Friction and mobility of many spheres in Stokes flow

B. Cichocki,a) B. U. Felderhof, and K. Hinsen
Institut für Theoretische Physik A, RWTH Aachen, Templergraben 55, D-52056 Aachen, Germany

E. Wajntyb and J. Bławzdziewicz
Institute of Fundamental Technological Research, Polish Academy of Sciences, Świetokrzyska 21, PL-00-049 Warsaw, Poland

(Received 23 June 1993; accepted 19 November 1993)

An efficient scheme is presented for the numerical calculation of hydrodynamic interactions of many spheres in Stokes flow. The spheres may have various sizes, and are freely moving or arranged in rigid arrays. Both the friction and mobility matrix are found from the solution of a set of coupled equations. The Stokesian dynamics of many spheres and the friction and mobility tensors of polymers and proteins may be calculated accurately at a modest expense of computer memory and time. The transport coefficients of suspensions can be evaluated by use of periodic boundary conditions.

I. INTRODUCTION

Many situations in science and technology involve the motion of solid particles immersed in a viscous fluid. The motion of each particle in the fluid causes a flow pattern, which in turn affects the motion of other particles. Hence, the dynamics of the system of particles is characterized by hydrodynamic interactions mediated by the fluid. On a sufficiently slow time scale the fluid may be neglected. The overall flow pattern is set up instantaneously, and perfectly follows the motion of particles. On this time scale the fluid velocity and pressure fields are described by the so-called creeping flow or Stokes equations.

The description and calculation of hydrodynamic interactions for creeping flow is beset by three fundamental difficulties. First, the interactions have long range. This is already evident from the Stokes solution for flow about a sphere. The velocity field decays as slowly as the inverse power of distance from the center. Second, the hydrodynamic interactions have many-body character. The calculation of the complete flow pattern for many particles has the nature of a multiple scattering expansion. Third, the friction functions diverge at short distances due to strong velocity gradients in the fluid set up by near particles in relative motion. The long range and many-body character of hydrodynamic interactions were noted already by Smoluchowski, who studied the resulting divergence problem in the theory of sedimentation.

A proper account of hydrodynamic interactions is required for the calculation of transport coefficients of suspensions, such as the sedimentation coefficient and the effective viscosity. The particles need not be freely moving. The permeability to flow of a rigid array of particles is a transport property of prime interest. Technically, the numerical calculation of such transport coefficients, the proper definition of which involves the limit of an infinite number of particles, requires the application of periodic boundary conditions. The calculation of flow properties for a finite number of particles is also of interest. For example, it is desirable to have an accurate method of calculation of the friction coefficients of polymers and proteins. We shall model such structures as rigid arrays of spheres.

Hydrodynamic interactions in a collection of spheres have been studied by many authors. It is natural to consider the flow pattern of a single sphere to be generated by a set of force multipoles. The lowest order force multipoles are the force and torque applied to the sphere. Higher order force multipoles are induced by the flow incident on the sphere. Numerical calculation of hydrodynamic interactions requires an account of a set of force multipoles including sufficiently high order. It is known, however, that a proper description of the short range divergence and the associated lubrication effect requires force multipoles of very high order. It was first suggested by Bossis and Brady that lubrication effects may be taken into account in the friction matrix in pair superposition approximation. Later the picture was completed by Durlofsky et al., who proposed that collective effects to the many-sphere friction matrix may be accounted for by force multipoles of relatively low order, combined with lubrication effects in pair superposition approximation. In their FTS scheme, Durlofsky et al. used only forces and torques in the first part of the calculation. They attempted to include stresslets in their FTS scheme, but this scheme is not readily extended to higher order. A systematic calculation involving higher order force multipoles was performed by Ladd. He handled lubrication effects in the same manner as Durlofsky et al.

It turns out that the method of truncation at finite multipole order requires delicate consideration. If in our calculation we use the rank of Cartesian force multipole tensor as the criterion for truncation then we run into a peculiar difficulty. Truncation at finite order by this method causes divergence of the two-sphere friction matrix in the physical regime. The same type of divergence must be expected for many spheres.

We have chosen a different method of truncation,
based on the angular dependence of the flow pattern about a single sphere. For this truncation the two-sphere friction matrix diverges in the unphysical regime. In the limit of infinite truncation order the divergence corresponds to the lubrication singularity at touching. We show in the following that with our method of truncation the elements of the friction matrix corresponding to collective motion converge rapidly with increasing order of truncation, even for touching spheres. The elements of the friction matrix describing relative motion are corrected for lubrication effects in pair superposition approximation.

The Stokesian dynamics of freely moving spheres requires updating of sphere configurations on the basis of calculated velocities. For this one needs the many-sphere mobility matrix, rather than the friction matrix. In the calculations of Durlofsky et al. and of Ladd the mobility matrix was calculated as the inverse of the friction matrix. Numerically this is an expensive procedure. We show in the following that the many-sphere mobility matrix may be calculated directly, in the same way as the friction matrix, from the solution of a system of equations. This procedure permits effective numerical calculation of the Stokesian dynamics of many spheres.

II. HYDRODYNAMIC INTERACTIONS

We consider a collection of $N$ spheres suspended in an incompressible fluid of shear viscosity $\eta$. The fluid is of infinite extent in all directions, or bounded by solid walls at which the flow satisfies prescribed boundary conditions, e.g., no slip. Alternatively we consider also $N$ spheres in a cubic volume $V$ with periodic boundary conditions applied at the surface of the cube. We assume a low Reynolds number, so that the fluid velocity field $v(r)$ and the pressure $p(r)$ satisfy the Stokes equations

$$\eta \nabla^2 v - \nabla p = 0, \quad \nabla \cdot v = 0. \quad (2.1)$$

We assume that the motion of the fluid is due entirely to the motion of the spheres. Thus if translational velocities $U_1,...,U_N$ and rotational velocities $\Omega_1,...,\Omega_N$ of the spheres are given, then for any configuration of centers $R_1,...,R_N$ there is a uniquely determined corresponding flow pattern $v(r)\hat{=p}(r)$. If the fluid is of infinite extent, then the velocity field $v(r)$ tends to zero at infinity, and the pressure $p(r)$ tends to a constant $p_0$. The spheres exert forces $F_1,...,F_N$ and torques $T_1,...,T_N$ on the fluid. These are related linearly to the velocities by the friction matrix $\xi$.

$$F_j = \sum_{k=1}^{N} (\xi_{jk}^T \cdot U_k + \xi_{jk}^R \cdot \Omega_k), \quad (2.2)$$

$$T_j = \sum_{k=1}^{N} (\xi_{jk}^T \cdot U_k + \xi_{jk}^R \cdot \Omega_k), \quad j=1,...,N,$$

where the superscripts refer to the translational and rotational components. We abbreviate Eq. (2.2) as

$$F = \xi \cdot U, \quad (2.3)$$

where the $6N$-dimensional vector $F$ comprises both forces and torques, and the $6N$-dimensional vector $U$ comprises both translational and rotational velocities.

