Minimising The Energy of Charged Particle Configurations on a Circular Surface by Means of Simulated Annealing

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Abstract
In this article, we explore the configurations of charged particles confined on a circular surface. In such a physical system, the configuration will tend towards a minimised energy state. Here, we try to find that configuration and, in particular, the global minimum. This was carried out by performing simulated annealing. We investigated the effect of different cooling schedules, i.e. linear, exponential logarithmic or sigmoidal, the length of the Markov chain, and the number of iterations run for each temperature. We found that a slow exponential cooling scheduls with a long enough Markov chain yields accurate results which confirm the theory. Additionally, we determined that it is important to do full exploration of the configuration space and choose a respective step size in order to avoid getting stuck in local minima. We found that the energy was the lowest with all particles on the edge of the circle up until eleven particles. For twelve particles, we found that the optimal energy configuration had one particle centered, while the rest remained on the rim. For future research, we suggest exploring the effect of adding forces between the particles in order for their movement to favour a direction and, therefore, converge more quickly.

1. Introduction

In 1904, the physicist J.J. Thomson investigated the stability and the minimum electrostatic potential energy configuration of N electrons in a constrained space such as the surface of a sphere (Thomson, 1904). The general Thomson problem can be applied to many domains involving the electrostatic properties of an electron such as Valence shell electron pair repulsion (VSEP) theory in chemistry, the structural arrangement of proteins and drugs in biochemistry or the analysis of superconducting metal in physics.
In this report, the Thomson problem is restricted to a circle with different numbers of electrons. According to the second law of thermodynamics, a system with charged particles seeks to reach a stable configuration by minimising the total energy. However, iterating through all the possible states in order to find the minimum energy is ineffective due to the infinite number of possibilities.

To circumvent this problem, simulated annealing can be used. The probabilistic technique locates the global optimum of a given problem by using a heuristic approach in order to avoid any local optimum.
In this report, we aim to find the minimum energy configuration by means of simulate annealing. We hypothesised that the principle of minimum energy forces the particle to spread evenly over the circle by first creating a polygon on the edge of the circle. A higher N would induce polygons forming towards the inner of the circle.
Furthermore, we hypothesise that for the simulated annealing a slow cooling and the displacement method of the particles is crucial to reach a global minimum. A slow cooling schedule would allow the system to stay in equilibrium with its phase space, furthermore the right displacement strategies would circumvent the possibility of getting stuck in a local minimum.

2. Background & Theory

This section consists of two main parts. Firstly, the electrostatic system will be discussed. Secondly, we will discuss a technique called the simulated annealing.

2.1. Electrostatic systems

An electrostatic system consists of charged particles interacting with each other. This interaction happens via the electrostatic force, which is described by Coulomb's law:

$$F_e = k_e \frac{q_1 q_2}{r^2}, \tag{1}$$

in which F_e is the electrostatic force, k_e is Coulomb's constant, the q's represent the signed magnitude of the charges and r is the distance between the charges. When opposite charges are present, i.e. negative and positive, they attract each other, while equal sign forces repel each other.

The energy that is stored between two charged particles as a result of the Coulomb force, is given by:

$$U_e = k_e \frac{q_1 q_2}{r}, \tag{2}$$

where U_e is the potential electric energy. Generalising this equation for the total electrostatic interaction energy U in a system of N electrons, renders:

$$U_{ij}(N) = k_e \sum_{i<j}^{N} \frac{e_i e_j}{r_{ij}} \tag{3}$$

where r_{ij} is the distance between electron e_i and e_j and e_i and e_j represent the magnitude of the electron charge:

$$r_{ij} = |r_i - r_j| \tag{4}$$

As a result of the electrostatic force between opposite charges, such as a system consisting of electrons, the charges will move to the configuration with the lowest energy. In an unbounded system, this would mean that the charges repel each other to infinity. However, in a confined system, the charges will settle into a system with the largest average distance between the charges in comparison to similar neighbouring configurations. First, a polygon of particles is formed on the surface of the circle. However, magic numbers such 12 forces the system into a configuration with an electron at the centre. Higher magic numbers even induce the formation of inner polygons (Wille & Vennik, 1985).

