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On the Calculation of Equilibrium Time Correlation Functions in Hard-Sphere Fluids

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We discuss in detail techniques that have been used to determine single-particle equilibrium time correlation functions in a hard-sphere fluid on the basis of kinetic theory. The accuracy of various procedures is assessed.

KEY WORDS: Time correlation functions; kinetic theory; hard spheres; Boltzmann equation; Enskog equation; BGK solution method.

1. INTRODUCTION

Equilibrium time correlation functions between local microscopic fluctuations of one-particle quantities in a hard-sphere fluid can be determined numerically on the basis of the revised Enskog theory[(1-17)] (for surveys see refs. 7). The results of explicit calculations for these functions have been reported in detail before,[(4,6,8-12)] in order to interpret neutron scattering data on simple one-component liquids[(8-10,13-19)] and molecular dynamics data for hard-sphere fluids.[(20-22)] In this paper, we report the technical details of our calculations on the equilibrium time (t) correlation functions in the revised Enskog theory.[(8-12,13)]

We consider the set of time correlation functions for $t \geqslant 0$ given by

$$F_{jl}(k, t) = \langle \phi_j(\mathbf{v}_1)\, e^{tL_E(\mathbf{k})} \phi_l(\mathbf{v}_1) \rangle_1 \tag{1.1}$$

where $\phi_j(\mathbf{v}_1)$ and $\phi_l(\mathbf{v}_1)$ are elements of a complete set $\{\phi_j(\mathbf{v}_1)\}$ of orthonormal polynomia in the one-particle velocity $\mathbf{v}_1$, which will be given below, The brackets denote the one-particle average

$$\langle \cdots \rangle_1 = \int d\mathbf{v}_1\, \phi(v_1) \cdots \tag{1.2}$$

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with $\phi(v_1)$ the normalized Maxwell velocity distribution function

$$\phi(v_1) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-mv_1^2/2k_B T} \tag{1.3}$$

T the temperature, k_B Boltzmann's constant, m the mass of the particles, and the inner product of any two functions $f(\mathbf{v}_1)$ and $g(\mathbf{v}_1)$ of $\mathbf{v}_1$ is defined by $\langle f(\mathbf{v}_1)\, g(\mathbf{v}_1)\rangle_1$. In Eq. (1.1), $L_E(\mathbf{k})$ is the Fourier transform of the linear symmetric inhomogeneous Enskog operator, introduced before.[23] $L_E(\mathbf{k})$ acts on functions of $\mathbf{v}_1$ and is

$$L_E(\mathbf{k}) = -i\mathbf{k}\cdot\mathbf{v}_1 + n\chi\bar{\Lambda}_\mathbf{k} + n\bar{A}_\mathbf{k} \tag{1.4}$$

Here $n = N/V$ is the number density, with N the number of particles and V the volume of the fluid. The linear Enskog operator $L_E(\mathbf{k})$ of Eq. (1.4) is a generalization of the corresponding linear Boltzmann operator that describes the time evolution in a dilute gas of hard spheres.

The first term $-i\mathbf{k}\cdot\mathbf{v}_1$ represents the free streaming of a particle and is also present in the linear Boltzmann operator. $\mathbf{k}$ is a wavevector with length $k = |\mathbf{k}|$.

The second term generalizes the binary collision operator of the Boltzmann equation. It contains, like the Boltzmann collision operator, only uncorrelated binary collision dynamics, but the statistical ansatz of the Boltzmann collision term has been modified in two respects to incorporate the higher density of the fluid. First, the frequency of binary collisions has been increased by a factor $\chi = g(\sigma)$, where $g(\sigma)$ is the radial distribution function for two hard spheres, with diameter σ, at contact. Second, the difference in position of two colliding hard spheres has been taken into account, which is neglected in the Boltzmann collision operator. This leads, in the revised Enskog theory, to a collision operator $\bar{\Lambda}_\mathbf{k}$ which depends on $\mathbf{k}$.

The operator $\bar{\Lambda}_\mathbf{k}$ acts on an arbitrary function $h(\mathbf{v}_1)$ as

$$\bar{\Lambda}_\mathbf{k} h(\mathbf{v}_1) = \Lambda_\mathbf{k} h(\mathbf{v}_1) - \langle \Lambda_\mathbf{k} h(\mathbf{v}_1)\rangle_1 \tag{1.5}$$

with the binary collision operator $\Lambda_\mathbf{k}$ given by

$$\Lambda_\mathbf{k} h(\mathbf{v}_1) = -\sigma \int d\hat{\sigma} \int d\mathbf{v}_2\, \phi(v_2)\, |\mathbf{v}_{12}\cdot\boldsymbol{\sigma}|\, \theta(\mathbf{v}_{12}\cdot\boldsymbol{\sigma}) \times \{h(\mathbf{v}_1) - h(\mathbf{v}_1') + e^{-i\mathbf{k}\cdot\boldsymbol{\sigma}}[h(\mathbf{v}_2) - h(\mathbf{v}_2')]\} \tag{1.6}$$

Here $\boldsymbol{\sigma} = \sigma\hat{\boldsymbol{\sigma}}$, where the unit vector $\hat{\boldsymbol{\sigma}}$ defines the geometry of the binary collision, $\mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2$, $\theta(x)$ is the Heaviside (step) function, and

$\mathbf{v}_1' = \mathbf{v}_1 - (\mathbf{v}_{12} \cdot \hat{\boldsymbol{\sigma}})\,\hat{\boldsymbol{\sigma}}$ and $\mathbf{v}_2' = \mathbf{v}_2 + (\mathbf{v}_{12} \cdot \hat{\boldsymbol{\sigma}})\,\hat{\boldsymbol{\sigma}}$ are the velocities of particles 1 and 2 after a binary collision with initial velocities $\mathbf{v}_1$ and $\mathbf{v}_2$, respectively. The operator $\chi \bar{\Lambda}_{\mathbf{k}}$ reduces to the linear Boltzmann collision operator Λ_0 in the limit $n\sigma^3 \to 0$ and $k\sigma \to 0$, since then $\langle \Lambda_0 h(\mathbf{v}_1) \rangle_1 = 0$, $\chi \to 1$, and $\exp(-i\mathbf{k} \cdot \boldsymbol{\sigma}) \to 1$ [cf. Eqs. (1.5), (1.6)].

The third term in Eq. (1.4), the mean field operator $\bar{\Lambda}_{\mathbf{k}}$, is not present in the linear Boltzmann operator. It is given by

$$n\bar{\Lambda}_{\mathbf{k}} h(\mathbf{v}_1) = \left(1 - \frac{1}{\sqrt{S(k)}}\right) \int d\mathbf{v}_2\, \phi(v_2)\, i\mathbf{k} \cdot (\mathbf{v}_1 + \mathbf{v}_2)\, h(\mathbf{v}_2) \tag{1.7}$$

Thus, $\bar{\Lambda}_{\mathbf{k}}$ depends on the static structure factor $S(k)$ and takes into account the average influence of the other particles on the free motion of a hard sphere because of excluded volume effects.

The functions $F_{jl}(k, t)$ will be evaluated here using the Bhatnagar–Gross–Krook (BGK) method.[24] In the BGK method the functions $F_{jl}(k, t)$ of Eq. (1.1) are calculated explicitly in successive orders M, where M is the order of the BGK approximation. In the BGK approximation of order M, $L_E(\mathbf{k})$ is replaced by[9]

$$L_{\mathrm{E}}(\mathbf{k}) = f(\mathbf{k}) + F(\mathbf{k}) \tag{1.8}$$

where

$$f(\mathbf{k}) = -i\mathbf{k} \cdot \mathbf{v}_1 + d(k) \tag{1.9}$$

is a function of $\mathbf{v}_1$, and $F(\mathbf{k})$, given by

$$F(\mathbf{k})\, h(\mathbf{v}_1) = \sum_{j=1}^{M} \sum_{l=1}^{M} \phi_j(\mathbf{v}_1)\, \mathscr{F}_{jl}(k) \langle \phi_l(\mathbf{v}_1)\, h(\mathbf{v}_1) \rangle_1 \tag{1.10}$$

is an operator acting on functions of $\mathbf{v}_1$. In Eqs. (1.9) and (1.10),

$$d(k) = n\chi \Omega_{M+1,M+1}(k) \tag{1.11}$$

and

$$\mathscr{F}_{jl}(k) = -d(k)\, \delta_{jl} + n\chi \Omega_{jl}(k) + ik \left(\frac{k_{\mathrm{B}} T}{m}\right)^{1/2} \times \left(1 - \frac{1}{\sqrt{S(k)}}\right) (\delta_{j,1} \delta_{l,2} + \delta_{j,2} \delta_{l,1}) \tag{1.12}$$

with

$$\Omega_{jl}(k) = \langle \phi_j(\mathbf{v}_1)\, \bar{\Lambda}_{\mathbf{k}} \phi_l(\mathbf{v}_1) \rangle_1 \tag{1.13}$$

The third term on the right-hand side of Eq. (1.12) is due to the mean field operator $\bar{\Lambda}_{\mathbf{k}}$ [cf. Eq. (1.7)], where the indices 1 and 2 of the Kronecker delta functions refer to the first two polynomia in the complete orthonormal set $\{\phi_j(\mathbf{v}_1)\}$, i.e.,

$$\begin{aligned}\phi_1(\mathbf{v}_1) &= 1\\ \phi_2(\mathbf{v}_1) &= (m/k_B T)^{1/2}\ \mathbf{v}_1 \cdot \mathbf{k}/k\end{aligned} \tag{1.14}$$

which represent the local density and longitudinal velocity, respectively.[23]

We remark that Eq. (1.8) for $L_{\mathrm{E}}(k)$ follows from Eq. (1.4) when $-i\mathbf{k}\cdot\mathbf{v}_1$ and $n\bar{\Lambda}_{\mathbf{k}}$ are taken into account exactly and when $\bar{\Lambda}_{\mathbf{k}}$ is approximated by the infinite BGK matrix $\Omega_{jl}^{\mathrm{BGK}}(k)$. In the BGK approximation of order M, the first $M\times M$ block of $\Omega_{jl}(k)$ is taken into account exactly, i.e., $\Omega_{jl}^{\mathrm{BGK}}(k)=\Omega_{jl}(k)$ for j or $l=1,\ldots, M$, while the remaining matrix elements $\Omega_{jl}^{\mathrm{BGK}}(k)$ are set equal to zero, except for the diagonal elements $j=l=M+1,\ldots,$ which are all set equal to $\Omega_{M+1,M+1}(k)=d(k)/n\chi$.[9] In order to determine the $F_{jl}(k, t)$, we shall use their Laplace transforms, defined by

$$G_{jl}(k, z)=\int_0^\infty dt\, e^{-zt}F_{jl}(k, t)=\langle\phi_j(\mathbf{v}_1)\frac{1}{z-L_{\mathrm{E}}(\mathbf{k})}\phi_l(\mathbf{v}_1)\rangle_1 \tag{1.15}$$

which are, for $j, l=1,\ldots, M$, given by

$$G_{jl}(k, z)=\left[\frac{1}{1-\mathscr{A}(k, z)\,\mathscr{F}(k)}\mathscr{A}(k, z)\right]_{jl} \tag{1.16}$$

Here $\mathscr{F}(k)$ is the $M\times M$ matrix with elements $\mathscr{F}_{jl}(k)$ defined in Eq. (1.12) and $\mathscr{A}(k,z)$ is the $M\times M$ matrix with elements $\mathscr{A}_{jl}(k,z)$ given by $(j, l=1,\ldots, M)$,

$$\begin{aligned}\mathscr{A}_{jl}(k, z) &= \langle\phi_j(\mathbf{v}_1)\frac{1}{z-f(\mathbf{k})}\phi_l(\mathbf{v}_1)\rangle_1\\ &= \left\langle\phi_j(\mathbf{v}_1)\frac{1}{z+i\mathbf{k}\cdot\mathbf{v}_1-d(k)}\phi_l(\mathbf{v}_1)\right\rangle_1\end{aligned} \tag{1.17}$$

We remark that Eq. (1.16) follows from Eq. (1.15) by applying the operator identity

$$\frac{1}{z-L_{\mathrm{E}}(\mathbf{k})}=\frac{1}{z-f(\mathbf{k})-F(\mathbf{k})}=\frac{1}{z-f(\mathbf{k})}+\frac{1}{z-f(\mathbf{k})}F(\mathbf{k})\frac{1}{z-f(\mathbf{k})-F(\mathbf{k})} \tag{1.18}$$

to the right-hand side of Eq. (1.15) and by solving the resulting identity for $G_{jl}(k, z)$ in terms of the $M \times M$ matrices $\mathscr{A}(k, z)$ and $\mathscr{F}(k)$.

Thus, the $G_{jl}(k, z)$ are obtained from $M \times M$ matrix multiplication and inversion [cf. Eq. (1.16)] and the $F_{jl}(k, t)$ from the inverse Laplace transforms of the $G_{jl}(k, z)$.

In this paper we derive expressions for the matrix elements $\mathscr{A}_{jl}(k, z)$ and $\mathscr{F}_{jl}(k)$ [or $\Omega_{jl}(k)$; cf. Eq. (1.12)] needed in Eq. (1.16) that have been used in previous publications.[8–12]

For the complete set of functions $\{\phi_j(\mathbf{v}_1)\}$ that determine the matrix elements $\mathscr{A}_{jl}(k, z)$ and $\Omega_{jl}(k)$ we chose the Burnett polynomia.[25] These polynomia are proportional to the product of c^l, a spherical harmonic $Y_l^{(m)}(\hat{\mathbf{c}})$, and an associated Laguerre polynomial $L_r^{(l+1/2)}(c^2)$, where $\mathbf{c} = (m/2k_B T)^{1/2}\mathbf{v}$ is a reduced dimensionless velocity and $\hat{\mathbf{c}} = \mathbf{c}/c$ is the unit vector in the direction of $\mathbf{c}$. Thus, each label j in $\phi_j(\mathbf{v}_1)$ stands for the three "quantum numbers" $(r_j, l_j, m_j) = j$.

We have chosen this set of polynomia for the following three reasons.

(i) The operator $L_E(\mathbf{k})$ is, for all $\mathbf{k}$, invariant for rotations around the $\mathbf{k}$ axis. Here and in the following, we shall take $\mathbf{k}$ in the z direction. This implies that m_j is a "good" quantum number. Therefore, $F_{jl}(k, t) = 0$ for all k and t when $m_j \neq m_l$, or, equivalently, correlations occur only between fluctuations which have the same quantum number $m_j = m_l$. We note here that in neutron scattering experiments one considers fluctuations with quantum number $m_j = 0$ and that the correlation functions with $m_j = \pm 1$ are relevant for calculations of the shear viscosity of the fluid. Correlation functions of the hard-sphere fluid with $|m_j| > 1$ have had, so far, no practical applications.

(ii) The operator $\bar{\Lambda}_\mathbf{k}$ in $L_E(\mathbf{k})$ [cf. Eq. (1.4)] is for $k = 0$ and $k = \infty$ rotationally invariant, so that l_j is a good quantum number for small and large k. Thus, $\Omega_{jl}(k)$ is diagonal in m_j and m_l for all k and, in addition, diagonal in l_j and l_l for $k \to 0$ and $k \to \infty$.

(iii) The elements of $\Omega_{jl}(k)$ with $r_j \neq r_l$ or $l_j \neq l_l$ are, for all k, far smaller than those with $r_j = r_l$ and $l_j = l_l$. Therefore, the eigenfunctions and eigenvalues of $\bar{\Lambda}_k$ are, in first approximation, given by ϕ_j and $\Omega_{jj}(k)$, respectively. This property is relevant for high fluid densities in particular, since then $n\chi\Lambda_\mathbf{k}$ in the expression (1.4) for $L_E(\mathbf{k})$ dominates the free streaming and mean field terms, so that the $\phi_j(\mathbf{v}_1)$ and $\Omega_{jj}(k)$ are also approximate eigenfunctions and eigenvalues of $L_E(\mathbf{k})$, respectively.[10,26]

At the end we will discuss the relationship of the BGK method to two other approaches that have been used to determine the $F_{jl}(k, t)$, each applicable in a limited k range, however, i.e., hydrodynamics,[7] valid for $k \to 0$; and the ideal gas description,[20] valid for $k \to \infty$. In fact, as has been noted before,[6,12,27] the BGK method interpolates between these two approaches and applies to all $0 \leqslant k < \infty$.

