Electrostatic Patterns in the Interior of a Circular Region

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Abstract

We examine the formation of symmetric patterns of N equal charges in static equilibrium, confined in the interior of a circular region by a harmonic oscillator potential. We develop a simulation procedure for the determination of their equilibrium positions. Initially, the charges are assumed to occupy random positions on the plane. The time evolution of the system is determined with a numerical integration of the equations of motion of the N charges. By imposing a proper kinetic energy dissipation mechanism, equilibrium configurations are obtained. They correspond to the absolute minimum (ground state) or to a secondary higher minimum (excited states) of the multidimensional potential energy surface. Ground state configurations are presented for N=5-30, 45 and 230. They involve arrangements of charges at the vertices of regular polygons inscribed in concentric circles. The sequence of occupation indicates a shell effect, similar to the one encountered in the occupation of the electron orbits of the atoms. With increasing N, the rotational symmetry tends to disappear, competing with the one of an infinite triangular lattice. Changes in the symmetry of the ground to the excited state(s) are discussed in typical cases. Interesting patterns of a greater complexity are produced by groups of unequal charges in the same confinement.

Introduction

Symmetry plays an important role in both Art and Science, with numerous interconnections [1]. In Physics, symmetry underlies in the conservation laws, which play a key role in the understanding of Nature. Furthermore, realizing the symmetries of a given problem facilitates its mathematical formulation and solution [2].

What are the equilibrium positions of a system of N equal point-charges in the interior of a conducting disk? For a long time, this problem of electrostatics was thought to have a trivial solution. In equilibrium, the Coulomb potential energy of the system

$$W = \sum_{i<j}^{N} \frac{q_i q_j}{r_{ij}}$$

has a minimum. Therefore, the distances between any two charges (r_{ij}) have to be maximal. Therefore, the solution to the problem should be: the two end-points of a diameter of the circle for N=2, the vertices of an equilateral triangle for N=3, the vertices of a square for N=4, and in general, the vertices of a regular polygon. This result seemed so obvious that nobody tried to verify with a direct calculation of the total electrostatic energy, for quite a long time.

In 1985, A. Berezin compared the electrostatic energy W_A of the above configuration with the energy W_B of a configuration in which one charge is placed at the center of the disk and the rest (N-1) are placed on the vertices of the inscribed regular polygon. With a great surprise, it was found that for N greater than 11, configuration B has a smaller energy (and, therefore, a greater stability) than A [3,4]. Theoretically, it was shown that this happens for any integer greater than 11 [5]. From this fact, a number of questions emerge.

Why does this happen? We know that in three dimensions, the charge on a conductor is distributed on its surface and not its interior. This paradox appears because we apply the three-dimensional Coulomb

interaction to a system confined in two-dimensions. If we consider a logarithmic interaction potential between the charges (which is the two-dimensional analogue of the Coulomb potential), we obtain an equilibrium configuration with all charges on the circumference of the circle. Thus, we establish a consistency with our three-dimensional experience [6].

Are there any other configurations with a still lower energy? From symmetry considerations, it follows that such configurations exist, for large N. They consist of charges arranged on the corners of regular polygons inscribed in equally spaced concentric circles [6].

Which one is the lowest-energy equilibrium configuration? In the limit of infinite N, the problem reduces to finding the charge distribution on the surface of a conducting disk. This is a well-known problem of electrostatics, whose solution can be expressed in an analytic form [7,8]. However, for a finite N, the answer to this problem is not trivial. The potential energy of the system is a function of the 2N Cartesian coordinates of the charges. This multi-dimensional surface may involve a large number of secondary shallow minima. Stable equilibrium configurations correspond to the absolute minimum (ground state) or the secondary minima (excited states). At the local maxima (saddle-points), states of unstable equilibrium may be found.

Theoretical studies are difficult and rather sparse in the bibliography [9]. However, this problem presents a challenge for the computational science as a complex minimization problem. In the last years, significant progress has been made with the development of sophisticated computational methods [10,11]. In physics, variations of this problem form the basis for simulations of finite classical systems localized in two-dimensions [12,13]. For this purpose, Monte-Carlo minimization [12,14] and molecular dynamics methods [15] have been developed. A fundamental issue of these investigations concerns the study of ground and excited state equilibrium configurations.