In case of all the charges being placed on the edge of the circle, one can use equation 3 to write the total energy as

$$U_{ij}(N) = \frac{n}{4} \sum_{k=1}^{n-1} \frac{1}{sin(k\pi/n)} \tag{5}$$

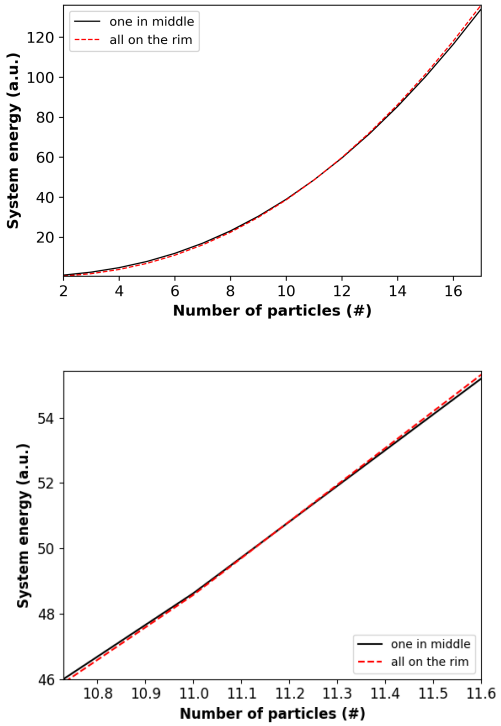

Figure 1: Shows the theoretical energy for the optimal configurations with all particles on the rim and with one particle in the middle.The bottom graph is a zoom-in of where the two curves overlap.

In case of one particle being placed in the centre, the total U can be expressed by

$$U_{ij}(N) = (n-1) + \frac{n-1}{4}\sum_{k=1}^{n-2}\frac{1}{sin(k\pi/n)} \quad (6)$$

Using these formulas, one finds the first magic number to be 12, as is shown by figure 1. In figure 1, we see that between 11 and 12 particles the energy of all particles on the rim becomes higher than the configuration with one particle in the middle.

Using formula 5 and 6, we find energies 38.624 a.u. and 38.923 a.u. for 10 particles, all on the rim and one in the middle respectively. For 11 particles, we find 48.576 a.u. and 48.624 a.u., respectively. Lastly, for 12 particles we find 59.807 a.u. and 59.576 a.u.

2.2. Simulated Annealing

The problem of finding the global minimum of a function is a well known challenge in computational problems. To this extent, simulated annealing can be applied.

Simulated annealing is a modification of the Metropolis-Hastings algorithm that was presented in 1953 by Metropolis (Metropolis et al., 1953). The algorithm was first applied by Kirkpatrick et al. (1983) as a method for solving the travelling salesperson problem.

Simulated annealing works by generating a Markov chain of states. For every step, a new state is randomly generated. If the newly generated state is more probable, i.e. has less energy in minimisation problems, we accept the state and move on to that state. If the newly configured state is less probable, there will be a chance of acceptance. This chance is given by the Boltzmann distribution:

$$P = e^{\frac{E_2 - E_1}{kT}} \quad (7)$$

where E_2 is the energy of newly generated state, E_1 the energy of the current state, k the Boltzmann constant and P is the chance of a state being accepted. T denotes the "temperature" and influences the probability of accepting the new state. By accepting transitional configurations (higher total energy U), one avoids getting stuck in local minima. By cooling the temperature T slowly, the probability P of accepting a non-favourable state decreases. Thus the system converges to a global optimum by gradually rejecting more non-favourable states. The outcome is dependent on the cooling procedure, which must be applied with care. The cooling procedure can be applied in, for example, a linear, exponential, logarithmic or sigmoidal fashion (Nourani & Andresen, 1998). Firstly, the linear method constantly

decreases the temperature by a constant α. Secondly, the exponential cooling schedule decreases the temperature according to

$$T(t) = T(0)\alpha^t \tag{8}$$

with t denoting the time step/state. Thirdly, the logarithmic cooling schedule is governed by the following function

$$T(t) = \frac{c}{log(t)} \tag{9}$$

with c set to the largest energy barrier or higher. Due to the logarithmic term the exponent in the Boltzmann term cancels. Consequently, the search for the global minimum is highly random and the convergence is slower. A fourth cooling schedule is sigmoidal cooling. The idea behind this method is a slow melting of the system, while retaining a large freezing stage. This cooling schedule follows

$$T(t) = \frac{a}{1 + e^{bx-c}} \tag{10}$$

However, the cooling procedure doesn't converge to a global minimum if the total system is not in equilibrium with its environment (Nourani & Andresen, 1998). In order words, it is important to take enough iterations at each temperature, i.e. Markov chain length, in order to avoid any disequilibrium.

An example of the effect of this algorithm is shown in figure 2.

3. Methodology

The aim of this paper is to analyse the minimum energy achieved for a given number of electrons confined in a circle using simulated annealing.

The electrons were randomly initialised, confined to an unit circle, with the python library random (McKinney, 2012). The random generator makes use of the Mersenne Twister algorithm (Matsumoto & Nishimura, 1998) to generate pseudo-random numbers.

