Thomson Problem on a Sphere

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Abstract

The study of this paper is about the mathematical computation to minimize the Coulomb energy of a system of N charged particles constrained to move on the surface of the unitary sphere. The method applied was the dynamical method, imposing a damped force proportional to the velocities of the particles and leaving evolve the system to reach the minimal energy.

Keywords: Thomson, Sphere, Coulomb energy, Polyhedrons /sep Minimal energy

1. Introduction

At the end of the 19th century the scientists understood very well electromagnetic phenomena at the macroscopic scale, thanks to electromagnetic theory by Maxwell. Moreover, Maxwell showed that the light is an electromagnetic wave composed of the magnetic and electric fields. In analogy with the mechanical waves of classical physics, they thought that there should be something to propagate the light in vacuum space, they called it: ether. However, the Michelson Morley experiment showed the ether do not exist. This experiment, the photoelectric effect and the blackbody radiation were some of the initiators of the Modern Physics and the study of the microscopic world.

Other important development was the improved vacuum pump which allowed the study of electrical discharges in the cathode rays. One of the most important experiments was carried out by Joseph John Thomson, a british physicist who discovered the ratio charge mass ($\frac{q}{m}$) of the electron using the cathode rays and measuring the deflections of these rays in the presence of electric and magnetic fields. "Thomson's measurement of $\frac{q}{m}$ showed that the particles in the cathode rays had either a much greater charge or a much smaller mass than the hydrogen atom"[1].

Thomson was interested in the atomic structure of nature, in order to explain the line spectra of the atoms he proposed his own atomic model. "Thomson held that atoms are uniform spheres of positively charged matter in which electrons are embedded. Popularly known as the plum-pudding model"[2].

Unfortunately his atomic model was valid only for a few years due the Rutherford scattering experiment, where the existence of the nucleus was discovered. However, nowadays

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the also called "Thomson problem" is very important for many aplications in computational science, microbiology, nanotechnology, maths, etc.

2. Problem

Given N charged particles that are moving on the surface of a unitary sphere, with constant initial velocities and in the presence of a damped force proportional to the velocities, find the minimum of the dimensionless Coulomb energy ($U(N)$) [3]

$$U(N) = \sum_{i=1}^{N} \sum_{j>i}^{n} \frac{1}{|\bar{r_i} - \bar{r_j}|}$$

using the dynamical method. Furthermore, compute the final configuration of the particles.

3. Method

To solve the problem, there were considered the following assumptions:

- The Coulomb force is the only interaction between the charged particles
- There is no energy emitted by the accelerated particles.
- Each particle has the same mass and charge ($m = q = 1$).
- The particles move on the surface of the sphere.
- There is a damped force between the particles and the surface, proportional to the angular velocities of them.

As the approach to solve the problem is a dynamical method, the first step is to find the kinetic and potential energy of the system. At a given time t, the coordinates (in spherical coordinates) of each charged particle are given by the vector

$$\bar{r}_\alpha(t) = (sin(\theta_\alpha(t))cos(\phi_\alpha(t)), sin(\theta_\alpha(t))sin(\phi_\alpha(t)), cos(\theta_\alpha(t)))$$

where $\alpha = 1, 2, ..., N$. If the kinetic energy is expressed in terms of the generalized coordinates $(\theta_\alpha, \phi_\alpha)$ the result is a quadratic function

$$T = \frac{1}{2} \sum_{\alpha=1}^{N} m_\alpha |\dot{\bar{r}}_\alpha|^2 \tag{1}$$

meanwhile the electric potential energy

$$U = \sum_{\alpha,\beta=1,\alpha<\beta}^{N} U_{\alpha,\beta}$$

where $U_{\alpha,\beta} = \frac{kq_\alpha q_\beta}{|\bar{r}\alpha - \bar{r}_\beta|}$, but as the interest is to find the final configuration, it is possible to set, without lose of generality, $k = 1$. Also for the electric potential energy $U_{\alpha,\beta} = U_{\beta,\alpha}$ and ignoring the self energy for each particle, $U_{\alpha,\alpha} = 0$, then

$$U = \frac{1}{2} \sum_{\alpha,\beta=1,\alpha\neq\beta}^{N} \frac{1}{|\bar{r}_\alpha - \bar{r}_\beta|} \tag{2}$$

