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Note on the direct calculation of mobility functions for two equal-sized spheres in Stokes flow

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A simple, direct method is presented for the calculation of mobility functions for the translational and rotational velocities and stresslets of two equal-sized spheres in unbounded low-Reynolds-number flow when the ambient velocity field is a superposition of a uniform stream, a vorticity and a rate-of-strain field. Our numerical procedure furnishes accurate values for touching spheres and coefficients for the near-field asymptotic expansions. The singular behaviour of the mobility functions is clarified. These results have been used to determine accurately the coefficient of the $O(c^2)$ term in the expression for the bulk stress in a suspension of spheres ($6.95c^2$ instead of $7.6c^2$).

1. Introduction

When two rigid spheres are set in motion in a Newtonian fluid in situations where the effect of inertial forces is negligible there exists a set of linear relations between the rigid-body motion of the spheres in the ambient field on one hand, and the moments (force, torque, stresslet) exerted on the spheres on the other. Such information is essential in the theoretical investigations of the behaviour of suspension of small particles, such as the trajectory analysis for colloid stability (van de Ven & Mason 1976; Zeichner & Schowalter 1977) and the calculation of bulk stress (Batchelor & Green 1972*b*; Batchelor 1977; Russel & Gast 1986). Following the general framework of Brenner & O'Neill (1972) we define the resistance problem as that in which the moments on the spheres are to be determined for the specified translational and rotational velocities of the spheres in a linear ambient field. The mobility problem is defined as that in which the forces and torques are prescribed in the ambient field and the particle motion and the stresslet are the unknowns. Historically, the solution of the mobility problem has lagged behind that of the resistance problem because the mobility problem is usually solved by inversion of the linear relations from the resistance problem.

Several methods have been developed for solving the Stokes equation for two spheres. Lin, Lee & Sather (1970) have used the bispherical coordinates to calculate the motion in a shear field. In their work the singular behaviour of some of the mobility functions at small separations raises the question of convergence in the evaluation of infinite series and Batchelor & Green (1972*a*) have observed the inconsistency with their asymptotic expressions. The case of two touching spheres in a shear field has been studied by Wakiya (1971, 1972) and Nir & Acrivos (1973) using the tangent-sphere coordinates. A more detailed analysis in a general linear field was done by Batchelor & Green (1972*a*). They used the method of reflections (Happel & Brenner 1983) to obtain the far-field analytic forms of the mobility functions valid when the separations are greater than sphere radius, and used the lubrication analysis (O'Neill & Majumdar 1970) for the near-field analytic forms. However, the information on the stresslet was limited to the far-field region and the values at touching. Although it is straightforward to apply the lubrication analysis to the resistance problem (Cox 1974), it should be noted that the mobility problem with the rate-of-strain ambient field requires the additional information on values for touching and almost-touching spheres. Batchelor & Green (1972*a*) used the values in Wakiya (1971) and Lin *et al.* (1970) for these purposes. As mentioned earlier, the solution of Lin *et al.* (1970) was not accurate enough at small separations and the information on the stresslets at small separations was unavailable, so that the calculation of the bulk stress in Batchelor & Green (1972*b*) contains $\pm 10\%$ uncertainty. Chen & Acrivos (1978) have used the multipole expansion technique to calculate mobility functions associated with the stresslet. Jeffrey & Onishi (1984) have used the method of twin multipole expansions and the lubrication analysis to obtain the expressions for resistance and mobility functions when the ambient velocity field is a superposition of a uniform stream and a vorticity field (no rate-of-strain field). For widely separated spheres they represented the mobility functions in the term of the polynomial of R^{-n}, where R is the dimensionless centre-to-centre distance between two spheres. They tested the convergence of the series at small separations and found that for certain mobility functions, the series solution did not coincide with the near-field asymptotic values even when summed to terms to $O(R^{-220})$. Recently, Kim & Mifflin (1985) have computed the entire set of functions using the boundary collocation methods of Ganatos, Pfeffer & Weinbaum (1978). They solved the resistance problems first and then used the relations between the resistance and mobility matrices to calculate the mobility functions. However, certain resistance functions are singular in the near field, the resistance matrix becomes ill-conditioned, and thus their method was successful only for dimensionless separations greater than 0.01. (The region between touching and 0.01 makes significant contributions to the bulk stress.)

