.26)}$$

which follows from the symmetry of $\mathcal{F}^{(n)}(a;c',c)$ in c and c'. Again, we have found that the use of a 100-point Gauss–Legendre quadrature set [mapped linearly onto the indicated integration interval, in the case of Eq. (A.21)] to perform the integrals in Eqs. (A.18) and (A.21) was sufficient.

Finally, we discuss our algorithms for computing the $\widehat{\mathcal{G}}^{(n)}(a;c',c)$ moments. We begin by noting that for $a = 1$ we can use Eqs. (A.2a), (A.2c) and (A.3b), along with Eqs. (A.7a) and (A.7c), to conclude that

$$\widehat{\mathcal{G}}^{(n)}(1;c',c) = (1/2)\widehat{\mathcal{P}}_1^{(n)}(c',c) - \widehat{\mathcal{P}}_2^{(n)}(c',c), \qquad \text{(A.27)}$$

where $\widehat{\mathcal{P}}_1^{(n)}(c',c)$ and $\widehat{\mathcal{P}}_2^{(n)}(c',c)$ are given, respectively, by Eqs. (A.12) and (A.15). It thus follows that essentially the same algorithm that was used to compute the $\widehat{\mathcal{P}}^{(n)}(c',c)$ moments can be used to compute $\widehat{\mathcal{G}}^{(n)}(a;c',c)$ for $a = 1$.

Now, turning our attention to the more important case of $a \neq 1$, we first note that we can combine the arguments of the exponential and the hyperbolic sine in Eq. (A.3a) with the argument $\{-c'^2\}$ of the exponential in Eq. (A.7c) to show

that $\widehat{\mathcal{G}}^{(n)}(a;c',c)$, $a \neq 1$, can be expressed as

$$\widehat{\mathcal{G}}^{(n)}(a;c',c) = \widehat{\mathcal{G}}_1^{(n)}(a;c',c) - \widehat{\mathcal{G}}_2^{(n)}(a;c',c), \tag{A.28}$$

where

$$\widehat{\mathcal{G}}_1^{(n)}(a;c',c) = \frac{(a+1/a)^2}{2a}\int_{-1}^{1}\frac{r(c',ac,\mu_0)}{\Delta(a;c',c,\mu_0)} \times\Big[\exp\big\{-2{c'}^2[c\mu_0-(a+1/a)c'/2]^2/A(a;c',c,\mu_0\big\} - \exp\big\{-2A(a;c',c,\mu_0)/(a-1/a)^2\big\}\Big]P_n(\mu_0)\mathrm{d}\mu_0 \tag{A.29a}$$

and

$$\widehat{\mathcal{G}}_2^{(n)}(a;c',c) = (2/a)\mathrm{e}^{-{c'}^2}\int_{-1}^{1} r(c',ac,\mu_0)P_n(\mu_0)\mathrm{d}\mu_0. \tag{A.29b}$$

We note that in Eq. (A.29a)

$$A(a;c',c,\mu_0) = (a-1/a)^2{c'}^2/2 + C(a;c',c,\mu_0) + \Delta(a;c',c,\mu_0), \tag{A.30}$$

and that $r(c',ac,\mu_0)$, $C(a;c',c,\mu_0)$, and $\Delta(a;c',c,\mu_0)$ are as defined by Eqs. (A.4)–(A.6). In addition, while the integral in Eq. (A.29a) must be performed numerically, it is clear that the integral in Eq. (A.29b) has an analytical result, since it is the same as that of Eq. (A.10b), except that the second argument of $r(c',c,\mu_0)$ in Eq. (A.10b) is changed to ac in Eq. (A.29b). Therefore, we can look at the result expressed by Eq. (A.15) and write

$$\widehat{\mathcal{G}}_2^{(n)}(a;c',c) = \frac{4c'\mathrm{e}^{-{c'}^2}}{(2n+1)a}\Big[\Big(\frac{1}{2n+3}\Big)\Big(\frac{c'}{ac}\Big)^{n+1} - \Big(\frac{1}{2n-1}\Big)\Big(\frac{c'}{ac}\Big)^{n-1}\Big], \quad c \geq c'/a. \tag{A.31}$$