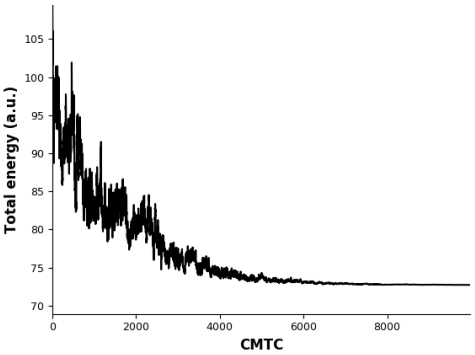

Figure 2: The freezing of the system. We see the total energy is lowered. This graph shows an exponential decrease in temperature.

In this report the electrons have equal charge. Therefore in equation 3, the charge e and Coulomb's constant can be set to 1 which results in the following formula

$$U_{ij}(N) = \sum_{i<j}^{N} \frac{1}{r_{ij}} \tag{11}$$

Thus the minimal energy is expressed by the maximal distance between each electron. An example of this phenomenon is shown in figure 3. It is clear from the example that after simulated annealing, i.e. the right state, the average distance between the particles is maximized.

Figure 3: The starting and ending configuration of electrons after simulated annealing. In the final state all particles are located at the edge of the circle, which is the state with the maximum average distance between particles.

The position of the electrons changed per iteration. First a hypothetical electron e_h was generated which potentially

Table 1: Parameters values of the general settings for the various experiments.

Parameter	Value
Markov chain length	100
Temperature range	0.5 - 10^{-6}
Iterations	100
Max step size	0.02
Cooling schedule	linear

replaces e_i. The position of e_h was defined by the location of $e_i \pm$ a random, exponentially distributed step with a mean value of 0.02. If the position of e_h yields a lower total energy U, e_h replaces e_i. Otherwise, the chance of acceptance is calculated by the equation 7. In this formula, the Boltzmann constant k was set to 1. This is done for all the electrons at each Markov state.

In order to investigate the importance of the different parameters such as the Markov chain length, the cooling procedure and the maximum displacement of the particle, a sensitivity analysis was conducted. As general parameters, the Markov chain length was set to a 100, the temperatures cooled from $0.5 - 1 \times 10^{-6}$ a.u. in a linear fashion over a 100 repetitions. This temperature range was chosen to make the average acceptance rate about 50% - 80% in the beginning of the algorithm and very low at the end of the simulation, as is shown in figure 4. The temperature changed each 100^{th} Markov state. The maximum step size was set to 0.02. For the sensitivity analysis only one parameter was modified at a time, doing the simulations for 10 particles. In these experiments, the measurement was repeated a 100 times in order to get a significant distribution of the final total potential energy U. An overview of the general parameter settings can be found in table 1.

The Markov chain length was tested for 1, 10, 100 and a 1000 states. The cooling procedure was tested for the linear, exponential, logarithmic and sigmoidal

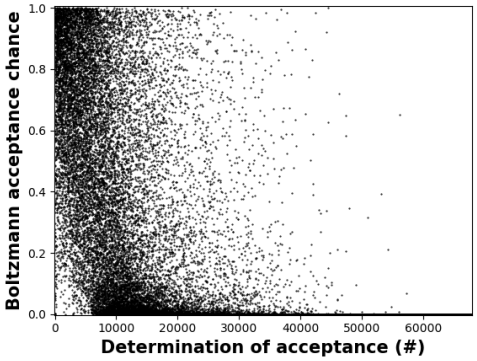

Figure 4: The chance of acceptance for generated configurations with higher energies than their prior configurations. It is clearly shown that the average acceptance chance is high in the beginning and decreases towards zero over the simulation. The simulation was done for a exponential cooling schedule.

schedule. The average step size was set to 1, 0.2 and 0.005. Finally, the best performing and computationally feasible parameters were used for 11 and 12 particles.

The results were plotted with the Python package Matplotlib (Hunter, 2007).

4. Results & Discussion

This paper researches the energy configurations of charged particles confined by a circular surface. To this extent, we ran simulations for various numbers of particles and observed the resulting configurations. In addition, we researched the influence of the cooling schedule, the length of the Markov chain, the number of Markov chains and the average step size.

First of all, we'll show the minimum energy configurations for N = 10, 11, 12, 23, i.e. number of particles. Figure 5 shows a uniform distribution of the particles on the rim for 10 and 11 particles. For N=12, the configuration contains one particle in the middle which indicates 12 to be a magic number. 23 particles generates a configuration with

a second inner circle composed of 5 particles. The visual inspection indicates that the annealing sampling is implemented correctly using the general parameters.