Using the equations (1) and (2) and doing the calculations required, the kinetic and potential energy of the system of N charged particles are

$$T = \frac{1}{2} \sum_{\alpha=1}^{N} (\dot{\theta}_\alpha^2 + \dot{\phi}_\alpha^2 sin^2(\theta_\alpha)) \tag{3}$$

$$U = \frac{1}{2\sqrt{2}} \sum_{\alpha,\beta=1,\alpha\neq\beta}^{N} \frac{1}{\sqrt{1 - cos(\theta_\alpha)cos(\theta_\beta) - sin(\theta_\alpha)sin(\theta_\beta)cos(\phi_\alpha - \phi_\beta) + \delta}} \tag{4}$$

Note a small constant, δ, was added by hand because if two particles are too close together they will feel a strong repulsive force, acquiring a lot of energy and it would take a long time to lose that energy by the friction. Therefore, the Lagrangian defined as $L = T - U$ is given by

$$L = \frac{1}{2} \sum_{\alpha=1}^{N} (\dot{\theta}_\alpha^2 + \dot{\phi}_\alpha^2 sin^2(\theta_\alpha)) - \frac{1}{2\sqrt{2}} \sum_{\alpha\neq\beta}^{N} \frac{1}{\sqrt{1 - cos(\theta_\alpha)cos(\theta_\beta) - sin(\theta_\alpha)sin(\theta_\beta)cos(\phi_\alpha - \phi_\beta) + \delta}} \tag{5}$$

To find the equations of motion for each particle, the Euler-Lagrange equations have to be solved:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\theta}_\rho} - \frac{\partial L}{\partial \theta_\rho} = 0 \qquad ; \qquad \frac{d}{dt}\frac{\partial L}{\partial \dot{\theta}_\rho} - \frac{\partial L}{\partial \theta_\rho} = 0$$

Note each particle has two Euler-Lagrange equations; then, there must be solved $2N$ coupled non-linear differential equations, which are

$$\ddot{\theta}_\alpha - \dot{\phi}_\alpha^2 sin(\theta_\alpha)cos(\theta_\alpha) + \frac{1}{4\sqrt{2}} \sum_{\alpha\neq\beta} \frac{cos(\theta_\alpha)sin(\theta_\beta)\cos(\phi_\alpha - \phi_\beta) - sin(\theta_\alpha)cos(\theta_\beta)}{\sqrt[3]{1 - cos(\theta_\alpha)cos(\theta_\beta) - sin(\theta_\alpha)sin(\theta_\beta)cos(\phi_\alpha - \phi_\beta) + \delta}} + \kappa\dot{\theta}_\alpha = 0 \tag{6}$$

and

$$\ddot{\phi}_\alpha + \frac{2\dot{\phi}_\alpha\dot{\theta}_\alpha cos(\theta_\alpha)}{sin(\theta_\alpha)} - \frac{1}{4\sqrt{2}} \sum_{\alpha\neq\beta} \frac{sin(\theta_\beta)sin(\phi_\alpha - \phi_\beta)}{sin(\theta_\alpha)\sqrt[3]{1 - cos(\theta_\alpha)cos(\theta_\beta) - sin(\theta_\alpha)sin(\theta_\beta)cos(\phi_\alpha - \phi_\beta) + \delta}} + \kappa\dot{\phi}_\alpha = 0 \tag{7}$$

The mathematical computation for the solutions of these 2N equations are presented below. It is important to consider that the Euler-Lagrange equations are of second order, that means two initial conditions are required for each generalized coordinate, then four initial conditions for each charged particle ($\theta_\alpha(0) = \theta_{\alpha 0}$, $\theta'_\alpha(0) = \theta'_{\alpha 0}$, $\phi_\alpha(0) = \phi_{\alpha 0}$, $\phi'_\alpha(0) = \phi'_{\alpha 0}$). In the Listing 1 these initial conditions were generated using the command RandomReal, also the initial states of each particle were plotted on the sphere.

Listing 1: Initial Conditions

```
(*Here the initial positions are generated randomly*)
Do[\[Theta]0[
i] = RandomReal[{0, Pi}, WorkingPrecision -> dgt];
\[Phi]0[i] = RandomReal[{0, 2 Pi}, WorkingPrecision -> dgt];
r0[i] = {Sin[\[Theta]0[i]] Cos[\[Phi]0[i]],
Sin[\[Theta]0[i]] Sin[\[Phi]0[i]], Cos[\[Theta]0[i]]};, {i, 1, n}]

(*Here the initial velocities are generated randomly*)
Do[
v\[Theta]0[i] = RandomReal[{0, 1}, WorkingPrecision -> dgt];
v\[Phi]0[i] = RandomReal[{0, 1}, WorkingPrecision -> dgt];, {i, 1, n}]
 initialpositions = Table[r0[i], {i, 1, n}];

(*Plot for the initial state*)
m1 = ListPointPlot3D[ initialpositions , PlotStyle -> PointSize[0.02],
PlotRange -> {{-1, 1}, {-1, 1}, {-1, 1}}];
m2 = Graphics3D[{Black, Opacity[.1], Sphere[{0, 0, 0}]}, Axes -> True,
PlotRange -> 1];
Show[m2, m1]
```

