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Electromagnetic instability of the Thomson problem

J. De Luca[1](*), S. B. Rodrigues[2](**) and Y. Levin[3](***)

[1] *Departamento de Física, Universidade Federal de São Carlos*
Rod. Washington Luiz km 235, 13565-905, Caixa Postal 676, São Carlos, SP, Brazil
[2] *Departamento de Matemática, Universidade Federal de São Carlos*
Rod. Washington Luiz km 235, 13565-905, Caixa Postal 676, São Carlos, SP, Brazil
[3] *Instituto de Física, Universidade Federal do Rio Grande do Sul*
Caixa Postal 15051, CEP 91501-970, Porto Alegre, RS, Brazil

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Abstract. – The classical Thomson problem of n charged particles confined to the surface of a sphere of radius a is analyzed within the Darwin approximation of electrodynamics. For $n < n_c(a)$, the ground state corresponds to a hexagonal Wigner crystal with a number of topological defects. However, if $n > n_c(a)$ the Wigner lattice is unstable with respect to small perturbations and the ground state becomes spontaneously magnetized for finite n.

The Thomson problem, finding the ground state of electrons inside a sphere with a uniform neutralizing background, has a time honored position in the history of modern physics [1–7]. The original question was posed by Thomson [8] after his discovery of the electron in 1897. Thomson conjectured that the knowledge of the positions of the electrons inside the atoms is essential to understanding the regularity of the chemical elements in the periodic table. At the time, however, the proton still had to wait 14 years to be discovered, so in order to keep his atom neutral, Thomson was forced to introduce a uniform neutralizing background. The model became known as the "plum pudding" atom and the question that needed to be answered was: What are the positions of the electrons inside a uniformly (positively) charged sphere? Surprisingly, after more than a century this problem still has no general solution.

If the background charge is made to vanish, the electrostatic energy will be a minimum only if all the electrons are located at the surface. This is a general consequence of the Earnshaw theorem [9] which precludes the existence of a stable equilibrium with purely electrostatic interactions. Curiously, the Coulomb potential is precisely on the borderline where this behavior is possible. If instead of $1/r$, the electrons interacted by a $1/r^{1+\epsilon}$ potential with $\epsilon > 0$, the bulk occupation of the sphere would be energetically favorable for a sufficiently large number of electrons [10]. Unfortunately, even the restricted-surface Thomson problem remains unsolved for an arbitrary number of electrons [11, 12].

In this letter we will show that if the relativistic corrections to the Coulomb law are properly taken into account, even our intuitive picture of the ground state as consisting of

(*) E-mail: deluca@df.ufscar.br
(**) E-mail: savio@dm.ufscar.br
(***) E-mail: levin@if.ufrgs.br

stationary particles located at fixed positions on the surface of a sphere must be abandoned. Instead, we find that for sufficiently large electron density, the energy is minimized by the particles undergoing a coherent motion and the sphere becomes spontaneously magnetized!

The starting point for our analysis is the well-known Darwin Lagrangian [13–23], which takes into account the relativistic corrections to the Coulomb law resulting from the particle motion,

$$L = -mc^2 \sum_i \sqrt{1 - \frac{v_i^2}{c^2}} - \frac{1}{2} \sum_{i \neq j} \frac{q_i q_j}{r_{ij}} + \frac{1}{4c^2} \sum_{i \neq j} \frac{q_i q_j}{r_{ij}} \left[\boldsymbol{v}_i \cdot \boldsymbol{v}_j + \left(\boldsymbol{v}_i \cdot \hat{\boldsymbol{r}}_{ij} \right) \left(\boldsymbol{v}_j \cdot \hat{\boldsymbol{r}}_{ij} \right) \right]. \quad (1)$$

Equation (1) is correct to order v^2/c^2. The velocity-dependent correction to the Coulomb energy arises from the electromagnetic coupling between the moving particles. Since the Lagrangian (1) does not contain explicit time dependence, the energy of the system

$$E = \sum_i \boldsymbol{v}_i \cdot \frac{\partial L}{\partial \boldsymbol{v}_i} - L \quad (2)$$

is a constant of motion,

$$E = \sum_i \frac{mc^2}{\sqrt{1 - \frac{v_i^2}{c^2}}} + \frac{1}{2} \sum_{i \neq j} \frac{q_i q_j}{r_{ij}} + \frac{1}{4c^2} \sum_{i \neq j} \frac{q_i q_j}{r_{ij}} \left[\boldsymbol{v}_i \cdot \boldsymbol{v}_j + \left(\boldsymbol{v}_i \cdot \hat{\boldsymbol{r}}_{ij} \right) \left(\boldsymbol{v}_j \cdot \hat{\boldsymbol{r}}_{ij} \right) \right]. \quad (3)$$

The ground state for n electrons on the surface of a sphere of radius a is then determined by the minimization of eq. (3).

