Generating, from scratch, the near-field asymptotic forms of scalar resistance functions for two unequal rigid spheres in low Reynolds number flow

Adam K. Townsend

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Adam K. Townsend\textsuperscript{a,b)}

AFFILIATIONS
Department of Mathematical Sciences, Durham University, Stockton Road, Durham DH1 3LE, United Kingdom
\textsuperscript{a)Author to whom correspondence should be addressed: adam.k.townsend@durham.ac.uk}
\textsuperscript{b)Work started while at Department of Mathematics, University College London, Gower Street, London WC1E 6BT, United Kingdom}

ABSTRACT
The motion of rigid spherical particles suspended in a low Reynolds number fluid can be related to the forces, torques, and stresslets acting upon them by 22 scalar resistance functions, commonly notated \(X_{11}^A, X_{12}^A, Y_{11}^A, Y_{12}^A, Y_{11}^B, Y_{12}^B, Y_{11}^C, Y_{12}^C\), etc. Near-field asymptotic forms of these resistance functions were derived in Jeffrey and Onishi \cite{Jeffrey1} and Jeffrey \cite{Jeffrey2}; these forms are now used in several numerical methods for suspension mechanics. However, the first of these important papers contains a number of small errors, which make it difficult for the reader to correctly evaluate the functions for parameters not explicitly tabulated. This short article comprehensively corrects these errors and adds formulas that were originally omitted from both papers, so that the reader can verify and implement the equations independently. The corrected expressions, rationalized and using contemporary nondimensionalization, are shown to match mid-field values of these scalars, which are calculated through an alternative method. A Python script to generate and evaluate these functions is provided.

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I. INTRODUCTION
The linearity of Stokes flow allows the forces, torques, and stresslets acting on particles suspended in a low Reynolds number fluid to be related to the particles’ velocities, angular velocities, and fluid background strain rate through a resistance or mobility matrix. For rigid spherical particles, the elements of the resistance matrix can be formed from scalar resistance functions, commonly notated as
\[X_{11}^A, X_{12}^A, Y_{11}^A, Y_{12}^A, Y_{11}^B, Y_{12}^B, X_{11}^C, X_{12}^C, Y_{11}^C, Y_{12}^C, Y_{11}^D, Y_{12}^D, Y_{11}^E, Y_{12}^E, Z_{11}^A, Z_{12}^A, Z_{11}^B, Z_{12}^B, Z_{11}^C, Z_{12}^C, Z_{11}^D, Z_{12}^D, Z_{11}^E, Z_{12}^E.\] (1)

The near-field asymptotic forms of the scalar resistance functions for two unequal rigid spheres were initially published in Jeffrey and Onishi\textsuperscript{1} and Jeffrey\textsuperscript{2}. The terms in the asymptotic forms themselves rely on recurrence relations, and, in the first of these two papers, there are a number of small errors. Furthermore, the reader may find it difficult to generate the required expressions (and therefore the value of these functions) in both papers independently, given the omission of intermediate formulas.

Some of these errors appear to have been noticed by authors, including indirectly by Kim and Karrila\textsuperscript{3} in corrected tabulations, and a partial list of errata has been published online by Ichiki\textsuperscript{4}. However, a comprehensive, fully corrected description of how to generate expressions for these functions, to enable verifiable calculation for arbitrary size ratios and separation distances, is yet to be published.

This short article is a compilation of the relevant equations, with those originally omitted now added, and with any errors fixed. Equations from Jeffrey and Onishi\textsuperscript{1} are labeled as (JO 1.1); similarly, equations from Jeffrey\textsuperscript{2} are labeled as (J 1), and those from the helpful Ichiki et al.\textsuperscript{5} are labeled as (I 1). Pages from Kim and Karrila\textsuperscript{3} are labeled as (K&K, p. 1).

At the end of the article, the questions of error identification and validation of the corrected forms are addressed.
Throughout this article, we use the same notation as the original papers. For two spheres of radius $a_1, a_2$ with centers a distance $s$ apart, we define the non-dimensional gap $\zeta$ and size ratio $\lambda$ as

$$\zeta = \frac{2s}{a_1 + a_2} - 2, \quad \lambda = \frac{a_2}{a_1}. \tag{2}$$

The near-field forms are valid for $\zeta \ll 1$ and $\zeta \ll \lambda$.

