Interaction potential of two spherical macroparticles at constant surface potentials

A A Pautov\textsuperscript{1,2}, M M Rodin\textsuperscript{1,2} and A V Filippov\textsuperscript{1}

\textsuperscript{1} State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovkykh Street 12, Troitsk, Moscow 108840, Russia
\textsuperscript{2} Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

E-mail: mikhail.rodin@phystech.edu

Abstract. Electrostatic interaction between two spherical macroparticles at constant charges of the particles and constant surface potentials is studied. The interaction potential of two spherical macroparticles as a function of surface separation distance $L$ is calculated using capacitance and potential coefficients. At small separation distances, the capacitance coefficients are defined by Russell’s asymptotical formulae; at large distances, the potential coefficients are calculated by approximate formulae obtained in this paper and, at intermediate distances, the capacitance and potential coefficients are found by smoothly joining the asymptotical and approximate formulae. A comparison of the data obtained in this paper with those of the previous papers is performed. It has been established that this technique provides the rather high precision in the interaction potential calculation for all interparticle distances.

1. Introduction

Interaction potential defines the rate constants of coagulation and agglomeration processes and also determines the conditions of phase transitions in dusty plasmas and electrolytes. For numerical simulation of the coagulation of nano- and micro-size particles a large matrix of coagulation constants is required (see, for example, [1]), thus a method of quick calculation of the interaction potential dependence on the surface separation distance is to be developed. The purpose of this paper is a search for a quick method to calculate the interaction potential of spherical particles on the condition that the charges or surface potentials of particles do not change with the interparticle distance. The latter is satisfied by conducting macroparticles in any medium and also by any macroparticles situated in a uniform plasma or electrolyte where the surface potential of macroparticles is equal to the floating plasma potential.

The interaction potential can be obtained by the integration of an interaction force [2] or with the use of capacitance or potential coefficients. Methods to find these quantities include the calculation in the spherical coordinate system [3,4], in the bispherical coordinate system [2,5–7] or the use of the method of images [5,8]. In the present paper the coefficients are determined according to Russell’s asymptotical formulae [9,10] for close approach of spheres and from the approximate formulae within the accuracy of $R^{-17}$ for large interparticle distances $R$. In the intermediate region the capacitance and potential coefficients are found by smoothly joining the asymptotical and approximate formulae.
2. Interaction potential. Capacitance and potential coefficients

When the surface potentials \( \phi_{1s}, \phi_{2s} \) do not depend on the interparticle distance, the interaction energy is written as \([2, 7, 11]\)

\[
U_\varphi = \frac{1}{2} (a_1 - C_{11}) \phi_{1s}^2 - C_{12} \phi_{1s} \phi_{2s} + \frac{1}{2} (a_2 - C_{22}) \phi_{2s}^2,
\]

(1)

where \( a_1, a_2 \) are the radii of the spherical macroparticles. This expression describes the interaction potential only without including the energies of isolated particles, so it goes to zero as the interaction distance goes to infinity. By definition \([8]\),

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

(2)

When the charges \( q_1, q_2 \) are constant, the interaction potential is expressed in terms of potential coefficients

\[
U_q = \frac{1}{2} \left( S_{11} - \frac{1}{a_1} \right) q_1^2 + S_{12} q_1 q_2 + \frac{1}{2} \left( S_{22} - \frac{1}{a_2} \right) q_2^2,
\]

(3)

which are defined similarly to (2)

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

(4)

It should be noted that from (3) using (2) we get

\[
U_q = \frac{1}{2} (C_{11} - a_1) \phi_{1s}^2 + C_{12} \phi_{1s} \phi_{2s} + \frac{1}{2} (C_{22} - a_2) \phi_{2s}^2 \equiv -U_\varphi
\]

(5)

(a discussion of this point is in \([11]\)).