Conversely, if external forces $F_1,...,F_N$ and torques $T_1,...,T_N$ are applied to the spheres, then these are caused to move with translational velocities $U_1,...,U_N$, and rotational velocities $\Omega_1,...,\Omega_N$. The velocities are linearly related to forces and torques,

$$U_j = \sum_{k=1}^{N} (\mu_{jk}^T \cdot F_k + \mu_{jk}^R \cdot T_k), \quad (2.4)$$

$$\Omega_j = \sum_{k=1}^{N} (\mu_{jk}^T \cdot F_k + \mu_{jk}^R \cdot T_k), \quad j=1,...,N.$$ We abbreviate Eq. (2.4) as

$$U = \mu \cdot F. \quad (2.5)$$

The mobility matrix $\mu$ is the inverse of the friction matrix

$$\mu = \xi^{-1}. \quad (2.6)$$

Both matrices depend on the configuration $X=(R_1,...,R_N)$ and on the geometry, i.e., the shape of the vessel or the periodicity of the system.

Our goal will be to develop an efficient scheme of numerical calculation of the friction matrix $\xi$ and the mobility matrix $\mu$. We must account for three important features of the hydrodynamic interactions. First, the interactions have long range. Second, they have many-body character. Third, they show singular behavior at short distances.

The long range is evident from the behavior of the Green function of the Stokes equations (2.1). This is given by the tensor field $T'(r,r')$ and the vector field $Q(r,r')$ which satisfy the following equations:

$$\eta \nabla^2 T - \nabla Q = -18(\delta(r-r')), \quad \nabla \cdot T = 0, \quad (2.7)$$

together with boundary conditions on the walls of the vessel. In infinite geometry the fields are translationally invariant and given by

$$T(r) = \frac{1}{8\pi \eta} \frac{1+\hat{r} \hat{r}}{r}, \quad Q(r) = \frac{1}{4\pi} \frac{\hat{r}}{r^2} \quad (2.8)$$

with $\hat{r} = r/r$. The tensor $T(r)$ is called the Oseen tensor.

The many-body character of the hydrodynamic interactions is evident from an approximate calculation of the translational friction matrix $\xi^T$ due to Kirkwood and Rice.

We assume for simplicity that the spheres have equal radius $a$ and are suspended in infinite fluid. The friction coefficient of a single sphere has the Stokes value $\xi_0 = 6\pi a \eta$. According to Faxen’s theorem the force exerted by sphere $j$ on the fluid is given by

$$F_j = \xi_0 \left(U_j - \nu_j^v(R_j) - \frac{1}{2} \eta \nabla^2 v_j^v(R_j) \right), \quad (2.9)$$

where $v_j^v(R)$ is the velocity field acting on sphere $j$ due to the flow patterns of the other spheres. Kirkwood and Rice approximated Eq. (2.9) by

$$F_j = \xi_0 \left(U_j - \sum_{k \neq j} T_{jk} \cdot F_k \right), \quad j=1,...,N, \quad (2.10)$$

where $T_{jk}$ is given by the Oseen tensor $T(R_j-R_k)$. Thus the last term in Eq. (2.9) is omitted and the flow pattern of each sphere is approximated by the contribution with slow-
est decay. Equation (2.10) represents a set of coupled equations for the forces which may be written in the abbreviated form
\[ \mathbf{F} = \mathbf{\zeta}(\mathbf{U} - \mathbf{\mathcal{F}} \cdot \mathbf{F}) \]  
with the $3N$ vectors $\mathbf{F}$ and $\mathbf{U}$, and the $3N \times 3N$-matrix $\mathbf{\mathcal{F}}$. The formal solution of Eq. (2.11) leads to the Kirkwood–Riseman approximation for the translational friction matrix
\[ \mathbf{\mathcal{F}}^{\mathcal{F}} = \mathbf{\mathcal{A}}(\mathcal{F})^{-1}, \]
where $\mathbf{\mathcal{A}}(\mathcal{F})$ is the Kirkwood–Riseman approximation to the friction matrix. Attempts have been made to improve on the Kirkwood–Riseman approximation to the friction matrix. Yamakawa\(^7\) used the complete Stokes flow pattern for a single translating sphere, and moreover included the last term in Eq. (2.9). Durlofsky et al.\(^{23}\) followed the same approach, but included also the torques and rotational velocities. They then evaluated the friction matrix by inversion as in Eq. (2.12). Subsequently they corrected for lubrication effects by adding the friction matrix calculated in pair approximation with the exact pair friction tensors, while avoiding double counting by subtracting an approximate pair contribution. As we shall see later, this scheme leads to quite reasonable results in many cases. However, a systematic approach to the problem of hydrodynamic interactions must include force multipoles of all orders. Ladd\(^{24-27}\) has performed computer simulations on systems of spheres in periodic boundary conditions including a large number of higher order multipole components. He followed Durlofsky et al.\(^{23}\) in correcting for lubrication effects.\(^{20,21}\)