In the Listing 2 the $2N$ Euler-Lagrange equations were written explicitly in two vectors. One for each generalized coordinate. Besides, the initial conditions computed in the Listing 1 were added.

Listing 2: Euler-Lagrange Equations

```
(*Euler-Lagrange Equation for \[Theta]*)
table1 = Table[{Subscript[\[Theta], i]''[
t] - (Subscript[\[Phi], i]'[t])^2*
Sin[Subscript[\[Theta], i][t]]*Cos[Subscript[\[Theta], i][t]] +
Sum[If[i != j,
1/(4 Sqrt[
2]) *((Cos[Subscript[\[Theta], i][t]]*
Sin[Subscript[\[Theta], j][t]]*
Cos[Subscript[\[Phi], i][t] - Subscript[\[Phi], j][t]] -
Sin[Subscript[\[Theta], i][t]]*
Cos[Subscript[\[Theta], j][t]]) /((1 -
Cos[Subscript[\[Theta], i][t]]*
Cos[Subscript[\[Theta], j][t]] -
Sin[Subscript[\[Theta], i][t]]*
Sin[Subscript[\[Theta], j][t]]*
Cos[Subscript[\[Phi], i][t] -
Subscript[\[Phi], j][t] + \[Delta])^(3/2))), 0], {j,
1, n}] + \[Kappa]*Subscript[\[Theta], i]'[t] == 0,
Subscript[\[Theta], i][0] == \[Theta]0[i],
Subscript[\[Theta], i]'[0] == v\[Theta]0[i]}, {i, 1, n}];

(*Euler-Lagrange Equation for \[Phi]*)
table2 = Table[{Subscript[\[Phi], i]''[
t]*(Sin[Subscript[\[Theta], i][t]])^2 +
2*Subscript[\[Phi], i]'[t]*Subscript[\[Theta], i]'[t]*
Cos[Subscript[\[Theta], i][t]]*Sin[Subscript[\[Theta], i][t]] -
```

```
27 Sum[
28  If[i != j,
29  1/(4 Sqrt[
30  2]) *((Sin[Subscript[\[Theta], i][t]]*
31  Sin[Subscript[\[Theta], j][t]]*
32  Sin[Subscript[\[Phi], i][t] -
33  Subscript[\[Phi], j][t]])/((1 -
34  Cos[Subscript[\[Theta], i][t]]*
35  Cos[Subscript[\[Theta], j][t]] -
36  Sin[Subscript[\[Theta], i][t]]*
37  Sin[Subscript[\[Theta], j][t]]*
38  Cos[Subscript[\[Phi], i][t] -
39  Subscript[\[Phi], j][t]] + \[Delta])^(3/2))), 0], {j,
40  1, n}] + \[Kappa]*Subscript[\[Phi], i]'[t] == 0,
41  Subscript[\[Phi], i][0] == \[Phi]0[i],
42  Subscript[\[Phi], i]'[0] == v\[Phi]0[i]}, {i, 1, n}];
43
44  (*Vector for the variables*)
45  vars1 = Table[{Subscript[\[Theta], i][t],
46  Subscript[\[Phi], i][t]}, {i, 1, n}];
47  vars = Flatten[Partition[Flatten[vars1], 1]];
```

The next step is to calculate numerically the equations using the command NDSolve (See Listing 3). As the solutions will be compared with the solutions obtained by Erber and Hockney[3] and they used an accuracy of eight digits, the results of the Listing 3 are given with the same precision.