In Section 2 we give the general expressions for the $\phi_j(\mathbf{v}_1)$, in Section 3 we derive the matrix elements $\mathscr{A}_{jl}(k, z)$, and in Section 4 we give the matrix elements $\Omega_{jl}(k)$. We end with a discussion of the previous results in Section 5. In addition, a comparison is made with results for $F_{11}(k, t)$ calculated by Yip *et al.*,[27] who also used the BGK method, but Hermite instead of Burnett polynomia as the basic set of complete orthonormal polynomia in $\mathbf{v}_1$.

2. A COMPLETE SET OF POLYNOMIA

In the explicit calculations to be performed below we use the reduced velocity $\mathbf{c} = (m/2k_B T)^{1/2} \mathbf{v}_1$ and write the velocity average $\langle \cdots \rangle_1$ as [cf. Eq. (1.2)]

$$\langle \cdots \rangle = \frac{1}{\pi^{3/2}} \int d\mathbf{c}\, e^{-c^2} \cdots \tag{2.1}$$

We use the Burnett polynomia given by[25]

$$\psi_{r,l,m}(\mathbf{c}) = N_{r,l} c^l L_r^{(l+1/2)}(c^2)\, Y_l^{(m)}(\hat{\mathbf{c}}) \tag{2.2}$$

with $r = 0, 1,..., \infty$; $l = 0, 1,..., \infty$; and $m = -l,..., 0,..., l$; which are orthonormal, i.e.,

$$\langle \psi^*_{r_1,l_1,m_1}(\mathbf{c})\, \psi_{r_2,l_2,m_2}(\mathbf{c}) \rangle = \delta_{r_1,r_2} \delta_{l_1,l_2} \delta_{m_1,m_2} \tag{2.3}$$

where the star denotes complex conjugation. In Eq. (2.2), $N_{r,l}$ is a normalization factor, given by

$$N_{r,l} = \left\{ \frac{4\pi r!}{(3/2)_{r+l}} \right\}^{1/2} \tag{2.4}$$

where we used Pochhammer's symbol $(a)_n$ defined by

$$(a)_n = \Gamma(a+n)/\Gamma(a) = a \cdot (a+1) \cdot \cdots \cdot (a+n-1) \tag{2.5}$$

with $\Gamma(x)$ the Γ function and $(a)_0 = 1$ for any a.

The associated Laguerre polynomia in Eq. (2.2) are given by[25]

$$L_r^{(l)}(x) = \frac{1}{r!} \left[\left(\frac{\partial}{\partial u} \right)^r (1+u)^{r+l} e^{-ux} \right]_{u=0} \tag{2.6}$$

and the spherical harmonics by[28,29]

$$Y_l^{(m)}(\hat{\mathbf{c}}) = y_{l,m}\left[\left(\frac{\partial}{\partial t}\right)^{l+m} [\mathbf{T}(t)\cdot\hat{\mathbf{c}}]^l\right]_{t=0} \tag{2.7}$$

where

$$y_{l,m} = \frac{(-)^{l+m}}{2^l l!}\left\{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right\}^{1/2} \tag{2.8}$$

and where the (complex) vector $\mathbf{T}(t)$ is given by

$$\mathbf{T}(t) = (1-t^2,\ -i-it^2,\ -2t) \tag{2.9}$$

The variables u and t in Eqs. (2.6), (2.7) are real and set equal to zero after differentiation.

From Eqs. (2.2), (2.6), and (2.7) it follows that

$$\psi_{r,l,m}(\mathbf{c}) = \frac{N_{r,l}\, y_{l,m}}{r!}\left\{\left(\frac{\partial}{\partial s}\right)^l \left(\frac{\partial}{\partial t}\right)^{l+m} \left(\frac{\partial}{\partial u}\right)^r (1+u)^{r+l+1/2} \right.$$
$$\left. \times \exp[-uc^2 + s\mathbf{T}(t)\cdot\mathbf{c}]\right\}_{s=t=u=0} \tag{2.10}$$

where the real variables s, t, and u are set equal to zero after differentiation. Thus, we obtain a complete set of orthonormal polynomia in $\mathbf{c}$ for which we will use the generating function $\exp[-uc^2 + s\mathbf{T}(t)\cdot\mathbf{c}]$ [Eq. (2.10)] in the explicit calculations to be performed below.

The polynomia with quantum number $m = 0$ are real, while the polynomia with $m \neq 0$ are complex and satisfy[28,29]

$$\psi^*_{r,l,m}(\mathbf{c}) = (-)^m\, \psi_{r,l,-m}(\mathbf{c}) \tag{2.11}$$

Therefore, fluctuations in the fluid with quantum number $m = 0$ are described by the complete set of *real* orthonormal polynomials

$$\Phi_{r,l}(\mathbf{c}) = \psi_{r,l,0}(\mathbf{c}) \tag{2.12}$$

with $r = 0, 1, \ldots, \infty$; $l = 0, 1, \ldots, \infty$. Similarly, fluctuations in the fluid with quantum number $|m| = 1$ are described by the complete sets of *real* orthonormal polynomials given by

$$\Phi^{(+)}_{r,l}(\mathbf{c}) = \frac{1}{\sqrt{2}}\{\psi^*_{r,l,1}(\mathbf{c}) + \psi_{r,l,1}(\mathbf{c})\} \tag{2.13}$$

and

$$\Phi^{(-)}_{r,l}(\mathbf{c}) = \frac{1}{i\sqrt{2}}\{\psi^*_{r,l,1}(\mathbf{c}) - \psi_{r,l,1}(\mathbf{c})\} \tag{2.14}$$

where $r = 0, 1, \ldots, \infty$ and $l = 1, \ldots, \infty$. The $(\pm)$ polynomia are orthogonal, i.e.,

$$\langle \Phi^{(+)}_{r_1, l_1}(\mathbf{c})\, \Phi^{(-)}_{r_2, l_2}(\mathbf{c}) \rangle = 0 \tag{2.15}$$

as follows from Eqs. (2.3) and (2.11).

In the next two sections, we use the (complex) representation for the $\psi_{r,l,m}(\mathbf{c})$ given by Eq. (2.10) to determine the matrix elements $\mathscr{A}_{jl}(k, z)$ and $\Omega_{jl}(k)$. In Section 5 we relate the labels j and r_j, l_j, m_j in $\phi_j(\mathbf{v}) = \psi_{r_j, l_j, m_j}(\mathbf{c})$.

3. THE MATRIX $\mathscr{A}$

We consider the matrix elements [cf. Eq. (1.17)]

$$\mathscr{A}_{jl}(k, z) = \left\langle \psi^*_{r_1, l_1, m_1}(\mathbf{c}) \frac{1}{z + i\mathbf{k} \cdot \mathbf{v}_1 - d(k)} \psi_{r_2, l_2, m_2}(\mathbf{c}) \right\rangle_1 \tag{3.1}$$

Here and in the next section we abbreviate the sets of quantum numbers (r_i, l_i, m_i) with $i = 1, 2$ by $(r_1, l_1, m_1) = j (i = 1)$ and $(r_2, l_2, m_2) = l$ $(i = 2)$. We note that $d(k)$ is real and negative for all k [cf. Eq. (1.11) and Ref. 9] and that z is a complex variable with Re $z \geqslant 0$ [cf. Eq. (1.15)], so that the real part of $z - d(k)$ is positive. Using the reduced velocity $\mathbf{c}$ instead of $\mathbf{v}_1$ yields

$$\mathscr{A}_{jl}(k, z) = -i \left(\frac{m}{2k_B T} \right)^{1/2} \frac{1}{k} A_{jl}(\zeta) \tag{3.2}$$

with

$$A_{jl}(\zeta) = \left\langle \psi^*_{r_1, l_1, m_1}(\mathbf{c}) \frac{1}{c_z - \zeta} \psi_{r_2, l_2, m_2}(\mathbf{c}) \right\rangle \tag{3.3}$$

where

$$\zeta = i \left(\frac{m}{2k_B T} \right)^{1/2} \frac{1}{k} [z - d(k)] \tag{3.4}$$

Therefore, ζ is a complex variable with Im $\zeta > 0$, since the real part of $z - d(k)$ is positive. Substituting Eq. (2.10) into Eq. (3.3) leads to

$$A_{jl}(\zeta) = P_1 P_2 Q_1 Q_2 \left\langle \frac{\exp(-\xi c^2 + \mathbf{X} \cdot \mathbf{c})}{c_z - \zeta} \right\rangle \tag{3.5}$$

where

$$\begin{aligned} \xi &= u_1 + u_2 \\ \mathbf{X} &= s_1 \mathbf{T}^*(t_1) + s_2 \mathbf{T}(t_2) \end{aligned} \tag{3.6}$$

and P_i and Q_i are differential operators defined by

$$P_i = y_{l_i m_i} \left(\frac{\partial}{\partial s_i}\right)_0^{l_i} \left(\frac{\partial}{\partial t_i}\right)_0^{l_i + m_i}$$
$$Q_i = \frac{1}{r_i!} N_{r_i l_i} \left(\frac{\partial}{\partial u_i}\right)_0^{r_i} (1 + u_i)^{r_i + l_i + 1/2} \tag{3.7}$$

with $i = 1, 2$. The subscript 0 in Eqs. (3.7) means that after differentiation with respect to s_i, t_i, and u_i, these variables are set equal to zero [cf. Eq. (2.10)], so that also $\xi = 0$ and $\mathbf{X} = 0$. The velocity integrals in Eq. (3.5) can be most conveniently evaluated successively in the x, y, and z directions, with the result

$$A_{jl}(\zeta) = P_1 P_2 Q_1 Q_2 \frac{1}{1+\xi} \exp\left(\frac{s_1 s_2 (1 + t_1 t_2)^2}{1+\xi}\right)$$
$$\times Z\left(\zeta(1+\xi)^{1/2} + \frac{s_1 t_1 + s_2 t_2}{(1+\xi)^{1/2}}\right) \tag{3.8}$$

where we have used the Gaussian integral

$$\int_{-\infty}^{+\infty} dx \exp(-\alpha x^2 + \beta x) = (\pi/\alpha)^{1/2} \exp(\beta^2/4\alpha)$$

for the x, y directions. In addition, we used that $\mathbf{T}(t) \cdot \mathbf{T}(t) = 0$, so that

$$\mathbf{X} \cdot \mathbf{X} = 2 s_1 s_2 \mathbf{T}^*(t_1) \cdot \mathbf{T}(t_2) = 4 s_1 s_2 (1 + t_1 t_2)^2$$

and $X_z = -2(s_1 t_1 + s_2 t_2)$ [cf. Eqs. (3.6) and (2.9)]. In Eq. (3.8), $Z(\zeta)$ is the plasma dispersion function resulting from the integral over the z direction, defined, for $\operatorname{Im} \zeta > 0$, by[30]

$$Z(\zeta) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} dx \frac{e^{-x^2}}{x - \zeta}, \qquad \operatorname{Im} \zeta > 0 \tag{3.9}$$

The function $Z(\zeta)$ can be analytically continued[30] in the whole complex ζ plane using the fact that for $\operatorname{Im} \zeta < 0$,

$$Z(\zeta) = -Z(-\zeta) + 2\pi^{1/2} i e^{-\zeta^2}, \qquad \operatorname{Im} \zeta < 0 \tag{3.10}$$

so that $Z(\zeta)$ is an analytic function of ζ for all ζ, i.e., no cuts or poles occur. There is, however, an essential singularity in $Z(\zeta)$ when $\operatorname{Im} \zeta \to -\infty$, due to the term $\exp(-\zeta^2)$ in Eq. (3.10).

When $|\zeta| \to \infty$ and $\mathrm{Im}\,\zeta > 0$, $Z(\zeta)$ decays to zero, according to the asymptotic expansion

$$Z(\zeta) = \frac{-1}{\zeta} \sum_{n=0,1,\dots}^{\infty} \left(\frac{1}{2}\right)_n \frac{1}{\zeta^{2n}}, \qquad \mathrm{Im}\,\zeta > 0 \tag{3.11}$$

while for any finite $\zeta, Z(\zeta)$ can be obtained, numerically, from the absolutely convergent series expansions

$$Z(\zeta) = i\pi^{1/2} \sum_{n=0}^{\infty} \frac{(i\zeta)^n}{\Gamma(n/2+1)} = i\pi^{1/2} e^{-\zeta^2} - 2\zeta \sum_{n=0}^{\infty} \frac{(-\zeta^2)^n}{(3/2)_n} \tag{3.12}$$

We also need that[30]

$$\frac{d}{d\zeta} Z(\zeta) = -2 - 2\zeta Z(\zeta) \tag{3.13}$$

for all ζ.

In Eq. (3.8) we evaluate the derivatives with respect to s_1, s_2, t_1, and t_2 and express the derivatives with respect to u_1 and u_2 in terms of $\partial/\partial\xi$. The result vanishes, except when $m_1 = m_2$, i.e.,

$$\begin{aligned} A_{jl}(\zeta) &= \delta_{m_1,m_2} C_{jl} \\ &\times \sum_{\lambda=|m_1|}^{\mathrm{Min}(l_1,l_2)} q(l_1, l_2; m_1; \lambda) \sum_{s=0}^{r_1+r_2} p(r_1, l_1; r_2, l_2; s) \\ &\times \left[\left(\frac{\partial}{\partial x}\right)^{l_1+l_2-2\lambda} \left(\frac{\partial}{\partial \xi}\right)^{s} (1+\xi)^{-(l_1+l_2+2)/2} Z(\zeta(1+\xi)^{1/2} + x) \right]_{x=\xi=0} \end{aligned} \tag{3.14}$$

Here, $\mathrm{Min}(l_1, l_2)$ is the minimum of l_1 and l_2,

$$C_{jl} = \frac{(-)^{l_1+l_2}}{2^{l_1+l_2}} \times \left(\frac{(3/2+l_1)_{r_1} (3/2+l_2)_{r_2} (l_1+m_1)!\,(l_1-m_1)!\,(l_2+m_1)!\,(l_2-m_1)!}{r_1!\,r_2!\,(1/2)_{l_1}(1/2)_{l_2}} \right)^{1/2} \tag{3.15}$$

$$q(l_1, l_2; m_1; \lambda) = \frac{4^{\lambda}(1/2)_{\lambda}}{(l_1-\lambda)!\,(l_2-\lambda)!\,(\lambda+m_1)!\,(\lambda-m_1)!} \tag{3.16}$$

and

$$p(r_1, l_1; r_2, l_2; s) = (-)^s \sum_{q=0}^{s} \frac{(-r_1)_q (-r_2)_{s-q}}{q!\,(s-q)!\,(l_1+3/2)_q (l_2+3/2)_{s-q}} \tag{3.17}$$

We remark that for the special cases when $r_1 = r_2 = 0$ and $l_1 = l_2 = m_1 = m_2$ one has from Eqs. (3.14)–(3.17) that $A_{jl}(\zeta) = Z(\zeta)$. For all other cases we calculated $A_{jl}(\zeta)$ in two ways, based on the expressions for $Z(\zeta)$ given by Eqs. (3.13) and (3.11), respectively, which are relevant for two different regions of ζ values.

