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Numerical and analytical verifications of the electrostatic attraction between two like-charged conducting spheres

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ABSTRACT

We calculate the capacitance coefficients for the problem of two conducting spheres using a numerical (boundary element) method as well as two analytical approaches. The consistency of the results serves as an independent verification of the counter-intuitive analytical result that like-charged spheres almost always attract at close approach. We further support this claim by reproducing the analytical surface charge density with the numerical method. Practical implementations are given in the Supporting Information.

1. Introduction

John Lekner's curious result of like-charged yet attracting spherical conductors [1] appears to defy our intuition and was aptly described by Grier as 'a wild result' [2]. Adding to the natural skepticism towards such results is the fact that the analytical derivation in Ref. [1] is not suited for the mathematically faint of heart—an assessment which holds for other publications [3,4] which reached the same conclusion using similarly involved methods. However, the importance of these results is indisputable since they provide an intermediate-distance attraction mechanism in the pair potential between like-charged polarisable particles. Accordingly, this is highly relevant for colloidal systems [5–7], where attraction is otherwise limited to short-distance van-der-Waals forces [8,9]; yet anomalous attraction was found experimentally [10]. Besides colloids, the electrostatic attraction is also of relevance to aerosols [11], as well as biological systems [12]. Nonetheless, experimental evidence of this attraction is sparse [7,10,13], and the need for verification of the theoretical results is relegated to numerical simulations. Murovec and Brosseau [14–16] carried out finite element modelling (FEM) and verified[1] Lekner's results concerning electrostatic energy and force between two conductors. In this contribution we provide another independent verification via two avenues: first, using the numerical boundary element method, also known as method of moments [17] (specifically, we use the open source software Scuff-Em [18] [2]), and second, using the independent analytical approach developed by Ciric & Kotuwage (C&K) [19]. Both serve to directly compute the capacitance coefficients, from which one can derive the electrostatic energy and thus the force; the numerical method also allows computation of the surface charge distributions, which we compare with Lekner's analytical result. Practical implementation details of the various methods used here are given in the Supporting Information (SI).

[1] Murovec and Brosseau[14] write that they can reproduce energy and force to within 0.1%, but do not elaborate any further.

[2] See http://homerreid.com/scuff-EM; we exclusively use the electrostatics module scuff-static.

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2. Capacitance coefficients and electrostatic energy

We briefly review the basic formulae of the problem. For two conductors with charges Q_a, Q_b the electrostatic potentials are given by

$$V_a = \frac{Q_a C_{bb} - Q_b C_{ab}}{C_{aa}C_{bb} - C_{ab}^2}\ , \quad V_b = \frac{Q_b C_{aa} - Q_a C_{ab}}{C_{aa}C_{bb} - C_{ab}^2}\ , \tag{1}$$

where C_{aa}, C_{bb} and $C_{ab} = C_{ba}$ are the self-capacitances and mutual capacitances [20]. The electrostatic energy associated with this system expands to

$$W = \frac{1}{2}(Q_a V_a + Q_b V_b) = \frac{1}{2}\frac{Q_a^2 C_{bb} - 2Q_a Q_b C_{ab} + Q_b^2 C_{aa}}{C_{aa}C_{bb} - C_{ab}^2}\ . \tag{2}$$

Using vector and matrix notations $\mathbf{V} = [V_a;V_b]$, $\mathbf{Q} = [Q_a;Q_b]$, and $\mathbf{C} = [C_{aa}\, C_{ab}\,;\, C_{ab}\, C_{bb}]$ leads to the general and succinct expressions

$$\mathbf{V} = \mathbf{C}^{-1}\mathbf{Q} \quad \text{and} \quad W = \frac{1}{2}\,\mathbf{Q}^T\mathbf{C}^{-1}\mathbf{Q}\ . \tag{3}$$

While the charges $\mathbf{Q}$ remain fixed, the potentials $\mathbf{V}$ and the total energy W solely depend on the geometric arrangement of conductors, which is fully captured by the capacitance coefficients $\mathbf{C}$. The electrostatic force between conductors is given by $F = -\partial W$, where (for constant charges) the derivative is to be taken over the spatial coordinate of interest.

Analytical expressions for the capacitances of two spheres are known [21] (see Eqn. 1.4 in Ref. [1]), and Lekner showed that these can be rewritten using Chebyshev polynomials (the first few terms of this solution are shown in Eqn. 2.1 in Ref. [1]). For our purpose we need expressions containing the full series, which we may write as follows:

$$\begin{aligned} C_{aa} &= a + ab\sum_{n=1}^{\infty}\left[aU_n(x) + bU_{n+1}(x)\right]^{-1}\ , \\ C_{bb} &= b + ab\sum_{n=1}^{\infty}\left[bU_n(x) + aU_{n+1}(x)\right]^{-1}\ , \\ -C_{ab} &= \frac{ab}{c}\sum_{n=1}^{\infty}U_n(x)^{-1}\ . \end{aligned} \tag{4}$$

Here $U_n(x)$ are Chebyshev polynomials of the second kind and $x = (c^2 - a^2 - b^2)/(2ab)$, with sphere radii a, b and center distance c (see Fig. 1 inset). An implementation of Eqn. (2) is given in the SI.

