Hydrodynamic interactions between spheres in a viscous fluid with a flat free surface or hard wall

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Citation: The Journal of Chemical Physics 126, 184704 (2007); doi: 10.1063/1.2724815
View online: http://dx.doi.org/10.1063/1.2724815
View Table of Contents: http://scitation.aip.org/content/aip/journal/jcp/126/18?ver=pdfcov
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Propagation of hydrodynamic interactions between particles in a compressible fluid
Hydrodynamic interactions between spheres immersed in a low-Reynolds-number fluid flow close to a flat free surface or hard wall are investigated. The spheres may have different or equal radii, and may be separated from the boundary or at contact with the free surface. A simple and useful expression is derived for the propagator (Green operator) connecting centers of two spheres. In the derivation, the method of images and the displacement theorems are used. Symmetry of the displacement operators is explicitly shown. The significance of these results in efficient Stokesian and Brownian dynamics simulations is outlined. An example of an application is shown. © 2007 American Institute of Physics. [DOI: 10.1063/1.2724815]

Hydrodynamic interactions between particles suspended in a fluid are significantly modified by the presence of a near boundary. For example, a flat hard wall or a free surface generates mutual hydrodynamic repulsion of two spheres approaching it side by side.\textsuperscript{1-3} Therefore, in a confined geometry, evaluation of suspension effective transport coefficients requires a special treatment.\textsuperscript{4,5} In particular, there is a lot of interest in quasi-two-dimensional suspensions. An example is a system of superparamagnetic colloidal spheres in water near to flat water-air interface. The particles are located at the bottom of a cylindrical water drop. When an external magnetic field is applied, the particles repel each other owing to dipole magnetic forces and move along the interface. The self-diffusion and collective diffusion, melting and freezing transitions have been extensively studied experimentally.\textsuperscript{6-8}

Effective transport coefficients of suspensions are theoretically derived and numerically simulated by statistical averaging of the corresponding mobility coefficients for groups of many suspended spherical particles.\textsuperscript{9} Therefore, it is essential to focus on efficient methods to evaluate many-body hydrodynamic interactions, i.e., the mobility (or, equivalently, friction) matrices.\textsuperscript{10} One of the most efficient methods is the multipole expansion of the stationary Stokes equations for the incompressible fluid flow.\textsuperscript{3,11} As the result, the multipole components $f_i$ of the stress exerted on the surface of sphere $i$, located at $R_i$, by the external fluid flow with the multipole components $v_{ij}$ (centered at sphere $j$, located at $R_j$) are determined as the following multiple scattering series:

$$f_i = Z_0(i) \sum_j \left[ \delta_{ij} - G_A(R_i, R_j)Z_0(j) + \sum_k G_A(R_i, R_k)Z_0(k)G_A(R_k, R_j)Z_0(j) + \cdots \right]v_{ij},$$

with the single-sphere friction operators $Z_0(j)$ and the Green operators $G_A(R_i, R_j)$, where the index $A=H$ for a flat hard wall, $A=F$ for a flat free surface, and $A=\infty$ for infinite unbounded fluid. Alternatively, Eq. (1) can be written as $f = (Z_0^{-1} + G_A)^{-1}v_0$, with the summation over particles included in the notation. The operator $Z_0(j)$, applied to the fluid flow incoming onto sphere $j$, results in the stress it exerts on this sphere, while $[-G_A(R_i, R_j)]$, applied to the stress on sphere $j$, results in the fluid flow generated at the center of sphere $i$. For unbounded fluid, $G_x(R_i, R_j)=0$ and $G_x(R_i, R_j) = G(R_i, R_j)$, if $i \neq j$, with $G$ denoting the Oseen tensor,\textsuperscript{10} and $R_j = R_i - R_i$. The Green operator connecting centers of different spheres $i \neq j$ is called a propagator and is denoted as $\tilde{G}_A(R_i, R_j)$. It does not depend on the sphere radii.