First, using Eq. (3.13) in Eq. (3.14), one finds

$$A_{jl}(\zeta) = \delta_{m_1,m_2} C_{jl}\{B_{jl}^{(1)}(\zeta) + B_{jl}^{(2)}(\zeta)\, Z(\zeta)\} \tag{3.18}$$

where $B_{jl}^{(1)}(\zeta)$ and $B_{jl}^{(2)}(\zeta)$ are polynomia in ζ given by

$$B_{jl}^{(1)}(\zeta) = \zeta \sum_{\substack{\mu = |l_1 - l_2| \\ \Delta\mu = 2}}^{l_1 + l_2 - 2|m_1|} \sum_{n \geqslant (\mu - 1)/2}^{r_1 + r_2 + \mu - 1} \times q\left(l_1, l_2; m_1; \frac{l_1 + l_2 - \mu}{2}\right) S^{(1)}(r_1, l_1; r_2, l_2; \mu, n)\, \zeta^{2n-\mu} \tag{3.19}$$

and

$$B_{jl}^{(2)}(\zeta) = \sum_{\substack{\mu = |l_1 - l_2| \\ \Delta\mu = 2}}^{l_1 + l_2 - 2|m_1|} \sum_{n \geqslant \mu/2}^{r_1 + r_2 + \mu} \times q\left(l_1, l_2; m_1; \frac{l_1 + l_2 - \mu}{2}\right) S^{(2)}(r_1, l_1; r_2, l_2; \mu, n)\, \zeta^{2n-\mu} \tag{3.20}$$

with the integer variables μ and n varying in steps of 2 and 1, respectively. In Eqs. (3.19) and (3.20)

$$S^{(1)}(r_1, l_1; r_2, l_2; \mu, n) = \sum_{k = n+1}^{r_1 + r_2 + \mu} S^{(2)}(r_1, l_1; r_2, l_2; \mu, k) \left(\frac{1}{2}\right)_{k-n-1} \tag{3.21}$$

and

$$S^{(2)}(r_1, l_1, r_2, l_2; \mu, k) = \frac{(-4)^k \mu!}{2^\mu} \sum_{p=0}^{r_1} \sum_{q=0}^{r_2} \sum_{t=0}^{p+q} \times \frac{(-r_1)_p\,(-r_2)_q\,(-p-q)_t\,[(\mu + l_1 + l_2)/2 + 1 - k + t]_{p+q-t}}{p!\,q!\,(l_1 + 3/2)_p\,(l_2 + 3/2)_q\,t!\,4^t(\mu - k + t)!\,(2k - 2t - \mu)!} \tag{3.22}$$

where it is understood that $1/n! = 0$ when n is a negative integer.

Thus, in Eq. (3.18), $B_{jl}^{(1)}(\zeta)$ is a polynomial in ζ of degree $2r_1+2r_2+l_1+l_2-2|m_1|-1$ and $B_{jl}^{(2)}(\zeta)$ a polynomial of degree $2r_1+2r_2+l_1+l_2-2|m_1|$. When l_1+l_2 is even, $B_{jl}^{(1)}(\zeta)$ contains only odd powers of ζ and $B_{jl}^{(2)}(\zeta)$ only even powers of ζ, while, when l_1+l_2 is odd, $B_{jl}^{(1)}(\zeta)$ contains only even powers of ζ and $B_{jl}^{(2)}(\zeta)$ only odd powers of ζ. We remark that Eq. (3.19) does not apply to the special cases discussed above, i.e., $r_1=r_2=0$, $l_1=l_2=m_1=m_2$, since $2r_1+2r_2+l_1+l_2-2|m_1|-1=-1$ then.

Second, we use Eq. (3.11) for $Z(\zeta)$ in Eq. (3.14). Then, for $\operatorname{Im}\zeta>0$,

$$A_{jl}(\zeta)=\delta_{m_1,m_2}C_{jl}\sum_{\substack{\mu=|l_1-l_2|\\ \Delta\mu=2}}^{l_1+l_2-2|m_1|}\sum_{n=0}^{\infty} \times q\left(l_1,l_2;m_1;\frac{l_1+l_2-\mu}{2}\right)T(r_1,l_1;r_2,l_2;\mu,n)\frac{1}{\zeta^{2n+\mu+1}} \tag{3.23}$$

with

$$T(r_1,l_1;r_2,l_2;\mu,n)=-\sum_{k\geqslant\mu/2}^{r_1+r_2+\mu} S^{(2)}(r_1,l_1;r_2,l_2;\mu,k)\left(\frac{1}{2}\right)_{k+n} \tag{3.24}$$

where the integer variables μ and n vary in steps of 2 and 1, respectively. Therefore, when $\operatorname{Im}\zeta>0$ and $\zeta\to\infty$, all $A_{jl}(\zeta)$ decay to zero proportional to $1/\zeta^{|l_1-l_2|+1}$.

We have used Eq. (3.18) to calculate $A_{jl}(\zeta)$ for finite, not too large, values of ζ. For very large ζ with $\operatorname{Im}\zeta>0$ both polynomia $B_{jl}^{(1)}(\zeta)$ and $B_{jl}^{(2)}(\zeta)$ in $A_{jl}(\zeta)$ diverge and Eq. (3.18) can no longer be used to obtain $A_{jl}(\zeta)$ in practice, since the $A_{jl}(\zeta)$ are very small then [cf. Eq. (3.23)]. Instead, when $\operatorname{Im}\zeta>0$ and $\zeta\to\infty$ we used Eq. (3.23) for $A_{jl}(\zeta)$. When $\operatorname{Im}\zeta<0$ and $\zeta\to\infty$ we used [cf. Eqs. (3.10) and (3.18)]

$$\begin{aligned}A_{jl}(\zeta)&=(-)^{l_1+l_2+1}A_{jl}(-\zeta)\\&\quad+\delta_{m_1,m_2}C_{jl}2\pi^{1/2}iB_{jl}^{(2)}(\zeta)\,e^{-\zeta^2},\qquad \operatorname{Im}\zeta<0\end{aligned} \tag{3.25}$$

where $A_{jl}(-\zeta)$ decays to zero for $\zeta\to\infty$ [cf. Eq. (3.23)], since $\operatorname{Im}-\zeta>0$. We remark that the second term on the right-hand side of Eq. (3.25) strongly diverges when $\operatorname{Im}\zeta\to-\infty$ and describes the approach to an essential singularity of $A_{jl}(\zeta)$ at $\operatorname{Im}\zeta=-\infty$. The relevance of these essential singularities at $\operatorname{Im}\zeta=-\infty$ in all $A_{jl}(\zeta)$ will be discussed in Section 4.4.

4. THE MATRIX Ω

In this section we determine the matrix elements $\Omega_{jl}(k)$ defined by Eq. (1.13), i.e., defined by

$$\Omega_{jl}(k) = \langle \psi^*_{r_1,l_1,m_1}(\mathbf{c})\, \bar{\Lambda}_{\mathbf{k}} \psi_{r_2,l_2,m_2}(\mathbf{c}) \rangle \tag{4.1}$$

where $j=(r_1, l_1, m_1)$ and $l=(r_2, l_2, m_2)$ and $\bar{\Lambda}_{\mathbf{k}}$ is given by Eqs. (1.5) and (1.6). We need the fact that the first two polynomia in the set $\{\phi_j(\mathbf{v}_1)\}$ are given by [cf. Eqs. (1.14) and (2.2)]

$$\phi_1(\mathbf{v}_1) = \psi_{0,0,0}(\mathbf{c}) = 1,$$
$$\phi_2(\mathbf{v}_1) = \psi_{0,1,0}(\mathbf{c}) = 2^{1/2} c_z = \left(\frac{m}{k_B T}\right)^{1/2} v_{1z} \tag{4.2}$$

Then, as discussed before,[23] the second term on the right-hand side of Eq. (1.5) contributes only to the 1,2 element of $\Omega_{jl}(k)$ in Eq. (1.13) and cancels the contribution of $\Lambda_{\mathbf{k}}$. In addition, it has been shown that[9,23]

$$\Omega_{j1}(k) = \Omega_{1j}(k) = 0 \tag{4.3}$$

for all $j = 1,\dots, \infty$. Thus, it suffices to consider the $\Omega_{jl}(k)$ with j or $l \geqslant 2$, which are given by

$$\Omega_{jl}(k) = \langle \psi^*_{r_1,l_1,m_1}(\mathbf{c})\, \Lambda_{\mathbf{k}} \psi_{r_1,l_1,m_1}(\mathbf{c}) \rangle, \qquad j, l \geqslant 2 \tag{4.4}$$

i.e., by Eq. (4.1) with $\bar{\Lambda}_{\mathbf{k}}$ replaced by $\Lambda_{\mathbf{k}}$, since the second term on the right-hand side of Eq. (1.5) does not contribute.

The binary collision operator $\Lambda_{\mathbf{k}}$ consists of four terms,

$$\Lambda_{\mathbf{k}} = -\Lambda^{(1)} + \Lambda^{(2)} - \Lambda^{(3)}_{\mathbf{k}} + \Lambda^{(4)}_{\mathbf{k}} \tag{4.5}$$

given by [cf. Eq. (1.6)]

$$\begin{aligned}
\Lambda^{(1)} &= \sigma \int d\hat{\boldsymbol{\sigma}} \int d\mathbf{v}_2\, \phi(v_2)\, |\mathbf{v}_{12}\cdot\boldsymbol{\sigma}|\, \theta(\mathbf{v}_{12}\cdot\boldsymbol{\sigma}) \\
\Lambda^{(2)} &= \sigma \int d\hat{\boldsymbol{\sigma}} \int d\mathbf{v}_2\, \phi(v_2)\, |\mathbf{v}_{12}\cdot\boldsymbol{\sigma}|\, \theta(\mathbf{v}_{12}\cdot\boldsymbol{\sigma})\, b_{\hat{\sigma}} \\
\Lambda^{(3)}_{\mathbf{k}} &= \sigma \int d\hat{\boldsymbol{\sigma}}\, [\exp(-i\mathbf{k}\cdot\boldsymbol{\sigma})] \int d\mathbf{v}_2\, \phi(v_2)\, |\mathbf{v}_{12}\cdot\boldsymbol{\sigma}|\, \theta(\mathbf{v}_{12}\cdot\boldsymbol{\sigma})\, P_{12} \\
\Lambda^{(4)}_{\mathbf{k}} &= \sigma \int d\hat{\boldsymbol{\sigma}}\, [\exp(-i\mathbf{k}\cdot\boldsymbol{\sigma})] \int d\mathbf{v}_2\, \phi(v_2)\, |\mathbf{v}_{12}\cdot\boldsymbol{\sigma}|\, \theta(\mathbf{v}_{12}\cdot\boldsymbol{\sigma})\, b_{\hat{\sigma}} P_{12}
\end{aligned} \tag{4.6}$$

where P_{12} replaces $\mathbf{v}_1$ by $\mathbf{v}_2$ in functions of $\mathbf{v}_1$, and $b_{\hat{\sigma}}$ replaces $\mathbf{v}_1$ and $\mathbf{v}_2$ by $b_{\hat{\sigma}}\mathbf{v}_1=\mathbf{v}'_1$ and $b_{\hat{\sigma}}\mathbf{v}_2=\mathbf{v}'_2$, respectively. Thus,

$$\Omega_{jl}(k) = -\Omega_{jl}^{(1)} + \Omega_{jl}^{(2)} - \Omega_{jl}^{(3)}(k) + \Omega_{jl}^{(4)}(k) \tag{4.7}$$

with

$$\Omega_{jl}^{(i)}(k) = \langle \psi^*_{r_1,l_1,m_1}(\mathbf{c})\, \Lambda_{\mathbf{k}}^{(i)} \psi_{r_2,l_2,m_2}(\mathbf{c})\rangle \tag{4.8}$$

where $i=1, 2, 3, 4$ and where for $i=1, 2$, $\Lambda_{\mathbf{k}}^{(i)}=\Lambda^{(i)}$ and $\Omega_{jl}^{(i)}(k)=\Omega_{jl}^{(i)}$ do not depend on k.

Next we substitute Eq. (2.10) into (4.8), so that

$$\Omega_{jl}^{(i)}(k) = P_1 P_2 Q_1 Q_2 G_k^{(i)}(s_1, t_1, u_1; s_2, t_2, u_2) \tag{4.9}$$

with the differential operators P_1, P_2, Q_1, and Q_2 given by Eq. (3.7) and

$$\begin{aligned} &G_k^{(i)}(s_1, t_1, u_1; s_2, t_2, u_2) \\ &\quad = \langle \{\exp[-u_1 c^2 + s_1 \mathbf{T}(t_1)^* \cdot \mathbf{c}]\}\, \Lambda_{\mathbf{k}}^{(i)} \exp[-u_2 c^2 + s_2 \mathbf{T}(t_2)\cdot \mathbf{c}]\rangle_1 \end{aligned} \tag{4.10}$$

with $\mathbf{c}=(m/2k_B T)^{1/2}\,\mathbf{v}_1$ as before [cf. Eq. (2.1)].

We substitute Eq. (4.6) into (4.10), use the reduced total velocity $\mathbf{V}=(m/8k_B T)^{1/2}(\mathbf{v}_1+\mathbf{v}_2)$ and the reduced relative velocity $\mathbf{v}=(m/2k_B T)^{1/2}(\mathbf{v}_1-\mathbf{v}_2)$ as integration variables, and introduce $\xi=u_1+u_2$ and $\mathbf{X}=s_1 T^*(t_1)+s_2\mathbf{T}(t_2)$ as before [cf. Eq. (3.6)]. The result is

$$\begin{aligned} &G_k^{(i)}(s_1, t_1, u_1; s_2, t_2, u_2) \\ &\quad = \frac{1}{nt_0(8\pi)^{1/2}} \int d\hat{\boldsymbol{\sigma}} \\ &\qquad \times \langle\!\langle |\mathbf{v}\cdot\hat{\boldsymbol{\sigma}}|\, \theta(\mathbf{v}\cdot\hat{\boldsymbol{\sigma}}) \exp[-\xi V^2 - \xi v^2/4 + \mathbf{X}\cdot\mathbf{V} + E^{(i)}(\mathbf{v},\mathbf{V})]\rangle_v\rangle_V \end{aligned} \tag{4.11}$$

where $t_0=m^{1/2}/[4n\sigma^2(\pi k_B T)^{1/2}]$ is the Boltzmann mean free time between collisions,

$$\begin{aligned} \langle\cdots\rangle_v &= (2\pi)^{-3/2}\int d\mathbf{v}\, e^{-v^2/2}\cdots \\ \langle\cdots\rangle_V &= (\pi/2)^{-3/2}\int d\mathbf{V}\, e^{-2V^2}\cdots \end{aligned} \tag{4.12}$$

and where

$$\begin{aligned}
E^{(1)}(\mathbf{v}, \mathbf{V}) &= -\xi \mathbf{v}\cdot\mathbf{V} + \tfrac{1}{2}\mathbf{X}\cdot\mathbf{v} \\
E^{(2)}(\mathbf{v}, \mathbf{V}) &= E^{(1)}(\mathbf{v}, \mathbf{V}) + 2u_2(\mathbf{v}\cdot\hat{\boldsymbol{\sigma}})(\mathbf{V}\cdot\hat{\boldsymbol{\sigma}}) - s_2[\mathbf{T}(t_2)\cdot\hat{\boldsymbol{\sigma}}](\mathbf{v}\cdot\hat{\boldsymbol{\sigma}}) \\
E^{(3)}(\mathbf{v}, \mathbf{V}) &= -i\mathbf{k}\cdot\boldsymbol{\sigma} + (u_2 - u_1)\,\mathbf{v}\cdot\mathbf{V} + \tfrac{1}{2}[s_1\mathbf{T}^*(t_1) - s_2\mathbf{T}(t_2)]\cdot\mathbf{v} \\
E^{(4)}(\mathbf{v}, \mathbf{V}) &= E^{(3)}(\mathbf{v}, \mathbf{V}) - 2u_2(\mathbf{v}\cdot\hat{\boldsymbol{\sigma}})(\mathbf{V}\cdot\hat{\boldsymbol{\sigma}}) + s_2[\mathbf{T}(t_2)\cdot\hat{\boldsymbol{\sigma}}](\mathbf{v}\cdot\hat{\boldsymbol{\sigma}})
\end{aligned} \tag{4.13}$$

We note that of the four $E^{(i)}(\mathbf{v}, \mathbf{V})$, only $E^{(3)}(\mathbf{v}, \mathbf{V})$ and $E^{(4)}(\mathbf{v}, \mathbf{V})$ depend on $\mathbf{k}$.