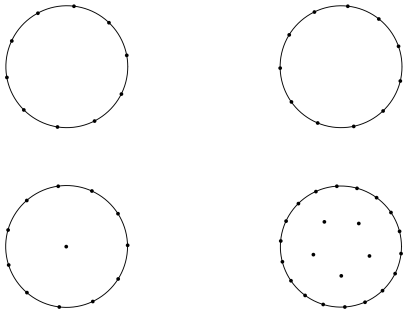

Figure 5: The optimal energy configurations for 10 and 11, 12 and 23 particles (TLBR).

4.1. Exploratory Measurements with 10 particles

In order to investigate the sensitivity of the simulation on the parameters, different measurements were carried out with 10 particles. Based on the theoretical calculations (figure 1), we chose to do the analysis with 10 particles in order to find the optimal parameters for more challenging configurations such as for 11 and 12 particles. For 11 particles the global minimum (all particles on the rim) is close to the local minimum (one particle to in the centre) energy-wise. Particle 12 represents the first magic number where the lowest energy is achieved by placing a particle in the centre.

4.1.1 Different numbers of repetitions of the Markov Chain

Figure 6 shows the minimum energy of a 100 simulations using the general parameters. Two distinct distributions can be seen with different intensity levels. Based on equation 5 & 6 and visual inspection of the configuration, we conclude the left peak corresponds to the global minimum configuration (38.62 a.u.) with all the particles on the rim. The right peak corresponds to the local minimum energy (38.92 a.u.) with one particle in the centre. In this report, we assumed that the theoretical values are the strict global/local minima achievable, due to the perfect uniform spreading of the particles. If an energy was below a theoretical local minimum, it was counted towards the global minimum energy configuration, since it is not possible to obtain lower energies with the local minimum than the theoretical value.

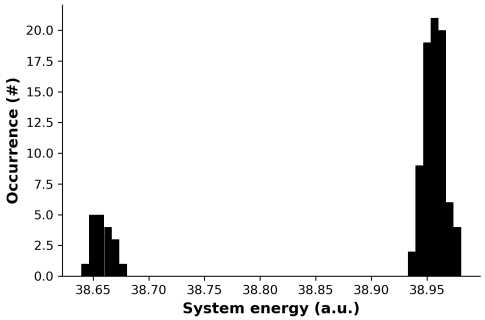

Figure 6: Minimum energy distribution with a Markov chain of 100 with a 100 repetitions, a linear cooling of 0.5- 1e-06 and a step size of 0.02 (general parameters). The global minimum was achieved 19 out of 100 simulations.

The sub-distributions emerge from a non-uniform spreading of the particles within the circle boundaries. However, the calculated minimum energy doesn't not cross the theoretical minimum energy due to the perfect arrangement assumed in theory. For the general parameters, the global minimum was achieved 19 times out of the 100 distinct simulations.

More numbers of repetitions of the Markov chains were analysed. This is equivalent to smaller temperature drops after every repetition. Figure 7 shows the distribution of a 100 system energies obtained with a Markov chain of length 100 and 10 repetitions.

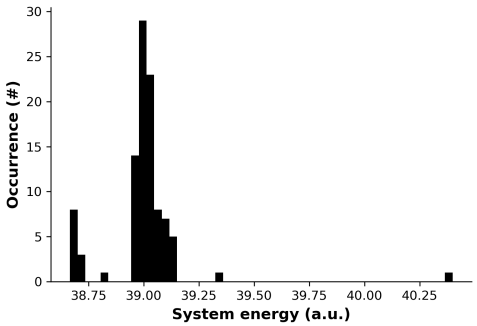

Figure 7: System energy distribution with general parameters and a Markov chain length of a 100 with 10 repetitions. The global minimum was achieved 12 out of a 100 simulations.

One can see that the distribution resembles the one from figure 6 with some additional spread at around 39.35 and 40.3. Here again, the distribution can be split in sub-distributions corresponding to the global and local minimum configurations. The global minimum configuration was achieved 12% of the time. Figure 8 represents the minimum energy distribution of a Markov chain of a 100 for a 100 repetitions. In comparison to figure 6 and 7, the two sub-distribution are more narrow.

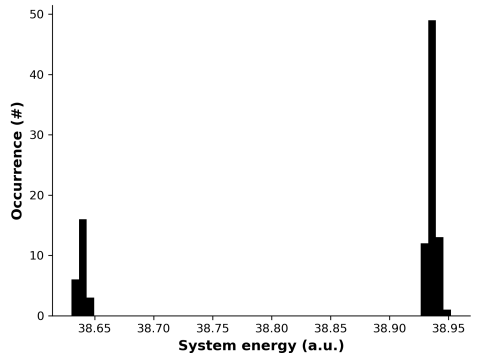

Figure 8: Minimum energy distribution with general parameters and a Markov chain of 100 for 100 repetitions. The global minimum configuration was achieved 25%.