Listing 3: Solutions

```
1
2  (*Solving Differential Equations*)
3  g = NDSolve[{table1, table2}, vars, {t, 0, 400},
4  WorkingPrecision -> dgt][[1]];
5  y[t_] := Evaluate[vars /. g]
6  result = Table[{Sin[y[t][[2*k - 1]]] Cos[y[t][[2*k]]],
7  Sin[y[t][[2*k - 1]]] Sin[y[t][[2*k]]], Cos[y[t][[2*k - 1]]]}, {k,
8  1, n}];
9
10 (*Paths of the charge particles*)
11  trayectories =
12 ParametricPlot3D[result, {t, 0, 400},
13 PlotRange -> {{-1, 1}, {-1, 1}, {-1, 1}}];
14 Show[trayectories, m2]
```

Once the Listing 3 have been executed, the interpolated functions are evaluated at the final time. Then, these solutions are displayed in two plots, the first one shows the charged particles at the equilibrium reached by the method (see Listing 4) and the last one shows the polyhedrons formed with the particles at the vertices (see Listing 5).

Listing 4: Final States

```
1   (*Positions at the equilibrium*)
2    final = 400;
3    finalpositions =
4   N[Table[{Sin[y[final][[2*k - 1]]] Cos[y[final][[2*k]]],
5   Sin[y[final][[2*k - 1]]] Sin[y[final][[2*k]]],
6   Cos[y[final][[2*k - 1]]]}, {k, 1, n}], dgt];
7   m3 = ListPointPlot3D[finalpositions,
8   PlotRange -> {{-1, 1}, {-1, 1}, {-1, 1}},
9    PlotStyle -> PointSize[0.02]];
10  Show[m2, m3]
```

Listing 5: Polyhedrons

```
Graphics3D[{EdgeForm[Red], Red, Specularity[White, 5],
Polygon[Part[ finalpositions , #] & /@
Subsets[Range[Length@finalpositions ], {3}]]}, Boxed -> True,
Axes -> True]
```

As a final step, for different number N of particles, the Coulomb dimensionles energies (equation (1)) were calculated and compared with the energies obtained bye Erber and Hockney[3].

Listing 6: Coulomb Dimensionless Energy

```
Sum[If[i != j, 1/2 1/Sqrt[ FullSimplify [ Expand[( finalpositions [[ i ]] - finalpositions [[ j ]]) .( finalpositions [[ i ]] -
    finalpositions [[ j ]]) ]]], 0], {i, 1, n}, {j, 1, n}]
```

4. Results

As it was mentioned before, the objective of this paper is to calculate the minimum of the electric potential energy and compare the results with the work of Erber and Hockney. To do that the Listings of the previous section were executed many times. The results for $N = 4$, $N = 12$, $N = 24$ and $N = 36$ are presented above. Then a more exhaustive comparison between these two works was done (see section 4.5).

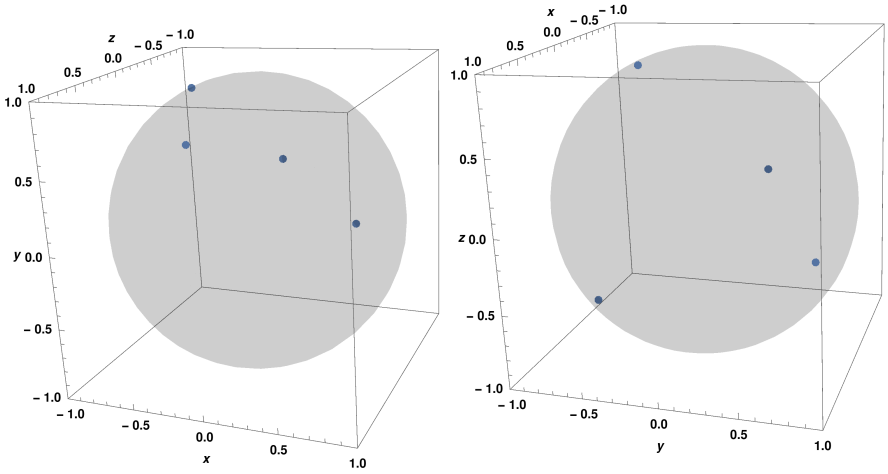
For all evaluations were considered the following values of the constants: $\delta = 0.1$ and $\kappa = 0.4$.

4.1. 4 Particles

It is important to remark that for the case four particles the polyhedron formed was the tetrahedron (see Figure 2(b)), composed by triangular faces and four vertices.