The propagators and the single-sphere friction operators are essential to determine the Stokesian dynamics of $N$ spheres located at $R_i$, which undergo external forces $F_j$:

$$\frac{dR_i}{dt} = \sum_j \mu_{ij} \cdot F_j,$$

with the translational-translational mobility matrix determined by all the positions, $\mu_{ij} = \mu_{ij}(R_1, \ldots, R_N)$, and evaluated as the inverse of the friction matrix, $\mu = \xi^{-1}$. Indeed, $\xi$ is evaluated directly from Eq. (1) by projecting the grand friction matrix $(Z_0^{-1} + G_A)^{-1}$ onto the lowest multipoles corresponding to $F_j$. The mobility matrix is also the basic element of the Brownian dynamics.\textsuperscript{12}

In this paper, we will prove properties of the propagators essential for evaluation of the hydrodynamic interactions: we will demonstrate symmetry of the displacement theorems from Ref. 13 for the propagators and we will show how to reformulate the scattering series in the presence of boundaries—how to express the propagator $\tilde{G}_A(R_i, R_j)$ in terms of $G(R_i, R_j)$ only.

To evaluate hydrodynamic interactions between two solid spheres centered at $R_i$ and $R_j$ in the fluid bounded by a flat free surface or hard wall at $z=0$, the mirror image
spheres $i'$, $j'$ are introduced at $\mathbf{R}_{i'}$, $\mathbf{R}_{j'}$, as illustrated in Fig. 1, and used to construct the propagator $\tilde{G}_{A}(\mathbf{R}_{i},\mathbf{R}_{j})$ for propagators for the unbounded fluid, 14,15

$$
\tilde{G}_{A}(\mathbf{R}_{i},\mathbf{R}_{j}) = \mathbf{G}(\mathbf{R}_{i}) + \mathbf{G}(\mathbf{R}_{j}) \cdot \mathcal{R}_{A}(\mathbf{z} \cdot \mathbf{R}_{jj}/2).
$$

(3)

In the multipole representation, 4 all the operators in the above relation (and their superposition) are represented by the multipole matrices (and their product), with the elements labeled by two sets of indices $lm\sigma$, which parametrize complete sets of regular and singular multipole solutions of the Stokes equations for an unbounded fluid, $v_{lm\sigma}$ and their adjoints, centered at the spheres $i,j$ and at their images $i', j'$, with the multipole indices $l,m$ related to the direction of the unit vector $\mathbf{z}$ normal to the boundary and pointing into the fluid. 4

For the free surface, $\mathcal{R}_{A}(z)=\mathcal{R}_{F}$ is the operator of mirror reflection with respect to the plane $z=0$ (independent of $z$), determined by its multipole elements,

$$
\mathcal{R}_{F,i'lm\sigma,lm\sigma} = (-1)^{l+m+\sigma} \delta_{ii'} \delta_{mm} \delta_{\sigma\sigma'}.
$$

(4)

For the hard wall, $\mathcal{R}_{A}(z)=\mathcal{R}_{j}(z)$ is the Lorentz reflection, 10 with the corresponding multipole elements $\tilde{R}_{H,i'lm\sigma,lm\sigma}(z)$ listed in Ref. 4.

To express the propagator $\tilde{G}_{A}(\mathbf{R}_{i},\mathbf{R}_{j})$ in terms of $\mathbf{G}(\mathbf{R}_{ij})$ only, $\mathbf{G}(\mathbf{R}_{ij})$ in Eq. (3) will now be expressed in terms of $\mathbf{G}(\mathbf{R}_{j})$. To this goal, the multipole centers are changed, and the multipole solutions are transformed according to the displacement theorems, derived in Ref. 13. In particular, for

$$
\mathbf{R} = \mathbf{R}_{+} + \mathbf{R}_{-},
$$

and

$$
|\mathbf{R}_{+}| > |\mathbf{R}_{-}|,
$$

(5)

Equation (3.3a) from Ref. 13 reads

$$
\mathbf{v}_{lm\sigma}(\mathbf{R}) = \eta \sum_{l'm'\sigma'} \mathbf{v}_{l'm'\sigma'}^{+}(\mathbf{R}_{+}) \mathbf{G}_{l'm'\sigma',lm\sigma}(\mathbf{R}_{-}),
$$

(6)

where $G_{l'm'\sigma',lm\sigma}(\mathbf{R})$ denotes the multipole matrix elements of the operator $\mathbf{G}(\mathbf{R})$,

$$
G_{l'm'\sigma',lm\sigma}(\mathbf{R}) = \frac{n_{l'm'}}{n_{lm}} S^{-}(\mathbf{R};l'm\sigma',lm\sigma),
$$

(7)

with $S^{-}$ evaluated in Ref. 13 and the normalization factors 18

$$
N_{lm} = \sqrt{\frac{4\pi(l+m)!}{(2l+1)(l-m)!}},
$$

(8)

introduced in Ref. 4 to obtain the symmetry

$$
\mathbf{G}^{\dagger}(\mathbf{R}) = \mathbf{G}(-\mathbf{R}),
$$

(9)

where $\dagger$ denotes the complex conjugate superposed with the transposition of the multipole indices $lm\sigma \rightarrow l'm\sigma'$ in Eq. (7).

