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A formulation of the linearized Boltzmann equations for a binary mixture of rigid spheres

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Abstract

Concise and explicit forms of the collision operators required to establish the linearized Boltzmann equations for a binary mixture of rigid spheres are reported for the case of isotropic scattering in the center-of-mass system.

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1. Introduction

In a fundamental paper [1] published in 1976, one of the authors (MMRW) of this work developed explicit expressions for the collision operators that are required in the linearized Boltzmann equations for a binary mixture of (somewhat) arbitrary particles. In that first work the differential-scattering cross sections were left arbitrary, and so the expressions used to define the collision operators were reported in explicit, but not very simple, forms. Here, as we wish to direct our attention to the scattering of rigid-sphere particles in the area of rarefied gas dynamics, we assume that the differential-scattering cross sections in Ref. [1] are constants so that Williams' previous results can now be reduced to more concise forms.

To start, we write the (coupled) linearized Boltzmann equations for a mixture of particles (labeled with subscripts $\alpha = 1$ and 2) in the form reported in Ref. [1], viz.

$$\mathbf{v} \cdot \nabla_{\mathbf{r}} G_{\alpha}(\mathbf{r}, \mathbf{v}) + S_{\alpha}(\mathbf{v}) G_{\alpha}(\mathbf{r}, \mathbf{v}) = \int S_{\alpha}(\mathbf{v}' : \mathbf{v}) G_{\alpha}(\mathbf{r}, \mathbf{v}') d^3 v' + \sum_{\beta=1}^2 \int S_{\alpha,\beta}(\mathbf{v}' : \mathbf{v}) G_{\beta}(\mathbf{r}, \mathbf{v}') d^3 v'. \quad (1)$$

Here the particle distribution functions have been expressed as

$$f_{\alpha}(\mathbf{r}, \mathbf{v}) = f_{\alpha,0}(\mathbf{v}) + G_{\alpha}(\mathbf{r}, \mathbf{v}), \quad (2)$$

where

$$f_{\alpha,0}(\mathbf{v}) = n_{\alpha} (\lambda_{\alpha} / \pi)^{3/2} e^{-\lambda_{\alpha} v^2}, \quad \text{with } \lambda_{\alpha} = m_{\alpha} / (2kT_0), \quad (3)$$

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is the Maxwellian distribution for n_α particles of mass m_α in equilibrium at temperature T_0 , and where $G_\alpha(\mathbf{r}, \mathbf{v})$ is used to denote the perturbation of the distribution function from equilibrium. In addition, k is the Boltzmann constant, \mathbf{r} is the spatial variable, \mathbf{v} is the velocity variable, and $v = |\mathbf{v}|$. Continuing, we let $\sigma_{\alpha,\beta}$ denote the constant differential-scattering cross sections and deduce from Ref. [1] that

$$S_\alpha(v) = n_1 \sigma_\alpha^{(1)}(v) + n_2 \sigma_\alpha^{(2)}(v), \tag{4}$$

$$S_\alpha(\mathbf{v}' : \mathbf{v}) = n_1 \sigma_1^{\alpha,1}(\mathbf{v}' : \mathbf{v}) + n_2 \sigma_1^{\alpha,2}(\mathbf{v}' : \mathbf{v}), \tag{5}$$

and

$$S_{\alpha,\beta}(\mathbf{v}' : \mathbf{v}) = n_\alpha [\sigma_{II}^{\alpha,\beta}(\mathbf{v}' : \mathbf{v}) - \sigma_{III}^{\alpha,\beta}(\mathbf{v}' : \mathbf{v})], \tag{6}$$

where

$$\sigma_\alpha^{(\beta)}(v) = 4\sigma_{\alpha,\beta}(\pi/\lambda_\beta)^{1/2} v(\lambda_\beta^{1/2} v), \tag{7}$$