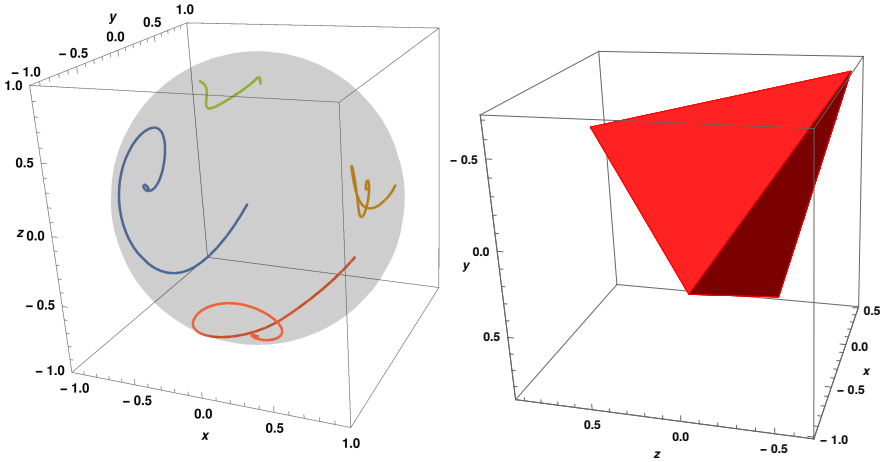
Table 1: Comparison minimum energy at the equilibrium state

Number of charges	Energy (Erber and Hockney)	Energy computed
4	3.67423461	3.674234614



(a) Initial state (b) Final state

Figure 1: Initial and final configurations of the system for 4 particles.



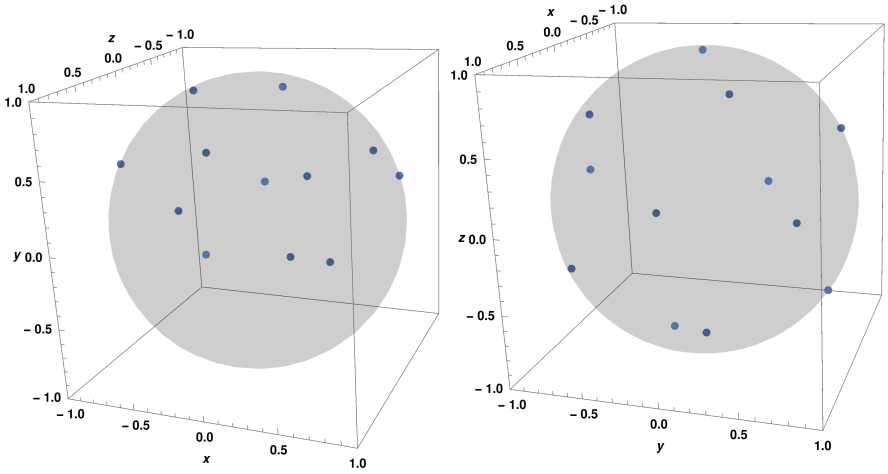
(a) Trayectories (b) Tetrahedron

Figure 2: (a) Trayectories of the 4 charged particles before reach the equilibrium. (b)Tetrahedron formed with the equilibrium state.

4.2. 12 Particles

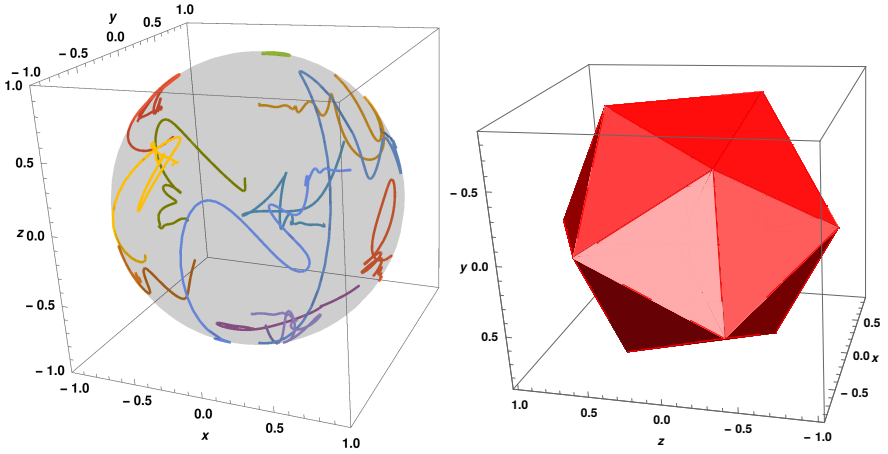
Table 2: Comparison minimum energy at the equilibrium state

Number of charges	Energy (Erber and Hockney)	Energy computed
12	49.16525306	49.1652531



(a) Initial state (b) Final state

Figure 3: Initial and final configurations of the system for 12 particles.