In the present paper, we investigate the patterns produced in equilibrium configurations of equal charges confined by a harmonic oscillator potential and indicate that a greater complexity of symmetric patterns arises in the case of groups of unequal charges held in the same confinement.

The Simulation Procedure

We have developed a simple simulation code, which allows us to follow the evolution of the system of N charges on its way to equilibrium. We start with an initial configuration of the 2N Cartesian coordinates, selected with random numbers from a uniform distribution within the unit circle. The charges are assumed to be at rest. There follows a coordinate transformation, which brings the center of mass of the system at the origin of the coordinate axes. This procedure reduces the total search time.

Each charge experiences the Coulomb force by the rest of the charges. Furthermore, we assume that all charges are attracted to the origin with a parabolic (harmonic oscillator) potential. This means that the force on each charge is proportional to its distance from the origin. It is like having attached springs, with the same spring constant k, to the charges.

Next, we allow the system to develop, according to the laws of Newtonian dynamics. The equations of motion are written in the form of difference equations, in Cartesian coordinates. The resulting system of equations was integrated numerically using Euler's method. Despite its simplicity, this method can provide sufficient accuracy, provided the step-size of time integration is sufficiently small. The step-size was set to a value ensuring that, in a free propagation of the system, the total energy is conserved.

In the following calculations, we use nuclear physics units. Length is measured in fm (Fermi), where $1fm=10^{-15}m$, energy in MeV and time in sec. The time scale was not fixed, since it is irrelevant in the present case. The charges are assumed to be point-like electrons, without loss of generality.

We demonstrate our simulation in the case of N=7 charges in a parabolic potential with a spring constant k = 50.0 MeV/fm^2. Initially, the charges are placed in the interior of a circle of radius R=1fm. Panel (a) of Figure 1 shows the potential and kinetic energy of the system as a function of time step. The potential energy (E_{pot}) of the system is a periodic function of time and shows two minima. The kinetic

energy (E_{kin}) is also a periodic function of time and shows opposite variations, in such a way that the total energy of this conservative system remains constant.

