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Many-particle jumps algorithm and Thomson's problem

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Abstract. We study Thomson's problem using a new numerical algorithm, valid for any interacting complex system based on the consideration of simultaneous many-particle transitions to reduce the characteristic slowing down of numerical algorithms when applied to critical or complex systems. We improve or reproduce all previous results on the Thomson problem, using much less computer time than the other numerical algorithms. We report ground-state energies for $101 \leq N \leq 135$, and study the stability of the ground state as a function of the number of charges considered. We associate this stability with how well defined are the charges surrounded by five nearest neighbours, whose number always seems to be equal to 12.

1. Introduction

The problem of finding the lowest-energy configuration of N charges distributed over the surface of a unit sphere has been studied by many authors since it was proposed by Thomson many years ago [1–6]. In spite of its apparent simplicity, it is a good example of a complex system, which includes disorder and interactions, with a non-trivial solution. The interest in the problem is partly due to the increasing importance of the carbon fullerenes [7–10] and to the 'magic' stability numbers exhibited by microclusters [11]. The problem is also relevant to the calculation of the electronic structure of anions, the difficulty of which is substantially overcome when they are surrounded by a charged sphere [6].

For systems with few charges, symmetry principles alone may be sufficient for determining the equilibrium configurations, as was demonstrated exactly by Leech for $N = 2-6, 12$ [12]. Many different numerical methods have been applied to finding the lowest minimum energy configurations. Erber and Hockney [2] obtained results for $N \leq 65$ by performing single-charge displacements in the direction of the electrostatic force. Simulated annealing [14] was used by Edmundson [4], who obtained the same results as Erber and Hockney, except for $N = 55$ and $N = 56$ for which only metastable states were obtained; although, on the other hand, he calculated low-energy configurations for $N = 72, 92$ and 100. The same author, using symmetry considerations [5], was able to calculate very stable configurations for many values of N up to 100.

The standard Monte Carlo technique allows us to obtain configurations at a given temperature, with the right probability, but it is inefficient near the critical temperature of a phase transition, because the correlation length diverges and transitions involve clusters of many particles [15]. New efficient Monte Carlo methods, based on cluster algorithms, have been designed to overcome the critical slowing down of phase transitions [16], but they cannot be applied to disordered systems, including Thomson's problem. Charges on a unit sphere also present the problem of slowing down, since to reach the lowest electrostatic

energy configuration, simultaneous many-particle movements are needed; metastable states act as energy barriers which lead to slowing down near the ground state.

There are some approaches which use cluster algorithms for spin glasses [17], but they are of limited efficiency. The main contribution in this field is the method of constrained global optimization [1], that iteratively uses a Glauber spin-flip probability and the Metropolis algorithm [13]. This method was applied to Thomson's problem and produced the best available results for $N \leq 100$, except for $N = 78$, where Edmundson's results [5], based on symmetry considerations, are better. Very recently, Erber and Hockney [18] improved the constrained global optimization results for $N = 69, 86$ and 87 .

This paper describes the application of a new numerical algorithm, specially designed for disordered interacting systems, to Thomson's problem with high- N values, giving the best results achieved by any other method for $N \leq 100$ and the ground-state configurations for $N \leq 135$. Our method consists of choosing a number of low-energy single-particle transitions, producing all possible combinations and then picking the one with the lowest energy. This procedure is iterated until there is no further reduction in energy. We also study the stability of the ground state and analyse the spatial correlations between charges as a function of the number of charges on the sphere.

2. Description of the numerical algorithm

We consider N charges disposed on the surface of a unit sphere, interacting through their Coulomb forces. We have to look for the positions of the charges that minimize the total dimensional electrostatic energy

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

where r_i is the position vector (x_i, y_i, z_i) of the charge i ($i = 1, \dots, N$), with the constraint $x_i^2 + y_i^2 + z_i^2 = 1$. We use Cartesian coordinates, since they are more convenient when moving the particles in the direction of the forces.

Our method, as applied to Thomson's problem, consists of the following. We first choose an arbitrary number n (we initially take $n = 3$ initially), which corresponds to the number of charges that will be considered moving in each step. We also select an initial angle ϑ , through which we will move each chosen charge. Then the following steps are performed:

(i) Look for the n charges suffering the greatest electrostatic forces and store their positions in an array. Initially, the N charges considered are placed at random on the unit sphere.

(ii) Calculate the positions of the n charges chosen if they are to be displaced by an angle ϑ in the direction of the corresponding force.