In Eq. (4.11) we perform the integrals over the three components of $\mathbf{V}$ and over the two components of $\mathbf{v}$ orthogonal to $\hat{\boldsymbol{\sigma}}$, which are all of the Gaussian type. For the integral over $\mathbf{v}\cdot\hat{\boldsymbol{\sigma}}$ we use

$$2\int_0^\infty dy\; y e^{-y^2 - 2xy} = {}_1F_1(1, 1/2; x^2) - \pi^{1/2} x e^{x^2} \tag{4.14}$$

where ${}_1F_1(1, 1/2; x^2)$ is the confluent hypergeometric function, defined in ref. 31. As a result,

$$\begin{aligned}
&G^{(1)}(s_1, t_1, u_1; s_2, t_2, u_2) \\
&\quad= \frac{(1+\xi/2)^{1/2}}{nt_0(1+\xi)^2}\, e^{(2+\xi)A^2} \\
&\qquad\times \frac{1}{4\pi}\int d\hat{\boldsymbol{\sigma}}\; {}_1F_1\left(-\frac{1}{2}, \frac{1}{2}; -(\mathbf{A}\cdot\hat{\boldsymbol{\sigma}})^2\right)
\end{aligned} \tag{4.15a}$$

$$\begin{aligned}
&G^{(2)}(s_1, t_1, u_1; s_2, t_2, u_2) \\
&\quad= \frac{(1+\xi/2)^{1/2}}{nt_0(1+\xi)(1+\xi+u_1u_2)}\, e^{(2+\xi)A^2} \\
&\qquad\times \frac{1}{4\pi}\int d\hat{\boldsymbol{\sigma}}\; \{\exp[-(\mathbf{A}\cdot\hat{\boldsymbol{\sigma}})^2]\}\; {}_1F_1\left(1, \frac{1}{2}; (\mathbf{B}\cdot\hat{\boldsymbol{\sigma}})^2\right)
\end{aligned} \tag{4.15b}$$

$$\begin{aligned}
&G_k^{(3)}(s_1, t_1, u_1; s_2, t_2, u_2) \\
&\quad= \frac{(1+\xi/2)^{1/2}}{nt_0(1+\xi+u_1u_2)^2} \\
&\qquad\times \frac{1}{4\pi}\int d\hat{\boldsymbol{\sigma}}\left\{\cos(\mathbf{k}\cdot\boldsymbol{\sigma})\; {}_1F_1\left(-\frac{1}{2}, \frac{1}{2}; -(\mathbf{B}\cdot\hat{\boldsymbol{\sigma}})^2\right)\right. \\
&\qquad\left. - i\pi^{1/2}\sin(\mathbf{k}\cdot\boldsymbol{\sigma})\, \mathbf{B}\cdot\boldsymbol{\sigma}\right\}
\end{aligned} \tag{4.16a}$$

$$G_k^{(4)}(s_1, t_1, u_1; s_2, t_2, u_2)$$
$$= \frac{(1+\xi/2)^{1/2}}{nt_0(1+\xi)(1+\xi+u_1u_2)}$$
$$\times \frac{1}{4\pi}\int d\hat{\boldsymbol{\sigma}} \left\{\cos(\mathbf{k}\cdot\boldsymbol{\sigma}) \exp[-(\mathbf{B}\cdot\hat{\boldsymbol{\sigma}})^2]\ {}_1F_1\left(1, \frac{1}{2}; (\mathbf{A}\cdot\hat{\boldsymbol{\sigma}})^2\right)\right.$$
$$\left. - i\pi^{1/2}\sin(\mathbf{k}\cdot\boldsymbol{\sigma})\ \mathbf{A}\cdot\hat{\boldsymbol{\sigma}} \exp[(\mathbf{A}\cdot\hat{\boldsymbol{\sigma}})^2 - (\mathbf{B}\cdot\hat{\boldsymbol{\sigma}})^2]\right\} \tag{4.16b}$$

where $G^{(1)} = G_k^{(1)}$ and $G^{(2)} = G_k^{(2)}$ do not depend on k and where

$$\begin{aligned} \mathbf{A} &= \tfrac{1}{2}(1+\xi)^{-1/2}(2+\xi)^{-1/2}\,\mathbf{X} \\ \mathbf{B} &= \tfrac{1}{2}(1+\xi+u_1u_2)^{-1/2}(2+\xi)^{-1/2} \\ &\quad \times [(1+u_2)\,s_1\mathbf{T}^*(t_1) - (1+u_1)\,s_2\mathbf{T}(t_2)] \end{aligned} \tag{4.17}$$

In Eqs. (4.15), (4.16) we have used the Kummer transformation[31]

$${}_1F_1(a, b; z) = \exp(z)\ {}_1F_1(b-a, b; -z)$$

with $a=1$ and $b=1/2$, to transform ${}_1F_1(1, 1/2; z)$ into ${}_1F_1(-1/2, 1/2; -z)$.

The angular integrations in the $G_k^{(i)}$ are performed in a different manner for $i = 1, 2, 3$, and 4, respectively. Therefore, in the remainder of this section, we consider the four $G_k^{(i)}$ and $\Omega_{jl}^{(i)}(k)$ with $i = 1, 2, 3$, and 4 separately.

(a) *The case $i=1$*

In Eq. (4.15a) for $G^{(1)}$ we directly perform the angular integration over $\hat{\boldsymbol{\sigma}}$, using that, for any $\mathbf{A}$,

$$\frac{1}{4\pi}\int d\hat{\boldsymbol{\sigma}}\ (\mathbf{A}\cdot\hat{\boldsymbol{\sigma}})^{2l} = \frac{1}{2l+1}(A^2)^l \tag{4.18}$$

so that, with Kummer's transformation,

$$G^{(1)}(s_1, t_1, u_1; s_2, t_2, u_2) = \frac{(1+\xi/2)^{1/2}}{nt_0(1+\xi)^2} e^{(1+\xi)A^2}\ {}_1F_1\left(2, \frac{3}{2}; A^2\right) \tag{4.19}$$

Then we use that

$$A^2 = \frac{s_1s_2(1+t_1t_2)^2}{(1+\xi)(2+\xi)} \tag{4.20}$$

as follows from Eqs. (4.17), (3.6), and (2.9).

Thus, $G^{(1)}$ depends on s_1, s_2, t_1, and t_2 only through $s_1 s_2(1+t_1 t_2)^2$. For any such functions f we have the relation [cf. Eq. (3.7)]

$$P_1 P_2 f(s_1 s_2(1+t_1 t_2)^2) = \delta_{l_1,l_2}\delta_{m_1,m_2}\frac{1}{4\pi}\left(\frac{3}{2}\right)_{l_1}\left[\left(\frac{\partial}{\partial x}\right)^{l_1} f(x)\right]_{x=0} \tag{4.21}$$

Therefore,

$$\Omega_{jl}^{(1)} = \frac{1}{4\pi n t_0}\left(\frac{3}{2}\right)_{l_1}\delta_{m_1,m_2}\,\delta_{l_1,l_2} Q_1 Q_2\left(\frac{\partial}{\partial x}\right)_0^{l_1}$$
$$\times\frac{(1+\xi/2)^{1/2}}{(1+\xi)^2}\,e^{x/(2+\xi)}\,{}_1F_1\left(2,\frac{3}{2};\frac{x}{(1+\xi)(2+\xi)}\right) \tag{4.22}$$

We write the result as

$$\Omega_{jl}^{(1)} = \frac{1}{n t_0}\,\delta_{m_1,m_2}\,\delta_{l_1,l_2} J^{(1)}(r_1,l_1;r_2,l_1) \tag{4.23}$$

where $J^{(1)}$ is dimensionless and does not depend on m_1 or m_2.

In order to perform the derivatives with respect to u_1 and u_2 in Eq. (4.22), we introduce, with $\xi = u_1 + u_2$,

$$D(r_1,\alpha_1;r_2,\alpha_2;k,q)$$
$$= \left(\frac{\partial}{\partial u_1}\right)_0^{r_1}\left(\frac{\partial}{\partial u_2}\right)_0^{r_2}\frac{(1+u_1)^{r_1+\alpha_1}(1+u_2)^{r_2+\alpha_2}}{(1+\xi)^k\,(1+\xi/2)^{q-1/2}}$$
$$= r_1!\,r_2!\sum_{t=0}^{\mathrm{Min}(r_1,r_2)}\sum_{j_1=0}^{r_1-t}\sum_{j_2=0}^{r_2-t}$$
$$\times (k)_t\left(-k-q+\alpha_1+\frac{3}{2}\right)_{j_1}\left(-k-q+\alpha_2+\frac{3}{2}\right)_{j_2}\left(q-\frac{1}{2}\right)_{r_1+r_2-j_1-j_2-2t}$$
$$\times\left[t!\,j_1!\,j_2!\,(r_1-t-j_1)!\,(r_2-t-j_2)!\,2^{r_1+r_2-j_1-j_2-2t}\right]^{-1} \tag{4.24}$$

so that one is led straightforwardly to the final result for $J^{(1)}$, i.e.,

$$J^{(1)}(r_1,l_1;r_2,l_1)$$
$$= l_1!\left[r_1!\,r_2!\left(\frac{3}{2}+l_1\right)_{r_1}\left(\frac{3}{2}+l_1\right)_{r_2}\right]^{-1/2}$$
$$\times\sum_{q=0}^{l_1}\frac{(-1/2)^q}{q!\,(l_1-q)!\,(3/2)_q}\left(-\frac{1}{2}\right)_q$$
$$\times D\left(r_1,l_1+\frac{1}{2};r_2,l_1+\frac{1}{2};l_1+2,q\right) \tag{4.25}$$

We remark that $J^{(1)}$ is real and symmetric in r_1 and r_2, i.e.,

$$J^{(1)}(r_1, l_1; r_2, l_1) = J^{(1)}(r_2, l_1; r_1, l_1)$$

(b) *The case* $i = 2$

We show in the Appendix that for any two (complex) vectors **A** and **B** one has that

$$\int d\hat{\boldsymbol{\sigma}} \exp[-(\mathbf{B}\cdot\hat{\boldsymbol{\sigma}})^2]\ {}_1F_1\left(1, \frac{1}{2}; (\mathbf{A}\cdot\hat{\boldsymbol{\sigma}})^2\right)$$

$$= [\exp(A^2 - B^2)] \int d\hat{\boldsymbol{\sigma}} \exp[-(\mathbf{A}\cdot\hat{\boldsymbol{\sigma}})^2]\ {}_1F_1\left(1, \frac{1}{2}; (\mathbf{B}\cdot\hat{\boldsymbol{\sigma}})^2\right) \tag{4.26}$$

Thus, for the special case that **A** and **B** are given by Eq. (4.17) one has [cf. Eqs. (4.17), (3.6), and (2.9)]

$$B^2 = -(1+\xi)\, A^2 \tag{4.27}$$

so that $A^2 - B^2 = (2+\xi)\, A^2$. Therefore,

$$G^{(2)}(s_1, t_1, u_1; s_2, t_2, u_2) = G^{(4)}_{k=0}(s_1, t_1, u_1; s_2, t_2, u_2) \tag{4.28}$$

as follows from Eqs. (4.15b), (4.16b), (4.26), and (4.27). As a consequence, the matrix elements $\Omega^{(2)}_{jl}$ are given by [cf. Eqs. (4.9) and (4.28)],

$$\Omega^{(2)}_{jl} = \Omega^{(4)}_{jl}(k=0) \tag{4.29}$$

i.e., by the matrix elements $\Omega^{(4)}_{jl}(k)$ for $k = 0$. The matrix elements $\Omega^{(4)}_{jl}(k)$ will be discussed below for general k, including $k = 0$.

(c) *The case* $i = 3$

To evaluate the angular integrations in Eq. (4.16) for the cases 3 and 4, we need the integral

$$I(k) = \int d\hat{\boldsymbol{\sigma}}\ [\exp(i\mathbf{k}\cdot\boldsymbol{\sigma})]\ f(s_1\mathbf{T}^*(t_1)\cdot\hat{\boldsymbol{\sigma}},\ s_2\mathbf{T}(t_2)\cdot\hat{\boldsymbol{\sigma}}) \tag{4.30}$$

where $f(x_1, x_2)$ is a function of $x_1 = s_1\mathbf{T}_1^*(t_1)\cdot\hat{\boldsymbol{\sigma}}$ and $x_2 = s_2\mathbf{T}(t_2)\cdot\hat{\boldsymbol{\sigma}}$. Then, in order to perform the derivatives with respect to s_1 and s_2, we use that

$$\left(\frac{\partial}{\partial s_1}\right)_0^{l_1}\left(\frac{\partial}{\partial s_2}\right)_0^{l_2} I(k) = \left(\frac{\partial}{\partial x_1}\right)_0^{l_1}\left(\frac{\partial}{\partial x_2}\right)_0^{l_2} f(x_1, x_2)$$

$$\times \int d\hat{\boldsymbol{\sigma}}\ [\exp(i\mathbf{k}\cdot\boldsymbol{\sigma})][\mathbf{T}^*(t_1)\cdot\hat{\boldsymbol{\sigma}}]^{l_1}\ [\mathbf{T}(t_2)\cdot\hat{\boldsymbol{\sigma}}]^{l_2} \tag{4.31}$$

We obtain from Eqs. (3.7) and (2.7) that

$$P_1 P_2 I(k) = \left(\frac{\partial}{\partial x_1}\right)_0^{l_1} \left(\frac{\partial}{\partial x_2}\right)_0^{l_2} f(x_1, x_2) \times \int d\hat{\boldsymbol{\sigma}}\, [\exp(i\mathbf{k}\cdot\boldsymbol{\sigma})]\, Y_{l_1}^{(m_1)*}(\hat{\boldsymbol{\sigma}})\, Y_{l_2}^{(m_2)}(\hat{\boldsymbol{\sigma}}) \tag{4.32}$$

Therefore, by expanding

$$\exp(i\mathbf{k}\cdot\boldsymbol{\sigma}) = \sum_{n=0}^{\infty} [4\pi(2n+1)]^{1/2}\, i^n j_n(k\sigma)\, Y_n^{(0)}(\hat{\sigma})$$

where the $j_n(x)$ are spherical Bessel functions,(29,31) we obtain

$$P_1 P_2 I(k) = \delta_{m_1,m_2} \left(\frac{\partial}{\partial x_1}\right)_0^{l_1} \left(\frac{\partial}{\partial x_2}\right)_0^{l_2} f(x_1, x_2) \times \sum_{\substack{n=|l_1-l_2| \\ \Delta n = 2}}^{l_1+l_2} M(l_1, l_2; m_1; n)\, j_n(k\sigma) \tag{4.33}$$

Here

$$M(l_1, l_2; m; n) = (-)^m [4\pi(2n+1)]^{1/2}\, i^n \int d\hat{\boldsymbol{\sigma}}\, Y_{l_1}^{(-m)}(\hat{\boldsymbol{\sigma}})\, Y_{l_2}^{(m)}(\hat{\boldsymbol{\sigma}})\, Y_n^{(0)}(\hat{\boldsymbol{\sigma}}) \tag{4.34}$$

Thus, the coefficients $M(l_1, l_2; m; n)$ are directly related to Wigner's 3-J symbols, which give the result of an angular integration over the product of *three* $Y_l^{(m)}(\hat{\boldsymbol{\sigma}})$ with total angular momentum $J = l_1 + l_2 + n$ and for which explicit expressions exist for all m.(28,29) We note that $M(l_1, l_2; m; n) = 0$ when $J = l_1 + l_2 + n$ is odd, that

$$M(l_1, l_2; m; 0) = \delta_{l_1, l_2} \tag{4.35}$$

and that(28)

$$M(l_1, l_2; 0; n) = i^n [(2l_1+1)(2l_2+1)]^{1/2} (2n+1) \times \frac{(J-2l_1)!\,(J-2l_2)!\,(J-2n)!}{(J+1)!} \left[\frac{(J/2)!}{(J/2-l_1)!\,(J/2-l_2)!\,(J/2-n)!}\right]^2 \tag{4.36}$$

when $J=l_1+l_2+n$ is even. As a consequence, the variable n in Eq. (4.33) varies in steps of *two* (i.e., $\Delta n=2$), being either even or odd depending on whether l_1+l_2 is even or odd, respectively.