$$\begin{aligned} \sigma_I^{\alpha,\beta}(\mathbf{v}' : \mathbf{v}) &= \frac{\sigma_{\alpha,\beta}}{8\pi^{1/2}} \frac{(m_\alpha + m_\beta)^4}{m_\beta^4} \lambda_\beta^{3/2} |\mathbf{v}' - \mathbf{v}| \\ &\times \exp\left\{-\lambda_\beta v'^2 - \frac{(m_\alpha + m_\beta)^2}{8kT_0 m_\beta} |\mathbf{v}' - \mathbf{v}|^2 - (\lambda_\alpha + \lambda_\beta) \mathbf{v}' \cdot (\mathbf{v} - \mathbf{v}')\right\} \int_0^\pi \frac{\sin \theta}{\sin^4(\theta/2)} \\ &\times \exp\left\{-\frac{(m_\alpha + m_\beta)^2}{8kT_0 m_\beta} |\mathbf{v}' - \mathbf{v}|^2 \cot^2(\theta/2)\right\} I_0\{(\lambda_\alpha + \lambda_\beta) |\mathbf{v} \times \mathbf{v}'| \cot(\theta/2)\} d\theta, \end{aligned} \tag{8}$$

$$\begin{aligned} \sigma_{II}^{\alpha,\beta}(\mathbf{v}' : \mathbf{v}) &= \frac{2\sigma_{\alpha,\beta}}{\pi^{1/2}} (m_\alpha + m_\beta)^4 \lambda_\alpha^{3/2} |\mathbf{v}' - \mathbf{v}| \exp\{-\lambda_\alpha v'^2\} \int_0^\pi \frac{\sin \theta}{D_{\alpha,\beta}^2(\theta)} \\ &\times \exp\left\{\frac{-\lambda_\alpha (m_\alpha + m_\beta)}{D_{\alpha,\beta}(\theta)} [(m_\alpha + m_\beta) |\mathbf{v}' - \mathbf{v}|^2 + 2(m_\alpha - m_\beta \cos \theta) \mathbf{v}' \cdot (\mathbf{v} - \mathbf{v}')] \right\} \\ &\times I_0\left\{\frac{2\lambda_\alpha |\mathbf{v}' \times \mathbf{v}| (m_\alpha + m_\beta) m_\beta \sin \theta}{D_{\alpha,\beta}(\theta)}\right\} d\theta, \end{aligned} \tag{9}$$

and

$$\sigma_{III}^{\alpha,\beta}(\mathbf{v}' : \mathbf{v}) = \frac{4\sigma_{\alpha,\beta}}{\pi^{1/2}} \lambda_\alpha^{3/2} |\mathbf{v}' - \mathbf{v}| \exp\{-\lambda_\alpha v'^2\}. \tag{10}$$

Here $I_0(x)$ is used to denote the modified Bessel function,

$$D_{\alpha,\beta}(\theta) = m_\alpha^2 + m_\beta^2 - 2m_\alpha m_\beta \cos \theta, \tag{11}$$

and

$$v(c) = \frac{2c^2 + 1}{c} \int_0^c e^{-x^2} dx + e^{-c^2}. \tag{12}$$

2. Alternative forms for the coupled Boltzmann equations

Having made the assumption that the differential-scattering cross sections are constants, we are now able to evaluate the integrals in Eqs. (8) and (9) to obtain more concise forms for those expressions. However, before reporting the new expressions, we introduce some variable changes. First of all, we rewrite Eq. (2) as

$$f_\alpha(\mathbf{r}, \mathbf{v}) = f_{\alpha,0}(v)[1 + H_\alpha(\mathbf{r}, \mathbf{v})], \tag{13}$$

so that

$$G_\alpha(\mathbf{r}, \mathbf{v}) = f_{\alpha,0}(v)H_\alpha(\mathbf{r}, \mathbf{v}), \tag{14}$$

and in order to introduce a dimensionless velocity variable, we let

$$\mathbf{v} = \mathbf{c}/\omega_\alpha \quad (15)$$

and

$$H_\alpha(\mathbf{r}, \mathbf{c}/\omega_\alpha) = h_\alpha(\mathbf{r}, \mathbf{c}), \quad (16)$$