The nondimensionalization in (JO 1.7) and (1.3) scales the resistance functions by factors of $(a_1 + a_2)/2$. As noted in Jeffrey, although this choice provides symmetry elsewhere, it leads to unwieldy factors of $(1 + \lambda)^{-3}$ in some of the expressions we are interested in. Here, we instead follow the convention of Kim and Karilla, Sec. 11.3, and scale all functions by factors of $a_i$. Specifically, to recover the dimensional forms, it is necessary to multiply the scalars in Eq. (1), derived as follows, by an appropriate factor:

A Python script implementing the corrected formulas is available on GitHub.\(^6\)

II. $X^4$ TERMS

Here, the $X^4$ formulas are given in full, with changes from the source material when noted. The same directions for alteration, when required, will be given for the other terms in later sections.

We first set up the recurrence relations from (JO 3.6–3.9),

$$P_{a00} = \delta_{1n}, \tag{5}$$

$$V_{a00} = \delta_{1n}. \tag{6}$$

$$V_{nq0} = P_{nq0} - \frac{2n}{(n + 1)(2n + 3)} \sum_{j=1}^{n} \binom{n + s}{n} P_{(q-j)(p-n-1)}, \tag{7}$$

$$P_{nq0} = \frac{n}{(n + 1)(n + 2(n + 1) + 2(n - n - s + 2)} \sum_{j=1}^{n} \binom{n + s}{n} P_{(q-j)(p-n+1)} - \frac{n}{2(n + 1)} P_{(q-j)(p-n-1)} - \frac{n}{2(n+1)} V_{(q-s)(p-n+1)}. \tag{8}$$

Then, we define the formulas from (JO 3.15 and 3.19),

$$f_k(\lambda) = 2^k \sum_{q=0}^{k} P_{(k-q)q2^k}, \tag{9}$$

$$g_1(\lambda) = 2\lambda^2(1 + \lambda)^{-3}, \tag{10}$$

$$g_2(\lambda) = \frac{1}{5} \lambda(1 + 7\lambda + \lambda^2)(1 + \lambda)^{-3}, \tag{11}$$

$$g_3(\lambda) = \frac{1}{42} (1 + 18\lambda - 29\lambda^2 + 18\lambda^3 + \lambda^4)(1 + \lambda)^{-3}, \tag{12}$$

$$m_1(m) = -2\delta_{m2} + (m - 2)(1 - \delta_{m2}). \tag{13}$$

We then define two intermediate functions, the first of which is given in (JO 3.22) as

$$A_{11}^X = 1 - \frac{1}{4}\zeta + \sum_{m = 2, \text{ even}}^{\infty} 2^{-m}(1 + \lambda)^{-m}f_m - \gamma_1 - 2m^{-1}g_2 + 4m^{-1}m_1^{-1}g_3. \tag{14}$$

The function $m_1$ is somewhat awkward as, despite being a toggle for whether $m = 2$, it is used in Jeffrey and Onishi\(^7\) for summation over both even and odd values of $m$. The later paper, Jeffrey,\(^7\) removes it by using instead a form of the summation that here would render the equivalent expression,

$$A_{11}^X = 1 - \frac{1}{4}\zeta + \sum_{m = 2, \text{ even}}^{\infty} 2^{-m}(1 + \lambda)^{-m}f_m - \gamma_1 - 2m^{-1}g_2 + 4m^{-1}(m + 2)^{-1}g_3. \tag{14a}$$

It is computationally convenient to have the same coefficients of $f_m, g_1, g_2, \text{ and } g_3$ (where they exist) in the summations for all functions of this type, so we choose to use this form when describing corrections going forward. Consistent coefficients also allow us to notice that all $f_m$ functions are defined with a factor of $2^m$, which cancels the $2^{-m}$ in the $f_m$ coefficient in the sum: these powers of 2 can therefore be left out of numerical implementations. In practice, we also find that moving the factor $(1 + \lambda)^{-m}$ inside the sum in the definition of $f_m$ can prevent the terms in the sum (specifically from $X^3$) from exceeding the maximum float size when $x$ and $m$ (and hence $q$) are large. However, we do neither of these things in this paper to remain consistent with the original texts.