It is plain that matrices of capacitance and potential coefficients are inverse to each other which makes it possible to obtain \( C_{ij} \) from \( S_{ij} \) and conversely. To find these quantities we can write electrostatic potentials generated by the spheres

\[
\phi_1(r_1, \mu_1) = \sum_{k=0}^{\infty} A_k \frac{P_k(\mu_1)}{r_1^{k+1}}, \quad \phi_2(r_2, \mu_2) = \sum_{k=0}^{\infty} B_k \frac{P_k(\mu_2)}{r_2^{k+1}},
\]

where \( r_{1,2} \) and \( \mu_{1,2} = \cos \theta_{1,2} \) are spherical coordinates with the origin in the center of the first and second macroparticles, respectively. Re-expansion of the Legendre polynomials \( P_k \) \([12]\) and substitution of the total potential in the boundary conditions lead to \([3]\)

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

(6)

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

(7)

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

Analysis of the system of equations (7) shows that the expansion coefficients can be presented in the form (see \([3]\) \( A_k = M_k q_1 + N_k q_2 \) with \( M_k \) and \( N_k \) only depending on ratios \( a_1/R \) and \( a_2/R \). Then one finds from (4) and (6)

\[
S_{11} = \frac{1}{R} + \frac{1}{R} \sum_{k=1}^{\infty} M_k \left( \frac{a_1}{R} \right)^k, \quad S_{22} = \frac{1}{a_2} + \frac{1}{R} \sum_{k=1}^{\infty} N_k \left( \frac{a_1}{R} \right)^k.
\]

(8)
From (6) and (7) with an accuracy up to and including terms of $R^{-17}$, we obtain

$$
S_{a,11} = \frac{1}{a_1} - \frac{a_1^3}{R^3} \left\{ \frac{R^2}{R^2 - a_2^2} - \frac{a_1 a_2^2 (R^2 + 2 a_1^2)}{R^6} + \frac{a_1 a_2^2 R^2}{(R^2 - a_1^2)^3} \left[ 1 + \frac{2 a_1 a_2^2 (1 + 2 a_1^2/R^2)}{R^2 - a_1^2} \right] \right\},
$$

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

$$
S_{a,22} = \frac{1}{a_2} - \frac{a_1^3}{R^3} \left\{ \frac{R^2}{R^2 - a_1^2} - \frac{a_1^3 a_2 (R^2 + 2 a_2^2)}{R^6} + \frac{a_1^3 a_2 R^2}{(R^2 - a_1^2)^3} \left[ 1 + \frac{2 a_1^3 a_2 (1 + 2 a_2^2/R^2)}{R^2 - a_1^2} \right] \right\}.
$$

(9)

When the macroparticles are close to each other so that the separation distance $L = R - a_1 - a_2$ is less than the least radius of particles, series entering into (8) are worse converged, thus the accuracy of (9) is decreased. In that region one can use of Russell’s asymptotical formulae [9,10]

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

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

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

(10)

Here $\psi(z)$ is the digamma function [13]: $\psi(z) = d \ln \Gamma(z)/dz$, and $\gamma$ is Euler’s constant: $\gamma = -\psi(1) \approx 0.5772$.

The data obtained by the above described methods were compared with results of calculation within the bispherical coordinates [2,7] where explicit expressions for the capacitance coefficients can be found. It can be seen from this comparison that domains of applicability of Russell’s asymptotical formulae (10) and approximate ones (9) do not overlap. To perform the transition from one region to the other a function $f(L)$ is introduced, and the smoothly joined capacitance coefficients are written as

$$
C_{ij} = C_{as,ij} f + C_{a,ij} (1 - f).
$$

(11)

In this paper, we use the function

$$
f(L) = \exp \left[ -\frac{4L (a_1 + a_2)}{a_1 a_2} \right].
$$

(12)

In figure 1, the interaction potential $U$ dependencies on $L$ calculated using smoothly joined capacitance coefficients (11) are compared with the results of calculation using the capacitance coefficients obtained with the bispherical coordinates in [2,7]. We set $\phi_1 = \phi_2 = \phi_0$ in the case of constant surface potentials and $q_1 = a_1 \phi_0$, $q_2 = a_2 \phi_0$ (so $q_i \propto a_i$) in the case of constant charges. Figure 1 shows that an attraction region is also apparent for different radii of macroparticles in the case of constant charges [14,15].

One can see that a discrepancy is only noticable in the region $L \sim \min(a_1, a_2)$ but is not more than 3% in the case of constant charges [figure 2(a)] and 1% in the case of constant surface potentials [figure 2(b)].

The relative error of the calculated values of the interaction potential is shown in figure 2. As the reference values, the data obtained with the bispherical coordinate system with an accuracy
Figure 1. The interaction potential dependencies on the separation distance for different ratios of the radii of macroparticles: $a_2/a_1 = 10$ (a), 5 (b), 2 (c) and 1 (d) with $a_2 = 10$ µm in each case. Solid curves 1 and triangles 2 are calculated for the case of constant charges from (3) using the bispherical [2, 7] and smoothly joined capacitance coefficients, respectively; similarly, dash curves 3 and circles 4 are calculated for the case of constant surface potentials (1).