where

$$\omega_\alpha = \lambda_\alpha^{1/2}. \quad (17)$$

It follows that we can now rewrite Eq. (1) as

$$\mathbf{c} \cdot \nabla_{\mathbf{r}} h_\alpha(\mathbf{r}, \mathbf{c}) + \varpi_\alpha(c) h_\alpha(\mathbf{r}, \mathbf{c}) = L_\alpha(\mathbf{r}, \mathbf{c}), \quad (18)$$

where

$$\varpi_\alpha(c) = \varpi_\alpha^{(1)}(c) + \varpi_\alpha^{(2)}(c), \quad (19)$$

with

$$\varpi_\alpha^{(\beta)}(c) = 4\pi^{1/2} n_\beta \sigma_{\alpha,\beta} (m_\alpha/m_\beta)^{1/2} v [(m_\beta/m_\alpha)^{1/2} c]. \quad (20)$$

In addition,

$$L_\alpha(\mathbf{r}, \mathbf{c}) = \int e^{-c'^2} f_\alpha(\mathbf{c}' : \mathbf{c}) h_\alpha(\mathbf{r}, \mathbf{c}') d^3 c' + \sum_{\beta=1}^2 \int e^{-c'^2} f_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) h_\beta(\mathbf{r}, \mathbf{c}') d^3 c', \quad (21)$$

where

$$f_\alpha(\mathbf{c}' : \mathbf{c}) = \omega_\alpha^{-2} e^{c^2} [n_1 \sigma_I^{\alpha,1}(\mathbf{c}'/\omega_\alpha : \mathbf{c}/\omega_\alpha) + n_2 \sigma_I^{\alpha,2}(\mathbf{c}'/\omega_\alpha : \mathbf{c}/\omega_\alpha)] \quad (22)$$

and

$$f_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = \omega_\alpha^{-2} e^{c^2} n_\beta [\sigma_{II}^{\alpha,\beta}(\mathbf{c}'/\omega_\beta : \mathbf{c}/\omega_\alpha) - \sigma_{III}^{\alpha,\beta}(\mathbf{c}'/\omega_\beta : \mathbf{c}/\omega_\alpha)]. \quad (23)$$

Evaluating the integral in Eq. (8), we find we can rewrite Eq. (22) as

$$f_\alpha(\mathbf{c}' : \mathbf{c}) = f_\alpha^{(1)}(\mathbf{c}' : \mathbf{c}) + f_\alpha^{(2)}(\mathbf{c}' : \mathbf{c}), \quad (24)$$

where

$$f_\alpha^{(\beta)}(\mathbf{c}' : \mathbf{c}) = \frac{n_\beta \sigma_{\alpha,\beta}}{\pi^{1/2}} \left(\frac{m_\beta}{m_\alpha}\right)^{1/2} \left(\frac{m_\alpha + m_\beta}{m_\beta}\right)^2 \frac{1}{|\mathbf{c}' - \mathbf{c}|} E_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}), \quad (25)$$

with

$$E_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = \exp \left\{ \frac{m_\beta}{m_\alpha} \frac{|\mathbf{c}' \times \mathbf{c}|^2}{|\mathbf{c}' - \mathbf{c}|^2} - \frac{(m_\alpha - m_\beta)^2}{4m_\alpha m_\beta} (c'^2 + c^2) - \frac{m_\beta^2 - m_\alpha^2}{2m_\alpha m_\beta} \mathbf{c}' \cdot \mathbf{c} \right\}. \quad (26)$$

Considering Eqs. (9) and (10), we find can write

$$f_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = f_{\alpha,\beta}^{(1)}(\mathbf{c}' : \mathbf{c}) - f_{\alpha,\beta}^{(2)}(\mathbf{c}' : \mathbf{c}), \quad (27)$$

where, in general,

$$f_{\alpha,\beta}^{(1)}(\mathbf{c}' : \mathbf{c}) = \frac{4n_\beta \sigma_{\alpha,\beta}}{\pi^{1/2}} |(m_\alpha/m_\beta)^{1/2} \mathbf{c}' - \mathbf{c}| J_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) \quad (28)$$

and

$$f_{\alpha,\beta}^{(2)}(\mathbf{c}' : \mathbf{c}) = \frac{4n_\beta \sigma_{\alpha,\beta}}{\pi^{1/2}} |(m_\alpha/m_\beta)^{1/2} \mathbf{c}' - \mathbf{c}|. \quad (29)$$