Using these results, we consider the matrix elements [cf. Eq. (4.9)]

$$\Omega_{jl}^{(3)}(k)=P_1P_2Q_1Q_2G_k^{(3)}(s_1,t_1,u_1;s_2,t_2,u_2) \tag{4.37}$$

with $G_k^{(3)}$ given by Eq. (4.16). $G_k^{(3)}$ is of the form given by Eq. (4.30) for $I(k)$, since

$$\mathbf{B}\cdot\hat{\boldsymbol{\sigma}}=\beta_1x_1+\beta_2x_2 \tag{4.38}$$

with $x_1=s_1\mathbf{T}^*(t_1)\cdot\hat{\boldsymbol{\sigma}}$, $x_2=s_2\mathbf{T}(t_2)\cdot\hat{\boldsymbol{\sigma}}$, and

$$\begin{aligned}\beta_1&=\tfrac{1}{2}(1+\xi+u_1u_2)^{-1/2}(2+\xi)^{-1/2}(1+u_2)\\ \beta_2&=-\tfrac{1}{2}(1+\xi+u_1u_2)^{-1/2}(2+\xi)^{-1/2}(1+u_1)\end{aligned} \tag{4.39}$$

Therefore,

$$\begin{aligned}&G_k^{(3)}(s_1,t_1,u_1;s_2,t_2,u_2)\\ &\quad=\frac{(1+\xi/2)^2}{nt_0(1+\xi+u_1u_2)^2}\\ &\quad\quad\times\frac{1}{4\pi}\int d\hat{\boldsymbol{\sigma}}\left[\cos(\mathbf{k}\cdot\boldsymbol{\sigma})_1F_1\left(-\frac{1}{2},\frac{1}{2};-(\beta_1x_1+\beta_2x_2)^2\right)\right.\\ &\quad\quad\left.-i\pi^{1/2}\sin(\mathbf{k}\cdot\boldsymbol{\sigma})(\beta_1x_1+\beta_2x_2)\right]\end{aligned} \tag{4.40}$$

Due to Eq. (4.33) we may write the result for $\Omega_{jl}^{(3)}(k)$ as

$$\begin{aligned}&\Omega_{jl}^{(3)}(k)\\ &\quad=\frac{1}{nt_0}\delta_{m_1,m_2}J^{(3)}(r_1,l_1;r_2,l_2)\\ &\quad\quad\times\sum_{\substack{n=|l_1-l_2|\\ \Delta n=2}}^{l_1+l_2}M(l_1,l_2;m_1;n)\,j_n(k\sigma)\end{aligned} \tag{4.41}$$

Then, when l_1+l_2 is *odd*, the $\Omega_{jl}^{(3)}(k)$ or $J^{(3)}(r_1,l_1;r_2,l_2)$ are determined by the second term on the right-hand side of Eq. (4.40) alone, i.e., by

$$\begin{aligned}&J^{(3)}(r_1,l_1;r_2,l_2)\\ &\quad=\frac{-1}{4\sqrt{\pi}}Q_1Q_2\left(\frac{\partial}{\partial x_1}\right)_0^{l_1}\left(\frac{\partial}{\partial x_2}\right)_0^{l_2}\\ &\quad\quad\times\frac{(1+\xi/2)^{1/2}}{(1+\xi+u_1u_2)^2}(\beta_1x_1+\beta_2x_2),\qquad(l_1+l_2\text{ is odd})\end{aligned} \tag{4.42}$$

It follows from this and Eqs. (3.6), (3.7), and (4.39) that $J^{(3)}$ is nonvanishing only when $r_1 = r_2 = 0$, $l_1 = 0$, $l_2 = 1$ or $r_1 = r_2 = 0$, $l_1 = 1$, $l_2 = 0$. Since these cases refer to the 1,2 and 2,1 elements of $\Omega_{jl}(k)$, we have

$$J^{(3)}(r_1, l_1; r_2, l_2) = 0$$
$$\Omega_{jl}^{(3)}(k) = 0, \qquad l_1 + l_2 \text{ odd}; j, l \geqslant 2 \tag{4.43}$$

for the part of the matrix $\Omega_{jl}^{(3)}(k)$ we are considering here, i.e., $j, l \geqslant 2$. Therefore $J^{(3)}$ and $\Omega^{(3)}$ are nonvanishing only when $l_1 + l_2$ is even. Then, $J^{(3)}$ is determined entirely by the first term on the right-hand side of Eq. (4.40). Hence, from Eqs. (4.37), (4.40), (4.41), and (4.33),

$$\begin{aligned} &J^{(3)}(r_1, l_1; r_2, l_2) \\ &\quad = \frac{1}{4\pi} Q_1 Q_2 \left(\frac{\partial}{\partial x_1}\right)_0^{l_1} \left(\frac{\partial}{\partial x_2}\right)_0^{l_2} \\ &\quad \times \frac{(1+\xi/2)^{1/2}}{(1+\xi+u_1 u_2)^2}\, {}_1F_1\left(-\frac{1}{2}, \frac{1}{2}; -(\beta_1 x_1 + \beta_2 x_2)^2\right), \qquad l_1 + l_2 \text{ even} \end{aligned} \tag{4.44}$$

which is evaluated straightforwardly, with the result

$$J^{(3)}(r_1, l_1; r_2, l_2) = \frac{(-)^{(l_1 - l_2)/2} \left(-\frac{1}{2}\right)_{r_1 + r_2 + (l_1 + l_2)/2}}{2^{r_1 + r_2 + (l_1 + l_2)/2} \left\{ \left(\frac{3}{2}\right)_{r_1 + l_1} \left(\frac{3}{2}\right)_{r_2 + l_2} r_1!\, r_2! \right\}^{1/2}} \tag{4.45}$$
$$(l_1 + l_2 \text{ is even})$$

We remark that $J^{(3)}$ is real and symmetric, i.e., $J^{(3)}(r_1, l_1; r_2, l_2) = J^{(3)}(r_2, l_2; r_1, l_1)$. In addition, for $k \to 0$ we have for $\Omega_{jl}^{(3)}(k)$ that [cf. Eqs. (4.41) and (4.35)],

$$\Omega_{jl}^{(3)}(0) = \frac{1}{nt_0} \delta_{m_1, m_2} \delta_{l_1, l_2} J^{(3)}(r_1, l_1; r_2, l_1) \tag{4.46}$$

since $j_0(0) = 1$ and $j_n(0) = 0$ for $n \geqslant 1$,[31] so that for $k = 0$, $\Omega_{jl}^{(3)}(0)$ is diagonal, not only in $m_1 = m_2$, but also in $l_1 = l_2$.

(d) *The case $i = 4$*

Here we consider

$$\Omega_{jl}^{(4)}(k) = P_1 P_2 Q_1 Q_2 G_k^{(4)}(s_1, t_1, u_1; s_2, t_2, u_2) \tag{4.47}$$

where $G_k^{(4)}$ is given by Eq. (4.16) and is of the form given by Eq. (4.30) for $I(k)$, using that

$$\mathbf{A} \cdot \hat{\boldsymbol{\sigma}} = \alpha(x_1 + x_2) \tag{4.48}$$

with $x_1 = s_1 \mathbf{T}^*(t_1) \cdot \hat{\boldsymbol{\sigma}}$, $x_2 = s_2 \mathbf{T}(t_2) \cdot \hat{\boldsymbol{\sigma}}$, and

$$\alpha = \tfrac{1}{2}(1+\xi)^{1/2}(2+\xi)^{-1/2} \tag{4.49}$$

Thus, we may write the result as

$$\Omega_{jl}^{(4)}(k) = \frac{1}{nt_0} \delta_{m_1, m_2} J^{(4)}(r_1, l_1; r_2, l_2) \times \sum_{\substack{n=|l_1-l_2| \\ \Delta n = 2}}^{l_1+l_2} M(l_1, l_2; m_1; n)\, j_n(k\sigma) \tag{4.50}$$

We distinguish between the cases that $l_1 + l_2$ is either odd or even.

First, when $l_1 + l_2$ is odd, we only need the second term on the right-hand side of Eq. (4.16) for $G_k^{(4)}$, so that

$$\begin{aligned} J^{(4)}&(r_1, l_1; r_2, l_2) \\ &= \frac{-1}{4\sqrt{\pi}} Q_1 Q_2 \left(\frac{\partial}{\partial x_1}\right)_0^{l_1} \left(\frac{\partial}{\partial x_2}\right)_0^{l_2} \\ &\quad \times \frac{(1+\xi/2)^{1/2}}{(1+\xi)(1+\xi+u_1 u_2)} \alpha(x_1+x_2) \\ &\quad \times \exp[\alpha^2(x_1+x_2)^2 - (\beta_1 x_1 + \beta_2 x_2)^2] \qquad (l_1 + l_2 \text{ is odd}) \end{aligned} \tag{4.51}$$

with α, β_1, and β_2 given by Eqs. (4.49) and (4.39). The derivatives in this equation can be performed straightforwardly, with the result

$$\begin{aligned} J^{(4)}(r_1, l_1; r_2, l_2) &= \left(\frac{\delta_{2r_1+l_1, 2r_2+l_2-1}}{(2r_2+2l_2+1)^{1/2}} + \frac{\delta_{2r_1+l_1, 2r_2+l_2+1}}{(2r_1+2l_1+1)^{1/2}} \right) \\ &\quad \times E\left(r_1, r_2; \frac{l_1+l_2-1}{2}\right) \qquad (l_1 + l_2 \text{ is odd}) \end{aligned} \tag{4.52}$$

where $(l_1 + l_2 - 1)/2$ is a nonnegative integer and

$$\begin{aligned} E(r_1, r_2; l) &= (-)^{r+1} \left(\frac{\pi(1+R)_r}{(3/2+R+l)_r} \right)^{1/2} \frac{(1+r)_{l+1}}{2^{r+l+1}(3/2)_l} \\ &\quad \times \sum_{j=0}^{R} \frac{(-R)_j\, ((r-l-1)/2)_j\, ((r-l)/2)_j}{j!\,(1+r)_j\,(1/2-R-l)_j} \end{aligned} \tag{4.53}$$

with $R = \mathrm{Min}(r_1, r_2)$, $r = |r_1 - r_2|$, and where l is an integer.

Second, when l_1+l_2 is even, we only need the first term on the right-hand side of Eq. (4.16) for $G_k^{(4)}$, so that

$$J^{(4)}(r_1,l_1;r_2,l_2) = \frac{1}{4\pi} Q_1 Q_2 \left(\frac{\partial}{\partial x_1}\right)_0^{l_1} \left(\frac{\partial}{\partial x_2}\right)_0^{l_2} \frac{(1+\xi/2)^{1/2}}{(1+\xi)(1+\xi+u_1u_2)} \times \exp[-(\beta_1 x_1+\beta_2 x_2)^2]\ {}_1F_1\left(1,\frac{1}{2};\alpha^2(x_1+x_2)^2\right) \quad (l_1+l_2 \text{ is even}) \tag{4.54}$$

Performing the derivatives leads to

$$\begin{aligned} J^{(4)}(r_1,l_1;r_2,l_2) &= \frac{(-)^{(l_1-l_2)/2}}{[2^{l_1+l_2} r_1!\, r_2!\, (3/2)_{r_1+l_1}(3/2)_{r_2+l_2}]^{1/2}} \\ &\times \sum_{n_1=0}^{l_1}{}' \sum_{n_2=0}^{l_2}{}' (-)^{(n_1-n_2)/2} (-l_1)_{n_1} (-l_2)_{n_2} \\ &\times \left(\frac{n_1+n_2}{2}\right)! \left(\frac{1}{2}\right)_{(l_1+l_2-n_1-n_2)/2} \frac{1}{n_1!\, n_2!} \\ &\times D\left(r_1, \frac{l_1+l_2+n_1-n_2-1}{2}; r_2, \frac{l_1+l_2-n_1+n_2-1}{2}; \frac{n_1+n_2}{2}, \frac{l_1+l_2}{2}\right) \\ &(l_1+l_2 \text{ is even}) \end{aligned} \tag{4.55}$$

where the primes on the summation signs mean that only terms with n_1+n_2 *even* have to be taken into account and where $D(r_1,\alpha_1;r_2,a_2;k,q)$ is given by Eq. (4.24).

We note that both for l_1+l_2 odd or even, $J^{(4)}(r_1,l_1;r_2,l_2)$ is real and symmetric, i.e., $J^{(4)}(r_1,l_1;r_2,l_2)=J^{(4)}(r_2,l_2;r_1,l_1)$. Also, from Eqs. (4.50) and (4.35) it follows that for $k\to 0$

$$\Omega_{jl}^{(4)}(0) = \frac{1}{nt_0}\delta_{m_1,m_2}\delta_{l_1,l_2} J^{(4)}(r_1,l_1;r_2,l_1) \tag{4.56}$$

where $J^{(4)}(r_1,l_1;r_2,l_1)$ is given by Eq. (4.55) with $l_1=l_2$.

Collecting the results obtained in this section yields for the matrix elements $\Omega_{jl}(k)$ with $j=(r_1,l_1,m_1)$ and $l=(r_2,l_2,m_2)$ that for j or $l\geqslant 2$,

$$\Omega_{jl}(k) = \frac{\delta_{m_1,m_2}}{nt_0}\left\{\delta_{l_1,l_2} J^s(r_1,l_1;r_2,l_1) + J^d(r_1,l_1;r_2,l_2) \sum_{\substack{n=|l_1-l_2| \\ \Delta n=2}}^{l_1+l_2} M(l_1,l_2;m_1;n)\, j_n(k\sigma)\right\} \tag{4.57}$$

where [cf. Eqs. (4.7), (4.23), (4.29), and (4.56)]

$$J^s(r_1, l_1; r_2, l_1) = -J^{(1)}(r_1, l_1; r_2, l_1) + J^{(4)}(r_1, l_1; r_2, l_1) \tag{4.58}$$

with $J^{(1)}$ and $J^{(4)}$ given by Eqs. (4.25) and (4.55), respectively, and

$$J^d(r_1, l_1; r_2, l_2) = -J^{(3)}(r_1, l_1; r_2, l_2) + J^{(4)}(r_1, l_1; r_2, l_2) \tag{4.59}$$

with $J^{(3)}$ given by Eqs. (4.43) and (4.45) and $J^{(4)}$ given by Eqs. (4.52) and (4.55) and where $M(l_1, l_2; m_1; n)$ in Eq. (4.57) is given by Eq. (4.34).

For $k \to 0$ one has

$$\Omega_{jl}(0) = \frac{1}{nt_0} \delta_{m_1,m_2} \delta_{l_1,l_2} J(r_1, l_1; r_2, l_1) \tag{4.60}$$

with

$$J(r_1, l_1; r_2, l_1) = J^s(r_1, l_1; r_2, l_1) + J^d(r_1, l_1; r_2, l_1) \tag{4.61}$$

the reduced matrix elements of the Boltzmann collision operator $\Lambda_B = \lim_{k \to 0} \Lambda_{\mathbf{k}}$ considered by Foch and Ford.[25] For $k \to \infty$, all spherical Bessel functions in Eq. (4.57) decay to zero, so that

$$\Omega_{jl}(\infty) = \frac{1}{nt_0} \delta_{m_1,m_2} \delta_{l_1,l_2} J^s(r_1, l_1; r_2, l_1) \tag{4.62}$$

where the J^s are the reduced matrix elements of the Lorentz–Boltzmann collision operator $\Lambda^s = \lim_{k \to \infty} \Lambda_{\mathbf{k}}$ relevant for the description of self-diffusion processes in the fluid.[9]

We conclude that the $\Omega_{jl}(k)$ are diagonal in $m_1 = m_2$ for all k, diagonal in $l_1 = l_2$ for $k = 0$ (i.e., the Boltzmann limit) and $k = \infty$ (i.e., the Lorentz–Boltzmann limit) and depend for intermediate k on $m_1 = m_2$ only through the coefficients $M(l_1, l_2; m_1; n)$ [cf. Eq. (4.57)].

