The Structure of Metastable States in The Thomson Problem

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Abstract. A practical numerical method for the effective solution of the Thomson Problem is proposed. The developed iterative algorithm allows to conduct theoretical researches such as study of the number of asymptotic solutions depending on the particle count. Metastable states of charged point systems on a unit sphere were considered and the probability of falling into the basin of each state was obtained. Founded upon the algorithm and dual lattice representation approach, the framework for rapid construction of capped carbon nanotubes was created.

1. Introduction

What configuration of N unit point charges on a unit sphere minimizes the electrostatic potential energy of the system? Mathematically it is required to minimize the following energy functional for given N:

$$W(r_1, \ldots, r_N) = \sum_{i<j} \frac{1}{|r_i - r_j|}, \tag{1}$$

where $r_i \in \mathbb{S}^2$ for $i = 1, \ldots, N$.

The given problem was initially presented 1904 by Thomson and nowadays is one of the unsolved problems of the 20th Century. The development of numerical optimization methods for solving the Thomson Problem draws close attention of professionals due to its high complexity [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. According to [2], the number of metastable configurations shows exponential asymptotic behavior with respect to N. Moreover, the region containing the global minimum is often small compared with those of other minima [4], which adds to the aforementioned difficulty of the Thomson problem. The Thomson problem has been tackled by several methods such as steepest descent [2], constrained global optimization (CGO) [3], generalized simulated annealing algorithm [5, 6], genetic algorithms [4], and variants of Monte Carlo [8, 11]. However, the lowest energy solutions were systematically catalogued only for $N < 400$ and for selected structures up to $N = 4000$ [8, 11]. Recent studies of the Thomson Problem revealed its significant application in the capped carbon nanotubes design [12, 13].

During the last decade a keen interest of researchers from various scientific fields has been caused by design and study of the properties of nanomaterials. Nanomaterials are generally

materials containing structural elements, that do not exceed 100 nm along one dimension and thus develop entirely new properties.

Recently, increasing interest is caused by carbon nanotubes (CNTs) [14]. CNTs offer new opportunities for biological and medical applications: visualization of molecular, cellular and tissue structures, design of biosensors and its base electrodes, targeted delivery of various substances, radiation and photothermal therapy.

The most promising property of CNTs within biomedical applications area is its ability to penetrate various tissues of the body and transport large doses of agents, resulting in diagnostic and therapeutic effects [15].

2. Dynamic Monte Carlo simulation method

2.1. Methodology

We introduce a new statistical approach to the problem that allows to find not only ground state but also stable charges configurations and measure the degree of sustainability.

The proposed algorithm consists of 2 main stages:

2.1.1. Stage 1

(i) Let $m := 0$.
M sets each of N independent and uniformly distributed on a unit sphere $\xi_i \in U(\mathbb{S}^2)$ points are constructed. For random number generation puprose the Mersenne Twister PRNG is used.

(ii) Let $r_1, \ldots, r_N$ be radius vectors of on sphere distributed points, i.e. $|r_i| = 1$.

2.1.2. Stage 2

(i) Let $m := m + 1$.
The next set $r_1, \ldots, r_N$ of independent and uniformly distibuted on a unit sphere points is considered.

(ii) If $m > M$ then Stop.

(iii) For each pair $(i, j : i \neq j)$ the Coulomb force is modeled:

$$F_{ij} = \frac{(r_j - r_i)}{|r_j - r_i|^3}, \qquad \forall i, j : i \neq j. \tag{2}$$

(iv) For each point r_i the resultant is calculated:

$$F_i \equiv F(r_i) = \sum_{j, j \neq i} F_{ij}, \qquad \forall i. \tag{3}$$

(v) Now, let us displace the points on each iteration so that the potential energy of the system would decrease, i.e. let us find such $r'_1, \ldots, r'_N$, that

$$W(r'_1, \ldots, r'_N) < W(r_1, \ldots, r_N), \qquad W(r_1, \ldots, r_N) = \frac{1}{2} \sum_{i \neq j} \frac{1}{|r_i - r_j|} \tag{4}$$

It can be accomplished in the following steps:

(a) Let us choose k_1 from the condition:

$$F_{k_1} = \max_i |F_i| \tag{5}$$

(b) The k_1-th point is chosen and displaced according to the rule

$$r'_{k_1} = \gamma(r_{k_1} + \alpha F_{k_1}), \tag{6}$$

where α is specially selected factor responsible for the method's rate of convergence, γ is a normalizing factor that meets the terms $|r'_i| = 1$, r'_i is a new position of the i-th point.