The Cartesian force multipole tensor of rank $p+1$ for a single sphere centered at the origin is defined by\(^{29}\)
\[ \mathbf{F}(p+1) = \frac{1}{p!} \int_{r < a} \mathbf{r} \mathbf{f}(\mathbf{r}) \, d\mathbf{r} , \]
where $\mathbf{f}(\mathbf{r})$ is the force density induced in the sphere.\(^{17-19}\) The tensor in Eq. (3.1) has $3p+1$ components. A smaller number suffices for a determination of the flow outside the sphere. It is sufficient to specify the set of irreducible multipole moments $\{ f_{l,m} \}$, where the subscript $l$ takes integer values $l = 1, 2, \ldots$, the subscript $m$ takes $2l+1$ integer values for each $l$, and the subscript $s$ takes the three values 0, 1, 2 for given $l,m$. Alternatively we shall use the more descriptive notation $S$, $T$, $P$ for the three values 0, 1, 2 of the index $s$ ($S$ standing for symmetric, $T$ for tangential, $P$ for pressure)\(^{30}\). The irreducible force multipole moments can be defined in spherical\(^{31}\) or in Cartesian coordinates.\(^{32}\) We need not quote the precise definition and merely note that the three components $f_{1,m}$ may be identified with the Cartesian components of the force $\mathbf{F}$, and the three components $f_{1,m}$ may be identified with the Cartesian components of the torque $\mathbf{T}$. We arrange the irreducible force multipole components for sphere $j$ as the infinite dimensional vector
\[ \mathbf{f}_h(j) = \begin{pmatrix} F_j \\ T_j \\ f_{kh}(j) \end{pmatrix} , \]
where $f_{kh}(j)$ denotes all higher order components. Correspondingly we define a projection operator $\mathcal{P}(j)$ on the $\mathcal{F}T$ subspace for sphere $j$ by
\[ \mathcal{P}(j) \mathbf{f}(j) = \begin{pmatrix} F_j \\ T_j \\ 0 \end{pmatrix} . \]

The translational and rotational velocity of the sphere and the value of the acting velocity field $\mathbf{v}_j(\mathbf{r})$ and its derivatives at the center of the sphere may be arranged in a similar multipole vector\(^{31}\)
\[ \mathbf{c}(j) = \begin{pmatrix} \mathbf{U}_j - \mathbf{v}_j(\mathbf{R}_j) \\ \mathbf{\Omega}_j - \mathbf{\omega}_j(\mathbf{R}_j) \end{pmatrix} |_{\mathbf{R}_j} , \]
where $\mathbf{\Omega}_j$ is the angular velocity of sphere $j$.
where \( \mathbf{c}_n(j) \) denotes all higher order components. The two multipole vectors \( \mathbf{f}(j) \) and \( \mathbf{c}(j) \) are related by the single-sphere extended friction matrix \( \mathbf{Z}_0(j) \)

\[
\mathbf{f}(j) = \mathbf{Z}_0(j) \mathbf{c}(j).
\]

The matrix \( \mathbf{Z}_0(j) \) may be constructed from the solution of the single sphere problem. Due to rotational symmetry the matrix is diagonal in the subscript \( l \).

Application of the projection operator \( \mathcal{P}(j) \) to the multipole vector \( \mathbf{c}(j) \) results in

\[
\mathcal{P}(j)\mathbf{c}(j) = \begin{pmatrix} 
U_j - v_j^f(R_j) \\
\Omega_j - \frac{1}{2} \mathbf{v} \times \mathbf{v}_j^f(r) |_{R_j} \\
0
\end{pmatrix}.
\]

We decompose the vector \( \mathbf{c}(j) \) as

\[
\mathbf{c}(j) = \mathbf{c}^u(j) - \mathbf{c}^+(j)
\]

with

\[
\mathbf{c}^u(j) = \begin{pmatrix} 
U_j \\
\Omega_j \\
0
\end{pmatrix}, \quad \mathbf{c}^+(j) = \begin{pmatrix} 
v_j^f(R_j) \\
\frac{1}{2} \mathbf{v} \times \mathbf{v}_j^f(r) |_{R_j} \\
-\mathbf{c}_n(j)
\end{pmatrix}.
\]

The second vector may be constructed from the flow pattern incident on sphere \( j \). In the absence of a flow pattern due to external sources it is linearly related by a Green matrix to the set of force multipole vectors

\[
\mathbf{c}^+(j) = \sum_{k=1}^{N} \mathbf{G}(j,k) \mathbf{f}(k).
\]

The Green matrix \( \mathbf{G} \) is determined completely by geometry. In infinite space the diagonal term \( \mathbf{G}(j,j) \) vanishes. Substituting Eqs. (3.7) and (3.9) into Eq. (3.5) we find the set of coupled multipole equations

\[
f(j) = \mathbf{Z}_0(j) \left( \mathbf{c}^u(j) - \sum_{k=1}^{N} \mathbf{G}(j,k) \mathbf{f}(k) \right), \quad j = 1, \ldots, N.
\]

This set of equations is exact. It is the analogue of the approximate Eq. (2.10) for the forces. Collecting the multipole components of all spheres into a single vector, we may write Eq. (3.10) in the abbreviated form

\[
f = \mathbf{Z}_0(\mathbf{c}^u - \mathbf{G} \mathbf{f}).
\]

The matrix \( \mathbf{Z}_0 \) is diagonal in particle labels and is composed of the friction matrices for the individual spheres. The formal solution of Eq. (3.11) is

\[
f = \mathbf{Z}_0[1 + \mathbf{G} \mathbf{Z}_0]^{-1} \mathbf{c}^u.
\]

Hence one finds the friction matrix \( \mathbf{\xi} \) by projection onto the \( \mathit{FT} \) subspace

\[
\mathbf{\xi} = \mathcal{P} \mathbf{Z}_0[1 + \mathbf{G} \mathbf{Z}_0]^{-1} \mathcal{P}.
\]

In the next section we show how this exact, but formal expression leads to a practical scheme of numerical calculation.

### IV. FRICTION MATRIX

In practical numerical calculations the infinite-dimensional multipole vectors must be truncated at finite order. From consideration of the angular dependence of the flow pattern about a single sphere it follows that it is natural to truncate at some maximum value \( L \) of the subscript \( l \). With truncation at order \( L \) the number of irreducible force multipole components per sphere is \( n_L = 3L(L+2) \). Thus upon truncation the infinite set of Eqs. (3.11) is replaced by the set of \( \mathit{Nn}_L \) equations

\[
f_L = \mathbf{Z}_0(L)(\mathbf{c}^u - \mathbf{G}_L \mathbf{f}_L).
\]

The Green matrix \( \mathbf{G}_L \) is the truncated version of the complete Green matrix \( \mathbf{G} \). In our explicit calculation the Green matrix \( \mathbf{G}_L \) is evaluated explicitly and exactly, either for infinite space or in periodic boundary conditions, in a representation with irreducible Cartesian multipole components up to order \( L \). After solving Eq. (4.1) as in Eq. (3.12) and projecting onto the \( \mathit{FT} \) subspace we find an approximation to the friction matrix

\[
\mathbf{\xi}_L = \mathcal{P} \mathbf{Z}_0(L)[1 + \mathbf{G}_L \mathbf{Z}_0(L)]^{-1} \mathcal{P}.
\]