In summary there are two major disadvantages in the previous methods of solving the mobility problem. Firstly, three separate solution methods are required for touching, near-field and far-field problems, respectively. In addition, the usual lubrication-type analysis for near-field problems is somewhat cumbersome and the information on the stresslets with this method is still unavailable. Secondly, the singular behaviour of the resistance functions at small separations makes the mobility problems ill-conditioned. Therefore, even with the accurate values of the resistance functions at small separations, the inversion process to the mobility functions becomes unstable.

Our purpose here is to introduce a simple, direct method which provides accurate information on the mobility functions of two equal-sized spheres at all separations including the case of touching. As shown in subsequent sections, the boundary collocation method as used by Kim & Mifflin (1985) can be modified to bypass the singularity problem and the inversion process. We have tested the method at small separations and, when possible, have compared the results with accurate asymptotic expressions from previous works. For illustrative purposes, we calculate here the mobility functions of two neutrally buoyant spheres. Details are shown for very small separations and the near-field asymptotic expressions analogous to those obtained from lubrication theory are presented. With this information we determine a more accurate value of Batchelor & Green's (1972*b*) $O(c^2)$ coefficient in the expression for the bulk stress in suspension.

2. Mobility functions

Two equal-sized spheres of radii a centred at $\boldsymbol{x}_\alpha(\alpha = 1,2)$ are immersed in an unbounded Newtonian fluid of viscosity μ. The Reynolds number of the flow is very small so that we may neglect the effect of inertial forces. The ambient flow field $\boldsymbol{v}^\infty = \boldsymbol{U}^\infty + \boldsymbol{\Omega}^\infty \times \boldsymbol{x} + \boldsymbol{E}\cdot\boldsymbol{x}$ is a superposition of a uniform stream, a vorticity and a rate-of-strain field. The boundary conditions on the surface are the rigid-body motion $\boldsymbol{U}^{(\alpha)} + \boldsymbol{\Omega}^{(\alpha)} \times (\boldsymbol{x}-\boldsymbol{x}_\alpha)$. No external force or torque acts on the spheres, and following Batchelor & Green (1972*a*), we define the mobility functions which appear in the expressions of the translational and rotational velocities and the stresslet as

$$U_i^{(1)} = v_i^\infty(\boldsymbol{x}_1) + \{\tfrac{1}{2}A\, d_i d_j + \tfrac{1}{2}B(\delta_{ij} - d_i d_j)\}\, r_k E_{jk}, \tag{2.1a}$$

$$U_i^{(2)} = v_i^\infty(\boldsymbol{x}_2) - \{\tfrac{1}{2}A\, d_i d_j + \tfrac{1}{2}B(\delta_{ij} - d_i d_j)\}\, r_k E_{jk}, \tag{2.1b}$$

$$\Omega_i^{(1)} = \Omega_i^{(2)} = \Omega_i^\infty + C\epsilon_{ijk} d_j d_l E_{kl}, \tag{2.2}$$

$$\begin{aligned} S_{ij}^{(1)} = S_{ij}^{(2)} &= \tfrac{20}{3}\pi a^3\mu\{(1+K)E_{ij} + L(d_i d_k \delta_{jl} + d_j d_k \delta_{il} - \tfrac{2}{3} d_k d_l \delta_{ij})E_{kl} \\ &\quad + M(d_i d_j - \tfrac{1}{3}\delta_{ij}) d_k d_l E_{kl}\}, \end{aligned} \tag{2.3a}$$

$$\begin{aligned} &= \tfrac{20}{3}\pi a^3 \mu\{E_{ij} + \tfrac{3}{2}P(d_i d_j - \tfrac{1}{3}\delta_{ij})(d_k d_l - \tfrac{1}{3}\delta_{kl})E_{kl} \\ &\quad + \tfrac{1}{2}Q(d_i \delta_{jl} d_k + d_j \delta_{il} d_k + d_i \delta_{jk} d_l + d_j \delta_{ik} d_l - 4 d_i d_j d_k d_l)E_{kl} \\ &\quad + \tfrac{1}{2}K(\delta_{ik}\delta_{jl} + \delta_{jk}\delta_{il} - \delta_{ij}\delta_{kl} + d_i d_j \delta_{kl} + \delta_{ij} d_k d_l \\ &\quad - d_i \delta_{jl} d_k - d_j \delta_{il} d_k - d_i \delta_{jk} d_l - d_j \delta_{ik} d_l + d_i d_j d_k d_l)E_{kl}\}, \end{aligned} \tag{2.3b}$$