The second intermediate function is from (JO 3.23), and indeed needs correcting to be

$$-\frac{1}{2} (1 + \lambda)A_{12}^X = \frac{1}{4}\zeta + 2\zeta \log 2 - 2\gamma_3 + \sum_{m = 1, \text{ odd}}^{\infty} 2^{-m}(1 + \lambda)^{-m}f_m - \gamma_1 - 2m^{-1}g_2 + 4m^{-1}(m + 2)^{-1}g_3, \tag{15}$$

noting the change from $m_1$ (which is identically $m = 2$ given that $m$ is odd) to $m + 2$.

Then the resistance scalars are given by

$$X_{11}^4 = g_1\zeta^{-1} + g_2 \log (\zeta^{-1}) + A_{11}^X + g_3\zeta \log (\zeta^{-1}), \tag{16}$$

$$X_{12}^4 = g_1\zeta^{-1} + g_2 \log (\zeta^{-1}) - \frac{1}{2} (1 + \lambda)A_{12}^X + g_3\zeta \log (\zeta^{-1}). \tag{17}$$

from (JO 3.17 and 3.18) up to $O(\zeta \log (\zeta^{-1}))$: note the different scaling on $X_{11}^4$ as we use the aforementioned convention from (K&K, p. 279).

III. $V^4$ TERMS

The recurrence relations are (JO 4.6–4.11), but with $V_{nq0}$ corrected to
\[ V_{n pq} = P_{n pq} + \frac{2n}{(n+1)(2n+3)} \sum_{i=1}^{q} \left( \frac{n+s}{n+1} \right) P_{i(q-1)(p-1)}, \quad (18) \]

noticing the sign change on the 1 in the last subscript.

The required intermediate formulas for the \( f, g, \) and \( m \) functions are Eq. (9), (JO 4.16–4.17), and Eq. (13), respectively.

Then the \( A' \) terms are given by (JO 4.17–4.18); if desired, these can be more conveniently written to remove \( m_{j} \) and the Jeffrey form by writing

\[ A'_{1z} = 1 - g_{5} + \sum_{m = -2}^{\infty} \left[ 2^{-m} (1 + \lambda)^{-m} f_{m} - 2m^{-1} g_{2} + 4m^{-1} (m + 2)^{-1} g_{5} \right], \quad (18a) \]

\[ -\frac{1}{2} (1 + \lambda) A'_{1z} = 2g_{2} \log 2 - 2g_{5} + \sum_{m = -1}^{\infty} \left[ 2^{-m} (1 + \lambda)^{-m} f_{m} - 2m^{-1} g_{2} + 4m^{-1} (m + 2)^{-1} g_{5} \right], \quad (18b) \]

but this does not constitute a correction.

Either way, we are left with the resistance scalar formulas

\[ Y'_{1z} = g_{5} \log (\xi^{-1}) + A'_{1z} + g_{3} \xi \log (\xi^{-1}), \quad (19) \]

\[ -Y'_{1z} = g_{5} \log (\xi^{-1}) - \frac{1}{2} (1 + \lambda) A'_{1z} + g_{3} \xi \log (\xi^{-1}) \]

from (JO 4.15–4.16), with a different scaling on \( Y'_{1z} \).

IV. \( Y' \) TERMS

The recurrence relations are the same as those for the \( Y^a \) terms except that the initial conditions are replaced by (JO 7.3–7.5).

The intermediate formula for the \( f \) function is

\[ f_{k}(\lambda) = 2^{k+1} \sum_{q=0}^{k} Q_{k(q-2)} \xi^{q}, \quad (21) \]

with the \( g \) formula given by (JO between 7.10 and 7.11), with the correction to \( g_{5} \) of

\[ g_{5}(\lambda) = 2 \frac{125}{2} \lambda (43 - 24 \lambda + 43 \lambda^{2}) (1 + \lambda)^{-4}. \quad (30) \]

Then the \( C' \) terms from (JO 7.11–7.12), correcting the latter [note the power of \((1 + \lambda)^{-1}\)] and writing both to avoid \( m_{j} \), are

\[ C'_{12} = 1 - g_{5} + \sum_{m = 2}^{\infty} \left[ 2^{-m} (1 + \lambda)^{-m} f_{m} - 2m^{-1} g_{2} + 4m^{-1} (m + 2)^{-1} g_{5} \right], \quad (31) \]

\[ C'_{12} = 2g_{4} \log 2 - 2g_{5} + \sum_{m = 1}^{\infty} \left[ 2^{1-m} (1 + \lambda)^{3-m} f_{m} - 2m^{-1} g_{2} + 4m^{-1} (m + 2)^{-1} g_{5} \right], \quad (32) \]

The resistance scalars are finally

\[ Y'_{11} = g_{5} \log (\xi^{-1}) + C_{11} + g_{3} \xi \log (\xi^{-1}), \quad (33) \]

\[ \frac{8}{(1 + \lambda)^{2}} Y'_{12} = g_{5} \log (\xi^{-1}) + C_{12} + g_{3} \xi \log (\xi^{-1}), \quad (34) \]

again with a different scaling on \( Y'_{11} \) compared to (JO 7.9–7.10).