(iii) Using the Gray code (see below), make all possible combined movements (2^n) of the chosen charges and pick up the movement which results in the configuration with the lowest energy.

(iv) If the previous step reduces the total energy, go back to the first step.

(v) In the opposite case, reduce the angle ϑ by a constant factor, which we choose to be equal to 2. Increase the number n with an algorithm that takes into account the energy reduction in the latest iteration and the computer time per iteration, as a function of n . Stop the program when the energy difference between the present configuration and the

configuration we were in the last time we performed this step is smaller than a prefixed value, which we choose to be equal to 10^{-10} .

(vi) The whole procedure is repeated (usually 100 times) for different initial random configurations of the charges. The energy of the different metastable or ground states obtained in each run is stored.

The Gray code was introduced in coding theory in order to minimize the effects of a single transmission error. A wrong bit in an integer number codified according to this code only changes the correct number in one unit. Successive integers only differ by one bit [19]. The energies of the 2^n combinations of charge movements are calculated sequentially with the Gray code, so that only one charge is displaced between any two combinations. Thus, the energy of each combination can be obtained from the energy of the previous one by adding a term that includes the effects of one sole charge movement.

The number of possible simultaneous transitions n is a crucial parameter. There is an optimum n that maximizes the energy reduction per iteration divided by the corresponding computer time. This optimum number increases as the energy approaches its absolute minimum. We modify n dynamically within the program, which helps to reduce the slowing down speeds up the process of reaching the minimum energy. The optimum n also increases with the total number of charges considered. We found that the best initial value of n is 3, independent of the number of charges N . The final value of n obtained with our dynamical algorithm depends on the particular configuration chosen, and on average is approximately equal to 9 for systems with a number of charges of the order of $N = 100$.

3. Ground-state energy

For $N \leq 100$ we are able to reproduce the better results that have been obtained by any other methods. In particular, for $N = 78$ we get the value of the energy obtained by Edmundson [5], with symmetry arguments that the constrained global optimization method was unable to find.

In table 1 we show our results for $101 \leq N \leq 135$. As Erber and Hockney pointed out, the number of distinct fairly stable low-energy configurations increases exponentially with the number of charges considered. Furthermore, the ground state is not necessarily the most easily reachable configuration, so the algorithm has to be repeated many times for different initial random configurations, and the speed of the numerical method is a critical factor. For each initial configuration, our algorithm takes less than 2 minutes for $N \sim 100$, and about 5 minutes for $N \sim 130$ in a R8000 CPU.

As a measure of the stability of the ground-state configuration, we calculate the frequency of appearance or 'capture basin' of the ground state as the final metastable stage of our algorithm for different random initial configurations. In figure 1, we show this frequency as a function of the number of charges on a semilogarithmic plot. We can see that the frequency tends to zero exponentially, but with very large fluctuations. The straight line in figure 1 corresponds to the function

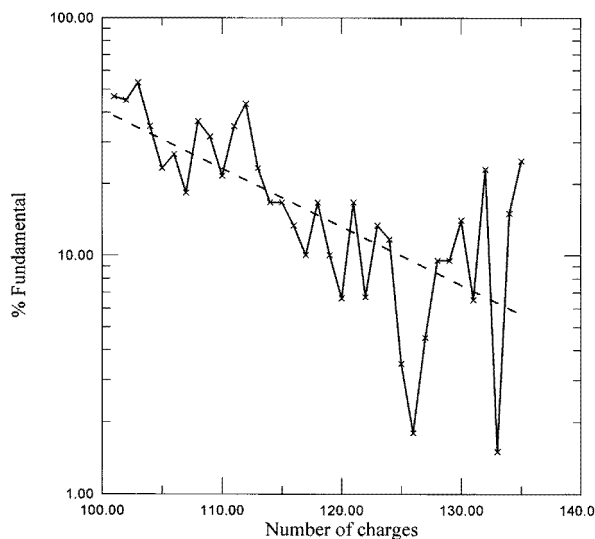
$$f = f_0 e^{-0.056N} . \quad (2)$$

This curve is a good indication of how many different initial configurations must to be attempted to be reasonably sure of obtaining the ground state. (What we call ground states here are the smallest energy configurations we reach for each N . There is no way to be sure that one has reached the true ground state of the system.) Erber and Hockney [18] found that the number of metastables states (M) depends on the number of charges in the form

$$M \propto e^{0.0497N} . \quad (3)$$

Table 1. Minimal-energy values obtained for Thomson's problem of N point charges on the surface of a unit sphere.