where $\boldsymbol{r} = \boldsymbol{x}_2 - \boldsymbol{x}_1$ is the centre-to-centre vector and $\boldsymbol{d} = \boldsymbol{r}/|\boldsymbol{r}|$. In addition to the contributions from the ambient field (the single-sphere solution), hydrodynamic interaction effects are described in terms of six mobility functions which are functions only of the dimensionless centre-to-centre distance $R = |\boldsymbol{r}|/a$. We define the dimensionless separation ξ as $\xi = R-2$ for later use. The axisymmetry about the centre-to-centre axis facilitates the decomposition of the translational velocity into the radial (A function) and circumferential (B function) components. Also, due to the axisymmetry, only three rate-of-strain fields out of five are independent, so that three functions are sufficient to express the stresslet. The first decomposition of the stresslet, (2.3*a*) is due to Batchelor & Green (1972*a*) and the second (2.3*b*), is as in Chen & Acrivos (1978) and Kim & Mifflin (1985). Simple relations exist between the two sets, i.e.

$$P = K + \tfrac{4}{3}L + \tfrac{2}{3}M, \quad Q = K + L, \tag{2.4}$$

so that we can recover one set from the other. We discuss the advantages and disadvantages of each decomposition in the subsequent section. The function J is also defined for later use:

$$J = K + \tfrac{4}{5}L + \tfrac{2}{15}M = \tfrac{1}{5}(P + 2Q + 2K). \tag{2.5}$$

3. Boundary collocation

The disturbance velocity field $\boldsymbol{v}(\boldsymbol{x}) - \boldsymbol{v}^\infty(\boldsymbol{x})$ satisfies the Stokes equation and the equation of continuity for incompressible flow,

$$-\nabla p + \mu\nabla^2 \boldsymbol{v} = 0, \quad \nabla\cdot\boldsymbol{v} = 0. \tag{3.1}$$

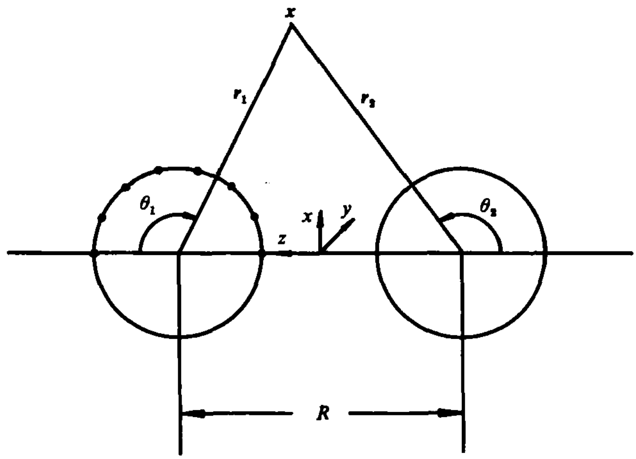

FIGURE 1. Two-sphere geometry with the position of collocation points.

The solution can be represented using Lamb's general solution, as in Happel & Brenner (1983):

$$v(x)-v^{\infty}(x)=\sum_{\alpha=1}^{2}\sum_{n=1}^{\infty}\left[\nabla\Phi_{-n-1}^{(\alpha)}+\nabla\times(r_\alpha\chi_{-n-1}^{(\alpha)})+\frac{(n+1)}{\mu n(2n-1)}r_\alpha p_{-n-1}^{(\alpha)}\right.$$
$$\left.-\frac{(n-2)}{\mu 2n(2n-1)}r_\alpha^2\nabla p_{-n-1}^{(\alpha)}\right]. \qquad (3.2)$$