The global minimum is achieved with 25% of the time. In order to compare the different parameters, the mean value including the variance was been computed. The existence of two distributions forced us to calculate the mean and variance of each peak separately. For the Markov chain length of a 100 with 10 repetition (figure 7, the outlier of 40.3 has been ignored for the variance calculation. This can be done as this measurement belongs to the second local minimum, for which the configuration has 2 particles in the middle. This claim is supported by the recurrence of measurements at 40.3 in other experiments, as well as by visual inspection of the configuration. The results of figures 6, 7 and 8 are summarised in table 2.

Table 2: Different numbers of repetitions of the Markov chains - Shows the average values of the peaks and their variance. Peak 1 is the left peak in the histogram and represents the lower system energy, peak 2 represents the right peak and higher energy value

Repetitions	Peak1 $\pm$ Var	Peak2 $\pm$ Var
10	38.7 $\pm$ 1.3e-03	39 $\pm$ 3.3e-03
100	38.66 $\pm$ 8.5e-05	38.99 $\pm$ 8.7e-05
1000	38.64 $\pm$ 1.5e-05	38.94$\pm$ 1.e-05

What stands out in this table is the difference in the mean minimum energy between the different repetition numbers. The more repetition are applied the closer one gets to the theoretical global/local minimum. Furthermore, the variance decreases accordingly. The larger number of repetitions also improves the performance of the algorithm to achieve the global minimum with a higher rate. An explanation for this phenomenon could be that more repetitions allow for a slow cooling, which positively affects the measurements. However, a 1000 repetitions with the remaining general parameters is computation expensive.

4.1.2 Different step sizes

In addition to a step size of 0.02, the values 1 and 0.005 were tested. Figure 9 shows the distribution of the minimum energy of a 100 simulations with a step size of 1.

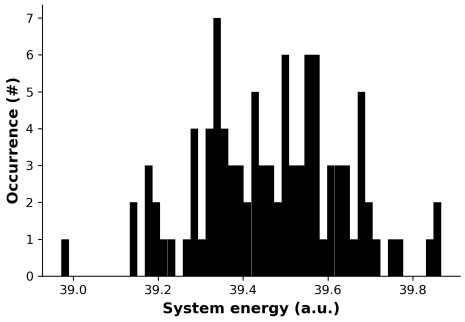

Figure 9: Minimum energy distribution with general parameters and a step size of 1. The global minimum configuration was not achieved.

The distribution has a high variance ranging from 39 to 40. By comparing with the theoretical values, we see that the global minimum is never achieved, which is clear from the fact that the energy is never below the local minimum. Figure 10 shows the distribution of the minimal energy of a 100 simulations with a step size of 0.005.

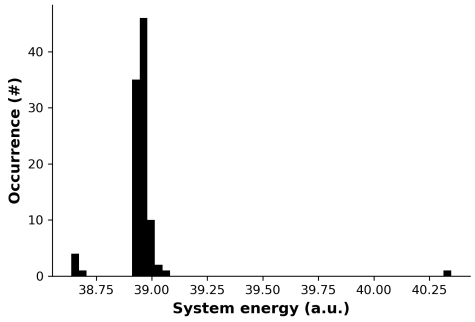

Figure 10: Minimum energy distribution with general parameters and a step size of 0.005. The global minimum configuration was achieved 5 out of 100 simulations.

One can see that the distribution is divided in two well defined sub-distributions which correspond to the different configurations. Once again the local minimum energy distribution has higher occurrence than the global minimum. In order to compare the impact of the different step sizes, table 3 compares the different mean values and their variance. For the energy distribution with a step size of 0.005, the outlier around 40.3 has been ignored for the aforementioned reason. Once again the mean and variance were calculated for the different peaks. The threshold for dividing the peaks was defined by the theoretical local minimum energy.

Table 3: Different step size - Shows the average values of the peaks and their variance. Peak 1 is the left peak in the histogram and represents the lower system energy, peak 2 represents the right peak and higher energy value

	Peak1 $\pm$ Var	Peak2 $\pm$ Var
1	/	39.47 $\pm$ 0.03
0.02	38.66 $\pm$ 8.5e-05	38.99 $\pm$ 8.7e-05
0.005	38.65 $\pm$ 2.5e-04	38.96 $\pm$ 5.5e-04

Table 3 exhibits the mean value and variance of the different step sizes. For a step size of 1, the global minimum was never achieved. Thus only one peak is formed. One can see that with an lower step size, the mean minimum energy gets closer to the global and local minimum energy. However, the variance increased with 0.005 in comparison to a step size of 0.02. Taking the ratio of global minimum achieved in a 100 simulations, a step size 0.02 generates better results with 12% in comparison to 0.05 with 5% and 1 with 0. A possible reasoning for the bad performance for a step size of 1 is the important random change in position of the electrons which doesn't allow for fine tuning. On the other hand, a small step size can results in particle get stuck in the centre. The small step size decrease the probability that the particle jumps out of the local minimum.

