Minimum Energy Configurations of Charges on a Conductive Disc

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Using simulated annealing, the global minima of N identical charges on a conductive disc was simulated up to N=29. Computational methods are discussed for accuracy and efficiency, solutions obtained agree with those obtained by Erko and Oymak[1] as well as Worley[2].

Keywords: Electrostatics, Simulated Annealing, Global Minimum, Charge Distributions

I. INTRODUCTION

Given N identical charges placed on a finite conductive surface they will diffuse in a manner as to minimise the potential energy of the system. Solutions to such optimisation problems were notably considered by J. J. Thomson when describing the plum pudding model[3] and more recently, for the study of manipulation of small semiconductor particles known as quantum dots which have potential applications in transistors, quantum computing[4] and medical imaging[5]. The configurations to the ground state minima are not necessarily trivial and various approaches since have been explored since the initial proposition put forward by Berezin in 1985[6].

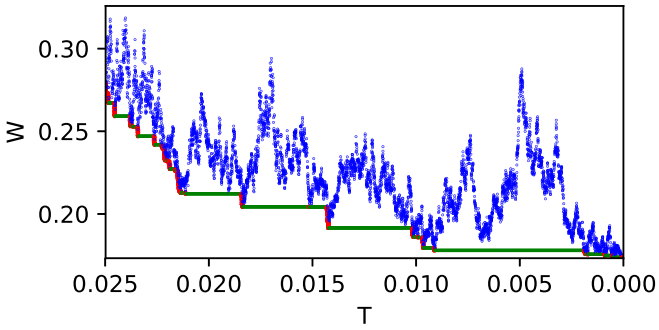

FIG. 1. The process of simulated annealing for N = 3, red points are new lowest found minimum energies.

II. COMPUTATIONAL DETAILS

A. Simulated Annealing

N identical charges were randomly generated within a radius r = 10 disc and allowed to diffuse through incremental motion. The total energy of the system was calculated through the sum of the non-dimensional equation for the electrostatic potential energies of each of the charges.

$$W = \frac{1}{2}\sum_i \sum_j \frac{1}{r_{ij}} \tag{1}$$

where r_{ij} is the distance between charge i and j and the factor of a half accounts for double counting. For calculations, a random moment was generated, ones that lowered the total energy were always accepted, while those that caused the total energy to increase were accepted with a probability proportional to

$$P \propto \exp(-\Delta W/T) \tag{2}$$

This process was repeated for a fixed value of temperature with the amount of runs proportional to the number of charges, this ensured that each charge had roughly an equal amount of moves irrespective of the total number of charges (~ 400 moves per charge). Initially, the increment of movement, dl, and the number of moves for each charge must be sufficiently large to allow the particles to be able to move across the entire solution space and thus a value of $dl = 0.4$ was chosen as $400 \times 0.4 = 160$ allowed a single charge to have the ability to move about the entire diameter of the disc.

At high temperatures, all possible motions are permitted except those that place the charges outside the disc, and configurations with notably low total energies were saved. After a set amount of movement iterations, the system was cooled and dl decreased by $\sim 4\%$, causing less configurations that raised the energy to be accepted and allowing the simulation to 'home in' on minima, an example of this process is depicted FIG. 1 .

B. Circumventing Local Minima

The choice of annealing, rather than other methods such as hill a climb algorithm, was chosen for solving for the minimum potentials as for higher N configurations (N > 11); which are discussed later, have the characteristic of having multiple solutions with similar energies but with discrete configurations as seen in FIG. 2. Traditional hill climb algorithms are strongly dependent on the initial conditions of the system and have no method to distinguish local minima from global minima.

Some solutions to getting trapped in these local minima include, reverting back to a previously found higher energy configuration if no new lower energies are found after a certain amount of runs, this can be computation-

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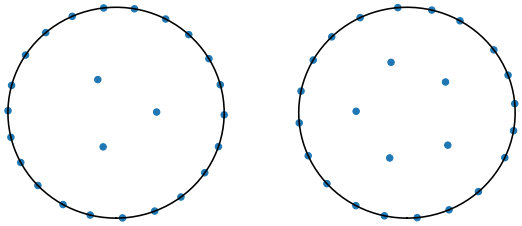

FIG. 2. Two configurations for N=25 with total energies $W_{Tot} = 32.20816$ and $W_{Tot} = 32.15070$ respectively. The configuration with three charges inside is a metastable local minima, while the other with five is the global minima.

ally intensive however it significantly lowers the probability of getting trapped in these suboptimal potential wells. Randomly regenerating the charges positions to see if they tend to a lower configuration or having a probability of a charges randomly moving by large increments in random directions in an attempt to get out of these holes.