Here p_{-n-1}, Φ_{-n-1} and χ_{-n-1} are exterior spherical harmonics and $r_\alpha = x - x_\alpha$ is the position vector in terms of the spherical coordinates $(r_\alpha, \theta_\alpha, \phi)$ for $\alpha = 1, 2$ as shown in figure 1. The spherical harmonics are expanded as

$$p_{-n-1}^{(\alpha)}=\sum_{m=0}^{n} r_\alpha^{-n-1}P_n^m(\cos\theta_\alpha)(a_{0n}^{(\alpha)}\delta_{0m}+a_{mn}^{(\alpha)}\sin m\phi), \qquad (3.3a)$$

$$\Phi_{-n-1}^{(\alpha)}=\sum_{m=0}^{n} r_\alpha^{-n-1}P_n^m(\cos\theta_\alpha)(b_{0n}^{(\alpha)}\delta_{0m}+b_{mn}^{(\alpha)}\sin m\phi), \qquad (3.3b)$$

$$\chi_{-n-1}^{(\alpha)}=\sum_{m=0}^{n} r_\alpha^{-n-1}P_n^m(\cos\theta_\alpha)\,c_{mn}^{(\alpha)}\cos m\phi, \qquad (3.3c)$$

where P_n^m is the associated Legendre function and $a_{mn}^{(\alpha)}$, $b_{mn}^{(\alpha)}$ and $c_{mn}^{(\alpha)}$ are unknown coefficients to be determined. The force, torque and stresslet exerted on sphere α are

$$F^{(\alpha)}=-4\pi\nabla(r_\alpha^3 p_{-2}),\quad T^{(\alpha)}=-8\pi\mu\nabla(r_\alpha^3\chi_{-2}),\quad S^{(\alpha)}=-\tfrac{2}{3}\pi\nabla\nabla(r_\alpha^5 p_{-3}). \qquad (3.4a, b, c)$$

Substituting (3.3) into (3.4) gives the simple expressions for force, torque and stresslet in terms of a single coefficient in spherical harmonics.

For each mobility function, we need only one particular value of m (0, 1 or 2) depending on the rate-of-strain field used as the applied ambient field. Figure 2 shows these three subproblems and the resulting non-zero components of the translational and rotational velocities and stresslet related to the mobility functions defined in the

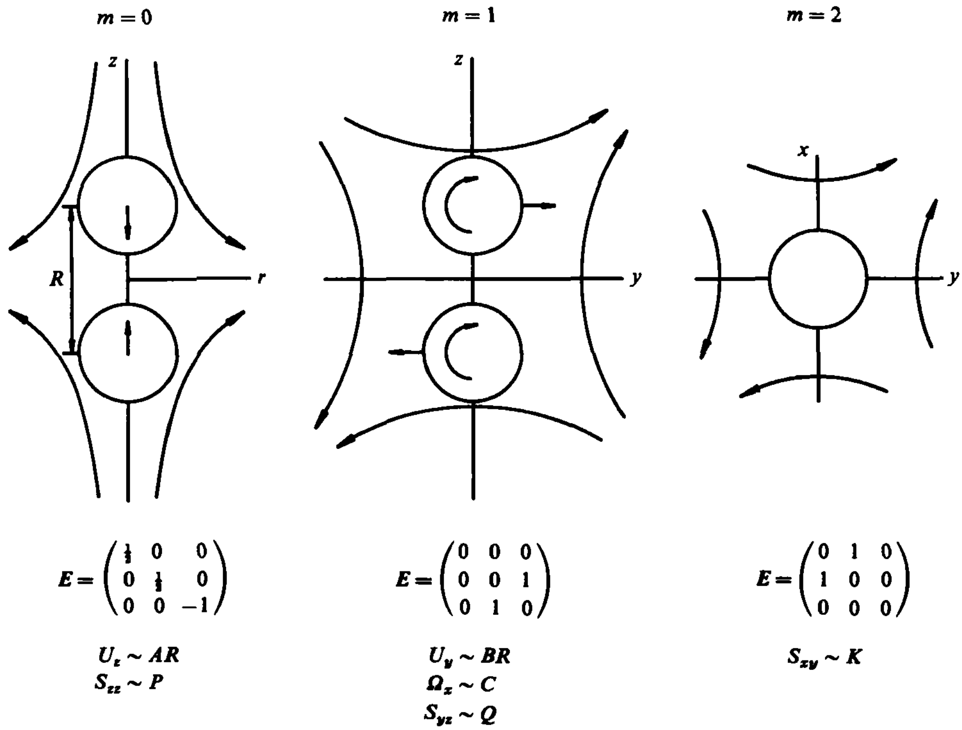

FIGURE 2. Three subproblems with the applied rate-of-strain fields and the resulting mobility functions of two neutrally buoyant spheres.

previous section. The decomposition of the stresslet by Kim & Mifflin (1985) in (2.3*b*) is a more natural and simpler choice than that of Batchelor & Green (1972*a*) because only one mobility function is associated with each subproblem.