The other displacement theorems, Eqs. (3.3b), (3.2a), and (3.2b) from Ref. 13, can be written as

$$
\mathbf{v}_{lm\sigma}(\mathbf{R}) = \sum_{l'm'\sigma'} \mathbf{v}_{l'm'\sigma'}^{+}(\mathbf{R}_{+}) S_{l'm'\sigma',lm\sigma}(\mathbf{R}_{-}),
$$

(10)

$$
\mathbf{v}_{lm\sigma}^{+}(\mathbf{R}) = \sum_{l'm'\sigma'} \mathbf{v}_{l'm'\sigma'}^{+}(\mathbf{R}_{+}) S_{l'm'\sigma',lm\sigma}(\mathbf{R}_{-}),
$$

(11)

and

$$
S_{l'm'\sigma',lm\sigma}(\mathbf{R}) = \frac{n_{l'm'}}{n_{lm}} S^{+}(\mathbf{R};l'm\sigma',lm\sigma),
$$

(12)

where $S_{l'm'\sigma',lm\sigma}(\mathbf{R})$ are the multipole matrix elements of the operator $\mathbf{S}(\mathbf{R})$,

$$
S_{l'm'\sigma',lm\sigma}(\mathbf{R}) = \frac{n_{l'm'}}{n_{lm}} S^{+}(\mathbf{R},l'm\sigma',lm\sigma),
$$

(13)

with $S^{+}$ evaluated in Ref. 13 (except the missing term corrected in Ref. 11). It can be checked that the coefficients $S^{+}$, evaluated in Ref. 13, satisfy the relation

$$
S_{l'm'\sigma',lm\sigma}(\mathbf{R}) = \frac{n_{l'm'}}{n_{lm}} S^{+}(\mathbf{R};l'm\sigma',lm\sigma).
$$

(14)

It is useful to specify how to displace the propagators. In particular, integrating Eq. (10) with an appropriate multipole function over spherical surface of radius $b \rightarrow 0$, and using Eq. (3.5) from Ref. 13, we obtain

$$
\mathbf{G}(\mathbf{R}) = \mathbf{G}(\mathbf{R}_{+}) \cdot \mathbf{S}(\mathbf{R}_{-}).
$$

(15)

Now we are going to represent the propagator defined in Eq. (3), using the displacement $\mathbf{R}_{ij} = \mathbf{R}_{ij} + \mathbf{R}_{jj}$ (see Fig. 1). From Eq. (15) it follows that $\mathbf{G}(\mathbf{R}_{ij}) = \mathbf{G}(\mathbf{R}_{ij}) \cdot \mathbf{S}(\mathbf{R}_{jj})$, if $\mathbf{R}_{ij} > \mathbf{R}_{jj}$. Therefore, the propagator has the form

$$
\tilde{G}_{A}(\mathbf{R}_{i},\mathbf{R}_{j}) = 2\mathbf{G}(\mathbf{R}_{ij}) \cdot \mathbf{P}_{A}(\mathbf{R}_{jj})
$$

(16)

for $\mathbf{R}_{ij} > \mathbf{R}_{jj}$, where

$$
\mathbf{P}_{A}(\mathbf{d}) = \frac{1}{2} [\mathbf{I} + \mathbf{S}(\mathbf{d}) \cdot \mathcal{A}_{A}(d/2)]
$$

(17)

is a projection operator,

$$
\mathbf{P}_{A}(\mathbf{d}) = \mathbf{P}_{A}(\mathbf{d}) \cdot \mathbf{P}_{A}(\mathbf{d}).
$$

(18)

Equation (18) results from the relation

$$
[\mathbf{S}(\mathbf{d}) \cdot \mathcal{A}_{A}(d/2)] = \mathbf{I}
$$

(19)

for $\mathbf{d} \perp \mathbf{S}$, which in turn follows from the properties of the operations $\mathcal{A}$ (mirror reflection) and $\mathcal{S}$ (Lorentz reflection), specified in Eqs. (12.4)–(12.6) in Chap. 12.2 of Ref. 10. For $A=F$ (free surface), Eq. (19) is just the multipole representation of the
identity \(M^2 = I\), and for \(A = H\) (hard wall)—of the identity \(u^{**} = u\).