The scheme is feasible only if \( L \) need not be too large to get accurate results. However, we know from the solution of the two-sphere problem that multipole components of very high order are required for an accurate description of the lubrication effects which dominate the friction between two near spheres in relative motion. Therefore we follow the procedure of Durlofsky et al. in correcting for lubrication effects. We add to the approximate friction matrix in Eq. (4.2) the matrix found in superposition approximation with the exact pair friction matrices,

\[
\mathbf{\xi}^\text{sup} = \sum_{i<j} \mathbf{\xi}(i,j).
\]

where the pair matrix \( \mathbf{\xi}(i,j) \) is defined as in Eq. (2.14). To avoid double counting we subtract the same expression with the pair friction matrices calculated with truncation at order \( L \)

\[
\mathbf{\xi}_{\text{sup, } L} = \sum_{i<j} \mathbf{\xi}_L(i,j).
\]

We denote the difference as

\[
\Delta \mathbf{\xi}_L = \mathbf{\xi}^\text{sup} - \mathbf{\xi}_{\text{sup, } L}.
\]

The exact friction matrix may be expressed as

\[
\mathbf{\xi} = \lim_{L \to \infty} (\mathbf{\xi}_L + \Delta \mathbf{\xi}_L).
\]

The matrix \( \mathbf{\xi}_L + \Delta \mathbf{\xi}_L \) will provide a good approximation for already fairly low values of \( L \). The contribution \( \Delta \mathbf{\xi}_L \) takes care of long-range and many-body effects, the matrix \( \mathbf{\xi}_L \) takes care of short distance lubrication effects. We denote our approximation at order \( L \) to the \( \mathit{N} \)-sphere friction matrix as

\[
\mathbf{\xi}_L = \mathbf{\xi}_L + \Delta \mathbf{\xi}_L.
\]

The main approximation in the above scheme is the assumption, suggested by Bossis and Brady, that lubrica-
tion effects are well accounted for in pair superposition approximation to the friction matrix. Durlofsky et al.\textsuperscript{23} have provided evidence to support this contention. However, the lubrication effect contributes only for relative motions which cause strong gradients in the flow field. As we shall show, for collective motions, which do not excite strong gradients, the friction matrix is well approximated by $\xi_L$, with truncation at relatively low $L$, even when the particles are very close. For such motions the correction $\Delta \xi_L$ is very small. On the other hand, close relative motion causes strong gradients and activates lubrication. Since the lubrication region is localized near the point of closest approach it is clear that for these motions the superposition approximation is appropriate. In the next section we analyze the collective motions in more detail.

V. COLLECTIVE MOTIONS

In this section we show that for collective motions, which do not excite a lubrication region, the exact friction matrix $\xi$ is well approximated by the friction matrix $\xi_L$, with truncation at relatively low multipole order $L$. The statement is true even for touching spheres. We demonstrate its validity by considering a pair and a triplet of spheres.

The short distance behavior of the friction functions for a pair of spheres was investigated in detail by Jeffrey and Onishi.\textsuperscript{20} They used lubrication theory to calculate the coefficients of singular and nonanalytic terms of the type exhibited in Eq. (2.16). The singular behavior gives rise to slow convergence of the series expansion of the friction functions in inverse powers of the distance between centers. Alternatively the singular behavior may be analyzed from the coefficients of the series expansion. An efficient recursion scheme for calculating a large number of coefficients was developed by Cichocki et al.\textsuperscript{31}

The presence of a lubrication region in the flow generated by the motion of two spheres is signaled by the presence of singular and nonanalytic terms in the friction functions, of the type shown in Eq. (2.16). There are four types of motion which excite a lubrication region. In the first motion the two spheres approach each other along the line of centers. In the second motion they rotate in opposite sense about the line of centers. In the third motion they rotate in parallel axes perpendicular to the line of centers. In the fourth motion they rotate in opposite directions perpendicular to the line of centers. In the third motion they rotate in the same sense about parallel axes perpendicular to the line of centers. In the fourth motion they rotate in the opposite sense about the line of centers. The friction functions corresponding to all other motions do not have singular or nonanalytical terms of the type shown in Eq. (2.16). This fact was recognized by Jeffrey and Onishi for the singular terms, but they did not find cancellation of the nonanalytic terms due to an error in one of the friction functions. The correct coefficient of the $\xi$ in $\xi$ term in the asymptotic expansion of the friction function $Y_{ij}$, as defined by Jeffrey and Onishi, is $31/500$ for equal spheres, rather than $31/250$, as was noted by Ladd.\textsuperscript{26} With correction of the error the singular and nonanalytical terms cancel from all friction functions describing collective motion. As a consequence of the cancellation we expect rapid convergence with $L$ of the friction matrix $\xi_L$ for this type of motion.

As an example of the speed of convergence we consider two touching spheres moving together either perpendicular or parallel to the line of centers. In Table I we list the drag coefficient $\xi_{11} + \xi_{12}$ in units $\xi_0$ for the two motions, as calculated from $\xi_L(1,2)$, and compare with the exact result. Again the convergence is quite rapid. As a second example we consider the collective motion of three equal spheres, touching with centers at the corners of an equilateral triangle, and moving with equal speed perpendicular to the plane of the triangle. Again this is a motion without lubrication region. In Table II we list the drag coefficient $\xi_{11} + \xi_{12} + \xi_{13}$ in units $\xi_0$ for this motion, as calculated from $\xi_L(1,2,3)$, and compare with the exact result. Again the convergence is quite rapid. We also list the contribution from $\Delta \xi_L(1,2,3)$ which rapidly decreases with increasing $L$. We note that this contribution can be calculated from the second column in Table I.

The exact result quoted in Table II has been derived in the following manner. We consider the friction function

$$Z(x) = (\xi_{11} + \xi_{12} + \xi_{13})/\xi_0$$

for three equal spheres of radius $a$ centered at the corners of an equilateral triangle with sides $R = 2ax$. By use of the spherical multipole representation and the displacement theorem\textsuperscript{13} one can solve Eq. (3.11) by iteration. This yields the function $Z(x)$ in the form of the series expansion.