The disturbance velocity field evaluated at the sphere surface must satisfy the no-slip boundary conditions so that it equals $\boldsymbol{U}^{(\alpha)}+\boldsymbol{\Omega}^{(\alpha)}\times(\boldsymbol{x}_s-\boldsymbol{x}_\alpha)-\boldsymbol{v}^{\infty}(\boldsymbol{x}_s)$, where $\boldsymbol{x}_s$ denotes the point on the surface (collocation point). As shown in Kim & Mifflin (1985), this fundamental collocation equation can be simplified further. Firstly, the ϕ-dependence can be factored so that the original two-dimensional collocation in θ and ϕ reduces to the one-dimensional collocation in θ. Secondly, the fore–aft mirror symmetry with respect to the (X, Y)-plane (figure 1) implies that the coefficients in spherical harmonics for sphere 1 are either equal or negative to the corresponding coefficients for sphere 2 depending on the type of ambient field. Thus, by truncating the spherical harmonics at N terms, the $3N$ unknown coefficients that result from equations at N collocation points (on the surface of sphere 1) are determined by solving the $3N\times 3N$ linear system of equations.

Kim & Mifflin (1985) first solve the resistance problem, where the information on the right-hand side of the collocation equation (the rigid-body motion and ambient field) is completely specified and the coefficients (the resistance functions) are determined. The mobility functions are then obtained by inversion of the linear relations between the resistance and mobility functions. However, the collocation equation may be modified to yield the mobility functions directly. Giving values for the forces and torques is equivalent to prescribing values for a_{m1} and c_{m1}. The resulting translational and rotational motions are the new unknowns. This is accomplished in the collocation equations by switching the column vectors that multiply a_{m1} and c_{m1} with the right-hand-side vectors that multiply the translational and rotational velocities. For the problem in §2, there are no external forces or torques, so the right-hand side of the modified collocation equation contains only the column for the ambient rate-of-strain field. It should be noted that whereas the original system of equations becomes singular and/or ill-conditioned at touching, the modified system contains (removable) poles and is well-conditioned.

The computations presented here were obtained with equidistant collocation with points at $\theta_1 = (k/(N-1))\pi$ for $k = 0, 1, 2, \ldots, N-1$. (See figure 1.)

4. Results and discussions

According to the near-field asymptotic analyses, the mobility functions have two different types of near-field asymptotic behaviour, i.e. $O(\xi)$ and $O(1/\ln \xi^{-1})$. The mobility functions of the latter type cause a more serious convergence problem at small separations, and in testing our method, we shall pay special attention to such mobility functions. Unfortunately, the exact asymptotic expressions of this type are not available for the mobility functions defined in §2. However, similar behaviour is exhibited by the mobility function which relates the circumferential component of the translational velocity of sphere 1 to the force imposed on sphere 1. (The function is denoted by y^a_{11} in Jeffrey & Onishi 1984). Figure 3 is a plot of y^a_{11} as a function of the number of collocation points (N = 72, 124, 198, 398). The broken line is the near-field asymptotic expression of Jeffrey & Onishi (1984) and the unfilled circle is the exact value for touching spheres (the broken line approaches this value logarithmically). The following general points are illustrated by this figure.

(i) The collocation solution produces accurate values for touching spheres. In fact, such values can be obtained with even fewer collocation points (e.g. $N = 12$ for this particular problem).