5. DISCUSSION

We have derived general expressions for the $M \times M$ matrices $\mathscr{A}_{jl}(k, z)$ [cf. Eqs. (3.2) and (3.18)] and $\Omega_{jl}(k)$ [cf. Eq. (4.57)] for $j = (r_1, l_1, m_1)$ and $l = (r_2, l_2, m_2)$. These matrices are needed to determine the one-particle time correlation functions $F_{jl}(k, t)$ in a hard-sphere fluid using the BGK method explicitly [cf. Eqs. (1.15) and (1.16)].

The results given here reduce to those used before[11,12,32] to calculate the nine correlation functions $F_{jl}(k, t)$ with j or $l = 1, 2, 3$. Here the label j or $l = 3$ refers to the third polynomial in the set $\{(\phi_j(\mathbf{v}_1))\}$, i.e.,

$$\phi_3(\mathbf{v}_1) = \psi_{1,0,0}(\mathbf{c}) = \left(\frac{2}{3}\right)^{1/2} \left(\frac{3}{2} - \mathbf{c}^2\right) = \frac{-1}{\sqrt{6}} \left(\frac{m}{k_B T} \mathbf{v}_1^2 - 3\right) \tag{5.1}$$

This function represents the local microscopic temperature fluctuations of the fluid. These nine correlation functions $F_{jl}(k, t)$ (which all have quantum number $m = 0$) are needed to understand the time behavior of the intermediate scattering function $F_{11}(k, t)$, which is the function relevant for neutron or light scattering experiments on simple dense fluids.[11,12,20,32]

We now discuss the properties of the $F_{jl}(k, t)$ as to: (1) their convergence with respect to the label M in the BGK method; (2) the transition to ideal gas behavior at large k; (3) the transition to hydrodynamic behavior at small k; and (4) their description in terms of eigenmodes.

5.1. Convergence

To study the convergence of the BGK method for the calculation of the nine $F_{jl}(k, t)$ with j or $l = 1, 2, 3$, one needs to order the polynomia $\Phi_{r,l}(\mathbf{c}) = \psi_{r,l,0}(\mathbf{c})$ [cf. Eq. (2.12)] with respect to the quantum numbers r and l. To do so, we have used three criteria.[9-12]

5.1.1. Lorentz–Boltzmann Ordering. In the Lorentz–Boltzmann ordering (LB), the label j in the set $\{\phi_j\}$ corresponds to the labels r, l in the set $\{\Phi_{r,l}(\mathbf{c})\}$ in such a manner that the reduced diagonal elements $J^s(r, l; r, l)$ of the Lorentz–Boltzmann operator Λ^s decrease with increasing $j = (r, l)$. In Fig. 1, we show the $J^s(r, l; r, l)$ as a function of r and l. We see that J^s decrease at fixed r with increasing l and at fixed l with increasing r.

Thus, the ordering of the $\Phi_{r,l}(\mathbf{c})$ can be read off from Fig. 1 and follows globally the rule that the "lowest" (r, l) come first and, more particularly, that the lowest $r + l$ come first (cf. Fig. 1). The results are summarized in Table I, where the first 24 polynomia in the Lorentz–Boltzmann ordering are given.

5.1.2. Boltzmann Ordering. In the Boltzmann ordering (B), the $\{\phi_j\}$ are ordered such that the reduced diagonal elements $J(r, l; r, l)$ of the Boltzmann operator Λ_B decrease with increasing $j = (r, l)$.

In Fig. 2, we show $J(r, l; r, l)$ as a function of r and l, where we see that J decreases at fixed r with increasing l and at fixed l with increasing r. Thus, again, the "lowest" (r, l) (but not the lowest $r + l$) come first. The results are also summarized in Table I.

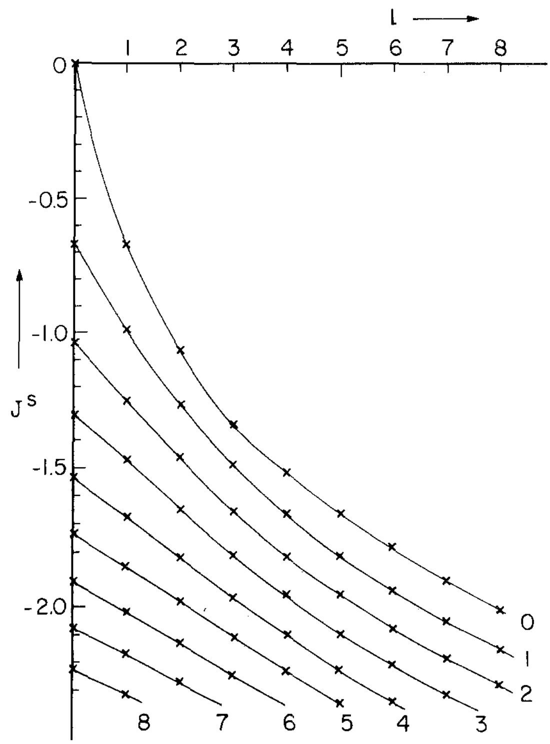

Fig. 1. The reduced diagonal elements $J^s = J^s(r, l; r, l)$ of the Lorentz–Boltzmann operator [cf. Eqs. (4.58) and (4.62)] as a function of l at various values of r (crosses). The curves connect the J^s with the same $r = 0, 1, 2, \ldots, 8$ as indicated at the end of each curve.

We observe in Table I that the LB and B orderings are very similar. Thus, for example, in the BGK approximation of order $M = 9$ all nine polynomia in the LB and B orderings are the same, or, when $M = 24$, 21 of the 24 polynomia are the same in the LB and B orderings (cf. Table I).

5.1.3. Alterman Ordering. In the Alterman ordering (A), the $\{\phi_j\}$ are ordered such that the eigenvalues $\lambda(r, l)$ of the reduced Boltzmann operator $nt_0\Lambda_B$, as computed by Alterman *et al.*,[33] decrease with increasing $j = (r, l)$.

In fact, for each $l = 0, 1, \ldots, 13$, the $\lambda(r, l)$ are the 30 eigenvalues $\lambda_i(l)$ with $i = 1, \ldots, 30$ of the 30×30 matrices $J(r_1, l; r_2, l)$ with r_1 or $r_2 = 0, 1, \ldots, 29$. Here the labels r in $\lambda(r, l)$ and i in $\lambda_i(l)$ are related to each other in such a manner that r refers to that polynomial $\Phi_{r,l}$ that contributes most to the eigenfunction corresponding to $\lambda_i(l)$. Therefore, in $\lambda(r, l)$, while l is a "good" quantum number, r is an "approximate" quantum number,

Table I. Quantum Numbers r and l of the Polynomials $\Phi_{r,l}(\mathbf{c}) = \psi_{r,l,0}(\mathbf{c})$ [Eq. (2.12)] and Corresponding Values of $J^s(r, l; r, l)$ (Fig. 1), $J(r, l; r, l)$ (Fig. 2), and $\lambda(r, l)$ (Section 5.1.3)[a]

r	l	$J^s(r, l; r, l)$	$J(r, l; r, l)$	$\lambda(r, l)$	j(LB)	j(B)	j(A)
0	0	0	0	0	1	1	1
0	1	−0.6667	0	0	2	2	2
1	0	−0.6667	0	0	3	3	3
1	1	−0.9833	−0.5333	−0.4975	4	4	5
2	0	−1.0333	−0.5333	−0.4746	5	5	4
0	2	−1.0667	−0.8000	−0.7593	6	6	8
2	1	−1.2478	−0.8571	−0.6994	7	7	7
1	2	−1.2619	−0.9762	−0.8353	8	9	11
3	0	−1.3076	−0.8857	−0.6866	9	8	6
0	3	−1.3286	−1.2000	−1.0023	10	13	21
2	2	−1.4607	−1.1795	−0.8981	11	12	14
3	1	−1.4733	−1.1224	−0.8173	12	10	10
1	3	−1.4871	−1.3135	−1.0229	13	14	23
0	4	−1.5175	−1.4540	−1.1120	14	18	43
4	0	−1.5347	−1.1623	−0.8096	15	11	9
3	2	−1.6467	−1.3758	−0.9484	16	16	16
2	3	−1.6514	−1.4600	−1.0430	17	19	26
0	5	−1.6665	−1.6349	−1.1703	18	25	>60
1	4	−1.6673	−1.5650	−1.1185	19	22	46
4	1	−1.6719	−1.3506	−0.8955	20	15	13
5	0	−1.7324	−1.3952	−0.8904	21	17	12
0	6	−1.7927	−1.7770	−1.2046	22	31	>60
3	3	−1.8111	−1.6133	−1.0614	23	24	30
1	5	−1.8147	−1.7558	−1.1727	24	29	>60

[a] Also given are the corresponding labels j of $\phi_j(\mathbf{v}_1) = \Phi_{r,l}(\mathbf{c})$ when one uses the Lorentz–Boltzmann [j(LB)], the Boltzmann [j(B)], or the Alterman [j(A)] orderings, respectively.

since it refers to the polynomial $\Phi_{r,l}$ only in as far as $\Phi_{r,l}$ gives the most important contribution to the eigenfunction of Λ_B corresponding to the eigenvalue $\lambda(r, l)$.

The result of the Alterman ordering of the polynomials $\Phi_{r,l}$ is given in Table I. We observe that the A ordering does not differ considerably from the B ordering, and that when $M = 24$, 17 of the 24 polynomia are the same in the LB and A orderings. We also see that, while the LB ordering stresses the importance of polynomia with low $r + l$, the A ordering emphasizes the importance of polynomia with low l alone.

5.1.4. Convergence of Correlation Functions. Of the nine correlation functions $F_{jl}(k, t)$ with j or $l = 1, 2, 3$, only three are independent.

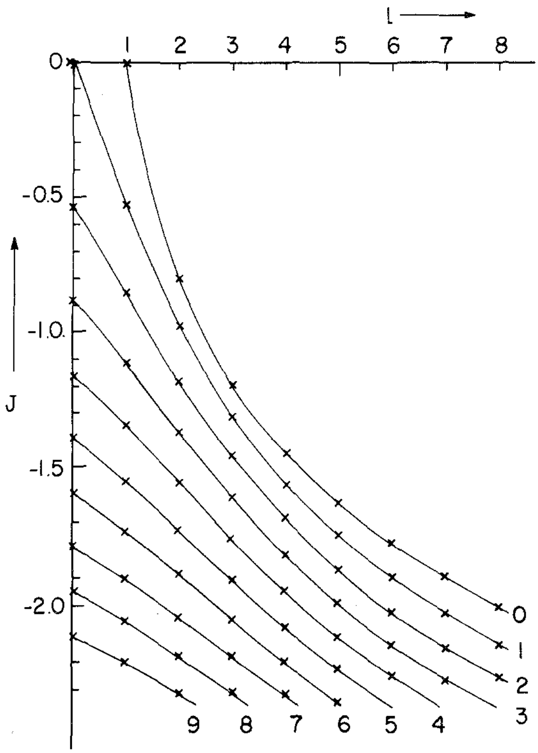

Fig. 2. The reduced diagonal elements $J = J(r, l; r, l)$ of the Boltzmann operator Λ_B [Eqs. (4.60) and (4.61)] as a function of l at various values of r (crosses). The curves connect the J with the same $r = 0, 1, 2, ..., 9$ as indicated at the end of each curve. Note that $J = 0$ for $r = 0$, $l = 0$; $r = 0$, $l = 1$; and $r = 1$, $l = 0$.

We have chosen before(11,12,32) to calculate the Fourier transforms of three independent correlation functions

$$S_{jl}(k, \omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt\, e^{-i\omega t} F_{jl}(k, t) \tag{5.2}$$

namely those for $(j, l) = (1, 1)$, $(1, 3)$, and $(3, 3)$. The $S_{jl}(k, \omega)$ are given by

$$S_{jl}(k, \omega) = \frac{1}{\pi} \operatorname{Re} G_{jl}(k, z = i\omega) \tag{5.3}$$

with $G_{jl}(k, i\omega)$ from Eq. (1.16). We consider now the convergence of the $S_{jl}(k, \omega)$ with respect to M and with respect to the ordering of the polynomia.

As to the convergence with respect to M, we find for all densities and all k that the convergence of the $S_{jl}(k, \omega)$ is slowest when $\omega = 0$. Therefore, it suffices to consider the results for the $S_{jl}(k, \omega)$ as functions of M for $\omega = 0$ alone. For three values of k we show $S_{jl}(k, 0)/t_E$ as a function of M in Fig. 3 for $V_0/V = 0.071$, in Fig. 4 for $V_0/V = 0.333$, and in Fig. 5 for $V_0/V = 0.625$, where $V_0/V = n\sigma^3/\sqrt{2}$ is a reduced density, with V_0 the volume of close packing of a hard-sphere fluid. The three densities considered here are the same as those in ref. 27 for $S_{11}(k, \omega) = S(k, \omega)/S(k)$, where $S(k, \omega)$ and $S(k)$ are the dynamic and static structure factors of the fluid, respectively.

We find that the convergence with respect to M of the $S_{jl}(k, 0)$ is almost independent of the density and is mainly determined by the value of kl_E (cf. Figs. 3–5). Here $l_E = l_0/\chi$ and $l_0 = (8k_B T/\pi m)^{1/2} t_0$ are the Enskog and Boltzmann values of the mean free path between collisions, respectively. The convergence is fastest at small k. Thus, for $kl_E \leqslant 0.5$ the $S_{jl}(k, 0)$ have converged for $M = 55$ to at least four significant figures (i.e., to 0.01%), both in the A ordering (shown) as well as in the LB ordering. The convergence becomes slower when kl_E increases. For $kl_E = 3$ the results at

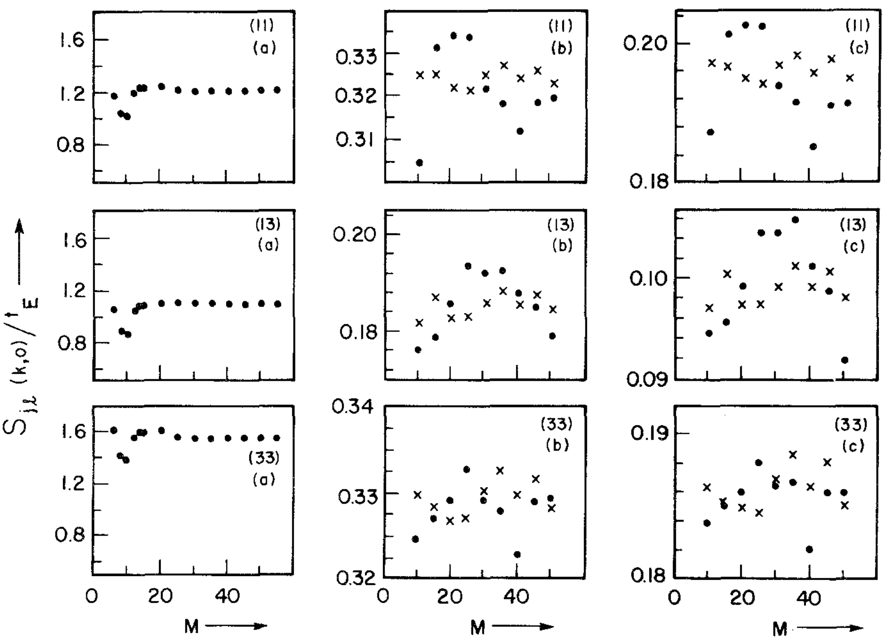

Fig. 3. The reduced $S_{jl}(k, 0)/t_E$ as a function of M at the reduced density $V_0/V = 0.0071$ for $j, l = 1, 1$; 1, 3; and 3, 3 (as indicated in parentheses), for (a) $kl_E = 0.5$, (b) 1.77, and (c) 3, using the Alterman ordering (dots) and the Lorentz–Boltzmann ordering (crosses).

