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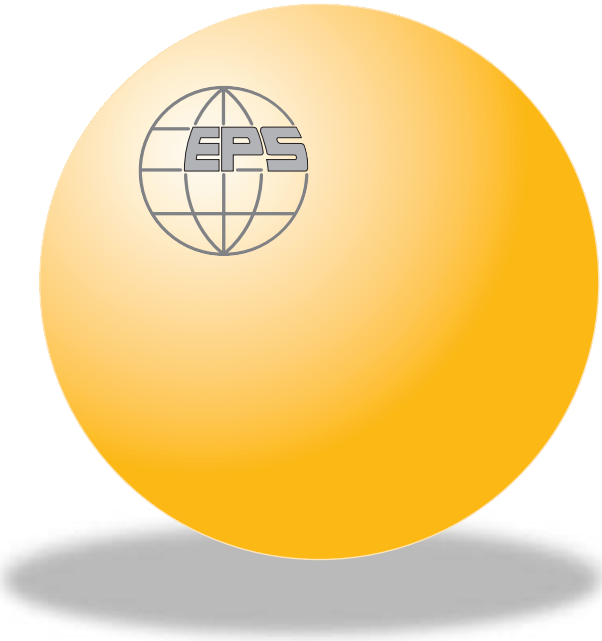

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Why charges go to the surface: A generalized Thomson problem

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Abstract. – We study a variant of the generalized Thomson problem in which n particles are confined to a neutral sphere and interacting by a $1/r^\gamma$ potential. It is found that for $\gamma \leq 1$ the electrostatic repulsion expels all the charges to the surface of the sphere. However, for $\gamma > 1$ and $n > n_c(\gamma)$ occupation of the bulk becomes energetically favorable. It is curious to note that the Coulomb law lies exactly on the interface between these two regimes.

In a recent paper [1], Bowick *et al.* studied a system of particles confined to the surface of a sphere and interacting by a repulsive $1/r^\gamma$ potential with $0 < \gamma < 2$. They called this "the generalized Thomson problem". It is interesting, however, to recall that the original Thomson problem was posed as a model of a classical atom [2]. Thus, n electrons were supposed to be confined in the *interior* of a sphere with a uniform neutralizing background, the so-called "plum pudding" model of an atom. The Thomson problem, which is still unsolved, is then to find the ground state of electrons *inside* the sphere.

In the absence of a neutralizing background, the electrostatic repulsion between the particles "dynamically" drives the charges to the surface. This significantly simplifies the calculations by reducing the search of the ground state from the three dimensions down to two [3]. But what if instead of the Coulomb potential electrons interacted by a $1/r^\gamma$ potential? Would they still go to the surface or prefer to stay in the bulk? This question was not addressed in the paper of Bowick *et al.* who have *a priori* confined their particles to reside on the surface.

It is clear that for a small number of charges, mutual repulsion will force them to the surface. What happens, however, as the concentration of particles increases? To answer this question we compare the electrostatic energy of the configuration in which all n particles are on the surface of a sphere with a configuration in which $n-1$ particles are at the surface and one particle is located at the center of a sphere. The electrostatic energy of n particles of charge q interacting through a generalized Coulomb potential $q^2/\epsilon r^\gamma$, with dielectric constant ϵ, confined to the surface of a sphere with radius a, can be obtained by considering the

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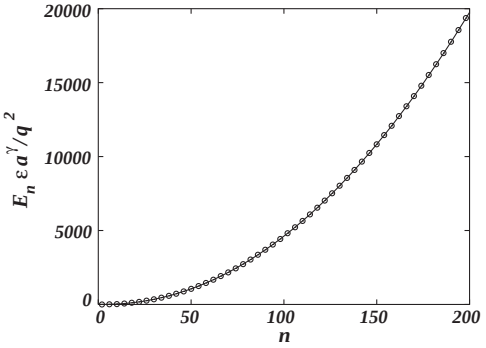

Fig. 1

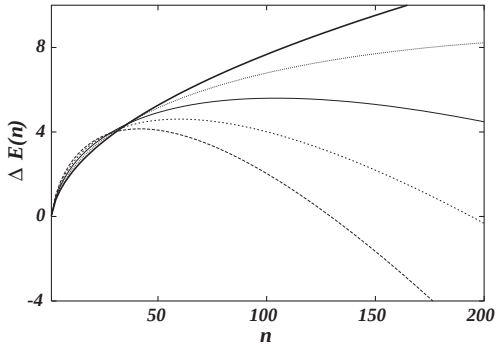

Fig. 2

Fig. 1 – Energy E_n for charges with $\gamma = 1.4$, eq. (4), as a function of the number n of particles, compared with the simulation data (points). The Madelung constant $M_\gamma \simeq 1.78$ gives a perfect fit to the data points over the whole range on n. 2000 sites were used for allowed positions of the charges on the surface of the sphere.