N	Energy	N	Energy
101	4540.590 05	119	6364.347 32
102	4633.736 57	120	6474.756 33
103	4727.836 62	121	6586.121 95
104	4822.876 52	122	6698.504 47
105	4919.000 64	123	6811.827 23
106	5015.984 59	124	6926.169 97
107	5113.953 55	125	7041.473 26
108	5212.813 51	126	7157.669 22
109	5312.735 08	127	7274.819 50
110	5413.549 29	128	7393.007 44
111	5515.293 21	129	7512.107 32
112	5618.044 88	130	7632.167 38
113	5721.824 98	131	7753.205 17
114	5826.521 57	132	7875.045 34
115	5932.181 29	133	7998.179 21
116	6038.815 59	134	8122.089 72
117	6146.342 45	135	8246.909 49
118	6254.877 03		

**Figure 1.** Logarithm of the frequency of occurrence of the ground state as a function of the number of the charges of the system.

The similar absolute value of both exponents confirms the hypothesis that the main factor affecting the frequency of occurrence of the ground state is the number of metastable states. We have calculated the dependence of the number of metastable states obtained with our method on the number of charges. We obtained the same exponent as in (3), but the constant of proportionality is smaller in our case by a factor of 0.8. Thus, the number of metastable states with respect to only one-electron transitions is about one quarter the number of metastable states with respect to more than one-electron transitions.

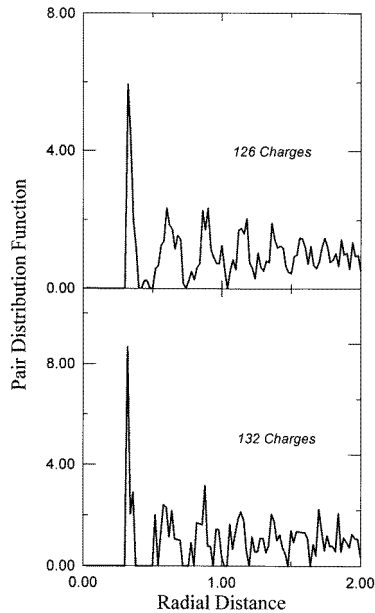


Figure 2. Pair distribution function versus distance for the ground state for $N = 126$ and $N = 132$.

4. Nearest-neighbour distribution

We study the pair distribution function (PDF) for a different number of charges. We found that in the ground state, when charges are disposed on their minimal-energy positions, the PDF presents both very pronounced peaks and forbidden distances. Even in the low-energy metastable state, the peaks and the gaps in the PDF are quickly smoothed out. The figure of the PDF in [3] is similar to our results for the metastable state considered. Thus we conclude that in the true ground state the PDF is more similar to that of a crystal than the results previously reported, at least for most values of N .

In figure 2 we show the PDF for $N = 126$ and for $N = 132$ which are very unstable and very stable systems, respectively. In both cases, the first peak corresponds to nearest-neighbour charges. The number of nearest-neighbour pairs can be counted, for most values of N . We plotted the spatial charge distribution and checked that the charges have either six or five nearest-neighbour charges. So, the number of charges with five nearest neighbours can be deduced from the total number of nearest-neighbour pairs. We found that all the ground-state configurations, for $N > 100$ have 12 charges with five nearest neighbours. Furthermore, we checked that these 12 charges are roughly arranged at the corners of an icosahedron, and their positions are extremely similar to those of a system of 12 charges on a sphere. When the ground state is very stable, the charges with five nearest neighbours are very well defined, meaning that the distance of all of them to their nearest neighbours are all practically the same, and so the first peak in the PDF is very sharp, as for $N = 132$ in figure 2. On the other hand, ground states with ill-defined nearest neighbours are difficult to reach, as for $N = 126$ in figure 2.

We also try to obtain correlations between the stability of the ground state and fluctuations in the total energy of the system, but with no success. The total energy of the system is roughly proportional to N^2 and presents extremely small fluctuations around this global tendency, which we believe is due to the long-range character of the interaction. The nearest-neighbour distribution (either distances or angles) is clearly the most sensitive

tool to study the ground-state stability.

5. Conclusions

We found that our many-particle jumps energy minimization technique is especially suited to Thomson's problem. We calculated the ground-state configurations for $N < 136$ and found that the charges arrange themselves on a triangular lattice with some 'defects', which correspond to charges surrounded by only five nearest neighbours. The number of defects is equal to 12 for $N > 100$ and these occupied the corners of an icosahedron, which constitutes an extremely stable configuration. The ground state for a given number of charges is very stable when its first peak in the PDF is well defined and vice versa.

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