4.1.3 Different cooling schedules

To examine the influence of different cooling schedules, we investigated the results yielded by a linear, an exponential, a logarithmic and a sigmoidal cooling schedule. Figure 11, 12, 13 show the minimum energy distribution of a 100 simulations using a sigmoidal, logarithmic and exponential cooling schedule using the remaining general parameters. All the methods yield two narrow sub-distribution which correspond to the different configurations. Table 4 presents the mean and variance of the sub-distributions for each cooling schedule. Apart from the linear cooling, all the other cooling methods yield the same mean close to the theoretical global/local minimum. However, the logarithmic technique generates results with a slightly higher variance than the sigmoidal and exponential one. The ratio with which the global minimum energy is achieved indicates that the exponential is the best performing method with 16 global minimum configuration achieved out of a 100 simulations.

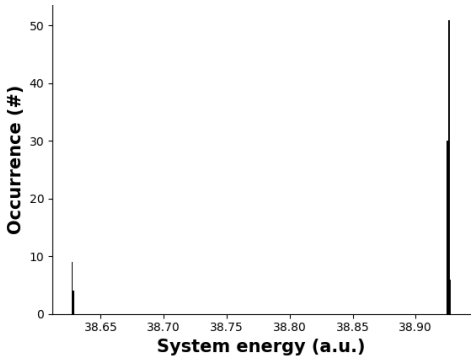

Figure 11: The system energy distribution for simulations with a sigmoidal cooling schedule and 10 particles. We find 13 simulations resulting in the global minimum and 87 in the local minimum.

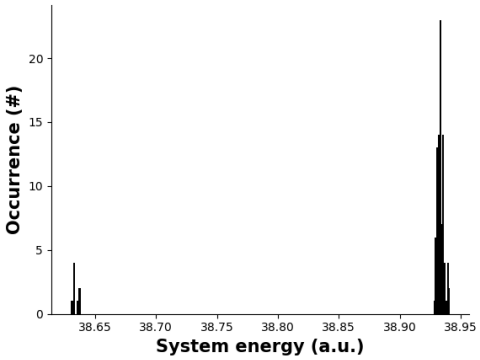

Figure 12: The system energy distribution for simulations with a logarithmic cooling schedule and 10 particles. We find 11 simulations resulting in the global minimum and 89 in the local minimum.

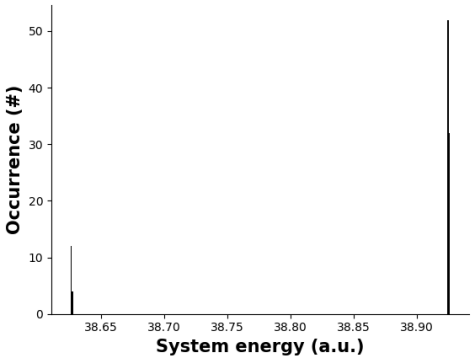

Figure 13: The system energy distribution for simulations with an exponential cooling schedule and 10 particles. We find 16 simulations resulting in the global minimum and 84 in the local minimum.

Table 4: Cooling Schedules for 10 particles - Shows the average values of the peaks and their variance. Peak 1 is the left peak in the histogram and represents the lower system energy, peak 2 represents the right peak and higher energy value. Using the exponential cooling we found the 2nd local minimum 3 three times, these were considered a 3rd peak and, therefore, not taken into account.

	Peak1 $\pm$ Var	Peak2 $\pm$ Var
Linear	38.66 $\pm$ 8.5e-05	38.99 $\pm$ 8.7e-05
Sigmoid	38.63 $\pm$ 2.7e-07	38.93 $\pm$ 4.5e-07
Exponential	38.63 $\pm$ 2.8e-07	38.93 $\pm$ 2.3e-07
Logaritmic	38.63 $\pm$ 6.3e-06	38.93 $\pm$ 7.1e-06

The exponential cooling reduces the temperature in a faster fashion than the

other method without bringing the system into a disequilibrium. At the end, the cooling decreases really slow which enables a more precise configuration of the particles.

4.1.4 Different Markov Chain lengths

To investigate the effect of changing the Markov Chain length, this parameter was varied, while the other parameters were kept to the general setting. This also means that the number of repetitions of the Markov chain was a 100 for every simulation, thereby keeping the temperature differences between the different chains constant. This experiment was carried out for a length of 1, 10, 100 and 1000, of which the results are shown in figure 14, 15, 8 and 16, respectively. A Markov chain of length 1 (figure 14) yields an energy distribution with high variance. Furthermore, the global minimum is never reached for a 100 simulations. Even though the cooling procedure is relative slow, the short Markov length doesn't allow to exploit the properties of the temperature to optimise the configuration. The random process dominates in this case.