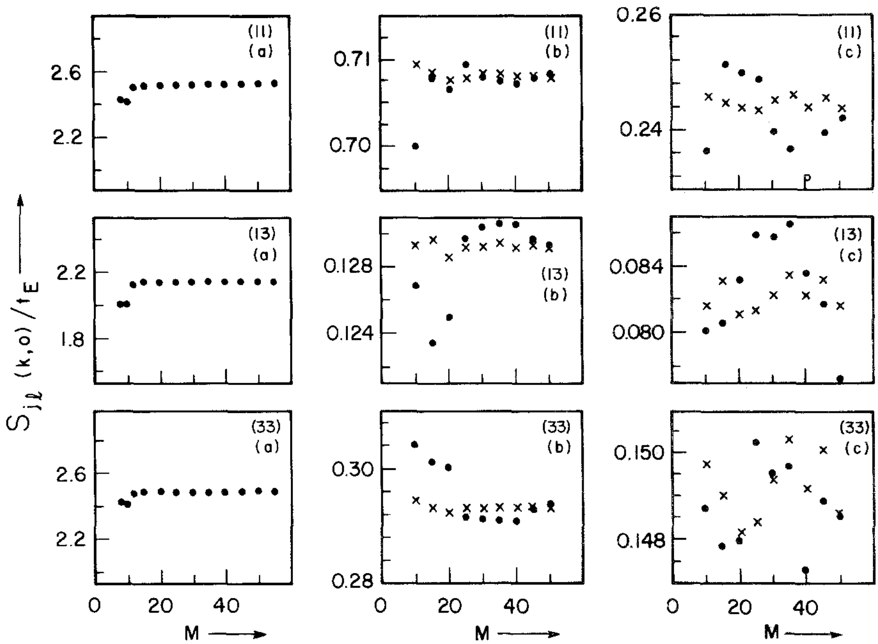

Fig. 4. The reduced $S_{jl}(k, 0)/t_E$ as a function of M at the reduced density $V_0/V = 0.33$ for $j, l = 1, 1; 1, 3;$ and $3, 3$ (as indicated in parentheses), for (a) $kl_E = 0.143$, (b) 1, and (c) 3, using the Alterman ordering (dots) and the Lorentz–Boltzmann ordering (crosses).

$M = 55$ have converged within about 1% for the LB ordering and within about 3% for the A ordering. The convergence improves again when kl_E increases further (e.g., in the LB ordering to about 0.5% at $kl_E = 50$).

Thus, the correlation functions $S_{jl}(k, \omega)$ can be calculated with the BGK method of order $M = 55$ for all k, all ω, and all densities with an accuracy of at least 1% in the LB ordering or 3% in the A ordering. That the results for the $S_{jl}(k, \omega)$ in the A ordering converge slower than those in the LB ordering implies that the polynomia with low quantum number l alone are less important for the computation of $S_{jl}(k, \omega)$ than the polynomia with low $r + l$.

We remark that the convergence of $S_{11}(k, 0)$ as a function of the number of Burnett polynomia used in the explicit calculation (i.e., M in Figs. 3–5) is faster than the convergence discussed in ref. 27, where Hermite polynomia were used. The reason for this is that Burnett polynomia are more economical than Hermite polynomia, since they incorporate the cylindrical symmetry in velocity space.

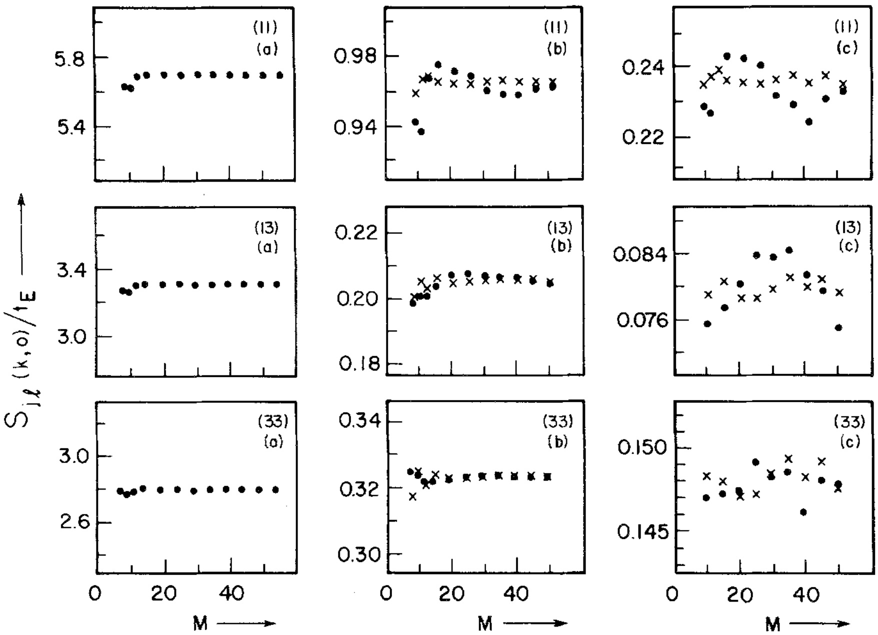

Fig. 5. The reduced $S_{jl}(k, 0)/t_E$ as a function of M at the reduced density $V_0/V = 0.625$ for $j, l = 1, 1; 1, 3$; and 3, 3 (as indicated in parentheses), for (a) $kl_E = 0.039$, (b) 1, and (c) 3, using the Alterman ordering (dots) and the Lorentz–Boltzmann ordering (crosses).

5.2. Ideal Gas Behavior

Next we consider the correlation functions $G_{jl}(k, z)$ with j or $l = 1, 2, 3$ in the BGK approximation of order M in the ideal gas limit $k \to \infty$. To study this limit, it is convenient to use the (complex) reduced frequency

$$z^* = \frac{2i}{\sqrt{\pi}} \frac{zt_E}{kl_E} = i\left(\frac{m}{2k_B T}\right)^{1/2} \frac{z}{k} \tag{5.4}$$

as a quantity of order 1 and $1/kl_E$ as a small expansion parameter around $1/kl_E = 0$. Here $t_E = t_0/\chi$ is the Enskog mean free time. We use that in Eq. (1.16) for $G_{jl}(k, z)$ all matrix elements of $\mathscr{A}(k, z)$ are small compared to those of $\mathscr{F}(k)$ for all z. For, the matrix elements $\mathscr{F}_{jl}(k)$ of the $M \times M$ matrix $\mathscr{F}(k)$ are finite for $k \to \infty$, so that $\mathscr{F}(k)$ is a quantity of order $(kl_E)^0$ [cf. Eq. (1.12) and ref. 9]. The elements $\mathscr{A}_{jl}(k, z)$ of the $M \times M$ matrix $\mathscr{A}(k, z)$ in Eq. (1.16), on the other hand, are given by [cf. Eq. (3.2)]

$$\mathscr{A}_{jl}(k, z) = \frac{-2it_E}{\sqrt{\pi}} \frac{1}{kl_E} A_{jl}(\zeta) \tag{5.5}$$

where $\zeta = z^* + O[(kl_E)^{-1}]$ [cf. Eqs. (3.4) and (5.4)]. Thus, $\mathscr{A}(k, z)$ is a quantity of order $(kl_E)^{-1}$ and small compared to $\mathscr{F}(k)$. Therefore, we can write [cf. Eq. (1.16)]

$$G_{jl}(k, z) = \{\mathscr{A}(k, z) + \mathscr{A}(k, z)\, \mathscr{F}(k)\, \mathscr{A}(k, z) + O[(kl_E)^{-3}]\}_{jl} \quad (5.6)$$

or, with Eq. (5.5),

$$G_{jl}(k, z) = \frac{-2it_E}{\pi^{1/2} kl_E}\left[A_{jl}(z^*) + \frac{g_{jl}^{(M)}(z^*)}{kl_E} + O(kl_E)^{-2})\right] \quad (5.7)$$

where

$$g_{jl}^{(M)}(z^*) = \frac{-2it_E}{\sqrt{\pi}}\left[d(\infty)\, A'_{jl}(z^*) + \sum_{j',l'}^{M} A_{jj'}(z^*)\, \mathscr{F}_{j'l'}(\infty)\, A_{l'l}(z^*)\right] \quad (5.8)$$

with $A'_{jl}(z) = dA_{jl}(z)/dz$.

Thus, the $G_{jl}(k, z)$ in Eq. (5.7) are given by series expansions in terms of inverse powers of kl_E, where the coefficients are functions of z^*. The leading term $\sim A_{jl}(z^*)$ in Eq. (5.7) is the Laplace transform of the ideal gas $F_{jl}(k, t)$, as given by Eq. (1.1), with $L_E(\mathbf{k})$ replaced by $-i\mathbf{k}\cdot\mathbf{v}_1$, i.e., by the free streaming contribution to $L_E(\mathbf{k})$ [cf. Eq. (1.4)]. From this it follows immediately that the BGK approximations of order M to the $G_{jl}(k, z)$ $(j, l = 1, 2, 3)$ reduce to their corresponding exact ideal gas values for $k \to \infty$ for any fixed M.

The approach of the $G_{jl}(k, z)$ to their ideal gas values is given by the second term on the right-hand side of Eq. (5.7) [i.e., by the $g_{jl}^{(M)}(z^*)$]. This term depends on M via $d(\infty)$ [cf. Eq. (1.11)] as well as via the three $M \times M$ matrix multiplications in Eq. (5.8). By evaluating the $g_{jl}^{(M)}(z^*)$ numerically in the BGK method with $M \leqslant 55$, we find that the results have converged within a few percent for $M = 55$. This has been reported before for $(jl) = (11)$, (13), and (33).[12,32]

To get an idea of how fast the approach to ideal gas behavior is, we evaluated the $g_{11}^{(\infty)}(z^*)$. To do this, we used that

$$g_{jl}^{(\infty)}(z^*) = \frac{-2it_E}{\sqrt{\pi}}\left\langle \phi_j(\mathbf{v}_1)\, \frac{1}{c_z - z^*}\, n\chi\Lambda^s\, \frac{1}{c_z - z^*}\, \phi_l(\mathbf{v}_1)\right\rangle_1 \quad (5.9)$$

and that

$$\frac{d}{dz} A_{jl}(z) = \sum_{j'=1}^{\infty} A_{jj'}(z)\, A_{j'l}(z) \quad (5.10)$$

Equation (5.9) follows from Eqs. (1.12), (3.3), and (5.8), while Eq. (5.10) follows from Eq. (3.3) and that the $\{\psi_{r,l,m}(\mathbf{c})\}$ form a complete set of polynomia in $\mathbf{c}$. The expression (5.9) has been evaluated analytically for $j=l=1$ in ref. 35. We find that our BGK result for $g_{11}^{(M)}(z^*)$ with $M=55$ does not differ by more than a few percent from the exact $g_{11}^{(\infty)}(z^*)$. Thus, it appears that the approach of the $G_{jl}(k, z)$ to ideal gas behavior can be described accurately by the BGK method, at least when $M \geqslant 55$.

5.3. Hydrodynamic Behavior

To study the hydrodynamic limit, i.e., the $k \to 0$ limit, of the nine $G_{jl}(k, z)$ in the BGK approximation of order M, we rewrite Eq. (1.16) in the equivalent but more convenient form

$$G_{jl}(k, z) = \left[\frac{1}{\mathscr{A}^{-1}(k, z) - \mathscr{F}(k)}\right]_{jl} \tag{5.11}$$

and consider $\mathscr{F}(k)$ and $\mathscr{A}^{-1}$ for $k \to 0$ and z of order k^0, k, or k^2.

(a) The $M \times M$ matrix $\mathscr{F}(k)$ in Eq. (5.11) is a quantity of order k^0 when $k \to 0$. For, the Boltzmann collision operator $\Lambda_{\mathrm{B}} = \lim_{k \to 0} \bar{\Lambda}_{\mathbf{k}}$ has three longitudinal ($m=0$) eigenfunctions with vanishing eigenvalue, i.e.,

$$\Lambda_{\mathrm{B}} \psi_j(\mathbf{v}_1) = 0 \tag{5.12}$$

where $j = 1, 2$, or 3. As a consequence of this and Eqs. (1.11)–(1.13), the vectors $(1, 0, 0,\ldots)$, $(0, 1, 0,\ldots)$, and $(0, 0, 1, 0,\ldots)$, which correspond to $\psi_1(\mathbf{v}_1)$, $\psi_2(\mathbf{v}_1)$, and $\psi_3(\mathbf{v}_1)$, respectively, are eigenvectors of the matrix $\mathscr{F}(0)$ with eigenvalue $d(0)$. Since $d(0)$ is finite for any $M \geqslant 3$ [cf. Eq. (1.11) and ref. 23], the matrix $\mathscr{F}(0)$ has (at least) three eigenvectors with non-vanishing eigenvalue.

(b) The $M \times M$ matrix $\mathscr{A}(k, z)$ is also a quantity of order k^0. For, it follows from the Eqs. (3.2)–(3.4) that

$$\mathscr{A}(k, z) = \frac{1}{z - d(k)}\left[1 + \frac{1}{\zeta}\mathscr{V} + \frac{1}{\zeta^2}\mathscr{E} + O(k^3)\right] \tag{5.13}$$

where the matrix elements V_{jl} of $\mathscr{V}$ and E_{jl} of $\mathscr{E}$ are given by

$$V_{jl} = \langle \Phi_{r_1, l_1}(\mathbf{c})\, c_z \Phi_{r_2, l_2}(\mathbf{c}) \rangle \tag{5.14}$$

$$E_{jl} = \langle \Phi_{r_1, l_1}(\mathbf{c})\, c_z^2 \Phi_{r_2, l_2}(\mathbf{c}) \rangle \tag{5.15}$$

respectively. Here we have used that the variable ζ in Eqs. (3.2)–(3.4) is *large* and of order $1/k$ [since $d(0)$ is finite], so that $1/\zeta$ is of order k and *small.* Thus, $\mathscr{A}^{-1}(k, z)$ is a quantity of order k^0, and given by [cf. Eq. (5.13)],

$$\mathscr{A}^{-1}(k, z) = [z - d(k)] \left[\mathbb{1} - \frac{1}{\zeta} \mathscr{V} + \frac{1}{\zeta^2} (\mathscr{V}^2 - \mathscr{E}) + O(k^3) \right] \quad (5.16)$$

where the leading term $-d(k)\,\mathbb{1}$ is the same as that in $\mathscr{F}(k)$ [cf. Eq. (1.12)].

Then, by subtracting the expressions (5.16) for $\mathscr{A}^{-1}(k, z)$ and (1.12) for $\mathscr{F}(k)$, one obtains

$$G_{jl}(k, z) = \left[\frac{1}{z - \mathscr{L}^E(k) + 2k_B T k^2 (\mathscr{V}^2 - \mathscr{E})/[md(0)] + O(k^3)} \right]_{jl} \quad (5.17)$$

Here $\mathscr{L}^E(k)$ is the $M \times M$ matrix with elements $L^E_{jl}(k)$,

$$L^E_{jl}(k) = \langle \Phi_{r_1, l_1}(\mathbf{c})\, L_E(\mathbf{k})\, \Phi_{r_2, l_2}(\mathbf{c}) \rangle \quad (5.18)$$

so that [cf. Eq. (1.4), (1.13), and (5.16)]

$$L^E_{jl}(k) = -ik \left(\frac{2k_B T}{m} \right)^{1/2} V_{jl} + n\chi \Omega_{jl}(k)$$
$$+ ik \left(\frac{k_B T}{m} \right)^{1/2} \left(1 - \frac{1}{\sqrt{S(k)}} \right) (\delta_{j,1} \delta_{l,2} + \delta_{j,2} \delta_{l,1}) \quad (5.19)$$

where the three terms on the right-hand side are due to the free streaming $(-i\mathbf{k} \cdot \mathbf{v}_1)$, the collision $(n\chi \bar{\Lambda}_{\mathbf{k}})$, and the mean field $(n\bar{A}_{\mathbf{k}})$ terms in Eq. (1.14) for $L_E(\mathbf{k})$, respectively.

We discuss the approach to hydrodynamic behavior of the $G_{jl}(k, z)$ through the spectral decomposition of $\mathscr{L}^E(k)$,

$$L^E_{jl}(k) = \sum_{i=1}^{M} z_i(k)\, \phi_j^{(i)}(k)\, \phi_l^{(i)}(k) \quad (5.20)$$

where the $z_i(k)$ are the M eigenvalues of $\mathscr{L}^E(k)$ and the $\phi_j^{(i)}(k)$ are the components of the corresponding M eigenvectors $\phi^{(i)}(k)$.