Here

$$J_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = \frac{2}{R_{\alpha,\beta}^2} \int_0^{u_{\alpha,\beta}} \exp\{-C_{\alpha,\beta}(\mathbf{c}' : \mathbf{c})u^2\} I_0\{2u|\mathbf{c}' \times \mathbf{c}|[1 - (u/u_{\alpha,\beta})^2]^{1/2}\} u du, \quad (30)$$

where

$$C_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = c'^2 + c^2 - 2\mathbf{c}' \cdot \mathbf{c} / R_{\alpha,\beta}, \tag{31}$$

$$u_{\alpha,\beta} = 2(m_\alpha m_\beta)^{1/2} / |m_\alpha - m_\beta|, \tag{32}$$

and

$$R_{\alpha,\beta} = 2(m_\alpha m_\beta)^{1/2} / (m_\alpha + m_\beta). \tag{33}$$

Following the discussion given in the Appendix, we find we can evaluate the integral in Eq. (30) to obtain

$$J_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = \frac{(m_\alpha + m_\beta)^2}{2V_{\alpha,\beta}(\mathbf{c}' : \mathbf{c})} \exp\left\{ \frac{-2m_\alpha m_\beta C_{\alpha,\beta}(\mathbf{c}' : \mathbf{c})}{(m_\alpha - m_\beta)^2} \right\} \sinh[2V_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) / (m_\alpha - m_\beta)^2], \tag{34}$$

where

$$V_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = \{ (m_\alpha m_\beta)^2 C_{\alpha,\beta}^2(\mathbf{c}' : \mathbf{c}) + m_\alpha m_\beta (m_\alpha - m_\beta)^2 |\mathbf{c}' \times \mathbf{c}|^2 \}^{1/2}. \tag{35}$$

For the special case of $\alpha = \beta$, we can evaluate the integral defined by Eq. (30) (or use Eq. (34)) to find from Eq. (28) that

$$f_{\alpha,\alpha}^{(1)}(\mathbf{c}' : \mathbf{c}) = \frac{4n_\alpha \sigma_{\alpha,\alpha}}{\pi^{1/2}} \frac{1}{|\mathbf{c}' - \mathbf{c}|} \exp\left\{ \frac{|\mathbf{c}' \times \mathbf{c}|^2}{|\mathbf{c}' - \mathbf{c}|^2} \right\}. \tag{36}$$

Continuing, we let

$$K_{1,1}(\mathbf{c}' : \mathbf{c}) = f_1(\mathbf{c}' : \mathbf{c}) + f_{1,1}^{(1)}(\mathbf{c}' : \mathbf{c}) - f_{1,1}^{(2)}(\mathbf{c}' : \mathbf{c}), \tag{37}$$

$$K_{1,2}(\mathbf{c}' : \mathbf{c}) = f_{1,2}^{(1)}(\mathbf{c}' : \mathbf{c}) - f_{1,2}^{(2)}(\mathbf{c}' : \mathbf{c}), \tag{38}$$

$$K_{2,1}(\mathbf{c}' : \mathbf{c}) = f_{2,1}^{(1)}(\mathbf{c}' : \mathbf{c}) - f_{2,1}^{(2)}(\mathbf{c}' : \mathbf{c}), \tag{39}$$

and

$$K_{2,2}(\mathbf{c}' : \mathbf{c}) = f_2(\mathbf{c}' : \mathbf{c}) + f_{2,2}^{(1)}(\mathbf{c}' : \mathbf{c}) - f_{2,2}^{(2)}(\mathbf{c}' : \mathbf{c}), \tag{40}$$

so that we can rewrite Eq. (18) as

$$\mathbf{c} \cdot \nabla_r h_\alpha(\mathbf{r}, \mathbf{c}) + \varpi_\alpha(c) h_\alpha(\mathbf{r}, \mathbf{c}) = \sum_{\beta=1}^2 \int e^{-c'^2} K_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) h_\beta(\mathbf{r}, \mathbf{c}') d^3 c'. \tag{41}$$