<table>
<thead>
<tr>
<th>$L$</th>
<th>$\xi_L$</th>
<th>$\Delta \xi_L$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.584 5</td>
<td>0.013 2</td>
</tr>
<tr>
<td>2</td>
<td>0.575 7</td>
<td>0.001 4</td>
</tr>
<tr>
<td>3</td>
<td>0.574 86</td>
<td>0.000 02</td>
</tr>
<tr>
<td>4</td>
<td>0.574 88</td>
<td>0.000 04</td>
</tr>
<tr>
<td>Exact</td>
<td>0.574 91</td>
<td>0</td>
</tr>
</tbody>
</table>
The coefficients $c_j$ may be calculated from the series we get at touching the precise value zero of the determinant of the mobility matrix, the elimination. Once the value $x_1$ has been determined one may cast the expansion in Eq. (5.2) was first studied by Kim. The first 22 coefficients are listed in Table III. The series with coefficients $C_j$ is rapidly convergent. We list the first 22 coefficients $C_j$ in Table III. With 85 terms of the series expansion, or more straightforwardly as a polynomial, leads to rapid convergence of the friction matrix.

We have calculated the first 85 expansion coefficients $b_j$. His value for $b_6$ does not agree with the exact value $b_6 = 5451/8192$ calculated by Pienkowska, whereas ours does. Nonetheless, Kim's observation that $(-1)^j b_j$, grows exponentially with $j$ is correct. The observation implies that the series is dominated by a pole at an unphysical value $x_1 < -1$. The value $x_1$ can be found by a Pade analysis of the series expansion, or more straightforwardly as a zero of the determinant of the mobility matrix, the elements of which can be found from a similar series expansion. Once the value $x_1$ has been determined one may cast the function $Z(x)$ in the form:

$$Z(x) = \sum_{j=0}^{\infty} b_j x^{-j}.$$  \hspace{1cm} (3.2)

We have calculated the first 85 expansion coefficients $b_j$. The first 22 coefficients are listed in Table III. The series expansion in Eq. (5.2) was first studied by Kim. However, his values for the coefficients $b_j$ for $j>6$ are incorrect. His value for $b_6$ does not agree with the exact value $b_6 = 5451/8192$ calculated by Pienkowska, whereas ours does. Nonetheless, Kim's observation that $(-1)^j b_j$ grows exponentially with $j$ is correct. The observation implies that the series is dominated by a pole at an unphysical value $x_1 < -1$. The value $x_1$ can be found by a Pade analysis of the series expansion, or more straightforwardly as a zero of the determinant of the mobility matrix, the elements of which can be found from a similar series expansion. Once the value $x_1$ has been determined one may cast the function $Z(x)$ in the form:

$$Z(x) = \frac{A}{x-x_1} + \sum_{j=0}^{\infty} c_j x^{-j}. \hspace{1cm} (5.3)$$

We have found the values:

$$A = 0.127522 \quad \text{and} \quad x_1 = -1.0939747. \hspace{1cm} (5.4)$$

The coefficients $c_j$ may be calculated from:

$$c_j = b_j - Ax_1^{j-1}, \quad j > 1. \hspace{1cm} (5.5)$$

The series with coefficients $c_j$ is rapidly convergent. We list the first 22 coefficients $c_j$ in Table III. With 85 terms of the series we get at touching the precise value:

$$Z(x=1) = 0.57491. \hspace{1cm} (5.6)$$

### Table III

<table>
<thead>
<tr>
<th>$j$</th>
<th>$(-1)^j b_j$</th>
<th>$(-1)^j c_j$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>0.75</td>
<td>0.3674337</td>
</tr>
<tr>
<td>2</td>
<td>0.5625</td>
<td>0.1439821</td>
</tr>
<tr>
<td>3</td>
<td>0.564875</td>
<td>0.0890270</td>
</tr>
<tr>
<td>4</td>
<td>0.6445313</td>
<td>0.1436572</td>
</tr>
<tr>
<td>5</td>
<td>0.6591797</td>
<td>0.1112361</td>
</tr>
<tr>
<td>6</td>
<td>0.6654035</td>
<td>0.0659689</td>
</tr>
<tr>
<td>7</td>
<td>0.6961670</td>
<td>0.0403987</td>
</tr>
<tr>
<td>8</td>
<td>0.7391739</td>
<td>0.0217800</td>
</tr>
<tr>
<td>9</td>
<td>0.8133872</td>
<td>0.0287764</td>
</tr>
<tr>
<td>10</td>
<td>0.8959279</td>
<td>0.0373648</td>
</tr>
<tr>
<td>11</td>
<td>0.9765689</td>
<td>0.0375225</td>
</tr>
<tr>
<td>12</td>
<td>1.0605121</td>
<td>0.0300004</td>
</tr>
<tr>
<td>13</td>
<td>1.1482364</td>
<td>0.0241646</td>
</tr>
<tr>
<td>14</td>
<td>1.2486853</td>
<td>0.0189792</td>
</tr>
<tr>
<td>15</td>
<td>1.3615966</td>
<td>0.0163292</td>
</tr>
<tr>
<td>16</td>
<td>1.4882580</td>
<td>0.0165695</td>
</tr>
<tr>
<td>17</td>
<td>1.6268937</td>
<td>0.0169037</td>
</tr>
<tr>
<td>18</td>
<td>1.7774661</td>
<td>0.017788</td>
</tr>
<tr>
<td>19</td>
<td>1.9423237</td>
<td>0.0155169</td>
</tr>
<tr>
<td>20</td>
<td>2.1219205</td>
<td>0.0140448</td>
</tr>
<tr>
<td>21</td>
<td>2.3195584</td>
<td>0.0135957</td>
</tr>
</tbody>
</table>

The experimental value $Z(x=1) = 0.574$ obtained by Lasso and Weidman agrees well with the exact result, but in view of the experimental uncertainty this is somewhat fortuitous. We note that an expansion of the type (5.3) can be used only for a small number of spheres since the number of poles in the unphysical regime with $x<1$ increases rapidly with the number of spheres. For four spheres we find six poles in this regime.

Even though the correction term $\Delta \xi L$ is small for collective motions we do include it in our numerical calculation. It is convenient to use the same expression for the approximate friction matrix for all types of motion.

## VI. TRUNCATION

We have shown in Sec. V for some simple examples of collective motion that our truncation at multipole order $L$ leads to rapid convergence of the friction matrix. We shall show later that for motions with lubrication the convergence is equally rapid. The rate of convergence depends on the method of truncation. We have based our truncation on the angular dependence of the flow field about a sphere. Here we show that a different method of truncation, based on the distance dependence of the flow field, gives rise to serious problems. In addition we shall discuss a modification of our scheme which uses less memory for almost identical results.