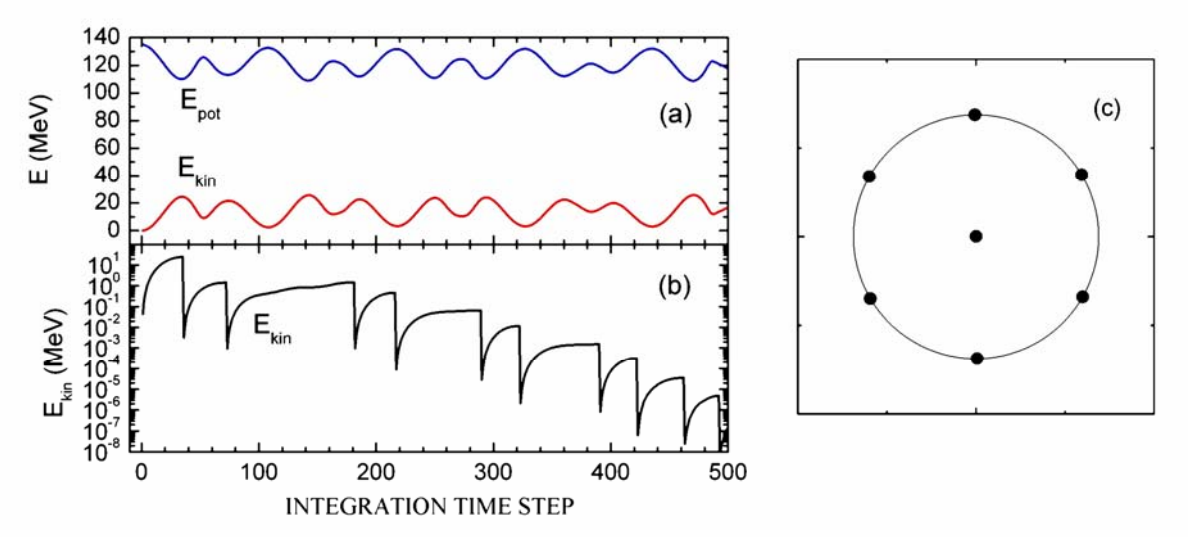

Figure 1: *(a) Time-development of the kinetic and potential energy of 7 equal charges under the influence of a parabolic potential. (b) Time-development of the kinetic energy with the dissipation procedure described in the text. (c) The resulting equilibrium configuration.*

In order to determine the equilibrium configuration of the system, we employ the following logic. The trajectories and total kinetic energy are stored in computer memory at all time steps. The system will be close to equilibrium whenever the potential energy shows a minimum, or the kinetic energy shows a maximum. After the third time-step, we compare the kinetic energy in the previous three steps. If we realize a maximum, we back-propagate the trajectories by one step and set all velocities equal to zero. If this is not an equilibrium configuration, the excess potential energy will be converted to kinetic. The system will evolve till the kinetic energy acquires a maximum. Then, the previous dissipation mechanism is applied, and so on. The above logic is repeated until the numerical integration exceeds 1500 steps. In Figure 1(b) we see that the kinetic energy (shown on a logarithmic scale) is reduced by 8 orders of magnitude after the first 500 integration steps. There follows the equilibrium configuration shown in Figure 1(c). One charge appears at the origin and the rest six charges are arranged at the vertices of a regular hexagon. The value of spring constant k represents a stiff potential. Weaker values of k allow for a kinetic energy increase and, consequently, a longer time scale for the system to reach equilibrium. An animation has been produced showing the evolution of the initial configuration on its way to equilibrium, as well as the impact of the spring constant to the dynamics of the system.

Since our initial configuration is drawn from a random distribution, the outcome of repeated runs is expected to produce a number of equilibrium configurations, each with a certain frequency of occurrence. These configurations correspond to the ground state (absolute minimum of the potential energy surface) and excited states (higher energy local minima). We find no correlation between the frequency of occurrence and the absolute energies of the minima.

Ground State Configurations

For a certain number of charges, the determination of the possible equilibrium configurations requires the execution of the simulation for a large number of times. The resulting energies of the potential energy

minima have to be sorted in ascending order. Thus, the ground state configuration (corresponding to the lowest energy) and excited-state configurations of various orders are obtained.