To write Eq. (32) in the Jeffrey's summation form, introduce \( \tilde{g}_{4} \) and \( \tilde{g}_{5} \) such that \( \tilde{g}_{4} = (1 + \lambda) g_{4}/8 \) (similarly for \( \tilde{g}_{5} \)). This changes Eq. (34) to become consistent with the other scalar definitions,

\[ Y'_{12} = \tilde{g}_{4} \log (\xi^{-1}) + \frac{8}{(1 + \lambda)^{2}} C'_{12} + \tilde{g}_{5} \xi \log (\xi^{-1}), \quad (34a) \]

which is the choice made in (K&K, p. 283). Note that the aforementioned error in \( \tilde{g}_{4} \) persists here; the "250" in the denominator of the \( \xi \log (\xi^{-1}) \) term in \( Y'_{12} \) (what we are calling \( \tilde{g}_{5} \)) should read "500."
VII. XG TERMS

The recurrence relations are the same as those for XA, and the f and g functions are given by (I 94) and (J between 19b and 20a). The Gx terms are given by (J 27), with a different scaling on the XG. This gives us expressions for X1G.

\[ X_{11}^G = g_1 \xi_{-1} + g_2 \log (\xi_{-1}) + G_{11}^X + g_3 \xi \log (\xi_{-1}), \]
(35)

\[ X_{12}^G = -g_1 \xi_{-1} - g_2 \log (\xi_{-1}) + \frac{1}{4} (1 + \lambda^2) G_{12}^Y - g_3 \xi \log (\xi_{-1}), \]
(36)

from (I 19), with a different scaling on the X12G.

VIII. YG TERMS

The recurrence relations are the same as those for YA, and the f and g functions are given by (I 115) and (J between 27b and 28a). The GY terms are given by (J 29), giving us expressions for YG.

\[ Y_{11}^G = g_1 \log (\xi_{-1}) + G_{11}^X + g_3 \xi \log (\xi_{-1}), \]
(37)

\[ Y_{12}^G = -g_2 \log (\xi_{-1}) + \frac{1}{4} (1 + \lambda^2) G_{12}^Y - g_3 \xi \log (\xi_{-1}) \]
(38)

from (J 27), with a different scaling on the Y12G.

IX. YH TERMS

The recurrence relations are the same as those for YH, and the f and g functions are given by (I 120) and (J between 35b and 36a). The HY terms are given by (J 37), giving us expressions for YH of

\[ Y_{11}^H = g_2 \log (\xi_{-1}) + H_{11}^X + g_3 \xi \log (\xi_{-1}), \]
(39)

\[ Y_{12}^H = g_3 \log (\xi_{-1}) + \frac{1}{8} (1 + \lambda^2) H_{12}^X + g_5 \xi \log (\xi_{-1}) \]
(40)

from (J 35), with a different scaling on the Y12H.

X. XM TERMS

The recurrence relations are the same as those for XA, but with different initial conditions (J 44). The f and g functions are given by (I 105) and (J between 48b and 49a). The XM terms are given by (J 50), giving us expressions for XM of

\[ X_{11}^M = g_1 \xi_{-1} + g_2 \log (\xi_{-1}) + M_{11}^X + g_3 \xi \log (\xi_{-1}), \]
(41)

\[ X_{12}^M = g_2 \xi_{-1} + g_3 \log (\xi_{-1}) + \frac{1}{8} (1 + \lambda^2) M_{12}^X + g_5 \xi \log (\xi_{-1}) \]
(42)

from (J 48), with a different scaling on the X12M.