(ii) At a fixed value of N, the collocation solution furnishes accurate values for ξ sufficiently large, as well as the exact value at touching. However, there is a neighbourhood near $\xi = 0$ where the collocation solution deviates from the asymptotic solution. This occurs because the collocation equations yield solutions that are analytic in ξ and since it is impossible to represent the transcendental behaviour of $O(1/\ln \xi^{-1})$ at small ξ as a finite sum in terms of the type ξ^{-n}. Consequently, on a logarithmic scale, the deviation manifests itself as premature jump to the 'plateau' at the value for touching and indeed, this premature jump may be exploited to determine the value for touching spheres.

(iii) The envelope for the family of curves obtained by increasing N is the near-field asymptotic solution.

For y^a_{11} our method reproduces the asymptotic results to within 0.1% difference down to the separation $\xi = 10^{-5}$. Our results also show that the asymptotic expression is valid for $\xi \leqslant 10^{-2}$. As one final comparison, we note that Jeffrey & Onishi (1984) have also calculated this function for small separations using the method of twin multipole expansions. Sums including terms to $O(R^{-220})$ were required to obtain reasonably accurate values for $\xi \geqslant 10^{-2}$. Here, we need 52 collocation points to achieve four-digit accuracy.

We now present the near-field results for the mobility functions of §2. In figure 4 we show plots of A, B, C, P, Q and K as functions of ξ for $0 \leqslant \xi \leqslant 0.01$. These plots are generated using 72 collocation points and the encircled points at $\xi = 0$ correspond to the computed values at $\xi = 10^{-7}$. Here again, these values are in agreement with prior works for touching spheres (to four-digit accuracy). The graphs show that the

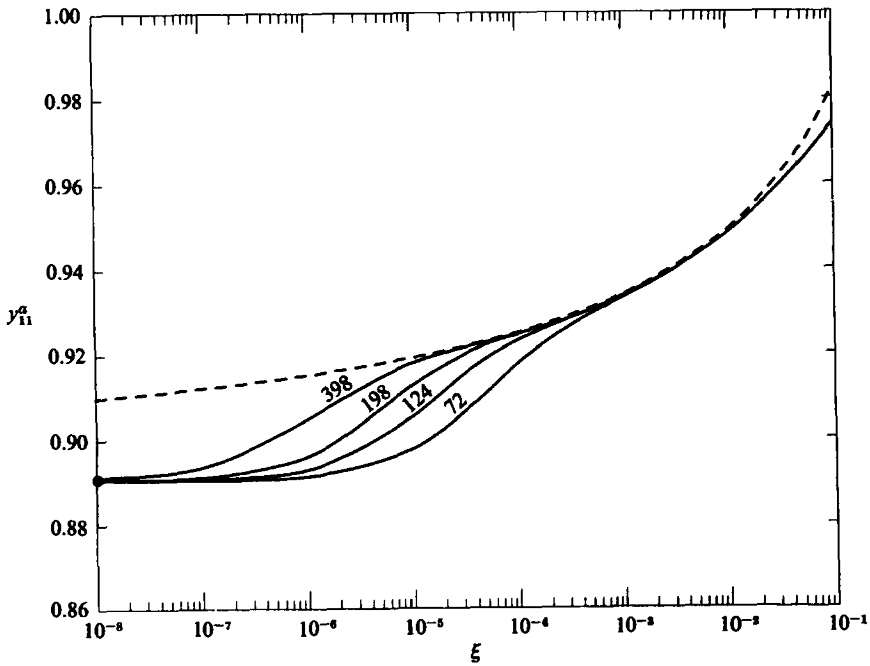

FIGURE 3. Graphs of the mobility function y^a_{11}. The numbers of collocation points are 72, 124, 198 and 398. The broken line is the near-field asymptotic expression in Jeffrey & Onishi (1984). The encircled point at $\xi = 10^{-8}$ corresponds to the exact value for touching spheres.