Figure 2. Relative errors of calculation of interaction potential using the smoothly joined ($U_{q,a}$ and $U_{\varphi,a}$) and bispherical capacitance coefficients ($U_{q,bsh}$ and $U_{\varphi,bsh}$) for the case of constant charges (a) and constant surface potentials (b). Curves 1–4 are for $a_1 = 1$ (1), 2 (2), 5 (3) and 10 µm (4); $a_2 = 10$ µm.

of 12 digits are taken. It is seen that in the case of constant charges, the errors increase with decreasing radius of the smallest macroparticle and reach the maximum at the 10-fold radii
difference. In the case of constant potentials of surfaces, errors, on the contrary, decrease with decreasing radius of the smallest macroparticle from 1% for equal radii to 0.2% for \( a_1 = 0.1a_2 \).

It is also seen from figure 2 that the deviations from the exact values are of a fairly regular nature and can in principle be reduced with the appropriate choice of the sewing function \( f(L) \), but this function will become a more complex function of the size of the macroparticles, than equation (12).

3. Conclusions

Electrostatic interaction of two conducting macroparticles in vacuum has been considered. The interaction potential has been calculated using the capacitance and potential coefficients for the case of both the constant surface potentials and the constant charges. A simple method for calculation of these coefficients is proposed. A comparison of the interaction potential dependencies on the separation distance of the surfaces, obtained by the proposed method and by using the bispherical coordinate system shows a sufficiently high accuracy of the proposed method. Further, the method for calculating the interaction potential developed in the present paper will be used to calculate the rate constants of coagulation of macroparticles taking into account the effects of screening of the electrostatic interaction by plasma in the framework of the approach proposed in [16–18].

Acknowledgments

The work is supported by the Russian Science Foundation (grant No. 16-12-10424).

References

[1] Belov I A, Ivanov A S, Ivanov D A, Pal’ A F, Starostin A N, Filippov A V, Dem’yanov A V and Petrushevich Y V 2000 J. Exp. Theor. Phys. 90 93–101
[2] Filippov A V 2009 J. Exp. Theor. Phys. 109 516–29
[3] Maxwell J C 1891 A Treatise on Electricity and Magnetism 3rd ed (Oxford: Clarendon Press)
[4] Bichoutskaia E, Boatwright A L, Khachatourian A and Stace A J 2010 J. Chem. Phys. 133 024105
[5] Thomson W 1884 On the mutual attraction or repulsion between two electrified spherical conductors Reprint of Papers on Electrostatics and Magnetism (London: Macmillan) pp 86–97
[6] Davis M H 1964 Q. J. Mech. Appl. Math. 17 499–511
[7] Filippov A V 2009 Contrib. Plasma Phys. 49 431–45
[8] Smythe W R 1950 Static and Dynamic Electricity 2nd ed (New York, Toronto, London: Taylor and Francis)
[9] Russell A 1909 Proc. R. Soc. A 82 524–31
[10] Lekner J 2011 J. Electrost. 69 11–4
[11] Landau L D and Lifshitz E M 1984 Electrodynamics of Continuous Media 2nd ed (Course of Theoretical Physics vol 8) (Oxford: Elsevier Butterworth–Heinemann)
[12] Hobson E W 1931 The Theory of Spherical and Ellipsoidal Harmonics (Cambridge: The University Press)
[13] Davis P J 1972 Gamma function and related functions Handbook of Mathematical Functions ed Abramowitz M and Stegun I A (New York: National Bureau of Standards) chapter 6 pp 253–96
[14] Lekner J 2012 Proc. R. Soc. A 468 2829–48
[15] Munirov V R and Filippov A V 2013 J. Exp. Theor. Phys. 117 809–19
[16] Filippov A V and Derbenev I N 2016 J. Exp. Theor. Phys. 123 1099–109
[17] Derbenev I N, Filippov A V, Stace A J and Besley E 2016 J. Chem. Phys. 145 084103
[18] Filippov A V, Derbenev I N, Pautov A A and Rodin M M 2017 J. Exp. Theor. Phys. 125 518–29