The Green matrix element between two force multipoles of order $l,m,s$, and $l',m',s'$, decays with distance as $R^{-l-l'-s-s'+1}$. This shows that with truncation at multipole order $L$ the contribution from $T$- and $P$-multipole components of order $L$ leads to faster decay with distance than that from $S$ components. It is tempting to omit the $T$ and $P$ components of highest multipole order from the calculation in order to save memory and computing time.

Truncation of the type discussed above corresponds to truncation at order $p_{max}$ in a Cartesian definition of the force multipole moments as in Eq. (3.1). As discussed earlier, our truncation at order $L$ includes $n_L = 3L(L+2)$ irreducible force multipole moments per sphere. In the formulation chosen by Ladd the reduced force multipole moments are defined by the replacement of the factor $r^p$ in Eq. (3.1) by its symmetric and traceless part $F^p$. This leads to reduced force multipole tensors of rank $p+1$. Ladd's tensor of order $p$ corresponds to a linear combination of $S$ moments of orders $l=p-1$ and $l=p+1$, our $T$ moments of order $l=p$, and our $P$ moments of order $l=p-1$. Thus with truncation at $p_{max}$ Ladd includes a total of $3p_{max}^2 + 6p_{max} + 2$ moments of types $S$, $T$, and $P$. In addition he includes the trace of the second rank force multipole tensor $F^{(2)}$. Thus with truncation at $p_{max}$ Ladd's description involves three more multipole components than our truncation at order $L=p_{max}$. Note that the trace of the second rank tensor $F^{(2)}$ does not contribute to the flow about a sphere. Ladd eliminates the trace from his system of equations.

From the above discussion it follows that truncation at $p_{max}$ corresponds in our formulation to truncation at order $L=p_{max}+1$ with omission of the $T$ and $P$ moments of...
order $L$ and the $P$ moments of order $L+1$. We shall denote this method of truncation as $p$ truncation. The difficulty with $p$ truncation becomes evident from consideration of the relative motion of two spheres along their line of centers. For this case the inverse matrix in Eq. (3.13) truncated by this method becomes singular in the physical regime. We consider the determinant of the matrix $I + GZ_0$ in the relevant subspace. In the notation of Ref. 31 this becomes

$$D(x) = \det [I - X'(1,2)T], \quad (6.1)$$

where $x = R/2a$ is the dimensionless distance between centers of two spheres of radius $a$. It suffices to consider only $S$ and $P$ components in the subspace with $m=0, m'=0$. We denote the determinant of the $4p_{\text{max}} \times 4p_{\text{max}}$-dimensional matrix obtained in $p$ truncation at rank $p_{\text{max}}$ by $D_p(x)$, and the determinant of the $4L \times 4L$-dimensional matrix truncated by our method at order $L$ by $D_L(x)$. In the first two columns of Table IV we list the largest positive zero $x_0$ of the functions $D_p(x)$ and $D_L(x)$ for truncation at various orders. It is clear that for $p$ truncation the zero is in the physical range $x > 1$ for all orders considered, whereas for our truncation the zero is in the unphysical range $x < 1$. In both cases in the limit of infinite order the zero will finally end up at the lubrication singularity at $x = 1$.

In Fig. 1 we plot the friction function $X_{12}'(R)/\zeta_0$ calculated with $p$ truncation at $p_{\text{max}} = 3$, and compare with the exact function. Some of the other two-sphere friction functions calculated with $p$ truncation show similar problems. The singularity difficulties make themselves felt both in the many-sphere truncated friction matrix and in the two-sphere correction matrix.

In Fig. 2 we plot the friction function $X_{12}'(R)/\zeta_0$ calculated with our truncation at orders $L = 1, 2, 3, 4$, and compare it with the exact function. The other two-sphere friction functions show similar behavior. The elements of the correction matrix $\Delta x_L$ are smooth functions of distance and nonvanishing only in a small range, which decreases with increasing $L$.

We emphasize that the form of the truncated matrix depends on the formulation of the problem. Ladd has used reduced force multipole moments truncated at $p_{\text{max}}$, as discussed above, but uses reduced velocity moments which differ from ours, and therefore has a different truncated matrix. Ladd's truncation does not lead to a singularity in the pair friction functions. The appearance of singularities resulting from the use of an approximated hydrodynamic interaction matrix has been noted earlier in Brownian dynamics simulations.

The choice of the order of truncation is based on a compromise between desired accuracy and requirements of memory and computing time. A minimum number of force multipole components must be kept to account for long range contributions. As mentioned above, the Green matrix element between two multipoles of orders $l,m,\sigma$ and $l',m',\sigma'$ decays with distance as $R^{-l-l'-\sigma-\sigma'+1}$. This shows that the $FT$ scheme of Durlofsky et al., which accounts only for multipole components with $l=1, \sigma=0,1$,
leaves out important long range contributions. The same is true of their \textit{FTS} scheme. At least all matrix elements which decay as slowly as \( R^{-3} \) should be kept for many-sphere systems, where large interparticle distances occur. Hence we must include at least the multipole with \( l=1, \sigma = -2, \text{with } l=2, \sigma = -1, \text{and } l=0, \sigma = 0 \), since these combine with \( l'=1, \sigma' = 0 \) to give decay as \( R^{-3} \). This suggests that we keep the multipole with \( l=1, \sigma = 0,1,2, \text{with } l=2, \sigma = 0,1, \text{and } l=3, \sigma = 0,1 \). However, this corresponds to \( p \) truncation at \( p_{\text{max}}=2 \), which leads to the singularity problem. Truncation at order \( L=2 \) requires 24 multipole components per sphere, but leaves out the \( l=3, \sigma = 0 \) multipole components. These are included with truncation at order \( L=3 \), which requires 45 multipole components per sphere. Truncation at this order yields satisfactory results. We have found for all configurations studied that truncation at order \( L=4 \) changes the results by less than one percent.

A slight modification of the truncation scheme at order \( L=3 \) leads to important savings of memory. We consider the truncation at order \( L=3 \), and delete all Green matrix elements connecting force multipoles of order \( l=3 \) with those of order \( l'=3 \). This allows us to express the force multipoles of order \( l=3 \) in terms of force multipoles of orders \( l=1 \) and \( 2 \). As a result we obtain a truncation of order \( L=2 \) with modified Green matrix elements which can be calculated straightforwardly. We find that the elements of the friction matrix calculated with the improved \( L=2 \) truncation scheme differs from those calculated with the original scheme of order \( L=3 \) by less than one percent.