(c) The transition from F_n to F'_n is carried out according to the rule

$$F_n{}' = F_n + \left(\frac{(r_j^{'} - r_n)}{|r_j^{'} - r_n|^3} - \frac{(r_j - r_n)}{|r_j - r_n|^3} \right), \qquad n \neq k_1, \quad F_{k_1}{}' = F(r_{k1}^{'}). \tag{7}$$

(d) The shift to the next iteration is performed by the change of notation

$$r'_1, \ldots, r'_N \to r_1, \ldots, r_N \tag{8}$$

and return to beginning of the iteration process.

(e) The exit of the iteration process is carried out by the following condition:

$$|W(r_1, \ldots, r_N) - W(r'_1, \ldots, r'_N)| < \epsilon, \tag{9}$$

where ϵ is the energy accuracy coefficient.

2.2. Computational framework

Based on the proposed algorithm and three-dimensional visualization the computational software suite was created. Primarily aimed at the Thomson Problem solution, the program makes it possible to compute metastable configurations of point charges not only on a unit sphere but also on an arbitrary convex surface, therefore creating many significant applications. One of them is capped carbon nanotubes construction.

NanoDesigner is a multifunctional framework extension for the computer design of low energy fullerene and capped nanotube structures. This software provides an ideal tool to accompany the study of the finite carbon molecules using atomistic computer simulation.

The computational core of the framework was written in C++11 using OpenMP and Intel C++ Compiler. Moreover, the dynamic calculation precision contributes to the better rate of convergence (see figure 1).

The results' analysis and visualization modules were implemented by MATLAB routines.

3. Results and conclusions

The aim of this study was to investigate metastable configurations and the convergence probability of a number of initial point system to each metastable state. The exponential asymptotic behavior of the metastable states number mentioned in [2] is confirmed (see figure 2). As mentioned in [16], the global minimum will most likely be obtained comparing to any metastable state. However, our computational experiments show the opposite for some N – the specific cases are presented in tables 1, 2. They illustrate also the complexity of metastable states distribution.

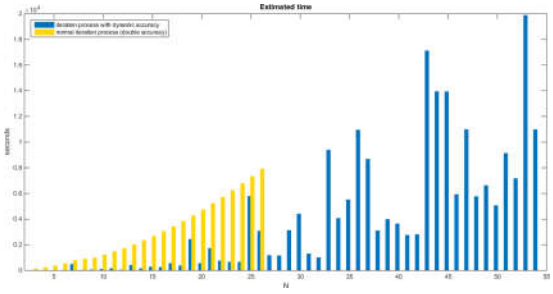


Figure 1. Comparison of the normal and dynamic iteration process (the computational precision grows near local extrema)