Our algorithm for computing $\widehat{\mathcal{G}}_2^{(n)}(a;c',c)$, $a \neq 1$ and $c \geq c'/a$, is thus based on Eqs. (A.28), (A.29a), and (A.31), and the use of a 100-point Gauss–Legendre quadrature to calculate the integral in Eq. (A.29a). When $c < c'/a$, we use Eqs. (A.28), (A.29a) and an appropriate alternative result for Eq. (A.29b), viz.

$$\widehat{\mathcal{G}}_2^{(n)}(a;c',c) = \frac{4c\,\mathrm{e}^{-{c'}^2}}{2n+1}\Big[\Big(\frac{1}{2n+3}\Big)\Big(\frac{ac}{c'}\Big)^{n+1} - \Big(\frac{1}{2n-1}\Big)\Big(\frac{ac}{c'}\Big)^{n-1}\Big], \quad c \leq c'/a. \tag{A.32}$$

At this point, having finished the discussion of our general algorithms for computing the Legendre moments of the scattering matrix for a binary mixture of rigid-sphere gases, we should add that the reported algorithms are not restricted to $n = 0, 1, \ldots, 8$, even though our testing procedure was focused on these values of n. It is recommended, however, that anyone wishing to use our algorithms with confidence for $n > 8$, should perform additional numerical tests in advance to be sure that the 100-point Gauss–Legendre quadrature set that we have used in this work will be adequate for the intended application.

To close this Appendix, we discuss next the special cases $c' = 0$ and/or $c = 0$ which were excluded from our general presentation. Considering first the case $c' = 0$ and $c \neq 0$, we find from Eqs. (A.1) and (A.2)

$$\widehat{\mathcal{P}}^{(0)}(0, c) = 4(2/c - c), \tag{A.33a}$$

$$\widehat{\mathcal{P}}^{(n)}(0, c) = 0, \quad n \geq 1, \tag{A.33b}$$

$$\widehat{\mathcal{F}}^{(0)}(a; 0, c) = \frac{4(a + 1/a)^2}{ac} \exp\big\{ -(a - 1/a)^2 c^2/4 \big\}, \tag{A.33c}$$

$$\widehat{\mathcal{F}}^{(n)}(a; 0, c) = 0, \quad n \geq 1, \tag{A.33d}$$

$$\widehat{\mathcal{G}}^{(0)}(a; 0, c) = (1/c)(a + 1/a)^2 \big\{ 1 - \exp\big[-4c^2/(a - 1/a)^2 \big] \big\} - 4c, \tag{A.33e}$$

and

$$\widehat{\mathcal{G}}^{(n)}(a; 0, c) = 0, \quad n \geq 1. \tag{A.33f}$$

Results for the case $c' \neq 0$ and $c = 0$ can be found from the above results for $c' = 0$ and $c \neq 0$ and the symmetry relations expressed by Eqs. (A.8), (A.26), and

$$\widehat{\mathcal{G}}^{(n)}(a; c', c) = (1/a) \mathrm{e}^{-(c'^2 - c^2)} \widehat{\mathcal{G}}^{(n)}(1/a; c, c'), \tag{A.34}$$

a relation that can be deduced from Eqs. (61) and (A.7c).

Finally, a few words about the case $c' = 0$ and $c = 0$. While we have found that the zeroth-order moments $\widehat{\mathcal{P}}^{(0)}(c', 0)$, $\widehat{\mathcal{F}}^{(0)}(a; c', 0)$, and $\widehat{\mathcal{G}}^{(0)}(a; c', 0)$ diverge as $1/c'$ when $c' \to 0$, the higher-order moments are all zero. Since only the $n = 1$ and $n = 2$ moments are required in this work, the fact that for $c = 0$ the $n = 0$ moments diverge when $c' \to 0$ is of no concern here. This issue is not important even for problems where the $n = 0$ moments are required, because these moments appear always as parts of integrands that include the factor c'^2, so that

$$\lim_{c' \to 0} c'^2 \widehat{\mathcal{P}}^{(0)}(c', 0) = 0, \tag{A.35a}$$

$$\lim_{c' \to 0} c'^2 \widehat{\mathcal{F}}^{(0)}(a; c', 0) = 0, \tag{A.35b}$$

and

$$\lim_{c' \to 0} c'^2 \widehat{\mathcal{G}}^{(0)}(a; c', 0) = 0. \tag{A.35c}$$

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