We have checked for the case of two spheres that with the above scheme of truncation with deletion the singularity \( x_0 \) is located in the unphysical range. In the last column in Table IV we list the value of the singularity for truncation and deletion at order \( L+1 \). It is clear that the resulting truncation scheme of order \( L \) yields significant savings of memory in comparison with the original scheme of order \( L+1 \), and that it provides a definite improvement on the original scheme of order \( L \). In practice the improved scheme of order \( L=2 \) is satisfactory.

### VII. MOBILITY MATRIX

In order to perform numerical computations of Stokesian dynamics, involving the updating of configurations of a set of freely moving spheres, it is necessary to know the sphere velocities for given forces and torques, as expressed by the mobility matrix \( \mu \). In a numerical scheme one could use as the approximate mobility matrix the inverse of the approximate friction matrix. This is the procedure followed by Durlofsky \textit{et al.} \cite{23} and by Ladd.\cite{24\textsuperscript{a},24\textsuperscript{b},24\textsuperscript{c},25\textsuperscript{a},25\textsuperscript{b}}. In our case this would imply that we use the relation

\[ \mu_L = Z_{\text{L}}^{-1}. \]  

(7.1)

However, the procedure requires inversion of a large matrix, which is numerically expensive. It is preferable to develop an alternative scheme which allows direct evaluation of the sphere velocities for given forces and torques from the solution of a system of equations.

We begin by deriving a formal expression for the exact mobility matrix, in analogy to Eq. (3.13) for the friction matrix. It is convenient to define

\[ \xi_0 = Z_0 \xi_0, \quad \mu_0 = Z_0^{-1} \xi_0. \]  

(7.2)

as the friction and mobility matrices valid for large separation of spheres in infinite space. Both matrices are diagonal, and are inverse to each other in the \textit{FT} subspace.

We define the convective extended friction matrix \( \hat{Z}_0 \) by

\[ \hat{Z}_0 = Z_0 - Z_\mu Z_0. \]  

(7.3)

It is easily checked that this expression agrees with the earlier definition in Ref. 39. The matrix \( \hat{Z}_0 \) differs from \( Z_0 \) only in the \( l=1 \) subspace. Note that the matrices \( \xi_0 \) and \( \mu_0 \) operate in the complete vector space. We shall prove that for any configuration of spheres the exact mobility matrix is given by the identity

\[ \mu = \mu_0 (I + Z_0 \hat{Z}_0 Z_0^{-1})^{-1} (I + Z_0 G) \xi_0. \]  

(7.4)

The matrix \( Z_0^{-1} \) is diagonal in the index \( l \) for each sphere, and is identical with the unit matrix for \( l>1 \).

In order to show the validity of Eq. (7.4) we multiply from the left by the friction matrix, as given by Eq. (3.13). Abbreviating

\[ A = Z_0 G, \quad B = Z_0 \hat{Z}_0 Z_0^{-1}, \]  

(7.5)

we then have

\[ \xi \mu = \xi_0 (I + A)^{-1} Z_0 \mu_0 (I + B)^{-1} (I + A) \xi_0. \]  

(7.6)

From Eqs. (7.2) and (7.3) we find

\[ \xi_0 \mu_0 = \xi_0, \quad A - B = A Z_0 \mu_0, \]  

(7.7)

which allows us to write

\[ \xi \mu = \xi_0 [I - (I + A)^{-1}(A - B)] (I + B)^{-1} (I + A) \xi_0. \]  

(7.8)

Using the matrix identity

\[ (I + A)^{-1}(B - A)(I + B)^{-1} = (I + A)^{-1} - (I + B)^{-1}, \]  

(7.9)

we therefore find \( \xi \mu = \xi_0 \), which equals the identity matrix in the \textit{FT} subspace, as it should.

It is evident upon expansion of the inverse matrix in Eq. (7.4) in a geometric series that it consists of a sum of terms with intermediate repeated products of \( G \hat{Z}_0 \). We may write alternatively

\[ (I + Z_0 \hat{Z}_0 Z_0^{-1})^{-1} = Z_0 (I + \hat{Z}_0) Z_0^{-1}. \]  

(7.10)

It is easy to show that the product in Eq. (7.4) may be cast in the form

\[ (I + Z_0 \hat{Z}_0 Z_0^{-1}) (I + Z_0 G) = I + Z_0 (I + \hat{Z}_0) (G Z_0 - \hat{Z}_0) Z_0^{-1}. \]  

(7.11)

Using Eqs. (7.3) and (7.4) we find that the mobility matrix is given by the alternative expression

\[ \mu = \mu_0 + \mu_0 Z_0 (I + \hat{Z}_0) G \hat{Z}_0 \mu_0. \]  

(7.12)
This is the expression derived earlier in operator form for bodies of arbitrary shape by one of us.\(^3\) It was used in theoretical analysis of sedimentation in a suspension of spheres.\(^{40,41}\) For present purposes, the expression (7.4) is more useful.

The procedure for calculating the sphere velocities directly for given forces and torques can now be indicated. From the given force multipole vector

\[
f = \begin{bmatrix} F \\ 0 \end{bmatrix}, \quad \mathcal{G} f = f,
\]

one first constructs the related multipole vector

\[
g = (1 + Z_0 G) \mathcal{G} f.
\]

One then solves the set of equations

\[
(1 + Z_0 G) \hat{Z}_0 \hat{Z}_0^{-1} h = g
\]

for the multipole vector \(h\). The translational and rotational velocities are found by multiplication by the diagonal mobility matrix \(\mu_0\)

\[
U = \mu_0 h.
\]

In Sec. VIII we show how this procedure can be turned into a practical and accurate scheme of numerical computation.