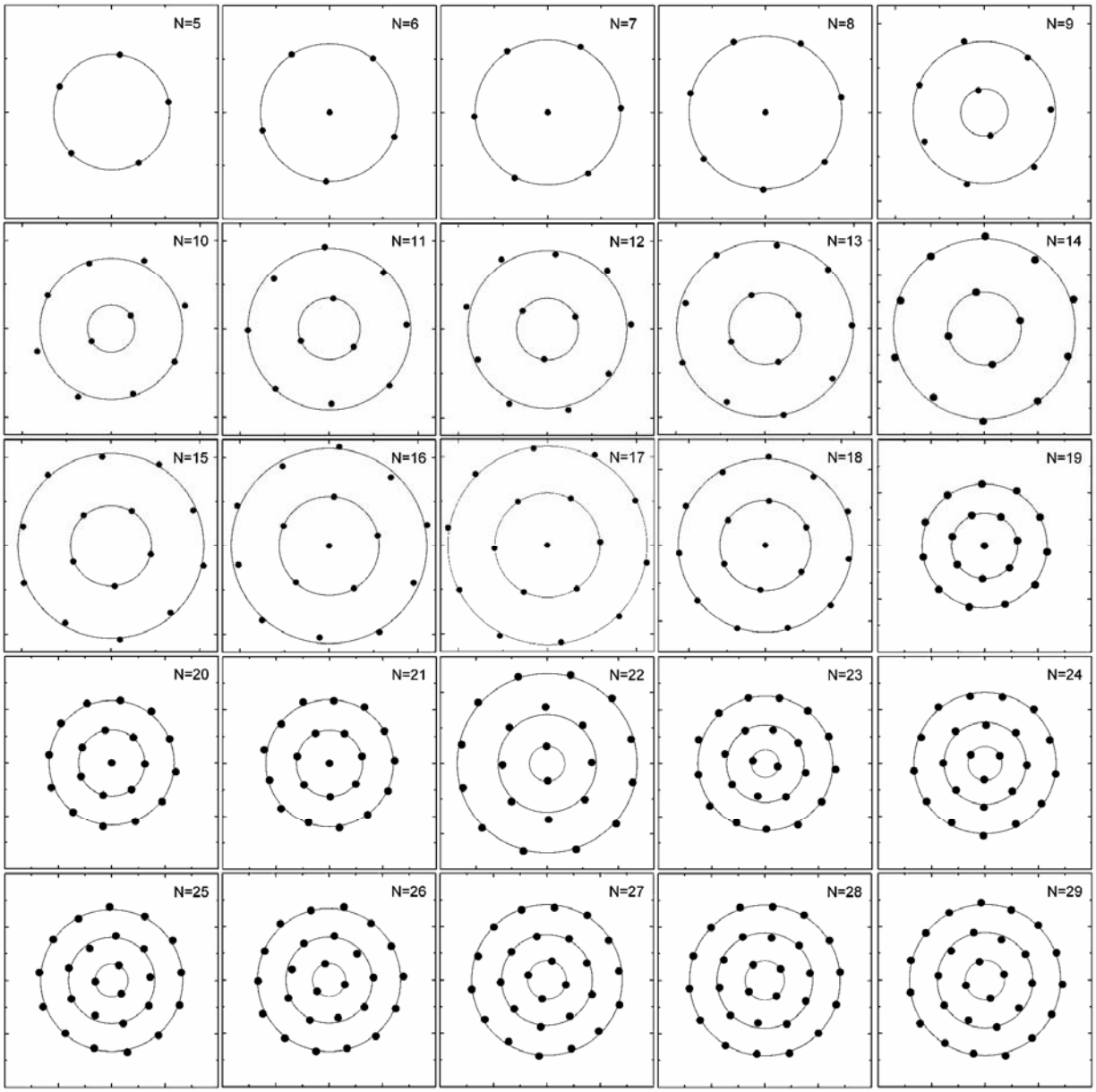

Figure 2: *Ground state equilibrium configurations of equal charges (N=5-29) in a parabolic potential.*

After 1000 runs of the simulation in each case, we determined the ground state configurations of N=5-29 charges in the parabolic potential. Our results are shown in Figure 2. The circles drawn guide the eye. We realize that for N=5, we get the charges arranged on the corners of a regular pentagon. For N=6-8 we get a regular polygon plus one charge at the origin. This seems to be in contrast with the original problem of Berezin [3,4]. However, the confining potential in our case is different. For N=9-15, we observe a small number of charges (n=2-5) on the circumference of an inner circle. Then, we have the appearance of a single charge at the origin (N=16-21). For N=22-19, we have the formation of a new inner circle. We note that as N increases, the number of perimeter charges increases and stabilizes to some value for a while, in order to support the inner charges. Then, it increases again. The same trend

appears in the next outmost inner circle, and so on. This is an analogue of a shell effect encountered in the occupation of the atomic orbitals by electrons in atoms, or of the nuclear orbitals by the nucleons in an atomic nucleus.

We note that the results shown in Figure 2 are in excellent agreement with the calculation of Ref. [15]. The only disagreement appears for N=19, for which Ref. [15] predicts a (5,10,14) configuration, as opposed to our (4,10,15). Many debates in the current literature concern configurations near shell closures, as in our case.

In Figure 2, we also see that charges in different shells do not always align perfectly on a circle. This is understood from the interplay between the two kinds of a potential (Coulomb and parabolic), where the system tries to establish equilibrium. If the system were infinite and unbounded, we would expect the charges to equilibrate in an infinite triangular lattice [12]. Therefore, our systems should show a tendency for a transition to some triangular symmetry, as N increases. This is illustrated in Figure 3, where minimum energy configurations are shown for N=30, 45 and 230.