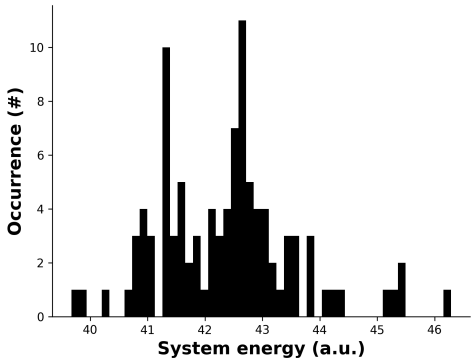

Figure 14: The system energy distribution for a simulation with a Markov chain length of 1 for 10 particles. There are no distinct peaks and the system energy is substantially higher than found in previous experiments.

A Markov chain of 10 (figure 15) shows three sub-distributions with smaller variance. In this case, the distribution around 40.4 corresponds to a local minimum with 2 particles in the middle.

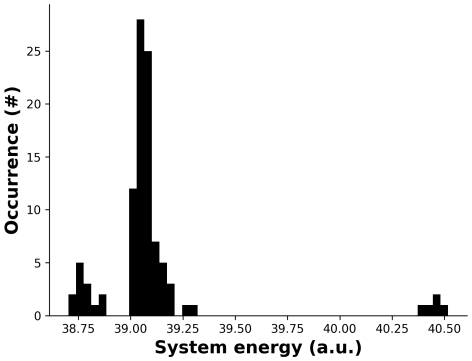

Figure 15: The system energy distribution for a simulation with a Markov chain length of 10 for 10 particles. We find 13 occurrences of the global minimum, 82 of the first local minimum and 5 of the second local minimum.

Figure 16 corresponds to a Markov chain of length a 1000 which yields two distinct distribution with little variance. In comparison to figure 14 and 15, a longer Markov chain allows to exploit the benefits of the different temperatures at each iteration which leads to a precise configuration.

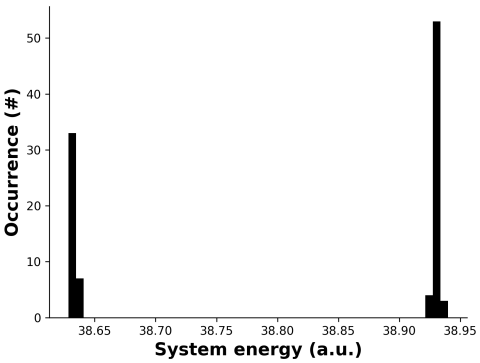

Figure 16: The system energy distribution for a simulation with a Markov chain length of 1000 for 10 particles. We find 40 occurrences of the global minimum and 60 of the first local minimum.

Table 5: Markov chain lengths for 10 particles - Shows the average values of the peaks and their variance. Peak 1 is the left peak in the histogram and represents the lower system energy, peak 2 represents the right peak and higher energy value. For a Markov chain length of 1, distinct peaks were not found.

	Peak1 $\pm$ Var	Peak2 $\pm$ Var
1	/	42.38 $\pm$ 1.4
10	38.78 $\pm$ 0.0018	39.08 $\pm$ 0.003
100	38.66 $\pm$ 8.5e-05	38.99 $\pm$ 8.7e-05
1000	38.63 $\pm$ 7.7e-06	38.93 $\pm$ 4.5e-06

Table 5 shows how a longer Markov chain improves the mean of the global and local minimum achieved with lower variance. Additionally, a Markov chain of 1000 yields 40 global minimum out of 100 simulations. However, this better performance comes at a substantial computational heavy.

4.2. Analysis on 11 & 12 particles

The goal of applying simulated annealing is finding the global minimum. However, when a local minimum is present with similar energy to the global minimum, locating the global minimum gets more difficult. In the case that two configurations are similar in energy, but far apart in configuration space, simulated annealing will have increased difficulty finding the global minimum. We find this to be the case for 11 particles. Based on the extensive analysis of the parameters, the best parameters were chosen for 11 particles. We define the best parameters as the settings that yield good results without compromising the computational running time. Therefore, based on the previous results we chose the general parameters with one difference. We use the exponential cooling schedule instead of the linear cooling fashion.

Figure 17 and 18 show the minimum energy distribution of 11 and 12 particles after a 100 simulations, respectively. Figure 17 shows 3 distinct peaks. The first two peaks correspond the global and first local minimum for 11 particles.