The operator \(P_A(d)\) projects onto the subspace of these solutions of the Stokes equations, which satisfy the corresponding boundary conditions at \(z = 0\).\(^\text{19}\)

Interchanging \(i\) with \(j\) in Eq. (16), applying \(^\dagger\), and taking into account the Lorentz reciprocity relation \(\) [see Eq. (26) in Ref. 4],

\[
\tilde{G}_\Lambda(R_i, R_j) = \tilde{G}_\Lambda(R_j, R_i),
\]

we obtain

\[
\tilde{G}_\Lambda(R_i, R_j) = 2P^T_i(R_{ji'}) \cdot G(R_{jj'}) \quad \text{for } R_{ij} > R_{i'i'},
\]

where the superscript \(T\) denotes transposition of the multipole indices \(l \sigma m' m'\). Note that \(P_A(d)\) is real if \(d \perp S\), therefore \(P_A(d) = P_A(d)\).

Equation (21) can be alternatively obtained in a similar way as Eq. (16), but with another displacement, \(R_{ij'} = R_{i'i'} + R_{i'j'}\) (see Fig. 1).

Combining Eqs. (16) and (21) with Eq. (18), we finally obtain the main result of this paper, i.e., the following expression for the propagator:

\[
\tilde{G}_\Lambda(R_i, R_j) = 2P^T_i(R_{ji'}) \cdot G(R_{jj'}) \cdot P_A(R_{ji'}),
\]

for \(R_{ij} > R_{i'i'}, R_{jj'}\).

Equation (22) simplifies evaluation of friction and mobility coefficients. Owing to this relation, the scattering sequence Eq. (1) can be alternatively calculated as the analogical superposition of modified single-sphere operators \(Z_0A(i) = 2P_A(i) [Z_0(i) + G(R_{ii'}) / R_{ii'}] \) \(\) [rather than \(Z_0(i)\)] and the propagators for the unbounded fluid, \(G(R_{ii'})\) \(\) [rather than \(\tilde{G}_\Lambda(R_i, R_i)\)]. In Eq. (1), the boundary conditions are taken into account in the Green operator \(G\), while the single-particle operator \(Z_0\) is the same as for the unbounded fluid. In the new formulation, the boundary conditions are taken into account in the modified single-particle operator \(Z_0A\), while the Green operator is just the simple Oseen tensor \(G\).

The new scheme has been applied in Ref. 11 for identical spheres touching a free surface, based on their Eq. (30). In this case, the modified friction operator characterizes a single dumbbell, made of a sphere and its touching mirror image. In particular, the method described in this work, was used in Ref. 11 to derive the asymptotic expressions for long-distance hydrodynamic interactions of the dumbbells (the analog of the Rotne-Prager formula), and in Ref. 16 this asymptotics was shown to be very accurate even for relatively close spheres. Both the asymptotic and the exact results can be used next to evaluate the self-diffusion and collective diffusion for the quasi-two-dimensional systems investigated experimentally in Refs. 6–8.

In this work, proving the relation Eq. (22), we have in particular shown the validity of Eq. (30), given without a proof in Ref. 11. The present result is more general. Equation (22) holds for spheres in general separated from the interface or hard wall (in particular they can also touch the free surface), and the sphere sizes may differ from one another.

Finally, let us mention that the displacement theorem for the propagators, Eq. (15), and the symmetry of the displacement operators, Eq. (14), are useful for developing new generation of fast numerical multipole procedures, following the ideas of Ref. 17.

This work was supported in part by the Polish Ministry of Science and Higher Education, Grant No. N501 020 32/ 1994.

\(^9\) J. K. G. Dhont, An Introduction to Dynamics of Colloids (Elsevier, Amsterdam, 1996).
\(^18\) In Ref. 11, there is a misprint in Eq. (B2) for \(n_{\sigma}\).
\(^19\) In Ref. 11, there is a misprint in Eq. (23), where the prime in the multipole function \(\dot{\gamma}' l m \sigma\) should be omitted.