We note that if the terms of order $1/c^2$ are neglected, we recover the classical formulation of the Thomson problem in which the electromagnetic coupling between the electrons is purely of the Coulomb form. In this case, the velocity-dependent contribution to the Hamiltonian is positive or zero, and the ground state corresponds to stationary particles residing at fixed positions on the surface of the sphere. For large n, this structure resembles a hexagonal Wigner crystal containing some topological defects. In general, however, the $1/c^2$ terms cannot be omitted and a full minimization of eq. (3) must be performed. To proceed, it is convenient to rewrite the energy in adimensional form. Defining the reduced displacement and velocity as $r^* = r/a$ and $v^* = v/c$, the reduced energy becomes

$$E^* \equiv E \frac{r_e}{q^2} = \sum_i \frac{1}{\sqrt{1 - v_i^{*2}}} + \frac{1}{2a^*} \sum_{i \neq j} \frac{1}{r_{ij}^*} + \frac{1}{4a^*} \sum_{i \neq j} \frac{1}{r_{ij}^*} \left[\boldsymbol{v}_i^* \cdot \boldsymbol{v}_j^* + \left(\boldsymbol{v}_i^* \cdot \hat{\boldsymbol{r}}_{ij} \right) \left(\boldsymbol{v}_j^* \cdot \hat{\boldsymbol{r}}_{ij} \right) \right], \quad (4)$$

where $r_e \equiv q^2/mc^2$ is the classical electron radius and $a^* = a/r_e$.

It is convenient to work in the spherical coordinate system with unit vectors $\hat{\boldsymbol{n}}$, $\hat{\boldsymbol{\theta}}$, $\hat{\boldsymbol{\phi}}$. The reduced velocity of electron i on the surface of the sphere is then $\hat{\boldsymbol{v}}_i^* = \hat{\boldsymbol{\theta}} v_{\theta i} + \hat{\boldsymbol{\phi}} v_{\phi i}$.

Minimization of E^*, eq. (4), is performed using a general-purpose quasi-Newton method where the Hessian update is given by the BFGS formula [24]. Gradients are computed analytically. A line search with cubic fit is used with the additional safeguard against evaluations beyond light speed. The procedure is highly non-trivial. In fact it is known that already for the classical Thomson problem, in the absence of relativistic corrections, there exists an exponentially large number of metastable states [25]. Thus, it is quite unlikely that any minimization procedure will be able to locate the exact ground state for a large number of electrons. This, however, is not of great importance since the metastable states have energies very close to that of the exact ground state [10,25]. Performing the minimization of E^* we find that for reduced

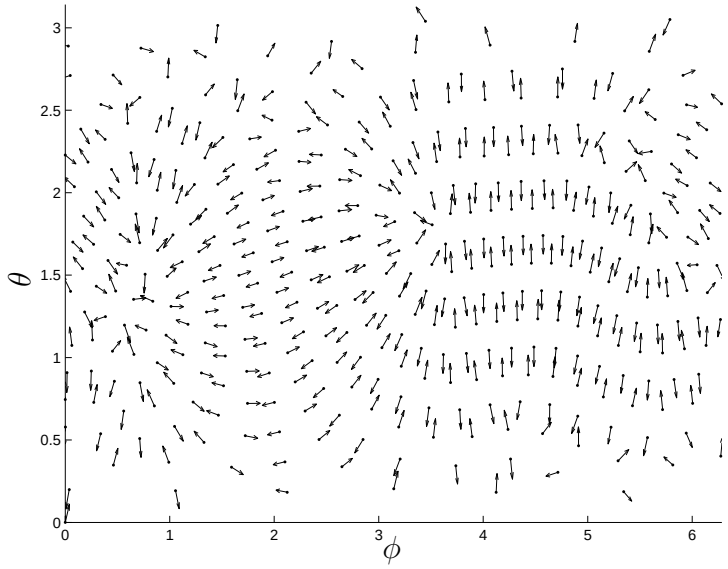

Fig. 1 – The velocity field of electrons in the supercritical region, $n = 400$ and $a = 0.7a_c$.