Making use of the explicit forms, we can now write

$$K_{1,1}(\mathbf{c}' : \mathbf{c}) = 4n_1 \sigma_{1,1} \pi^{1/2} \mathcal{P}(\mathbf{c}' : \mathbf{c}) + n_2 \sigma_{1,2} \pi^{1/2} \mathcal{F}_{1,2}(\mathbf{c}' : \mathbf{c}), \tag{42}$$

$$K_{1,2}(\mathbf{c}' : \mathbf{c}) = 4n_2 \sigma_{1,2} \pi^{1/2} \mathcal{G}_{1,2}(\mathbf{c}' : \mathbf{c}), \tag{43}$$

$$K_{2,1}(\mathbf{c}' : \mathbf{c}) = 4n_1 \sigma_{2,1} \pi^{1/2} \mathcal{G}_{2,1}(\mathbf{c}' : \mathbf{c}), \tag{44}$$

and

$$K_{2,2}(\mathbf{c}' : \mathbf{c}) = 4n_2 \sigma_{2,2} \pi^{1/2} \mathcal{P}(\mathbf{c}' : \mathbf{c}) + n_1 \sigma_{2,1} \pi^{1/2} \mathcal{F}_{2,1}(\mathbf{c}' : \mathbf{c}). \tag{45}$$

Here

$$\mathcal{P}(\mathbf{c}' : \mathbf{c}) = \frac{1}{\pi} \left(\frac{2}{|\mathbf{c}' - \mathbf{c}|} \exp\left\{ \frac{|\mathbf{c}' \times \mathbf{c}|^2}{|\mathbf{c}' - \mathbf{c}|^2} \right\} - |\mathbf{c}' - \mathbf{c}| \right) \tag{46}$$

is the basic kernel for the single-species gas, the spherical harmonics expansion of which has already been reported by Pekeris [2]. The additional (new) quantities we require here for the considered binary mixture of rigid spheres are

$$\mathcal{F}_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = \frac{1}{\pi} \left(\frac{m_\beta}{m_\alpha} \right)^{1/2} \left(\frac{m_1 + m_2}{m_\beta} \right)^2 \frac{1}{|\mathbf{c}' - \mathbf{c}|} \exp\left\{ \frac{m_\beta |\mathbf{c}' \times \mathbf{c}|^2}{m_\alpha |\mathbf{c}' - \mathbf{c}|^2} - \frac{(m_1 - m_2)^2}{4m_1 m_2} (c'^2 + c^2) - \frac{m_\beta^2 - m_\alpha^2}{2m_1 m_2} \mathbf{c}' \cdot \mathbf{c} \right\} \tag{47}$$

and

$$\mathcal{G}_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = \frac{1}{\pi} |(m_\alpha / m_\beta)^{1/2} \mathbf{c}' - \mathbf{c}| [J_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) - 1]. \tag{48}$$

Since $J_{\alpha,\beta}(\mathbf{c}' : \mathbf{c})$, for $\alpha \neq \beta$, is independent of α and β , we can rewrite Eq. (48) as

$$\mathcal{G}_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = \frac{1}{\pi} |(m_\alpha/m_\beta)^{1/2} \mathbf{c}' - \mathbf{c}| [J(\mathbf{c}' : \mathbf{c}) - 1]. \quad (49)$$

Here

$$J(\mathbf{c}' : \mathbf{c}) = \frac{(m_1 + m_2)^2}{2V(\mathbf{c}' : \mathbf{c})} \exp\left\{ \frac{-2m_1 m_2 C(\mathbf{c}' : \mathbf{c})}{(m_1 - m_2)^2} \right\} \sinh[2V(\mathbf{c}' : \mathbf{c})/(m_1 - m_2)^2], \quad (50)$$

where

$$V(\mathbf{c}' : \mathbf{c}) = \{(m_1 m_2)^2 C^2(\mathbf{c}' : \mathbf{c}) + m_1 m_2 (m_1 - m_2)^2 |\mathbf{c}' \times \mathbf{c}|^2\}^{1/2}, \quad (51)$$

$$C(\mathbf{c}' : \mathbf{c}) = \mathbf{c}'^2 + \mathbf{c}^2 - 2\mathbf{c}' \cdot \mathbf{c}/R, \quad (52)$$

and

$$R = 2(m_1 m_2)^{1/2}/(m_1 + m_2). \quad (53)$$

We consider that to obtain spherical harmonics expansions, in the manner of Pekeris [2], for the expressions listed as Eqs. (47) and (49) will require a major effort.