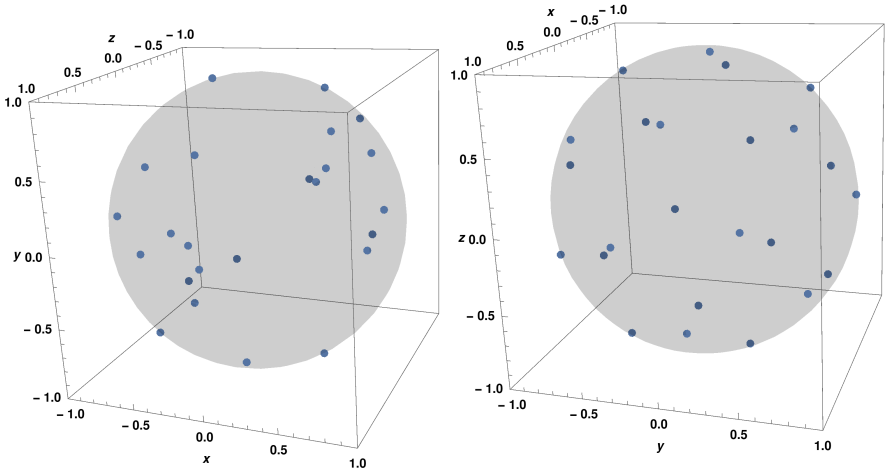
(a) Trayectories (b) Polyhedron

Figure 4: (a) Trayectories of 12 the charged particles before reach the equilibrium. (b)Polyhedron formed with the equilibrium state.

4.3. 24 Particles

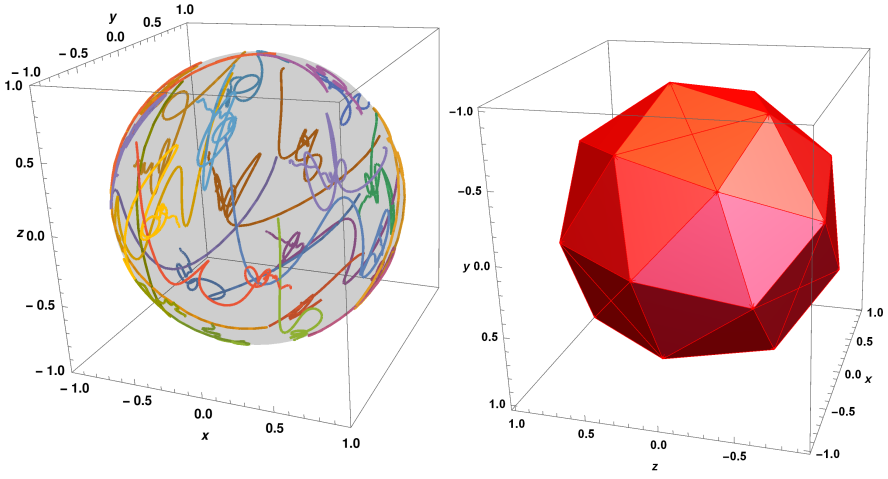
Table 3: Comparison minimum energy at the equilibrium state

Number of charges	Energy (Erber and Hockney)	Energy computed
24	223.34707405	223.348766



(a) Initial state (b) Final state

Figure 5: Initial and final configurations of the system for 24 particles.



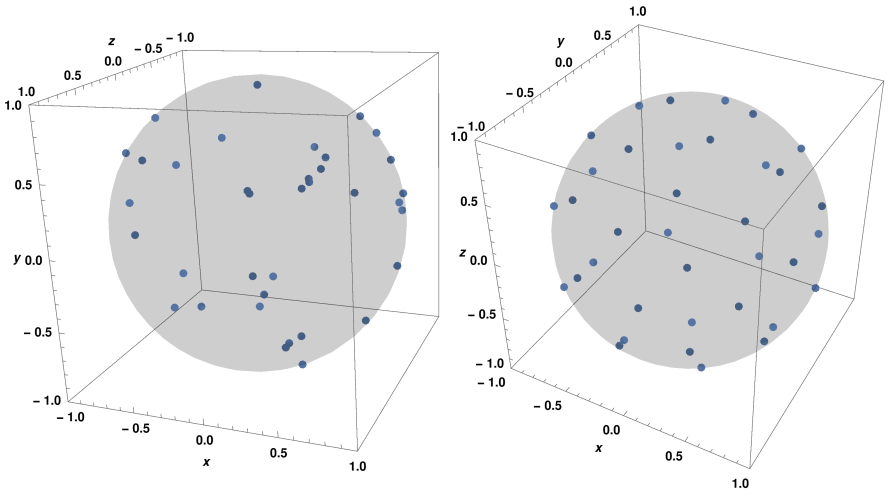
(a) Trayectories (b) Polyhedron

Figure 6: (a) Trayectories of the 24 charged particles before reach the equilibrium. (b)Polyhedron formed with the equilibrium state.