There is no sure way to know if a given solution is the global maximum without trying every possible combination, however we can assess to a degree of certainty using the above method, coupled with some sensible intuition to determine whether or not a given solution is correct.[7]

C. Program Optimisation

Each additional charge increases the computational time, therefore optimising the task of calculating the total energy is of special interest. One method is storing the total energy as a sum of energies each of the individual particles, and storing the energies of the individual particles as partial sums of the inter-particle energies. This means that when calculating a positional change of one particle, the corresponding new $\frac{1}{r_{ij}}$ value can be replaced in each of the partial sums and the total energy can be recalculated by summing the list. This is in contrast with recalculating the total energy explicitly at every step.

A possible method to reduce the total amount of iterations required would be to manually generate the initial positions based upon theorised underlying geometry, this however bares the problem of excluding the possibility of states existing that do not fit the hypothesised model as possibly found by Worley for N=185.[2]

Cerkaski and Nazmitdinov[8] approached the same problem by using a theoretical semi-analytical approach by means of analysing the actual coulomb interactions between the particles themselves, thereby removing the random and probabilistic parts from the computational analysis and speeding up the process dramatically, they claim remarkably accurate configurations upto N = 400.

III. RESULTS AND DISCUSSIONS

A. Results for N = 2 to 29

Simulations up to N=29 were conducted, all plots are found in VI appendices, and the following observations were made for the minimum energy ground states are shown in TABLE I.

TABLE I. Results for $2 \leq N \leq 29$.

N	Outer Shell	Inner Shell	Energy (W)
2	2	0	0.050004 ± 0.000001
3	3	0	0.173232 ± 0.000018
4	4	0	0.382930 ± 0.000084
5	5	0	0.688452 ± 0.000031
6	6	0	1.097088 ± 0.000044
7	7	0	1.614198 ± 0.000123
8	8	0	2.245100 ± 0.000444
9	9	0	2.994453 ± 0.000250
10	10	0	3.864899 ± 0.000291
11	11	0	4.861904 ± 0.000390
12	11	1	5.960433 ± 0.000574
13	12	1	7.185563 ± 0.000749
14	13	1	8.541193 ± 0.000718
15	14	1	10.02891 ± 0.000479
16	15	1	11.65662 ± 0.003831
17	15	2	13.41861 ± 0.008185
18	16	2	15.33275 ± 0.027040
19	16	3	17.34612 ± 0.018671
20	17	3	19.41057 ± 0.043897
21	18	3	21.67380 ± 0.034671
22	18	4	24.13014 ± 0.012186
23	19	4	26.67799 ± 0.068790
24	20	4	29.32740 ± 0.017570
25	20	5	32.15070 ± 0.017150
26	21	5	34.95413 ± 0.041319
27	22	5	38.04146 ± 0.028454
28	22	6	41.18431 ± 0.042809
29	23	6	44.50067 ± 0.018105

The uncertainty in the energy (W) was calculated via the standard deviation (σ) and standard error ($SE_{\overline{W}}$) with the use of three repeats (n) for each value of N. The full list with all values is found in VI Appendices. However due to the nature of the process, the calculated errors are incredibly small and can be neglected in most cases, they are presented here for completeness.

For values $N = 1$ to $N = 11$, the charges concentrated in an equidistant fashion around the circumference of the disc as in FIG. 3. $N = 12$ was the first configuration that did not fit the pattern of having the charges distribute around the circumference of the disc, instead the 12th charge was positioned at the center of the disc, as seen in FIG. 4. Berezin[6] proposes that possible solutions for this could be explained using catastrophe theory, and fundamentally arises from the fact that there cannot be a fully symmetrical placing of charges around the disc except for N = 1, 2, 3, 4, 6, 8,12 and 20, therefore other number of charges cause a finite degree of structural instability

resulting in non trivial configurations.

The single central charge configuration continues upto $N = 16$, then for $N = 17$ an additional charge is added at the centre, this continues to occur as shown in TABLE I upto $N = 29$ where 6 charges form a ring in the center FIG. 5.

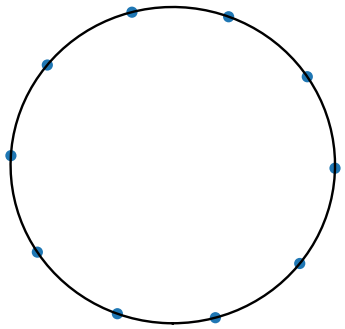

FIG. 3. Configuration for N=10.

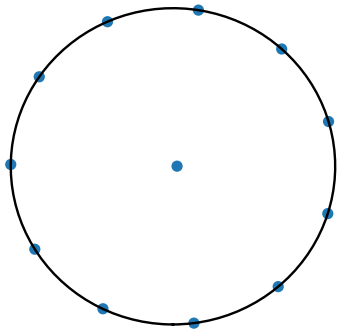

FIG. 4. Configuration for N=12.

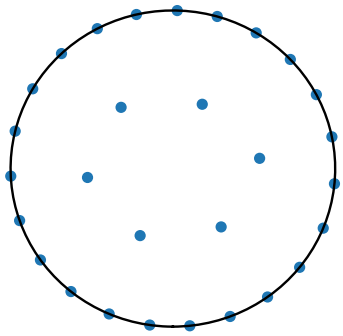

FIG. 5. Configuration for N=29. The asymmetry is due to limited computational time for the simulated annealling process.

