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Generalized Thomson problem in arbitrary dimensions and non-euclidean geometries

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HIGHLIGHTS

- The confinement of equally charged particles in the S^{d-1}-sphere is analyzed.
- The generalization of the so-called *Thomson problem* is performed.
- Compact structures appear in higher dimensions. $d \to \infty$ is addressed.
- New discrete systems are also studied: circumscribed and inscribed polygons.
- Non-Euclidean geometries are also considered.

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ABSTRACT

Systems of identical particles with equal charge are studied under a special type of confinement. These classical particles are free to move inside some convex region S and on the boundary of it Ω (the $S^{d-1}-$sphere, in our case). We shall show how particles arrange themselves under the sole action of the Coulomb repulsion in many dimensions in the usual Euclidean space, therefore generalizing the so called *Thomson problem* to many dimensions. Also, we explore how the problem varies when non-Euclidean geometries are considered. We shall see that optimal configurations in all cases possess a high degree of symmetry, regardless of the concomitant dimension or geometry.

1. Introduction

The seminal work of Wigner's predicting the crystallization of electrons [1] has had a continuation in recent years in different branches of science. At the beginning the attention was focused in solid state physics, regarding electron crystals, in the same vein as Wigner's original work. However, the concomitant *de facto* realization of the experimental setting has proved to be very challenging, like – among others – the creation of a Wigner crystal on the surface of superfluid Helium [2] or the achievement of Wigner crystals in GaAs/GaAlAs quantum wells [3]. Very recently a 1D Wigner crystal was produced in carbon nanotubes [4].

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Posterior research on the original Wigner problem triggered a diverse literature on both experimental and theoretical work regarding properties of ionic Coulomb crystals, and that is where we encounter the classical *Thomson problem* [5]. The original goal of the Thomson problem is the following: given N charges confined to the surface of a sphere, what is the arrangement of charges which minimizes the total electrostatic energy? In essence, the Thomson problem is concerned with finding the minimal energy ground state of a cluster of charges in an arbitrary geometries and nature of confinements, not only on the S^2-sphere.

Also, the Thomson problem is widely regarded as one of the most important unsolved packing problem in mathematics. On the one hand, it plays a central role in the field of strongly correlated Coulomb systems such as dusty plasmas, quantum dots and colloidal crystals. On the other hand, the Thomson problem yields geometrical and topological insights in ordered systems.

Specifically, systems with planar geometry have been studied previously [6–9]. The Thomson problem has been extensively studied also from very different perspectives in the literature [10–13].

Since the original case was initially intended for the S^1 (2D) and S^2 (3D) spheres in the usual Euclidean space, it is the aim of the present work to generalize the problem to those systems which live in

- higher dimensional S^{d-1}-spheres, d being the dimension of the concomitant Euclidean space,
- and systems where the metric space is changed so that it is no longer Euclidean (Elliptic $\mathbb{E}^d$ or Hyperbolic $\mathbb{H}^d$).

Recent remarkable work deal with methodology of random points on the sphere [14] as well as the study on entanglement in the $(d-1-)$spherium [15].

The study of non-Euclidean geometries and the Thomson problem bears great significance as far as geometry and physics are concerned. The way optimal energies E_N, as we shall see, behave differently for distances are measured using distinct metrics. As expected, minimal configurations and regular bodies will be intimately related. There is a physical reason for that since regular bodies are such that the sum of their respective vector positions $\sum_i \mathbf{r}_i$ is zero, which implies that there is no net dipole moment.

Let us briefly discuss the numerical methods for obtaining the exact energies and configurations for any confinement throughout this work. When working in the definite plane or space according to some metric, we will have k degrees of freedom per charged particle. Thus, the total number of variables will be kN. A minimization will take place for the whole set of parameters in every given configuration of the particles, finding the optimal Coulombian energy E_N^*.

The Thomson problem is certainly the kind of example of an NP hard problem and so progress in this area has only been possible thanks to the use of computational techniques. In our case, we have performed a two-fold search employing (i) an amoeba optimization procedure, where the optimal value is obtained at the risk of falling into a local minimum and (ii) the so called simulated annealing [16] well-known search method, a Monte Carlo method, inspired by the cooling processes of molten metals. The advantage of this duplicity of computations is that we can be quite confident about the final result reached. Indeed, the second recipe contains a mechanism that allows a local search that eventually can escape from local optima.

The purpose of this paper is to provide a semi-analytical approach to describe the ground state properties of charged particles in different geometries. Specially in the case of the S^{d-1}-sphere, we shall consider the minimal energies and concomitant configurations or arrangements of charged particles in different dimensions and, eventually, reach the limit for $d \to \infty$. We consider particles interacting by means of the Coulomb interaction at zero temperature. Finally, some conclusions are drawn in the last section.

2. The Thomson problem in arbitrary dimensions

2.1. One dimension

As explained previously, the only interaction between particles is electrostatic in nature. This implies that all particles interact with each other until an energetic equilibrium is reached, which is the one we are interested in. Suppose that we want to study the system composed by charged particles along a line segment between $[-R_0, R_0]$ (the radius R_0 will be 1 from now on). Due to symmetry reasons, the system is symmetric with respect to the center. For N even, no particle lies at the origin, whereas for N odd there is always one charge. Even though the physical system is quite simple, the optimal configuration of the charges for a minimum energy E_N is not analytical.

However, we can obtain an excellent upper bound by considering that, for large N, particles more or less arrange themselves in equally spaced divisions of the line segment containing them. Thus, defining the linear charge density $\lambda = \frac{L}{N-1}$ ($L = 2$ in our case), we have

$$E_N \approx \sum_{i<j} \frac{1}{\epsilon} \frac{1}{(j-i)\lambda} = \frac{N-1}{2\epsilon_r} \sum_{i<j} \frac{1}{j-i} \tag{1}$$

where $\epsilon_r = \epsilon/\epsilon_0$ is the relative dielectric constant of the medium. We shall use units so that $e^2/4\pi\epsilon_0 = 1$ from now on. The sum is performed between distinct pairs, so that it is equal to $1 + (H(N-1) - 1)N$, where $H(N-1)$ is the sum of the