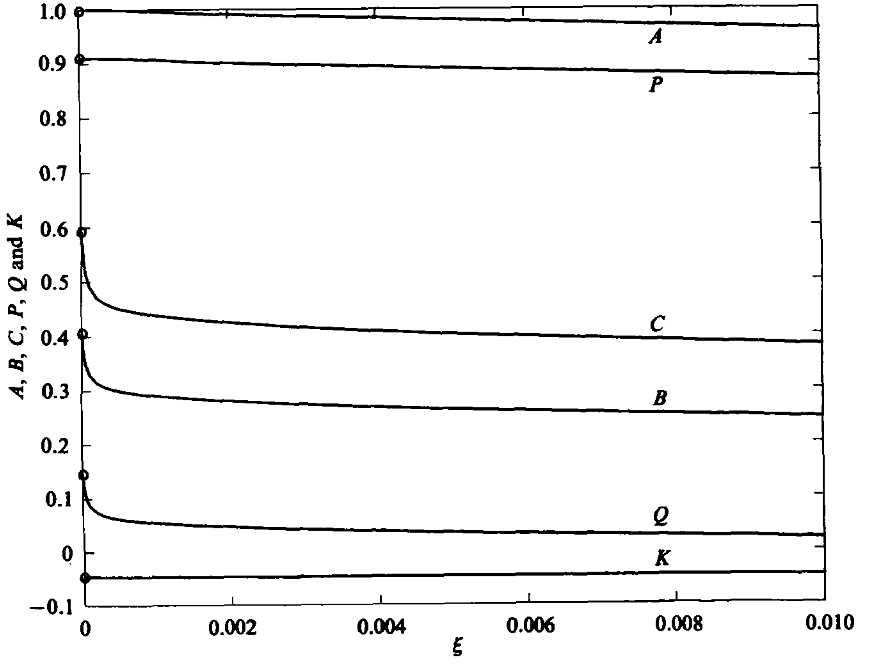

FIGURE 4. Graphs of the mobility functions A, B, C, P, Q and K of two neutrally buoyant equal sized spheres. The number of collocation points is 72 and the encircled points at $\xi = 0$ correspond to the computed values at $\xi = 10^{-7}$.

functions A, P and K have finite slope at $\xi = 0$, whereas the functions B, C and Q have infinite slope at $\xi = 0$. It is interesting to note that only the mobility functions in the subproblem for $m = 1$ have the singular behaviour at $\xi = 0$. Batchelor & Green (1972a) have shown the $O(\xi)$ behaviour of P (or $K+\frac{4}{3}L+\frac{2}{3}M$) function for small ξ using the lubrication analysis and presumed similar behaviour for K, L and M functions. This error is due to the lack of accurate information on K, L and M functions at small separations. In fact, the singular behaviour of L and M functions cancel each other exactly at small separations. The leading-order terms in L and M are $O(1/\ln \xi^{-1})$ and the coefficient for M is (-2) times that for L. To elucidate $O(1/\ln \xi^{-1})$ behaviour at small separations we plot B, C, Q and J as functions of $1/\ln \xi^{-1}$for $10^{-9} \leqslant \xi \leqslant 10^{-1}$ in figure 5. We increase the number of collocation points up to 398 where the convergence is obtained for $\xi \geqslant 10^{-5}$.

We have determined the near-field asymptotic expressions following the functional forms suggested by the lubrication analysis for future applications. Similar expressions valid for different ranges of ξ-values are available in Batchelor & Green (1972a), Arp & Mason (1977) and Chen & Acrivos (1978). The following expressions for A, P and K are obtained using the least-squares-curve fit with points at $\xi = 0$ and $10^{-3} \leqslant \xi \leqslant 10^{-2}$, and B, C, Q and J with the points at $\xi = 0$ and $10^{-5} \leqslant \xi \leqslant 10^{-2}$:

$$A = 1.000 - 4.148\xi + 3.290\xi^{\frac{3}{2}}, \tag{4.1a}$$

$$P = 0.9105 - 4.335\xi + 3.714\xi^{\frac{3}{2}}, \tag{4.1b}$$

$$K = -0.04722 + 0.08117\xi + 0.1273\xi^{\frac{3}{2}}, \tag{4.1c}$$

$$B = 0.4060 - \frac{0.9121}{\ln \xi^{-1}} + \frac{0.7804}{(\ln \xi^{-1})^2}, \tag{4.1d}$$

$$C = 0.5940 - \frac{1.238}{\ln \xi^{-1}} + \frac{1.135}{(\ln \xi^{-1})^2}, \tag{4.1e}$$

$$Q = 0.1454 - \frac{0.7250}{\ln \xi^{-1}} + \frac{0.6956}{(\ln \xi^{-1})^2}, \tag{4.1f}$$

$$J = 0.2214 - \frac{0.2630}{\ln \xi^{-1}} + \frac{0.02828}{(\ln \xi^{-1})^2}. \tag{4.1g}$$

It should be noted that slightly different values of the coefficient may be obtained if we use a different set of points. We observe that by excluding the points from $\xi = 10^{-2}$ to $\xi = 0$ in the least-squares-curve fit, the coefficient of ξ in A approaches the value in Batchelor & Green (1972a). Also, A and P functions behave similarly at small separations so that the coefficients of ξ in both expressions are the same at small separations.