surface charge density $\sigma^* = n/a^{*2}$ such that $\sigma^* < \sigma_c^*$ (subcritical region), the electrons form a stationary Wigner crystal with some topological defects. Above the critical charge density $\sigma^* > \sigma_c^*$ (supercritical region), the Wigner crystal, however, becomes unstable and a new ground state with moving electrons is formed. In fig. 1 we show the characteristic distribution of particles in this new ground state. The arrows indicate the relative magnitude and direction of the particle velocities. The figure shows bands of correlated antiferromagnetic velocities that try to adapt to the topology of the sphere. We stress that when the instability occurs, $v_i/c \ll 1$ for all the particles, so that the Darwin Lagrangian remains valid, up to quantum corrections. The melting of the Wigner crystal is an example of a classical zero-temperature phase transition.

To better understand the nature of the instability of the Wigner lattice, it is convenient to rewrite the Darwin energy in a matrix form. Defining a $2n$ component velocity vector $\boldsymbol{V} = \{\boldsymbol{v}_1^*, \boldsymbol{v}_2^*, \ldots \boldsymbol{v}_n^*\}$, eq. (4) can be rewritten to order $1/c^2$ as

$$E^* \approx n + \frac{1}{2}\boldsymbol{V}^T \mathbf{I}\, \boldsymbol{V} + \frac{1}{2a^*}\boldsymbol{V}^T \mathbf{D}\, \boldsymbol{V} + \frac{3}{8}\sum v_i^{*4} + \frac{1}{2a^*}\sum_{i\neq j}\frac{1}{r_{ij}^*}\,, \tag{5}$$

where $\mathbf{I}$ is a $2n \times 2n$ identity matrix and $\mathbf{D}$ is a position-dependent matrix constructed from the last term of eq. (4). The quadratic term in velocity is non-negative if all the eigenvalues of the matrix

$$\mathbf{A} = \mathbf{I} + \frac{1}{a^*}\mathbf{D} \tag{6}$$

are positive. In this case the ground state will have $\boldsymbol{V} = 0$ and the electrons will be organized into a Wigner crystal. On the other hand, as soon as one of the eigenvalues of $\mathbf{A}$ becomes negative, the Wigner lattice will lose stability, and a new ground state, with energy below that of the Wigner crystal, will be established. The phase transition occurs when $\lambda_{min}^{\mathbf{A}} = 0$, where $\lambda_{min}^{\mathbf{A}}$ is the minimum eigenvalue of the matrix $\mathbf{A}$.

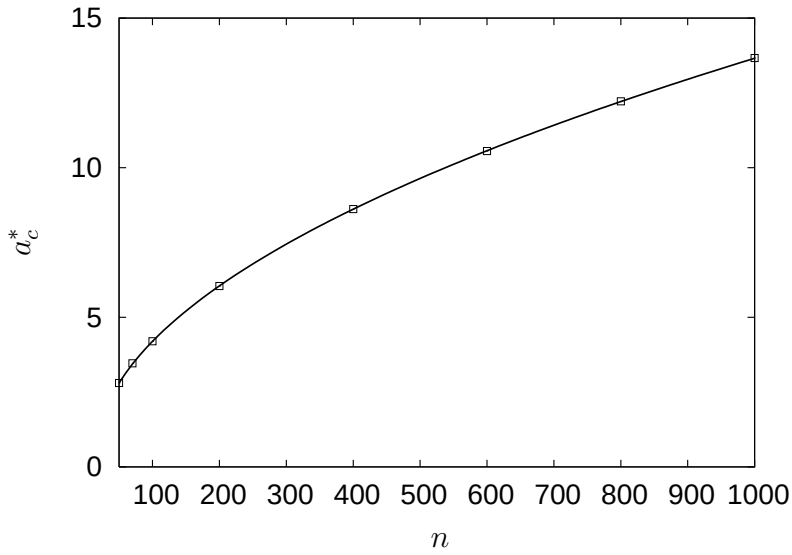

Fig. 2 – The reduced critical radius as a function of n. The solid line is a fit given by eq. (7).

It is important to note that the energetic bifurcation of eq. (5) is simultaneous with the dynamical instability of the Wigner lattice. If the Euler-Lagrange equations of motion are linearized around the stationary positions of the Wigner lattice, one can show that the Lyapunov instability occurs precisely when $\mathbf{A}$ loses convexity. Unfortunately, in the supercritical region, the equations of motion are differential-algebraic and due to the singularity of $\mathbf{A}$ are very difficult to integrate numerically [26].