4.4. 36 Particles

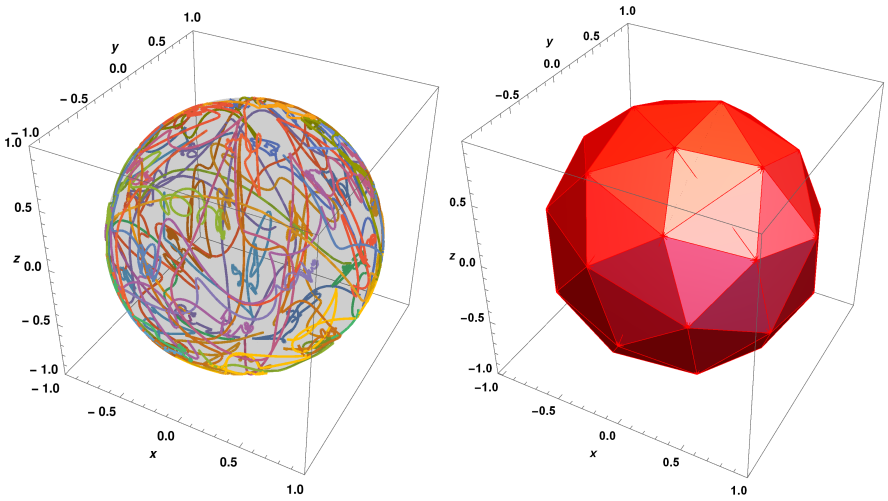
Table 4: Comparison minimum energy at the equilibrium state

Number of charges	Energy (Erber and Hockney)	Energy computed
36	529.12240842	529.1271244



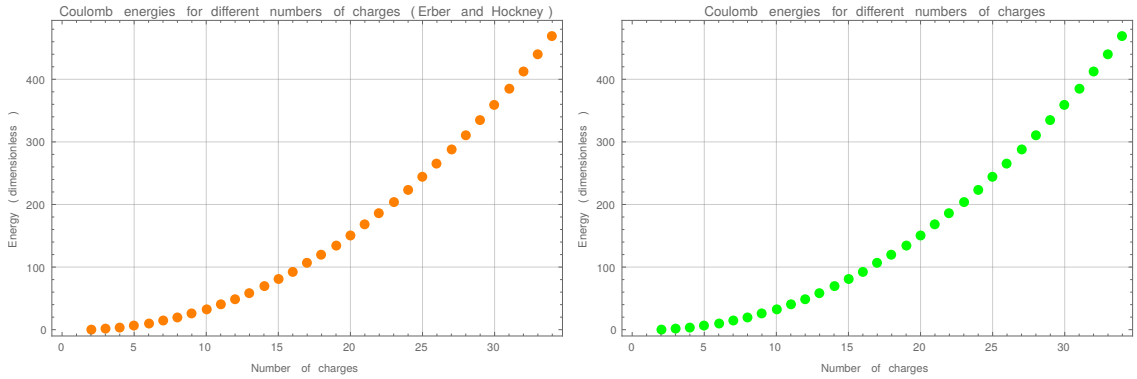
(a) Initial state (b) Final state

Figure 7: Initial and final configurations of the system for 36 particles.