B. Comparison to Theoretical Models

Erko and Oymak[1] propose a theoretically derived relationship between the total energy and the number of charges in the system given by

$$W(N) = \frac{\pi}{4}N^2 - 1.5599728N^{\frac{3}{2}} + 0.9509338N \qquad (3)$$

The above equation is for a disc of unit radius, and so to compare this to our $r = 10$ disc we must multiply our values of energy by a factor of 10.

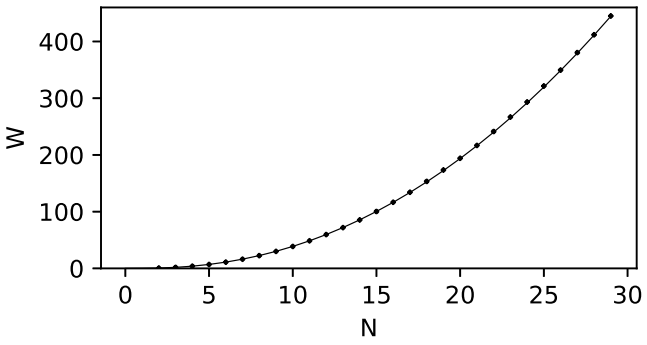

FIG. 6. Graph showing $10W$ plotted against N, the solid line is eq. 3.

Plotting the energies in table I multiplied by 10 against eq. 3 we obtain FIG. 6, we expect to find the simulated energies calculated by eq. 1 to coincide with this formula exactly as stated by Erko, and indeed, they do.

IV. CONCLUSION

Through on the process of simulated annealing, we have obtained conjectural estimates for the global minima configurations for the first 29 systems of N charges on a conductive disc. These are in agreement with pre-existing literature

Further extensions to higher values of N are possible but would require exponentially larger computational power, and so more efficient alogorithms than basic simulated annealling could prove more useful. Extensions to three dimensions have been studied in great detail and remains a problem of interest to mathematical researchers, as well as professionals working in the firlds of viral morphology, crystallography, molecular structure and quantum computing[9].

V. REFERENCES

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VI. APPENDICES

The following equations were used to calculate the standard deviation and standard error given in TABLE II.

$$\sigma = \sqrt{\frac{\sum \left(W - \overline{W}\right)^2}{(n-1)}} \tag{4}$$

$$SE_{\overline{W}} = \frac{\sigma}{\sqrt{n}} \tag{5}$$

TABLE II. Results for 2 ≤ N ≤ 29.

N	W1	W2	W3	$\overline{W}$	σ	SE
2	0.050008	0.050007	0.050004	0.050006	0.000002	0.000001
3	0.173232	0.173274	0.173293	0.173267	0.000031	0.000018
4	0.38293	0.38301	0.383214	0.383051	0.000146	0.000084
5	0.688555	0.688452	0.688524	0.68851	0.000053	0.000031
6	1.09712	1.097232	1.097088	1.097147	0.000076	0.000044
7	1.614546	1.614582	1.614198	1.614442	0.000212	0.000123
8	2.245657	2.2451	2.246621	2.245793	0.000769	0.000444
9	2.994864	2.99532	2.994453	2.994879	0.000433	0.00025
10	3.865333	3.865904	3.864899	3.865378	0.000504	0.000291
11	4.861904	4.863185	4.862169	4.862419	0.000676	0.00039
12	5.960541	5.962206	5.960433	5.96106	0.000994	0.000574
13	7.185869	7.187947	7.185563	7.18646	0.001297	0.000749
14	8.543614	8.542896	8.541193	8.542568	0.001244	0.000718
15	10.03044	10.02891	10.02912	10.02949	0.000829	0.000479
16	11.65662	11.66894	11.65849	11.66135	0.006635	0.003831
17	13.41861	13.43918	13.4458	13.43453	0.014177	0.008185
18	15.3464	15.41983	15.33275	15.36632	0.046835	0.02704
19	17.4103	17.34612	17.37132	17.37591	0.032339	0.018671
20	19.55182	19.41057	19.43243	19.46494	0.076032	0.043897
21	21.67379	21.74277	21.79343	21.73666	0.060052	0.034671
22	24.13014	24.16038	24.17077	24.15377	0.021106	0.012186
23	26.71513	26.67799	26.90041	26.76451	0.119147	0.06879
24	29.32747	29.38015	29.3274	29.34501	0.030431	0.01757
25	32.1507	32.2084	32.19179	32.18363	0.029704	0.01715
26	34.95413	35.041	35.09608	35.03041	0.071567	0.041319
27	38.04146	38.14001	38.09231	38.09126	0.049284	0.028454
28	41.33209	41.2689	41.18431	41.26177	0.074147	0.042809
29	44.50067	44.56285	44.52462	44.52938	0.031359	0.018105