XI. YM TERMS

The recurrence relations are the same as those for YA, but with different initial conditions (J 58). The f and g functions are given by (I 125) and (J between 64b and 65a). The YM terms are given by (J 66), giving us expressions for YM of

\[ Y_{11}^M = g_2 \log (\xi_{-1}) + M_{11}^X + g_3 \xi \log (\xi_{-1}), \]
(43)
FIG. 2. Values of the scalar resistance functions over non-dimensional gap, $\zeta$, for size ratio $\lambda = 0.1$. Those generated from the near-field formulas are represented by blue hollow circles, and those generated from Lamb's solution are blue filled circles. The dashed vertical line appears at $\zeta = \lambda$, recalling that the near-field formulas are only valid for $\zeta \ll \lambda$.

FIG. 3. Values of the scalar resistance functions over non-dimensional gap, $\zeta$, for size ratio $\lambda = 0.01$. Those generated from the near-field formulas are represented by blue hollow circles, and those generated from Lamb's solution are blue filled circles. The dashed vertical line appears at $\zeta = \lambda$, recalling that the near-field formulas are only valid for $\zeta \ll \lambda$. Discrepancies at the meeting point of the near-field and mid-field values are consistent with the near-field series expansion ignoring terms of $\mathcal{O}(\zeta)$. 
\begin{equation}
Y_{12}^M = g_M \log (\xi^{-1}) + \frac{1}{8} (1 + \lambda)^3 M_{12}^M + g_0 \xi \log (\xi^{-1}) \tag{44}
\end{equation}

from (J 64), with a different scaling on the $Y_{12}^M$.

XII. ZM TERMS

The recurrence relations are (J 73–76). The $f$ and $g$ functions are given by (I 131) and (J between 79b and 80a). The $M^M$ terms are given by (J 81), giving us expressions for $Z^M$ of

\begin{equation}
Z_{11}^M = M_{11}^M + g_M \xi \log (\xi^{-1}), \tag{45}
\end{equation}
\begin{equation}
Z_{12}^M = \frac{1}{8} (1 + \lambda)^3 M_{12}^M - g_0 \xi \log (\xi^{-1}) \tag{46}
\end{equation}

from (J 79), with a different scaling on the $Z_{12}^M$.

XIII. ERROR IDENTIFICATION

The original articles provide tabulated values of the intermediate scalars $A_{11}^N$, etc. The easiest way for the reader to confirm mistakes in the formulas is to confirm that the values computed from these formulas do not match those tabulated. Consider the following example:

<table>
<thead>
<tr>
<th>Value from (JO)</th>
<th>Value in (JO)</th>
<th>Correct value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{12}^N (\lambda = 1)$</td>
<td>$-0.24300$</td>
<td>$-0.35022$, $-0.2390$</td>
</tr>
<tr>
<td>$B_{11}^N (\lambda = 1)$</td>
<td>$-0.8355$</td>
<td>$-0.2390$</td>
</tr>
</tbody>
</table>

Happily, the errors in the formulas for the intermediate scalars appear not to extend greatly to the tabulation of their values for a small range of size ratios in Kim and Karrila,1 Sec. 11.3, where we find agreement with values calculated from the expressions in this article to at least the second significant figure (and often more).

Nonetheless, errors in the formulas can also be spotted by either deriving the equations independently or observing that the values derived do not match those in the mid-field; both methods are described as follows.

XIV. VALIDATION OF CORRECTED EXPRESSIONS

The reader is invited to derive and confirm the above formulas themselves, should they wish. The method is perhaps best explained in Jeffrey, Sec. II (starting at the paragraph containing the definition of $\xi$) and Secs. III B and III C, where $X^N$ is used as an example.

We can also confirm that the formulas produce values of the resistance scalars, which match those in the mid-field. Figures 1–3 demonstrate the near-field values matching to the mid-field values, which have been computed independently for $\lambda \approx 0.014$ using the two-sphere method of Wilson,1 based on the solution to Stokes flow given by Lamb.1 In computing the near-field values, infinite sums in the expressions [e.g., in Eq. (14)] are truncated after 100 nonzero terms; the addition of further terms does not change the appearance of the graphs. Recall that the near-field series expansions are valid only for $\xi \ll \lambda$ and ignore terms of $O(\xi)$.

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AUTHOR DECLARATIONS

Conflict of Interest

The author has no conflicts to disclose.

Author Contributions

Adam K. Townsend: Writing – original draft (equal).

DATA AVAILABILITY

The data that support the findings of this study are openly available in GitHub at https://github.com/Pecnut/stokesian-dynamics, Ref. 6.

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