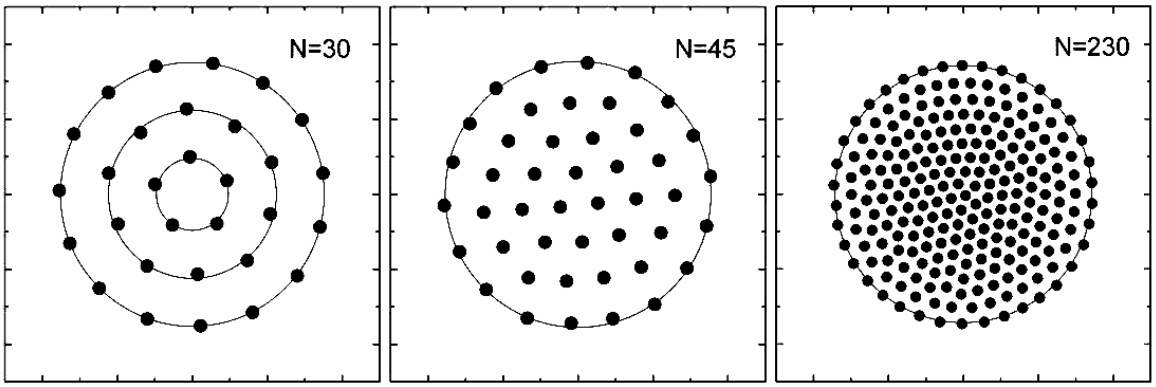

Figure 3: *Ground state equilibrium configurations of N=30, 45 and 230 equal charges.*

Excited State Configurations

In our simulations, we did not observe any excited states for N=7 and 11. In the rest of the cases, we observe an increasing complexity of excited states, with increasing N. Some typical cases of the evolution from the ground to the first few excited states are shown in Figure 4.

For N=5, the pentagonal ground state becomes a square with one charge at the center. For N=6, the central charge of the ground state moves to the periphery. For N=8, the opposite happens. One of the peripheral charges moves to the interior and forms a pair with the central one. For N=9, the inner pair of charges of the ground state breaks apart and a single central charge appears in the first excited state. For N=12, we have a different situation. The three inner charges of the ground state, change orientation in the first excited state and attract a fourth one in their shell, in the second excited state. A rotation of the inner shell is also observed in the first excited state for N=15. In its second excited state, a central charge appears.