To determine the critical charge concentration at which the Wigner crystal loses stability, we adopt the following procedure. For a given number of electrons n, the Coulomb energy is minimized to determine the positions of all the particles. For purely Coulombic interactions, the ground-state location of the electrons is independent of the size of the sphere, since a scales out of the expression for the electrostatic energy. Once the ground state coordinates are known, the eigenvalues $\lambda^{\mathbf{D}}$ of the matrix $\mathbf{D}$ can be calculated numerically. The criticality condition $\lambda^{\mathbf{A}}_{min} = 0$ is then equivalent to the requirements that $\lambda^{\mathbf{D}}_{min} = -a^*$. In fig. 2 we show the result of this procedure.

The points in fig. 2 can be very well fitted by

$$a_c^* = 0.4323\, n^{\frac{1}{2}} - \frac{12.680}{n}\,. \tag{7}$$

Equation (7) implies existence of a well-defined thermodynamic limit for the phase transition, $\lim n \to \infty$, $a_c^* \to \infty$ and $\sigma_c^* \to 5.35$.

To further explore the nature of the ground state for $\sigma > \sigma_c$, we define an order parameter

$$\boldsymbol{\mu}^* = \sum_i r_i^* \times \boldsymbol{v}_i^*\,. \tag{8}$$

Clearly, $\boldsymbol{\mu}^*$ is just proportional to the total magnetic moment of the sphere. In the subcritical region, the electron velocities are zero and $\boldsymbol{\mu}^* = 0$. The value of the magnetic moment in the supercritical region is plotted in fig. 3. We find that if the magnetic moment is scaled with

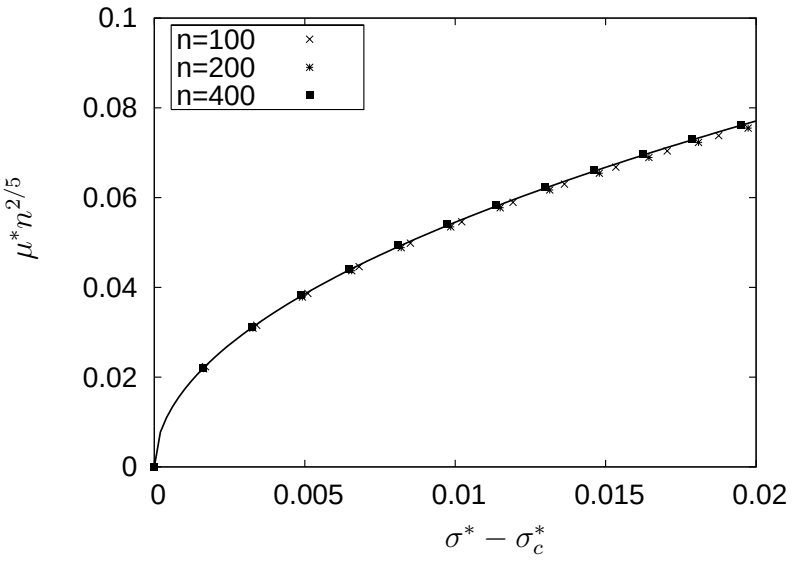

Fig. 3 – Magnetic moment in the supercritical region, the data points are the averages over five random initial configurations.

$n^{-2/5}$ and is plotted as a function of the reduced surface charge concentration $\sigma^* - \sigma_c^*$, all the points for different values of a^* and n fall on the same universal curve,

$$g(x) = 0.545\, x^{1/2}. \tag{9}$$

Thus, although locally the orientation of the velocity vectors is antiferromagnetic, globally the symmetry is broken and the sphere acquires a net magnetic moment. The magnetic moment is sub-extensive and vanishes with a square-root singularity as $\sigma \to \sigma_c^+$.

We next proceed to study the extensive property of the electromagnetic energy E^*. For $\sigma < \sigma_c$, a very accurate expression for the ground state of the Thomson problem [27, 28] can be obtained using a simple argument. Consider a uniformly *positively* charged spherical shell on which n electrons move. This problem defines a spherical one-component plasma (SOCP). The electrostatic (Coulomb) energy can be written as

$$F_{SOCP} = E_C + \frac{q^2 n^2}{2a} - \frac{q^2 n^2}{a}\,. \tag{10}$$

The first term is the Coulomb energy of interaction between n electrons on the surface of the sphere, the second term is the self-energy of the positive background charge, and the third term is the energy of interaction between n electrons and the background. At zero temperature, the classical SOCP will freeze into a hexagonal Wigner crystal (with some topological defects) whose energy is