### VIII. NUMERICAL COMPUTATION OF MOBILITIES

In numerical computation we must truncate the multipole vectors at finite order. The equations of the preceding section remain valid with truncated vectors and matrices. In particular the mobility matrix \(\mu_L\), given by

\[
\mu_L = \mu_0 (1 + Z_0 G \hat{Z}_0 \hat{Z}_0^{-1})^{-1} (1 + Z_0 G L) \mathcal{G} f,
\]

is the inverse of the friction matrix \(\xi_L\). The corrected mobility matrix \(\bar{\mu}_L\) with lubrication correction built in, defined in Eq. (7.1), is given by

\[
\bar{\mu}_L = [1 + \mu_L \Delta \xi_L]^{-1} \mu_L.
\]

We may find this matrix directly by modifying the set of equations to be solved. Let \(U_L\) be the velocities calculated with the matrix \(\mu_L\), and let \(\bar{U}_L\) be the corresponding velocities calculated with lubrication correction, so that

\[
U_L = \mu_L F, \quad \bar{U}_L = \bar{\mu}_L F.
\]

We can find the corrected velocities by solving the set of equations

\[
(1 + \mu_L \Delta \xi_L) \bar{U}_L = \mu_L F.
\]

However, this would require that we have the complete matrix \(\mu_L\) at our disposal. Instead we substitute the expression (8.1). It is then evident that the corrected velocities may be constructed from

\[
\bar{U}_L = \mu_0 \bar{f}_L,
\]

where the multipole vector \(\bar{f}_L\) is found as the solution of the set of equations

\[
[1 + Z_0 G L \hat{Z}_0 \hat{Z}_0^{-1} + (1 + Z_0 G L) \Delta \xi_L \mu_0] \bar{f}_L = g_L.
\]

The procedure allows fast computation of Stokesian dynamics, both for a finite number of spheres in infinite space, and in the thermodynamic limit with periodic boundary conditions.

### IX. NUMERICAL EXAMPLES

In the following, we present some examples, which demonstrate the accuracy and efficiency of our method. As in the calculation of the drag coefficient of three touching spheres, presented in Sec. V, we find that there is rapid convergence with increasing multipole order \(L\).

In the numerical implementation we have preferred a Cartesian representation of the reduced force multipoles. A complete set of Cartesian vector spherical harmonics, which appear in the definition of the multipoles,\(^{31}\) may be constructed from the scalar harmonics.\(^{42}\) Subsequently one may evaluate the elements of the Green matrix by use of the results for the two-sphere problem,\(^{31}\) or by using the displacement theorem.\(^{33}\) For systems with periodic boundary conditions we use the Cartesian representation.\(^{43}\)

As a first example we consider the mobility of six equal spheres of radius \(a\), located at the corners of a regular hexagon, as shown in Fig. 3. Let \(d\) be the distance between two neighboring centers expressed in units of the sphere diameter \(2a\), so that \(d=1\) corresponds to touching spheres. We choose coordinates such that the hexagon lies in the plane \(x=0\) with sphere 1 centered at the origin and with the center of sphere 4 on the positive \(z\) axis. We consider a force applied to sphere 4 in the \(y\) direction. All spheres move, but we calculate only the \(y\) component of the velocity of sphere 1, i.e., the element \(\mu_{1y4y}\) of the mobility matrix. In Fig. 4 we plot the reduced mobility \(\mu = 6a \eta q \mu_{1y4y}\) as a function of the distance \(d\), calculated with truncation at different orders \(L\). It is evident that truncation at order \(L=3\) yields sufficient accuracy, and that the mobility with truncation at \(L=3\) differs significantly from that with truncation at \(L=1\). We have found similar behavior for other elements of the mobility matrix, and for different...
Friction and mobility in Stokes flow

FIG. 4. Plot of the reduced mobility $\mu/\mu_0 = 6\pi\eta a_1 \rho_1$ for the configuration shown in Fig. 3. The reduced mobility is plotted as a function of reduced distance $d=R/2a$ between neighboring centers, as calculated with truncation at various multipole orders $L$.

FIG. 5. Plot of the reduced transverse mobility $\mu/\mu_0$ of a rod of $N$ spheres (squares). We compare with the Riseman–Kirkwood approximation (dashed curve), as given by the first term in Eq. (9.1). The drawn curve is a fit to the data given by the complete expression in Eq. (9.1) with values of the coefficients $a_i = 0.97$, $b_i = -0.72$.

X. DISCUSSION

We have presented an efficient scheme of numerical calculation of hydrodynamic interactions between many spheres. The nature of the scheme is such that in principle any desired accuracy can be attained. In practice we get satisfactory results by truncation at relatively low force multipole order with account of lubrication effects in pair superposition approximation. In our numerical implementation we use a Cartesian formulation. Both the many-sphere friction matrix and the mobility matrix are found

with $\mu_0 = 1/6\pi\eta a$. The leading terms were found by Riseman and Kirkwood by use of the approximation discussed in Sec. II. The coefficients $a_{ij}$ and $b_{ij}$ involve contributions of multipoles of all orders and analytic calculation is difficult. We have evaluated the mobilities $\mu_i$ and $\mu_j$ for rods of up to 100 spheres. In Fig. 5 we plot the reduced mobility $\mu_i/\mu_0$ as a function of $N$. We compare with the Riseman–Kirkwood approximation given by the first term in Eq. (9.1). The complete expression with coefficients $a_i = 0.97 \pm 0.01$, $b_i = -0.72 \pm 0.01$ gives an excellent fit to the numerical results over a wide range. In Fig. 6 we show a similar plot for the reduced mobility $\mu_j/\mu_0$. In this case we find a fit to the data for values $a_i = -0.12 \pm 0.01$, $b_i = 0.37 \pm 0.05$. The above results were calculated with truncation at orders $L=3$ and $L=4$. Truncation at $L=1$ would lead to significantly different values for the coefficients.
from the solution of a set of equations. As a consequence, in the Stokesian dynamics of $N$ spheres the number of operations is significantly reduced, and can even be made to be of order $N^2$ with suitable algorithms. A number of operations of order $N^3$ is always required if the mobility matrix is calculated as the inverse of the friction matrix. In our explicit examples we have calculated the friction matrix and the mobility matrix for a finite number of spheres in infinite space. The general formulation applies equally well to infinite systems with periodic boundary conditions. It can be extended to include the computation of particle stress, which is needed in a calculation of effective viscosity. Explicit calculations of sedimentation coefficient, effective permeability, and effective viscosity will be presented elsewhere.

ACKNOWLEDGMENTS

We thank Dr. I. Pienkowska for communicating the exact result quoted below Eq. (5.2), and Dr. A. J. C. Ladd for correspondence concerning the problem of truncation.

35. I. Pienkowska (private communication).
37. A. J. C. Ladd (private communication).