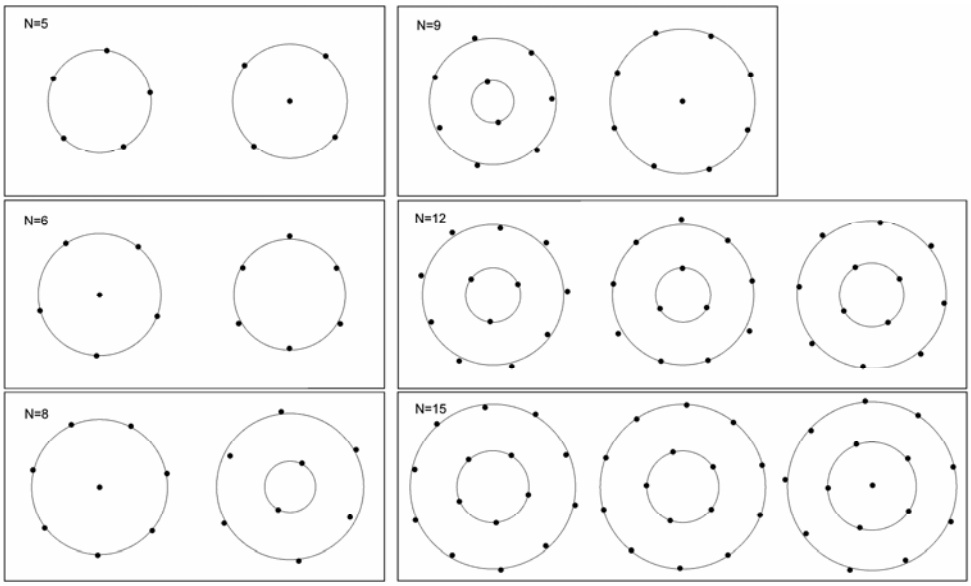

Figure 4: *Ground and excited state equilibrium configurations of N=5, 6, 8, 9, 12 and 15 equal charges, indicating changes in symmetry occurring at different minima of the potential energy surface.*

Patterns Involving Unequal Charges

We now examine some exotic configurations involving groups of unequal charges in a parabolic potential. The following configurations involve 5 or 6 big charges and a number of smaller ones. A larger number of big charges does not improve the effect. On the left of Figure 5, we show the case of N=42 unequal charges. Six of them have a charge of Q=30e and the rest 36 have a Q=10e (e=electron charge). The six outer charges produce a focusing effect for the smaller ones, ordered in concentric circles. On the right, we have N=40 charges arranged in three groups: 6 with Q=50e, 6 with Q=30e and 28 with Q=3e. We get two aligned hexagons, while the small charges order in concentric circles.

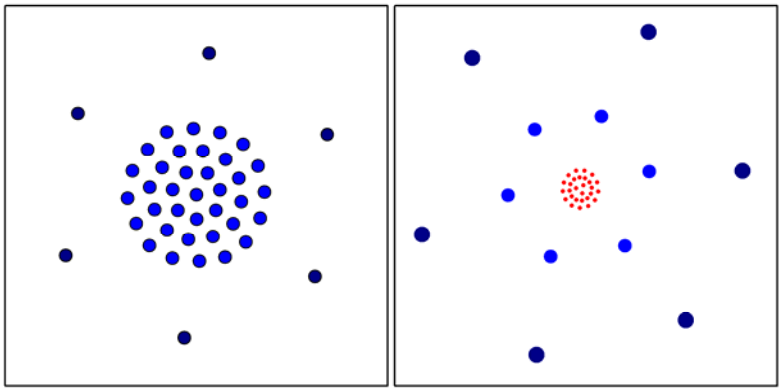

Figure 5: *Minimum energy configurations of N=42 and N=40 unequal charges (see the text).*

On the left of Figure 6, we show a configuration with N=12, involving 6 charges with Q=10e and 6 with Q=e. We obtain the formation of a small pentagon with a central charge inside the hexagon. The configuration on the right seems more impressive. We have a total of N=24 charges, involving three

groups: 6 charges with Q=10e, 6 with Q=e and 12 with Q=5e. The lines stress the symmetry of the configuration.

Using 5 big charges with Q=10e and 29 charges with Q=e and 10 times smaller spring constant, we get the configuration on the left of Figure 7. The small charges align in concentric circles. The small spring constant for the small charges causes this circular arrangement. On the right of Figure 7, we have a total of N=30 unequal charges in three groups, and the same spring constant for all of them. We have 5 charges with Q=80e, 15 charges with Q=30e, and 10 charges with Q=2e. The middle charges align in two parallel pentagons. Nine of the ten small charges align on a small circle and the tenth one appears at the center of the configuration.

The possibilities seem unlimited. Yet, the exploration of the resulting configurations under different assumptions on the symmetry of the confining potential, although interesting, lies beyond the scope of the present work.