$$F_{SOCP} = -M\frac{q^2 n}{d}\,, \tag{11}$$

where M is the Madelung constant and d is the characteristic size of the Wigner-Seitz cell, $\pi d^2 n = 4\pi a^2$. Combining eqs. (10) and (11), we arrive at a very simple expression for the Coulomb energy of n electrons on the surface of the sphere,

$$E_C = \frac{n^2 q^2}{2a} - M\frac{q^2 n^{3/2}}{2a}\,. \tag{12}$$

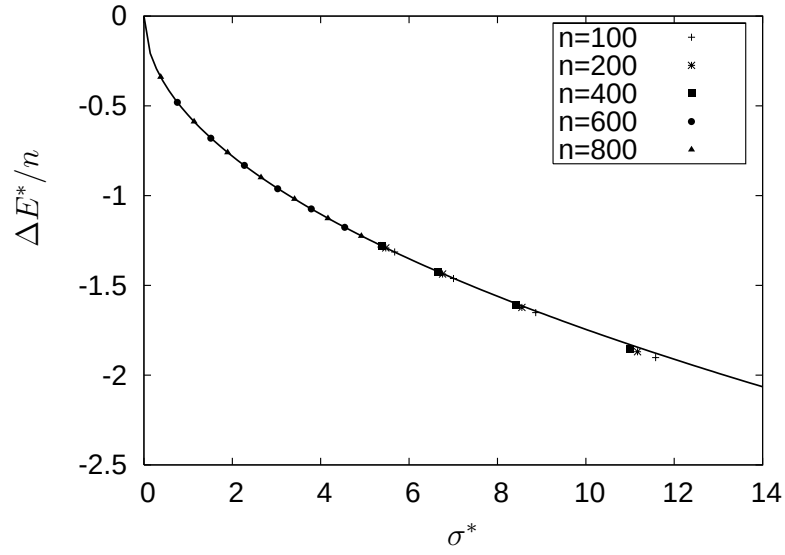

Fig. 4 – The $\Delta E^*/n$ as a function of σ^* for various combinations of n and a^*.

Equation (12) with $M = 1.1046$ gives a very accurate fit to the ground-state energy of the surface Thomson problem with purely Coulomb interactions [10, 27]. Note that for a planar OCP [29] $M = 1.1061$, so that the topological defects affect very little the value of the Madelung constant. It is also important to notice that although E_C is not extensive,

$$\Delta E_C \equiv \frac{1}{q^2}\left(E_C - \frac{n^2q^2}{2a}\right) \tag{13}$$

is. Therefore, if $\Delta E_C/n$ is plotted as a function of n/a^2 for different combinations of n and a, all points should fall onto one universal curve,

$$f(x) = -\frac{M}{2}\sqrt{x}. \tag{14}$$

We can now check if this universality also holds for the Thomson problem with the Darwin coupling between the particles. That is if

$$\Delta E^* \equiv E^* - 1 - \frac{n^2}{2a^*} \tag{15}$$

is such that $\Delta E^* = nf(\sigma^*)$, with $f(x)$ given by eq. (14). In fig. 4 $\Delta E^*/n$ is plotted as a function of σ^* for various combinations of n and a^*. It is quite surprising that even in the supercritical region $\sigma^* > 5.4$, the deviation of E^* from the energy of a stationary Wigner crystal remains very small. This is in spite of the fact that for $\sigma > \sigma_c$, the velocities of individual particles can be quite large. Evidently, the local antiferromagnetic ordering of the velocity vectors leads to significant cancellations which diminish the overall contribution of the Darwin term to the total energy.

We have shown that if the relativistic corrections are taken into account, the classical Thomson problem of the electrons confined to the surface of a sphere exhibits an electromagnetic instability. While for $\sigma < \sigma_c$, the ground state of electrons is a Wigner crystal with

some topological defects, for $\sigma > \sigma_c$, the Wigner lattice is unstable and a small perturbation can make the system evolve to a new ground state. This ground state is characterized by a local antiferromagnetic order [21–23], but finite net magnetic moment. The surface charge concentration at the phase transition has a well-defined thermodynamic limit $n \to \infty$, $a \to \infty$, while $\sigma_c^* \to 5.4$. This surface charge density, however, is so large that quantum effects must be taken into account [30,31]. The relativistic corrections to the Coulomb energy should not, therefore, affect the stability of a normal plasma.

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