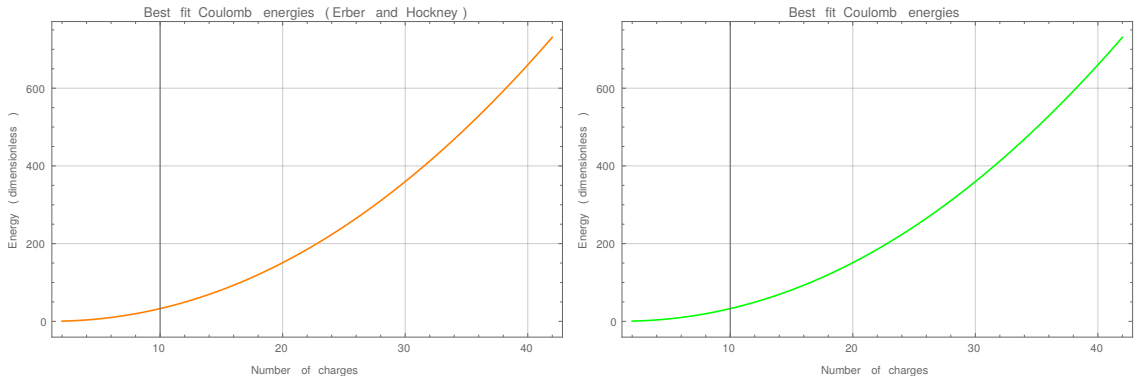
(a) Trayectories (b) Polyhedron

Figure 8: (a) Trayectories of the 36 charged particles before reach the equilibrium. (b)Polyhedron formed with the equilibrium state.



(a) Erber and Hockney data (b) Dynamical method data

Figure 9: Data of the energies for different number of charged particles.



(a) Erber and Hockney fit (b) Dynamical method fit

Figure 10: Best fits using the mathematica command Fit.

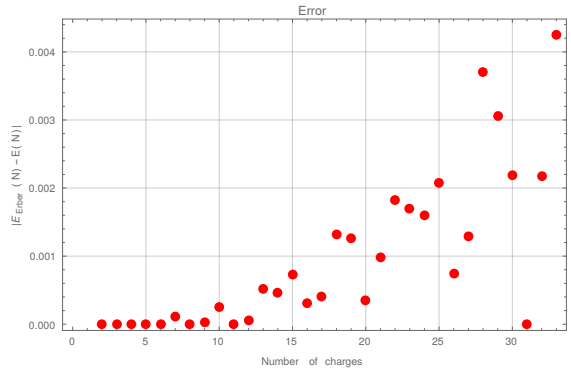


Figure 11: Absolute value of the diference of energies for each number of particles.

Table 5: Comparison minimum energy at the equilibrium state

Number of charges	Energy (Erber and Hockney)	Energy computed
2	0.50000000	0.500000000
3	1.73205081	1.7320508076
4	3.67423461	3.67423461
5	6.47469149	6.474691495
6	9.98528137	9.98528137
7	14.45297741	14.452977431
8	19.67528786	19.67539562
9	25.759986530	25.75999330
10	32.71694946	32.7169774
11	40.59645051	40.59670773
12	49.16525306	49.1652531
13	58.85323061	58.853290680
14	69.30636330	69.3068842
15	80.67024411	80.67071383
16	92.91165530	92.9123854
17	106.05040483	106.05071369
18	120.08446745	120.0848708
19	135.089467560	135.09079279
20	150.88156833	150.882827316
21	167.64162240	167.6419753
22	185.28753615	185.2885181
23	203.930190660	203.9320202
24	223.34707405	223.3487659
25	243.81276030	243.8143661
26	265.13332632	265.1354032
27	287.30261503	287.3033539
28	310.49154236	310.4928308
29	334.63443992	334.6381400
30	359.60394590	359.6070077
31	385.53083806	385.5330279
32	412.261274650	412.2612747
33	440.20405745	440.2062345
34	468.90485328	468.9091069

5. Conclusions

The difference between the dynamical method and another implementations of the problem is that in the first one we do not need an specific point to start the minimization of the function and it is sufficient leave evolve the system with time. Also with the dynamical method the minimum is always reached; or at least, it is not difficult to choose a suitable choice for the values of the damped factor κ and the constant δ such that at an interval of time $[0, t]$ the system is near the equilibrium at the final time t.

However, when the number of particles increases the paths followed by the charges are more complicated due the short distance between them and the Coulomb interaction, which transfers energy to the closest particles and then, they acquire kinetic energy to move in those complicated trayectories. If the choice for the final time t is small probably the system is not going to reach the equilibrium. Another complication to use the dynamical method is when the number of charges increases, the execution time increases as well; which is due that 2N second order, coupled, non-linear differential equations must be solved. Also the execution time increases if you are worry about the precision of the results and you demand an accuracy of m digits.

Nevertheless, taking care the values of the constants and giving sufficient time for the system to evolve, you are going to obtain a good approximation for the minimum energy (see Table 5 and Figure 11). In fact, for N small the error of the calculus is almost zero. Also, it is important to note that the error obtained by the program increase when the number of charges increases; that is due when N is large there are more degrees of freedom, then the error for each particle is accumulated, and there are more configurations for the minimum.

To find the energies of the section 4.5 (see Table 5), there were some problems due that sometimes the results corresponded to local minima and the program had to be executed many times until the global minima were reached.

References

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