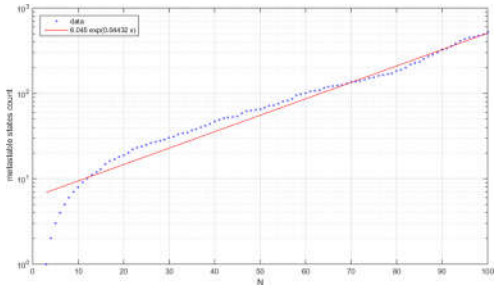


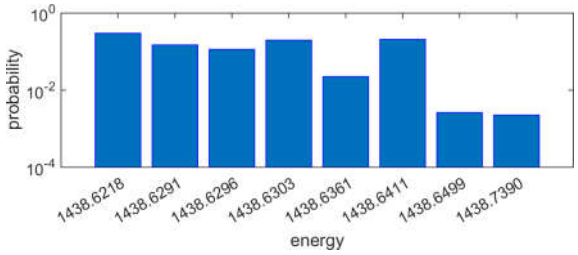
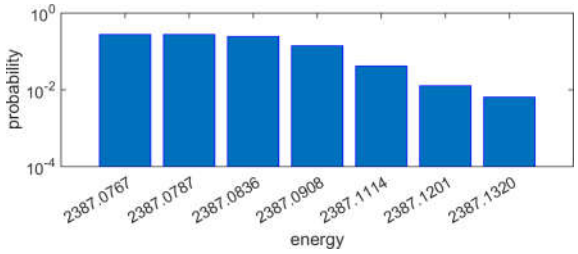
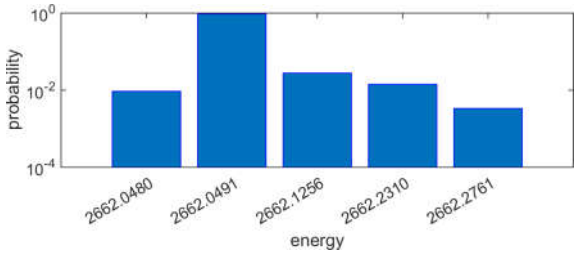
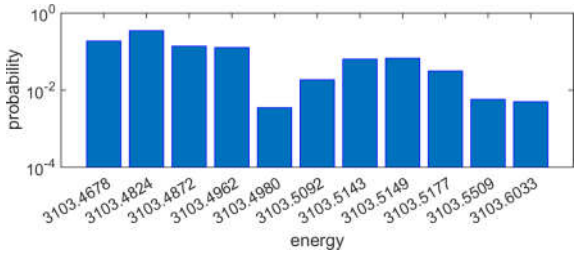
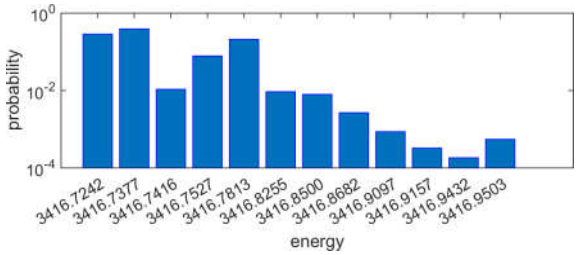
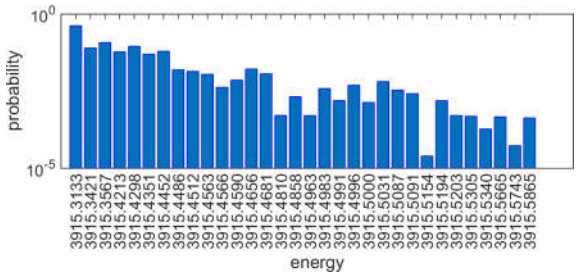
Figure 2. The metastable states number integral function and its exponential approximation

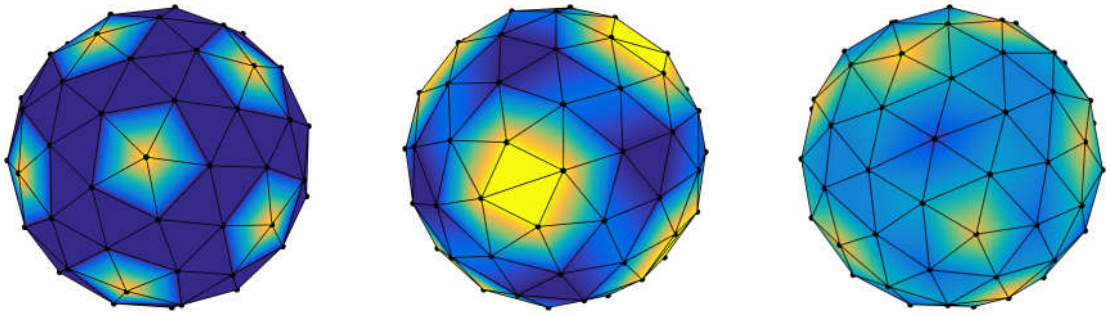
Table 1. Metastable states structure. It is important to note that already for $N = 37$ the global minimum is less likely to be obtained.

N	Stable state index	Occurence probability	Potential energy
16	1	0.75108	92.9125
16	2	0.24892	92.921
32	1	0.98558	412.2613
32	2	0.01442	412.469
37	1	0.24495	560.6213
37	2	0.75505	560.6295
46	1	0.15752	886.1687
46	2	0.67819	886.1716
46	3	0.15982	886.179
46	4	0.004477	886.2521

Despite the fact that numerical iterative methods aimed at the Thomson Problem solving have been intesively developing during last decade, the construction of the numerical algorithm that effectively enables us to find all solutions for $N > 500$ is a desirable goal for many applied researchers. Perhaps, our research provides another step in the right direction.

Table 2. Metastable states structure. The complexity grows rapidly as N increases.

N	Number of metastable states	Configurations structure
58	8	
74	7	
78	5	
84	11	
88	12	
94	32	



$E = 2255.00237$ $E = 2255.133326$ $E = 2255.26606$

Figure 3. Stable point configurations for $N = 72$ (force absolute value distribution coloring)

Acknowledgments
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