Fig. 2 – The difference in energy $\Delta E(n)$ between the configurations in which one particle is at the center of a sphere and $n-1$ particles are at the surface, and the configuration in which all n charges are on the surface. The values of γ range from 1 for the topmost curve to 1.4 for the bottommost curve, in intervals of 0.1. The topmost curve $\gamma = 1$ is a monotonically increasing function of n, while for $\gamma > 1$ the curves after reaching a maximum decline.

electrostatic energy of the two-dimensional one-component plasma (OCP) $F_n^{\rm OCP}$, *i.e.* charges on the surface of a sphere with a neutralizing background [4–7],

$$F_n^{\rm OCP} = E_n + \frac{q^2}{2\epsilon a^\gamma}\frac{2^{1-\gamma}}{2-\gamma}n^2 - \frac{q^2}{\epsilon a^\gamma}\frac{2^{1-\gamma}}{2-\gamma}n^2. \tag{1}$$

The first term E_n is the electrostatic energy of mutual repulsion between the charges, the second term is the self-energy of the neutralizing background, and the third term is the energy of interaction between the charges and the background. The advantage of working with the one-component plasma is that its ground-state energy can be estimated by considering the interaction of an individual charge with the background inside its Wigner-Seitz cell. The characteristic distance d between the charges on the sphere is such that $\pi d^2 n = 4\pi a^2$, and

$$d = \frac{2a}{\sqrt{n}}\,. \tag{2}$$

The ground-state energy of a Wigner crystal of charges interacting by a $1/r^\gamma$ potential is, therefore,

$$F_n^{\rm OCP} = -M_\gamma n \frac{q^2}{\epsilon d^\gamma}\,, \tag{3}$$

where M_γ is the Madelung constant. Of course, there is no perfect crystalline order of charges on the surface of the sphere and some topological defects must be present [8]. Nevertheless, we expect that the topological defects will not modify the scaling form of eq. (3), but will only affect the numerical value of the Madelung constant. Equation (1) can now be rewritten as

$$E_n = \frac{q^2}{2\epsilon a^\gamma}\left[\frac{2^{1-\gamma}}{2-\gamma}n^2 - \frac{M_\gamma}{2^{\gamma-1}}n^{1+\frac{\gamma}{2}}\right]. \tag{4}$$

This is equivalent to eq. (4) of ref. [1]. For the case of Coulomb interaction, $\gamma = 1$, it has been known for some time [9] that eq. (4) with $M_1 \approx 1.102$ gives an excellent approximation to the ground-state energy of electrons on the surface of a sphere. This value of M_1 is, indeed, very close to the Madelung constant of a planar Wigner crystal which is 1.1061. To test the accuracy of eq. (4) for different values of γ, we have simulated the distribution of charges on the surface of a sphere and calculated their electrostatic energy. To speed up the simulations, instead of using the full continuum algorithm for the surface Thomson problem, we have studied its discrete version. Thus, a number of sites were randomly placed on the surface of the sphere with a uniform probability density. The charges were then restricted to move only on these sites. There is a significant gain in the simulation time since all the electrostatic interactions can be tabulated once at the beginning of the simulation.

In fig. 1 we compare the result of numerical simulation with the analytic expression given by eq. (4). The agreement is perfect for the whole range of n.

Since the number of metastable states grows exponentially [10] with increase in n, our simulation is not able to locate the exact ground state for a large number of charges. However, the energy of nearly degenerate metastable states is very close to that of the ground state, and the error thus accrued is minimal. This can be clearly seen from the absence of any visible fluctuations in the data points plotted in fig. 1.

We are now in a position to compare the electrostatic energy of the configuration in which all the electrons are at the surface, with the configuration in which $n-1$ particles are on the surface and one charge is at the center of the sphere,

$$\Delta E(n) = E_{n-1} + \frac{q^2(n-1)}{\epsilon a^\gamma} - E_n. \tag{5}$$

From fig. 2 we see that for $\gamma > 1$, $\Delta E(n)$ starts positive, so that the charges are driven to the surface. However, as the surface particle population increases, $\Delta E(n)$ reaches a maximum and begins to decline. At the threshold number of charges $n = n_{\rm c}(\gamma)$ it becomes energetically favorable for the particles to penetrate into the bulk. For $\gamma \to 1^+$ the critical number of charges diverges as

$$n_{\rm c} \sim \frac{1}{(\gamma-1)^2}\,. \tag{6}$$

It is very curious that the Coulomb law is precisely at the border line of the two regimes. For the potentials with $\gamma \leq 1$ repulsion is strong enough to drive all the charges to the surface, while for $\gamma > 1$ and $n > n_{\rm c}(\gamma)$ the charges will penetrate into the bulk. Unlike for Coulomb charges, for particles interacting by $1/r^\gamma$ potential, the *Thomson problem* requires a full three-dimensional analysis of the distribution of particles inside the sphere. The *generalized* Thomson problem is, therefore, much more complex than its classical counterpart.

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