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Accurate and approximate methods to calculate capacitance and potential coefficients of two-particle system

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Abstract. Accurate and approximate methods to calculate the capacitance and potential coefficients of a system consisting of two macro-particles are considered. A technique of their calculation with sufficient accuracy for physical and technological applications is proposed. Based on them interaction potential and force as functions inter-particle distance are obtained.

1. Introduction
Interaction potential plays a valuable role in microparticle coagulation and agglomeration processes. When the capacitance coefficients of a particle system are determined one can calculate the potential in vacuum or uniform dielectric. From this perspective the purpose of the article is a search for a simple method to obtain these quantities for further calculation of the interaction potential and force.

2. Methods of calculating the capacitance coefficients
Let us consider two conducting spheres of radii that in general must not be neglected in the calculation. These macro-particles are situated in vacuum or uniform dielectric in the absence of an external electric field. In case if electric potentials are independent of the angular coordinates, which is also satisfied by spheres situated in plasma or electrolyte, we can define potential and capacitance coefficients \[1\]

\[\phi_{1s} = S_{11}q_1 + S_{12}q_2,\quad \phi_{2s} = S_{12}q_1 + S_{22}q_2,\]

\[q_1 = C_{11}\phi_{1s} + C_{12}\phi_{2s},\quad q_2 = C_{12}\phi_{1s} + C_{22}\phi_{2s}.\]

According to \[2\] (see also \[3\]) the total electrostatic potential generated by the system of two conducting spheres of radii \(a_1\) and \(a_2\) is given by

\[\phi(r_1, \mu_1) = \sum_{n=0}^{\infty} \left\{ A_n \frac{a_1^n}{r_1^{n+1}} + \sum_{k=0}^{\infty} B_k \frac{(n+k)!}{n!k!} \frac{r_1^n a_2^k}{R^{n+k+1}} \right\} P_n(\mu_1)\]
where \( r_1 \) and \( \mu_1 = \cos \theta_1 \) are respectively the radius and the polar angle cosine in the spherical coordinates relative to the first particle center with \( z \)-axis directed to the second particle center, \( R \) is the distance between them, \( P_n(\mu_1) \) are the Legendre polynomials. Turning to the coordinate system with the pole in center of the second particle, we obtain a similar expression. Each of them must fulfill its own pair of boundary equations

\[
\phi|_{r_1=a_1} = \phi_{1s}, \quad -\frac{a_1^2}{2} \int_0^\pi \frac{\partial \phi}{\partial r} |_{r_1=a_1} \sin \theta_1 d\theta_1 = q_1, \\
\phi|_{r_2=a_2} = \phi_{2s}, \quad -\frac{a_2^2}{2} \int_0^\pi \frac{\partial \phi}{\partial r} |_{r_2=a_2} \sin \theta_2 d\theta_2 = q_2,
\]

resulting in the following equations for the coefficients \( A_n \) and \( B_n \) \((n \neq 0) \) [2]

\[
A_n + \left( \frac{a_1}{R} \right)^{n+1} \sum_{k=1}^\infty B_k \frac{(n+k)!}{n!} \left( \frac{a_2}{R} \right)^k + q_1 \left( \frac{a_1}{R} \right)^{n+1} = 0, \\
B_n + \left( \frac{a_2}{R} \right)^{n+1} \sum_{k=1}^\infty A_k \frac{(n+k)!}{n!k!} \left( \frac{a_1}{R} \right)^k + q_2 \left( \frac{a_2}{R} \right)^{n+1} = 0.
\]

(3)

Considering the zeroth harmonic one finds [2]

\[
\phi_{1s} = \frac{q_1}{a_1} + \frac{q_2}{a_1 R} + \frac{1}{R} \sum_{k=1}^\infty B_k \left( \frac{a_2}{R} \right)^k, \\
\phi_{2s} = \frac{q_2}{a_2} + \frac{q_1}{a_2 R} + \frac{1}{R} \sum_{k=1}^\infty A_k \left( \frac{a_1}{R} \right)^k.
\]

(4)

One can see from expressions (1), (3), (4) how to obtain the potential coefficients \( S_{11}, S_{12} \) and \( S_{22} \). We should first solve system (3) providing \( q_2 = 0 \) to find \( A_n, B_n \) and then calculate the surface potentials \( \phi_{1s}, \phi_{2s} \) from (4) that yield \( S_{11} \) and \( S_{12} \) according to (1). Then, taking \( q_1 \) equal to zero, we obtain \( S_{22} \) in a similar way. This procedure can be abbreviated as

\[
S_{11} = \left. \frac{\phi_{1s}}{q_1} \right|_{q_2=0}, \quad S_{12} = \left. \frac{\phi_{2s}}{q_1} \right|_{q_2=0}, \quad S_{22} = \left. \frac{\phi_{2s}}{q_2} \right|_{q_1=0}.
\]

(5)

The potential coefficients can also be found analytically. We can see from (3) that the expansion coefficient \( A_k \) is expressed in terms of \( q_1 \) and \( q_2 \) as \( A_k = M_k q_1 + N_k q_2 \) and we can get \( M_k \) and \( N_k \) that are only determined of ratios \( a_1/R \) and \( a_2/R \). Then one finds from (5)

\[
S_{12} = \frac{1}{R} + \frac{1}{R} \sum_{k=1}^\infty M_k \left( \frac{a_1}{R} \right)^k, \quad S_{22} = \frac{1}{a_2} + \frac{1}{R} \sum_{k=1}^\infty N_k \left( \frac{a_1}{R} \right)^k.
\]

(6)

On the basis of symmetry, we can obtain \( S_{11} \) from \( S_{22} \) by permutation of \( a_1 \) and \( a_2 \).