Finally, and to be clear, we note that we have used $\sigma_{\alpha,\beta}$ to denote the differential-scattering cross section used in Ref. [1]; however, since we intend to continue this work within the context of a binary gas mixture (rigid-sphere collisions) we can follow Chapman and Cowling [3] and write, for this application,

$$\sigma_{\alpha,\beta} = \frac{1}{4} \left(\frac{d_\alpha + d_\beta}{2} \right)^2, \quad (54)$$

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

3. Concluding remarks

Given that we now have explicit forms for the collision operators for the coupled linearized Boltzmann equations for a binary mixture of rigid spheres, we intend next to investigate the possibility of obtaining spherical harmonics expansions of the scattering kernels that could be important generalizations of the work done by Pekeris [2] for the case of a single-species gas. We consider that such a generalization would be of significant value as we proceed to solve basic problems in rarefied gas dynamics for binary mixtures of rigid spheres.

In reviewing Refs. [1] and [4], we found that an error in the normalization of a certain form of the scattering kernel was made in both of those works, but a compensating error in later sections of those works rendered the normalization error non-consequential. In addition, we note that an alternative derivation of Williams' basic results [1] has been reported [5], but we have concluded that an error (in a basic definition) was made in the final steps of that work [5].

There are three ways in which the linearized Boltzmann equation for a binary mixture can be reduced to the single-species case: (1) the particles have equal masses and diameters, or (2) $n_2 = 0$, or (3) $n_1 = 0$. We can see that our results reduce to the correct forms for each of these three special cases. First, consider the case $m_1 = m_2 = m$ and $d_1 = d_2 = d$. We find from Eqs. (47) and (49)

$$\mathcal{F}_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = 2\mathcal{P}(\mathbf{c}' : \mathbf{c}) + \frac{2}{\pi} |\mathbf{c}' - \mathbf{c}|, \quad m_1 = m_2, \quad (55)$$

and

$$\mathcal{G}_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = \frac{1}{2} \mathcal{P}(\mathbf{c}' : \mathbf{c}) - \frac{1}{2\pi} |\mathbf{c}' - \mathbf{c}|, \quad m_1 = m_2. \quad (56)$$

Since $h_1(\mathbf{r}, \mathbf{c})$ and $h_2(\mathbf{r}, \mathbf{c})$ can be replaced by $h(\mathbf{r}, \mathbf{c})$, each component of Eq. (41) reduces, after we note Eq. (54), to

$$\mathbf{c} \cdot \nabla_{\mathbf{r}} h(\mathbf{r}, \mathbf{c}) + \varepsilon_0 v(\mathbf{c}) h(\mathbf{r}, \mathbf{c}) = \varepsilon_0 \int e^{-\mathbf{c}'^2} \mathcal{P}(\mathbf{c}' : \mathbf{c}) h(\mathbf{r}, \mathbf{c}') d^3 c', \quad (57)$$

where $\varepsilon_0 = n\pi^{1/2}d^2$, with $n = n_1 + n_2$. Eq. (57) is precisely the form [6] of the linearized Boltzmann equation for a collection of identical rigid spheres. For the case $n_2 = 0$, it is easy to see that Eq. (41) for $\alpha = 1$ reduces to the form of Eq. (57) for $h_1(\mathbf{r}, \mathbf{c})$ and Eq. (41) for $\alpha = 2$ is irrelevant. Similarly, for the case $n_1 = 0$, Eq. (41) for $\alpha = 2$ reduces to the form of Eq. (57) for $h_2(\mathbf{r}, \mathbf{c})$.