Our goal is to independently confirm these expressions, since the energy and force follow directly, as laid out above. For this we follow two approaches, i) the numerical method SCUFF-EM [18] and ii) the analytical C&K approach.

The first, SCUFF-EM, is an implementation of the boundary element method [17] for arbitrary geometries [22]. In practice this first requires the generation of discrete surface meshes describing our geometry, before invoking SCUFF-EM on those. For our electrostatic problem, SCUFF-EM then solves (using standard numeric tools) the linear matrix problem $\mathbf{M}\boldsymbol{\sigma} = \mathbf{V}$, where the electrostatic interactions between pairs of mesh elements are captured by matrix elements $(\mathbf{M})_{ij} = \int_i\int_j \frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|}\mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x}$, and $\boldsymbol{\sigma}$ and $\mathbf{V}$ are vectors of the mesh element charge densities and potentials. Setting the potentials of the two spheres to [1,0] (and [0,1]), and computing the overall induced charges, yields the capacitance coefficients [C_{aa},C_{ab}] (and [C_{ab},C_{bb}]).

The second method, C&K, is an analytic-numeric hybrid in the sense that an analytical expression is used to cast the problem into a matrix equation, which then must be solved with standard numerical tools. The somewhat lengthy analytical expression (Eqn. 4.2 in Ref. [19]) is reproduced in the SI. In a nutshell, the C&K approach builds and solves a similar matrix equation as SCUFF-EM, however, here the matrix elements are interactions between multipole expansion terms of non-concentric spheres.

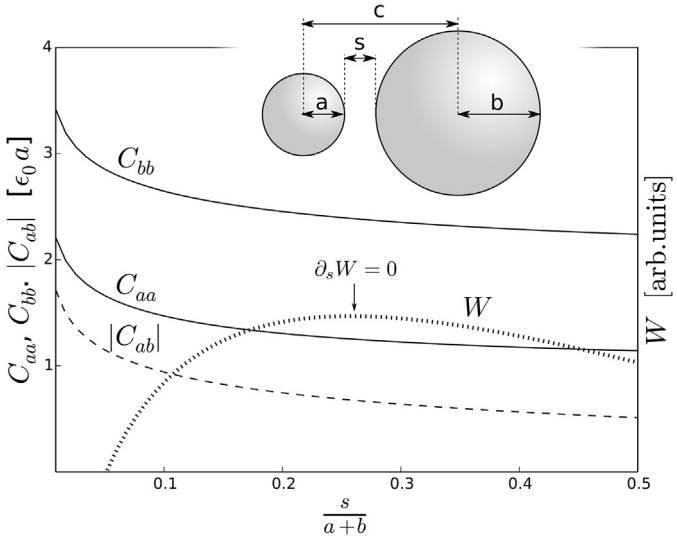

Fig. 1. Capacitance coefficients C_{aa}, C_{bb} (solid lines), C_{ab} (dashed line), and electrostatic energy $W\left(Q_a = 1, Q_b = \frac{1}{2}\right)$ of two conducting spheres for separations $\frac{s}{a+b} > 0.01$ (geometry shown in inset). The different methods, SCUFF-EM, C&K, and Lekner yield virtually identical capacitances and are not distinguishable here.

We now evaluate the capacitance coefficients using SCUFF-EM, C&K, and Lekner's result (Eqn. (2)). The same geometry as in Ref. [1] is used (see inset Fig. 1): sphere A with radius a, sphere B with radius $b = 2a$, centre-to-centre distance c, and gap $s = c - a - b$. Fig. 1 shows, as a function of $\frac{s}{a+b}$, the self-capacitances C_{aa} and C_{bb} (solid lines), the absolute inter-sphere capacitance $|C_{ab}|$ (dashed line), and the resulting energy W given charges $Q_a = 1$, $Q_b = ½$

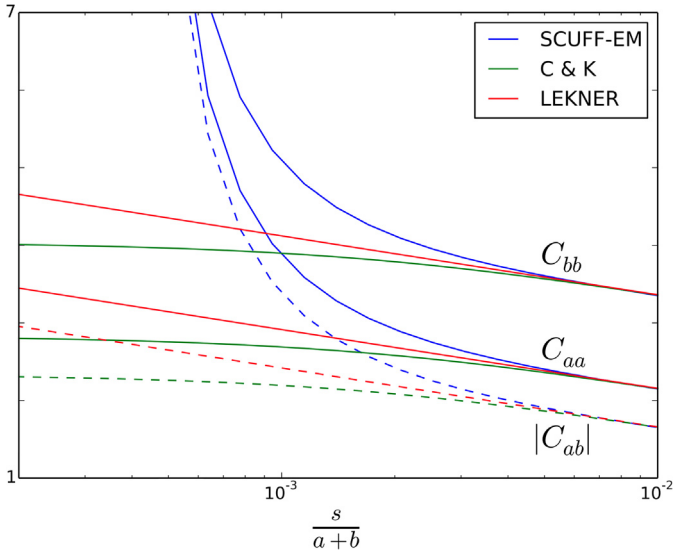

Fig. 2. Capacitance coefficients C_{aa}, C_{bb}, and C_{ab} (solid, dashed, and dotted lines) of two conducting spheres in close approach, computed via SCUFF-EM (blue), C&K (green) and with Lekner's series expansion as given in Eqn. (2) (red). Note the logarithmic abscissa. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)