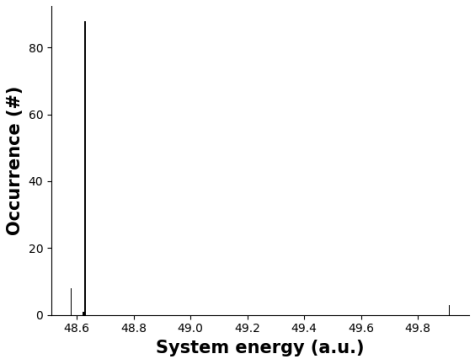

Figure 17: The system energy distribution for simulations with an exponential cooling schedule and 11 particles. We find 8 simulations resulting in the global minimum and 89 in the first local minimum and 3 in the second local minimum.

Figure 18 shows two distinct distributions, the global minimum and a local minimum. A system with 12 particles has a global minimum if one particle is in the centre (59.57 a.u.) of the circle. The configuration with no particle in the centre has an energy of (59.8 a.u.). However, the second peak around 60.7 corresponds to a configuration with 2 particles in the middle, while its energy is higher than the local minimum with no particle in the middle. This fact can possibly be explained by the width of the peaks of both configurations in phase space. For the configuration which features all particles on the rim, a slight deviation from symmetry increases the system energy a lot. Therefore, this system is unstable in comparison to a configuration with two particles in the middle, since this configuration is less sensitive to slight movements of the particles.

Table 6: 11 & 12 particles - Shows the average values of the peaks and their variance. Peak 1 is the left peak in the histogram and represents the lower system energy, peak 2 represents the right peak and higher energy value.

	Peak1 $\pm$ Var	Peak2 $\pm$ Var
11	48.58 $\pm$ 1.2e-07	48.63 $\pm$ 2.6e-07
12	59.58 $\pm$ 1e-06	60.69 $\pm$ 6.6e-07

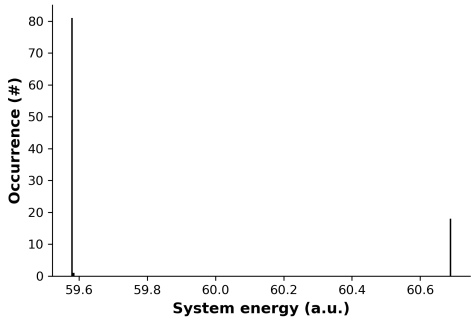

Figure 18: The system energy distribution for simulations with an exponential cooling schedule and 11 particles. We find 82 simulations resulting in the global minimum.

Table 6 presents the statistical analysis of the energy distribution with 11 and 12 particles. One can see that with the optimised parameters, the global minimum can be achieved with a low variance. However, for the challenging system with 11 particles, the global minimum is achieved only 8 times out of a 100 simulations. The reason is the fine line between global and local minimum in a system of 11 particles. On the other hand, for 12 particles the global minimum was achieved 82% of the simulations. Due to the phase space, the annealing sampling tends to place a particle at the early stage in the centre which results in a particle getting stuck in the local minimum due to the interaction of the particle on the rim pushing the particle to the centre. Therefore, for 12 particles the global minimum is reached with an high rate.

5. Limitations

The system energy does exactly not match the theoretical value and is always higher. This is the case since the theoretical value is the perfect configuration with minimal energy. Our simulation will approach this value, but will only reach it in the limit of an MCMC with an infinite length and infinitely slow cooling.

Secondly, in case of for example 11 particles, we often find the local minimum instead of the global minimum. Although this is a known problem in simulated annealing when the minima are close together, we were not able to significantly reduce the occurrence rate of the local minimum. As we expect to find better results for slower cooling, we would try to do longer Markov chains, which was not done here as a result of a lack of computational power.

For future research, we suggest looking into variable cooling schedules, which adjust their cooling speed by looking at energy drops. Additionally, one could investigate the effect of differently distributed step sizes.

6. Conclusion

In this investigation, the aim was to assess the global minimum energy configuration for N particles using the simulated annealing. The main goal was to determine the necessary parameters for simulated annealing in order to obtain a robust method for finding the optimal configurations. Our research has shown that a slow cooling is crucial for a robust outcome. The step size is an additional criterium which is crucial for avoiding local minimum. Different cooling schedules also influence the results, with exponential cooling outperforming logarithmic, linear and sigmoidal cooling. When the Markov chain length was increased, it yielded a better

global-to-local minimum ratio. Increasing the Markov chain length also increases the computational time. For future research, we suggest looking into longer Markov chain to see whether it can further improve the global-to-local minimum ratio. To make this feasible, we suggest using variable cooling schedules. Lastly, we suggest incorporating the Coulomb force, which could be used to guide the configuration in the right direction, although one should be careful as to not counter the qualities of simulated annealing.

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