As one application we have determined a more accurate estimate of the coefficient of the $O(c^2)$ term in the expression for the bulk stress (Batchelor & Green 1972b). At the time of their work, information on J was limited to the far-field region and the value at touching. For the near-field region they drew a smooth curve with an assumption of $O(\xi)$ behaviour. The triangles in figure 5 correspond to the values of J used in their bulk-stress calculation. They divided the range of integration into three parts, $0 \leqslant \xi \leqslant 0.0025$, $0.0025 \leqslant \xi \leqslant 1$ and $\xi \geqslant 1$. As shown in figure 5, the

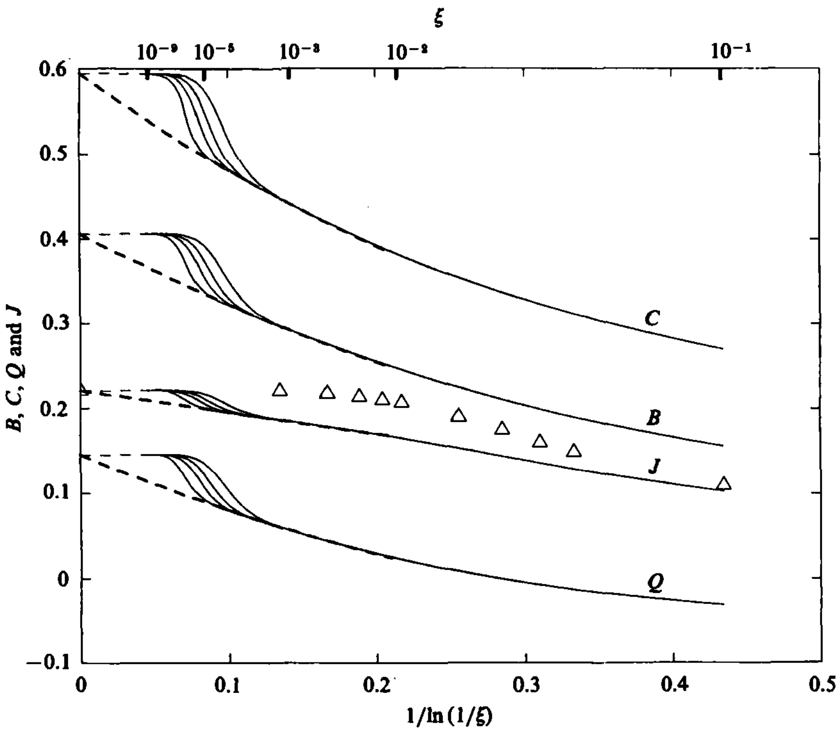

FIGURE 5. Graphs of the mobility functions B, C, Q and J. The numbers of collocation points are 72, 124, 198 and 398. The broken lines are near-field asymptotic forms by the least-squares-curve fit with polynomials in $1/\ln \xi^{-1}$. The triangles correspond to the values of the J function used in Batchelor & Green (1972*b*) for their bulk-stress calculation.

interpolation of J function in the regions $0 \leqslant \xi \leqslant 0.0025$ and $0.0025 \leqslant \xi \leqslant 1$ was the source of uncertainty in their final numerical result. We have also checked the values of the probability-density-distribution function and found that their near-field asymptotic expression was sufficiently accurate for the bulk-stress calculation. For the part of the range $0 \leqslant \xi \leqslant 0.0025$ we obtain 0.113 instead of their 0.132, and for $0.0025 \leqslant \xi \leqslant 1$ we obtain 0.387 instead of 0.449 (0.384 in Kim & Mifflin 1985). Thus the coefficient of the $O(c^2)$ term is 6.95 instead of 7.6.

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