Previously [2] system (3) was solved with regard for all the terms up to and including \( R^{-21} \). In this case, in (6) we should ignore all the terms higher than eighth term. After canceling the
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use for terms and letting again to infinity we have a range of geometrical series that converges to

\[ S_{a,11} = \frac{1}{a_1} - \frac{a_1^2}{R^3} \left\{ \frac{R^2}{R^2 - a_1^2} \right\}, \]

\[ S_{a,12} = \frac{1}{R} + \frac{a_1 a_2}{R^3} \left\{ 1 - \frac{R^2}{R^2 - a_1^2} \right\}, \]

\[ S_{a,22} = \frac{1}{a_2} - \frac{a_2^2}{R^3} \left\{ \frac{R^2}{R^2 - a_2^2} \right\}. \]

(7)

Transition from the potential coefficients to the capacitance coefficients is given by [1]

\[ C_{11} = \frac{S_{22}}{\Delta}, \quad C_{12} = -\frac{S_{12}}{\Delta}, \quad C_{22} = \frac{S_{11}}{\Delta} \]

(8)

where \( \Delta = S_{11} S_{22} - S_{12}^2 \) is a determinant of system (1). In the present paper to obtain the capacitance coefficients \( C_{11}, C_{12} \) and \( C_{22} \) we have numerically solved system (3) putting \( n_{\text{max}} = 500 \). However, when the macroparticles are far apart so that \( R \gg \max(a_1, a_2) \) one can use approximate analytical expressions including monopole and dipole terms. Neglecting there \( a_1 \) and \( a_2 \) with respect to \( R \) there we have well-known asymptotics \( C_{11} \rightarrow a_1, C_{12} \rightarrow -a_1 a_2 / R, C_{22} \rightarrow a_2 \).

When the spheres are close together the accuracy of computation in the spherical coordinates decreases significantly. In this limiting case we can use asymptotic formulae [4, 5]

\[ C_{11} = \frac{a_1 a_2}{a_1 + a_2} \left[ \frac{1}{2} \ln \left( \frac{a_2}{a_1 + a_2} \frac{1}{L} \right) - \psi \left( \frac{a_2}{a_1 + a_2} \right) + O \left( L^2 \right) \right], \]

\[ C_{12} = -\frac{a_1 a_2}{a_1 + a_2} \left[ \frac{1}{2} \ln \left( \frac{a_2}{a_1 + a_2} \frac{1}{L} \right) + \gamma + O \left( L^2 \right) \right], \]

\[ C_{22} = \frac{a_1 a_2}{a_1 + a_2} \left[ \frac{1}{2} \ln \left( \frac{a_2}{a_1 + a_2} \frac{1}{L} \right) - \psi \left( \frac{a_1}{a_1 + a_2} \right) + O \left( L^2 \right) \right], \]

where \( L = R - a_1 - a_2 \) is the separation distance, \( \psi(z) \) is the logarithmic derivative of the gamma function [6], \( \gamma = \psi(1) = 0.5772\ldots \) is the Euler’s constant.

Results obtained by the described methods were compared with data obtained using the bispherical coordinate system [7, 8], as illustrated in Figure 1. One can see from the figure that the use of the bispherical coordinates provides the most accurate picture of the capacitance coefficients behaviour for all \( L \). This is also given by asymptotical results for near approach of the macroparticles, but when \( L > 0.1 \, \mu m \) a discrepancy is noticeable. Numerical solving of (3) deals with \( n_{\text{max}} \times n_{\text{max}} \) matrix and slowly convergent series that provides computational problems when \( L \) is small. However, the results obtained from there are wholly satisfactory up to \( L = 10^{-3} \, \mu m \). The approximate expressions are seen from the figure to be only possible to use for \( L \) being greater than a micrometer.
3. Interaction potential and force between two macroparticles

With potential or capacitance coefficients, one can express the interaction potential of particles in terms of their charges or electric potentials respectively. As the charges are defined the interaction potential is [9]

\[ U = \frac{1}{2} \left( S_{11}q_1^2 + 2S_{12}q_1q_2 + S_{22}q_2^2 \right). \]  (9)
Differentiation of (9) with respect to \( R \) yields the interaction force with the sign reversed. Figure 3 shows the desired force \( F_{21} \) taken relative to the Coulomb force \( F_C \) describing the interaction between point charges.

![Graph showing the reduced force between macroparticles](image)

Figure 3: The reduced force between macroparticles of equal \( a_1 = a_2 = 10 \mu m \), left) and different radii \( a_1 = 1 \mu m, a_2 = 10 \mu m \), right) versus \( L \). Symbols 1 denote numerical differentiation of (9) where the potential coefficients are obtained from the capacitance coefficients shown in Figure 2. Curves 2 and circles 3 give respectively the results obtained in the bispherical coordinates and through the use of (7) and (9). The dashed lines denote the equality \( F_{21} = F_C \). The charges are \( q_1 = 10^2 e \), \( q_2 = 10^3 e \) in both cases.

4. Conclusions
Accurate and approximate calculation methods have been considered for the capacitance and potential coefficients of two conducting macroparticles. The limits of each approach applicability have been defined. Based on the data obtained the interparticle force has been calculated. It has been shown that the use of the asymptotical formulae for small interparticle distances and the analytical expressions for large ones provides good agreement with the results obtained in the bispherical coordinate system. The proposed method is not concerned with summation of infinite series and thus seems to be advantageous on the computational side.

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