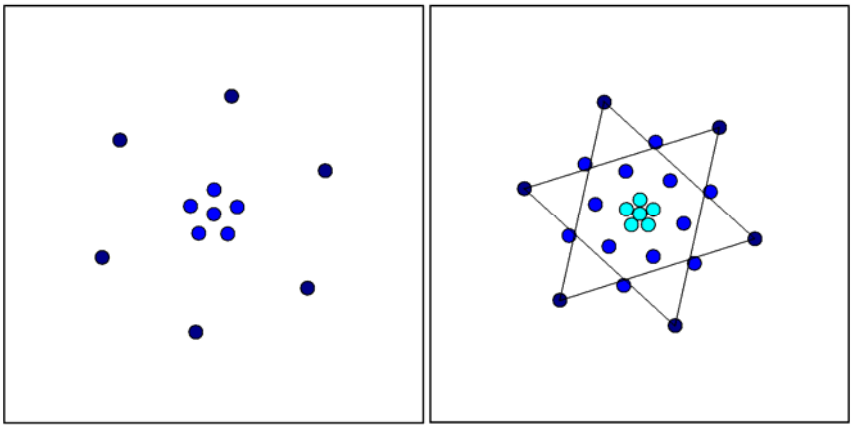

Figure 6: *Minimum energy configurations of N=12 and N=24 unequal charges (see the text).*

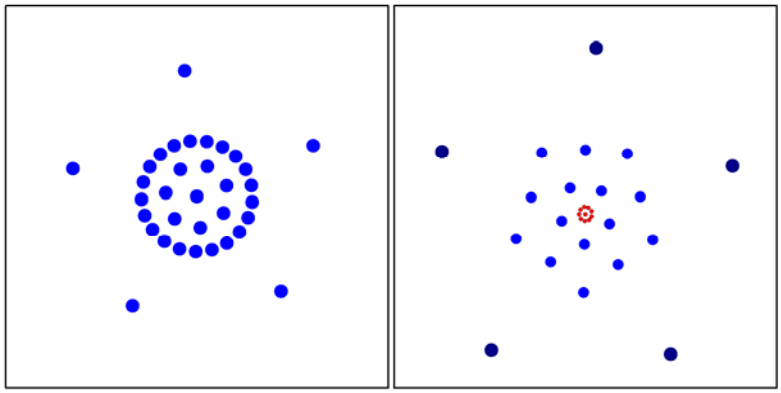

Figure 7: *Minimum energy configurations of N=34 and N=30 unequal charges (see the text).*

Related Problems

The original problem of Berezin originated from his desire to explain the shape of snowflakes [3]. It is also interesting in other disciplines, such as stereochemistry, botany, virology, information theory, nuclear theory, and elsewhere (see, Refs. [4,10]). A related mathematical problem in two-dimensions is the one of packing circles on a disk [10].

In three dimensions, the corresponding problem on the equilibrium positions of charges on the surface of a sphere has been studied for a long time and is known as the Thomson's problem. It originated from the early works of J.J. Thomson, on a mathematical model for the atom [16]. His plum pudding model considered the electrons (the plums) embedded in a spherical positively charged sphere (the pudding), in such a way that the atom appeared to be electrically neutral, in a macroscopic sense. Although, this model failed to explain the experimental evidence, the corresponding mathematical problem continues to be a challenge [10].

An experiment with a number (N=5-30) of small conducing stainless steel balls in the interior of a charged circular frame has been reported in Ref. [13]. Many of the equilibrium configurations look the same as the ones of charged particles in a parabolic potential. However, it was realized that a better overall agreement could be obtained if the interaction between the balls had a slower dependence on the distance than the Coulomb potential. Another related experiment was performed with small cylindrical bar magnets on an air table [17]. The authors were able to observe symmetrical and nonsymmetrical configurations for N up to 19. Furthermore, they observed oscillations around the equilibrium configurations and transitions between equilibrium configurations.

Summary

In the present work, we investigated the results of a numerical simulation on the problem of N equal charges in a harmonic oscillator potential. We presented ground state configurations for N=5-30, 45 and 230, exhibiting regular arrangements of the charges in concentric equidistant circles. We discussed changes in symmetry occurring in typical configurations as a given system equilibrates in higher-energy minima. We indicated the appearance of interesting symmetric configurations in the case of groups of unequal charges confined by the same potential.

This problem shows a continuing interest for the basic and computational science. It also has a value as an interdisciplinary problem, where one can develop physics intuition and aesthetics using a combination of skills on electrostatics, laws of classical motion, numerical methods and graphics.

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