Finally, it is our opinion that the compact and explicit forms (that contain no integrals) for the scattering kernels developed in this work are a significant improvement over the representations in terms of multi-dimensional integrals (that also include elliptic integrals) that are listed in Appendix B of Ref. [7] — especially for workers who employ some mathematical analysis before implementing a numerical code. We note also that the expressions in Ref. [5] that correspond to our Eqs. (47) and (49) were left as integrals (that contain a Bessel function), and thus they were not reduced to the compact forms we found.

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Appendix. An integral

In this appendix we report the transformations used to obtain Eq. (34) from Eq. (30). We first let

$$u^2 = (1/2)u_{\alpha,\beta}^2 [1 - (1 - \tau^2)^{1/2}], \quad \text{for } u \in [0, 2^{-1/2}u_{\alpha,\beta}], \tag{A.1a}$$

and

$$u^2 = (1/2)u_{\alpha,\beta}^2 [1 + (1 - \tau^2)^{1/2}], \quad \text{for } u \in [2^{-1/2}u_{\alpha,\beta}, u_{\alpha,\beta}], \tag{A.1b}$$

so that we can rewrite Eq. (30) as

$$J_{\alpha,\beta}(c' : c) = \frac{u_{\alpha,\beta}^2 e^{-\eta}}{R_{\alpha,\beta}^2} \int_0^1 \cosh[\eta(1 - \tau^2)^{1/2}] I_0(u_{\alpha,\beta}|c' \times c|\tau) \frac{\tau d\tau}{(1 - \tau^2)^{1/2}}, \tag{A.2}$$

where

$$\eta = (u_{\alpha,\beta}^2/2)C_{\alpha,\beta}(c' : c). \tag{A.3}$$

We next let

$$a\tau = x, \tag{A.4}$$

with

$$a = u_{\alpha,\beta}|c' \times c|, \tag{A.5}$$

and use integration by parts to rewrite Eq. (A.2) as

$$J_{\alpha,\beta}(c' : c) = \frac{2e^{-\eta}}{R_{\alpha,\beta}^2 C_{\alpha,\beta}(c' : c)} \left\{ \sinh(\eta) + \int_0^a \sinh[(\eta/a)(a^2 - x^2)^{1/2}] I_1(x) dx \right\}. \tag{A.6}$$

Now, in an often used table of integrals [8] there is listed (as # 6.667.1) the expression (for the case $\nu = 1/2$)

$$\int_0^a (a^2 - x^2)^{-1/2} \cosh[\sinh(t)(a^2 - x^2)^{1/2}] I_1(x) dx = (\pi/2) I_{1/2}[(a/2) e^t] I_{1/2}[(a/2) e^{-t}], \tag{A.7}$$

which we can differentiate with respect to t to obtain

$$\int_0^a \sinh[\sinh(t)(a^2 - x^2)^{1/2}] I_1(x) dx = \frac{f'(t)}{\cosh(t)}, \tag{A.8}$$

where

$$f(t) = (\pi/2) I_{1/2}[(a/2) e^t] I_{1/2}[(a/2) e^{-t}] \tag{A.9}$$

or

$$f(t) = (2/a) \sinh[(a/2) e^t] \sinh[(a/2) e^{-t}]. \tag{A.10}$$

We find we can write

$$f'(t) = \sinh(t) \sinh[a \cosh(t)] - \cosh(t) \sinh[a \sinh(t)], \quad (\text{A.11})$$

which we can use with Eq. (A.8) to find from Eq. (A.6), with $\sinh(t) = \eta/a$, our final result:

$$J_{\alpha,\beta}(\mathbf{c}' : \mathbf{c}) = \frac{(m_\alpha + m_\beta)^2}{2V_{\alpha,\beta}(\mathbf{c}' : \mathbf{c})} \exp\left\{\frac{-2m_\alpha m_\beta C_{\alpha,\beta}(\mathbf{c}' : \mathbf{c})}{(m_\alpha - m_\beta)^2}\right\} \sinh[2V_{\alpha,\beta}(\mathbf{c}' : \mathbf{c})/(m_\alpha - m_\beta)^2]. \quad (\text{A.12})$$

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