Using Eqs. (5.17) and (5.20), one finds that the $G_{jl}(k, z)$ are, for $k \to 0$, given by

$$G_{jl}(k, z) = \sum_{i=1}^{M} \phi_j^{(i)}(k)\, \phi_l^{(i)}(k) \frac{1}{z - z_i(k)} \quad (5.21)$$

i.e., by a sum of M Lorentzians in z.

We remark that the term $2k_B Tk^2(\mathscr{V}^2 - \mathscr{E})/md(0)$ in Eq. (5.17) can be neglected for $M \to \infty$, since $\lim_{M \to \infty}(\mathscr{V}^2 - \mathscr{E}) = 0$ [cf. Eqs. (5.14) and (5.15)]. We find in practice that the contributions of this term to the $G_{jl}(k, z)$ are negligible when $M \geqslant 10$. Therefore, the $G_{jl}(k, z)$ are given by the M discrete eigenmodes [i.e., eigenvalues $z_i(k)$ and eigenfunctions $\phi^{(i)}(k)$] of the $M \times M$ matrix $\mathscr{L}^E(k)$ up to order k^2.

For any $M \geqslant 3$, $\mathscr{L}^E(k)$ has eigenmodes that can be called extended hydrodynamic modes,[9-12] since for $k \to 0$ they tend to the three hydrodynamic modes. For these modes, the eigenvalues $z_i(k)$ $(i = 1, 2, 3)$ tend to zero for $k \to 0$ and the corresponding eigenvectors $\phi^{(i)}(0)$ are linear combinations of the three vectors that correspond to the $\psi_j(\mathbf{v}_1)$ with $j = 1, 2$, or 3 [cf. Eqs. (5.12), (5.14), (5.19), and (1.13)]. They are the heat mode $(i = h)$, for which $z_h(k)$ is real, and the two sound modes $(i = \pm)$, for which $z_+(k)$ and $z_-(k)$ are each other's complex conjugates.[9,32] The other $M - 3$ eigenvalues $z_i(k)$ of $\mathscr{L}^E(k)$ $(i = 4, \ldots, M)$ are kinetic modes, since they approach finite negative values for $k = 0$, with corresponding eigenfunctions $\phi^{(i)}(k)$ that have vanishing components $\phi_j^{(i)}(k)$ for $j = 1, 2$, and 3 and $k = 0$.

Thus, in the BGK approximation of order $M \geqslant 3$, the nine $G_{jl}(k, z)$ with j or $l = 1, 2$, or 3 are described for $k \to 0$ by the three hydrodynamic modes of $\mathscr{L}^E(k)$ only, i.e., by

$$G_{jl}(k, z) = \sum_{i = h, \pm} \phi_j^{(i)}(k)\, \phi_l^{(i)}(k) \frac{1}{z - z_i(k)} \tag{5.22}$$

The hydrodynamic description given by Eq. (5.22) for all nine $G_{jl}(k, z)$ includes in particular the Landau–Placzek triplet of Lorentzians for $G_{11}(k, z)$, or equivalently for $S_{11}(k, \omega)$ [cf. Eq. (5.3)].[9,32]

5.4. Eigenmodes

In the BGK approximation of order M for $L_E(\mathbf{k})$ [cf. Eqs. (1.8)–(1.10)] the nine $F_{jl}(k, t)$ of Eq. (1.1) with $j, l = 1, 2, 3$ are for any finite value of k given by a sum of M discrete eigenmodes and, in addition, an essential singularity contribution. Here we discuss the relative importance of these two contributions to $F_{jl}(k, t)$ and $S_{jl}(k, \omega)$ as functions of k and M.

The $F_{jl}(k, t)$ are the inverse Laplace transforms of the $G_{jl}(k, z)$, i.e. [cf. Eq. (1.15)],

$$F_{jl}(k, t) = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} dz\, e^{zt} G_{jl}(k, z) \tag{5.23}$$

where, in the BGK approximation of order M, the $G_{jl}(k, z)$ are given by Eq. (1.16). The $G_{jl}(k, z)$ have M discrete singularities (i.e., poles) in the complex z plane at finite, k-dependent, values $z = z_i(k)$, have one essential singularity at $\text{Re}\, z = -\infty$, and are analytic anywhere else. Therefore

$$F_{jl}(k, t) = \sum_{i=1}^{M} M_{jl}^{(i)}(k)\, e^{z_i(k)t} + F_{jl}^{(\text{es})}(k, t) \tag{5.24}$$

Here the discrete eigenvalues $z_i(k)$ are associated with those M values of z for which the determinant of the $M \times M$ matrix $1 - \mathscr{A}(k, z)\, \mathscr{F}(k)$ vanishes, i.e.,

$$D(k, z) = \text{Det}[1 - \mathscr{A}(k, z)\, \mathscr{F}(k)] = 0 \tag{5.25}$$

and where the corresponding amplitudes $M_{jl}^{(i)}(k)$ are given by

$$M_{jl}^{(i)}(k) = \frac{1}{D'(k, z_i)} [\mathscr{T}(k, z_i)\, \mathscr{A}(k, z_i)]_{jl} \tag{5.26}$$

$\mathscr{T}$ is the transpose of the $M \times M$ matrix of cofactors of $1 - \mathscr{A}\mathscr{F}$ and $D'(k, z) = \partial D(k, z)/\partial z$.

The (M-dependent) second term on the right-hand side of Eq. (5.24) is given by

$$F_{jl}^{(\text{es})}(k, t) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} dz\, e^{zt} G_{jl}(k, z) \tag{5.27}$$

where γ is real and negative and smaller than all real parts of the eigenvalues $z_i(k)$ for all k. Thus, the $F_{jl}^{(\text{es})}(k, t)$ decay to zero for $t \to +\infty$, faster than $\exp(\gamma t)$ for any negative real γ. In fact, the $F_{jl}^{(\text{es})}(k, t)$ decay in a Gaussian-like manner, i.e., for large t they are proportional to $\exp(-at^2)$, where a is a k-dependent parameter.

We remark that for $k \to 0$ the essential singularity contribution in Eq. (5.24) vanishes and that the $M_{jl}^{(i)}(k)$ and $z_i(k)$ tend to the $\phi_j^{(i)}\phi_l^{(i)}$ and $z_i(k)$ of Eq. (5.21), respectively. Thus, while for $k \to 0$, the $F_{jl}(k, t)$ are described by M discrete eigenmodes alone, one needs for finite k in addition the contribution of an essential singularity [cf. Eq. (5.24)]. To study the importance of the essential singularity we consider the Fourier transforms of the three $F_{jl}(k, t)$ with $j, l = (1, 1)$, $(1, 3)$, and $(3, 3)$ given by [cf. Eq. (5.24)]

$$S_{jl}(k, \omega) = \frac{1}{\pi} \text{Re} \sum_{i=1}^{M} \frac{M_{jl}^{(i)}(k)}{i\omega - z_i(k)} + S_{jl}^{(\text{es})}(k, \omega) \tag{5.28}$$

where

$$S_{jl}^{(\text{es})}(k, \omega) = (2\pi)^{-1} \int_{-\infty}^{+\infty} dt\, \exp(-i\omega t)\, F_{jl}^{(\text{es})}(k, t)$$

is the Fourier transform of the essential singularity contribution $F_{jl}^{(es)}(k, t)$ in $F_{jl}(k, t)$. For all densities and fixed $M \geqslant 10$ we find that the $S_{jl}^{(es)}(k, \omega)$ increase with increasing k to at most 5% of $S_{jl}(k, \omega)$ when $kl_E = 20$.

To show this, we have determined all ten discrete eigenmodes of $L_E(\mathbf{k})$ in the BGK method with $M = 10$ for all densities and k values [cf. Eqs. (5.25) and (5.26)], using the A-ordering. Thus, we obtained the complete first term on the right-hand side of Eq. (5.28) for $M = 10$. We also calculated the $S_{jl}(k, \omega)$ [i.e., the left-hand side of eq. (5.28)] in the BGK method with $M = 10$, using 10×10 matrix inversion [cf. Eqs. (5.3) and (1.16)]. The difference between these two terms determines the second term on the right-hand side of Eq. (5.28), i.e., the essential singularity contribution $S_{jl}^{(es)}(k, \omega)$ for $M = 10$.

For all densities we find that $S_{jl}^{(es)}(k, \omega)$ increases from zero at $k = 0$ to values of the order of 1 and 5% of $S_{jl}(k, \omega)$ when $kl_E \approx 6$ and 20, respectively. We show this in Fig. 6 for the low-density (Boltzmann) limit of $S_{11}(k, \omega) = S(k, \omega)$.[36] In Figs. 6a and 6b we plot for $M = 10$ the full BGK values of $S_{11}(k, \omega)$ and the contributions to $S_{11}(k, \omega)$ of all ten discrete eigenmodes when (a) $kl_E = 6$ and (b) $kl_E = 20$. We conclude from this and

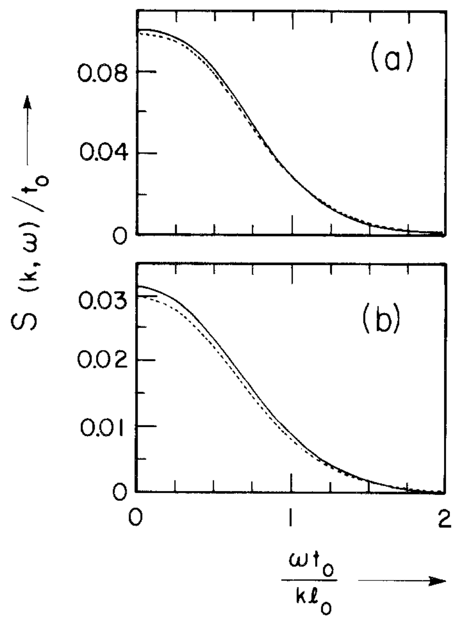

Fig. 6. (—) The reduced $S(k, \omega)/t_0$ in the low-density (Boltzmann) limit as a function of the reduced frequency $\omega t_0/kl_0$ for (a) $kl_0 = 6$ and (b) $kl_0 = 20$ in the BGK approximation of order $M = 10$, using the Alterman ordering. (– –) The contribution of all ten discrete BGK eigenmodes to $S(k, \omega)/t_0$. The difference is the contribution of the essential singularity.

the foregoing that for $kl_E \lesssim 20$ the $S_{jl}(k, \omega)$ can be described by considering the discrete eigenmodes of $L_E(\mathbf{k})$ alone and that, when $M = 10$, the essential singularity at Re $z = -\infty$ is relevant only for $kl_E \gg 20$.

For fixed values of kl_E up to $kl_E = 20$ we verified numerically up to $M = 55$ that, for all densities, the contributions $S_{jl}^{(es)}(k, \omega)$ to the $S_{jl}(k, \omega)$ decrease with increasing M, implying that the $S_{jl}(k, \omega)$ are increasingly better described by the discrete modes of $L_E(\mathbf{k})$ alone. However, the convergence in M is too slow to conjecture that for fixed kl_E and $M \to \infty$ the $S_{jl}(k, \omega)$ can be represented by an infinite sum of discrete eigenmodes only.

APPENDIX

We consider the integral [cf. Eq. (4.26)]

$$I(\mathbf{B}; \mathbf{A}) = \frac{1}{4\pi} \int d\hat{\boldsymbol{\sigma}} \exp[-(\mathbf{B} \cdot \hat{\boldsymbol{\sigma}})^2] \, {}_1F_1\left(1, \frac{1}{2}; (\mathbf{A} \cdot \hat{\boldsymbol{\sigma}})^2\right) \tag{A.1}$$

for any two (complex) vectors $\mathbf{A}$ and $\mathbf{B}$. Expanding the exponential and the confluent hypergeometric function yields

$$I(\mathbf{B}; \mathbf{A}) = \sum_{t=0}^{\infty} \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \frac{(-)^{q+t} (1/2)_{q+t} (1)_{p+t}}{t! \, p! \, q! \, (1/2)_t \, (3/2)_{p+q+2t}} \times (A^2)^p (B^2)^q (\mathbf{A} \cdot \mathbf{B})^{2t} \tag{A.2}$$

where we have used that

$$\frac{1}{4\pi} \int d\hat{\boldsymbol{\sigma}} \, (\mathbf{A} \cdot \hat{\boldsymbol{\sigma}})^{2l} (\mathbf{B} \cdot \hat{\boldsymbol{\sigma}})^{2m} = (A^2)^l (B^2)^m \, l! \, m! \frac{(1/2)_l (1/2)_m}{(3/2)_{l+m}} \times \sum_{j=0}^{\mathrm{Min}(l,m)} \frac{1}{j! \, (l-j)! \, (m-j)! \, (1/2)_j} \left(\frac{\mathbf{A} \cdot \mathbf{B}^2}{A^2 B^2}\right)^j \tag{A.3}$$

In Eq. (A.2) we use that the sum over p is a confluent hypergeometric series, i.e.,

$$I(\mathbf{B}; \mathbf{A}) = \sum_{t=0}^{\infty} \sum_{q=0}^{\infty} \frac{(-)^{q+t} (1/2)_{q+t}}{q! \, (1/2)_t \, (3/2)_{q+2t}} (B^2)^q (\mathbf{A} \cdot \mathbf{B})^{2t} \times {}_1F_1\left(1 + t, \frac{3}{2} + q + 2t; A^2\right) \tag{A.4}$$

Then, applying Kummer's transformation

$$
{}_1F_1\left(1+t, \frac{3}{2}+q+2t, A^2\right) = \exp(A^2)\, {}_1F_1\left(\frac{1}{2}+q+t, \frac{2}{3}+q+2t; -A^2\right)
$$

one finds

$$
I(\mathbf{B}; \mathbf{A}) = e^{A^2} \sum_{t=0}^{\infty} \sum_{q=0}^{\infty} \sum_{p=0}^{\infty} \frac{(-)^{p+q+t}\,(1/2)_{q+t}\,(1/2+q+t)_p}{p!\,q!\,(1/2)_t\,(3/2)_{q+2t}\,(3/2+q+2t)_p}
\times (A^2)^p\,(B^2)^q\,(\mathbf{A}\cdot\mathbf{B})^{2t} \tag{A.5}
$$

The sum over q, again, is a confluent hypergeometric series, i.e.,

$$
I(\mathbf{B}; \mathbf{A}) = e^{A^2} \sum_{t=0}^{\infty} \sum_{p=0}^{\infty} \frac{(-)^{p+t}\,(1/2)_{p+t}}{p!\,(1/2)_t\,(3/2)_{p+2t}}
\times (A^2)^p\,(\mathbf{A}\cdot\mathbf{B})^{2t}\, {}_1F_1\left(\frac{1}{2}+p+t; \frac{3}{2}+p+2t; -B^2\right) \tag{A.6}
$$

for which we use Kummer's transformation, so that

$$
I(\mathbf{B}; \mathbf{A}) = e^{A^2-B^2} \sum_{t=0}^{\infty} \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \frac{(-)^{p+t}\,(1/2)_{p+t}\,(1+t)_q}{p!\,q!\,(1/2)_t\,(3/2)_{p+2t}\,(3/2+p+2t)_q}
\times (A^2)^p\,(B^2)^q\,(\mathbf{A}\cdot\mathbf{B})^{2t} \tag{A.7}
$$

Equivalently,

$$
I(\mathbf{B}; \mathbf{A}) = e^{A^2-B^2} \sum_{t=0}^{\infty} \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \frac{(-)^{p+t}\,(1/2)_{p+t}\,(1)_{q+t}}{t!\,p!\,q!\,(1/2)_t\,(3/2)_{p+q+2t}}
\times (A^2)^p\,(B^2)^q\,(\mathbf{A}\cdot\mathbf{B})^{2t} \tag{A.8}
$$

Then, when in these summations the variables p and q are interchanged, one obtains the summations on the right-hand side of Eq. (A.2) with $\mathbf{A}$ and $\mathbf{B}$ interchanged. Hence,

$$
I(\mathbf{B}; \mathbf{A}) = e^{A^2-B^2} I(\mathbf{A}; \mathbf{B}) \tag{A.9}
$$

which directly leads to the equality given by Eq. (4.26).

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