Distribution of Point Charges on 2D Disks in Classical Electrostatics

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Abstract

The distribution of electric point charges on a conducting sphere can be calculated using energy minimisation techniques via the coulomb interaction of point charges. Stable states will be found when the coulomb potential between the charges is at a global minimum. Probabilistic global optimisation in the form of a simulated annealing algorithm is applied to N point charges confined to a 2D disk. This paper explores the minimum energy configurations of charge numbers up to 56 charges, optimisation of the parameters and algorithm, stability testing the minimum energy configurations and generated packing geometry of electrons close to the origin of the disk.

Introduction

The earliest work looking at configurations of electrons in confined regions was Wigner in 1934 (Wigner, 1934), with the prediction of the Wigner Crystal. Electrons moving in a non-interacting medium crystalise forming a lattice based on minimising the Coulomb potential.

Berezin then further suggested the idea that electrons confined to a disk would not follow the previously assumed configuration of N charges distributed on the edge of a disk in an N sided polygon (Berezin, 1985). By simple calculation it can be shown that for N = 12 charges the energy minimum occurs when the configuration has one charge expelled to the centre of the disk. Rees then took this further to show that for $12 \leq N \leq 16$, the minimum energy configurations have one charged expelled to the centre (Rees, 1985). Then for N = 17 it is more stable to have 2 charges distributed opposite each other at $r = 0.31R$ where R is the radius of the disk. The problem has been studied further using numerical calculations and simulated annealing methods to calculate the distributions for $N > 1000$ charges (Mughal & Moore, 2007).

The problem is a generalisation of the Thompson problem (Thomson F.R.S., 1904) which has wide ranging applications in biology with the geometries of viruses (Caspar & Klug, 1962). With advances in nanoscale physics, such confined systems can be realised in the form of quantum dots (Ciftja, 2013). This also appears when electrons are trapped on the surface of liquid Helium (Grimes & Adams, 1979).

Point charges follow the Coulomb potential for energy. The coulomb potential is spherically symmetric and is inversely proportional to the distance between 2 charges. The question, what is the minimum energy configuration of electrons confined to a disk, can be treated numerically by minimising the potential between all the charges.

As there exist many local minimum energy configurations, gradient descent and local optimisation algorithms are not suitable for this problem. The simulated annealing algorithm works well to find the global minimum in the 2N dimensional system of coordinates of N charges. In this work, I study the parameters and optimisation of the simulated annealing algorithm and I explore the minimum energy configurations of point charges on a 2D disk up to 56 charges. I look at the possibility of testing the stability of final configurations to avoid local minima and the generated geometries found within the minimum energy configurations.

Method

Simulation via simulated annealing

Simulated annealing algorithm for charges on a disk

Simulated annealing can be used to find the global minimum of a function that has many local minima. The

coulomb potential can be measured between the charges by a simple equation:

$$E = \frac{1}{2}\sum_{i,j}\frac{q_i q_j}{r_{ij}}, i \neq j$$

Equation 1 The energy of a set of N charges, where q_i, q_j represent the charge of the I'th and j'th charge respectively and r_{ij} is the distance between the I'th and j'th charge.

This equation will be at a minimum when the charges are distributed in the configuration that the electrons would fall into in a physical system.

The computation cost of the energy function can be decreased as in the sum $r_{ij} = r_{ji}$. Hence, the equation can be rewritten,

$$E = \sum_{i<j}\frac{q_i q_j}{r_{ij}}$$

The simulated annealing algorithm for this problem works through simple steps:

1. Randomly distribute N charges across the disk.
    a. Calculate the energy of the system
2. Choose randomly one charge and move it a small distance in a random direction.
    a. The chosen way to do this was to draw from a random uniform distribution between $-1 \rightarrow 1$ for the x and y coordinate and multiply the value by some chosen value δ
3. Calculate the new energy of the system
    a. If the energy of the system decreases, accept the change.
    b. If the energy of the system increases, accept the change with probability,

$$P(\Delta E, T) = e^{-\frac{\Delta E}{T}}$$

    Where ΔE is the energy change and T is a chosen temperature that changes the probability over the simulation.

4. After some chosen number of charge movements decrease the value of T to reduce the probability of accepting a higher energy configuration.
5. Reduce the temperature and run the simulation until the change in energy is negligible, to a chosen degree of accuracy.

I made the decision to diverge away from discretising the disk by limiting the change in the x and y coordinate of the charges to set step lengths. Instead, I used a random uniform distribution between $-1 \rightarrow 1$ scaled by some δ to move the charge. With this change the accuracy of the program falling into the final state increases as when the temperature decreases accepted movements for each charge will naturally decrease. The program will not accept large movements as these can increase the energy, moving away from the found minima. Instead, the simulation will reach the general minimum energy state and then randomly spiral closer to the true minimum energy configuration. This change means that the simulation naturally increases in accuracy with higher number of iterations and increases the possible states that can be explored by the charges as the movements are not limited to a set of possible moves determined by the resolution of the step lengths of a discretised disk.

Initial conditions and parameter optimisation

Initial temperature

An initial temperature, T, needs to be chosen. In order to calculate a reasonable initial value of T, the system was initialised many times and the energy calculated. I then calculated the standard deviation of the energies and the initial probability chosen according to the equation:

$$T_{initial} = -\frac{3\sigma}{\ln(P_{initial})}$$

Equation 2 P is the desired probability of accepting the energy change and σ is the standard deviation

The value of σ is the standard deviation of energies derived by initialising the system multiple times and randomly distributing the charges then calculating the energy and finding the standard deviation of all those energies. This equation gives an initial temperature that accepts a higher energy state that is 3 standard deviations away from the average with probability P.

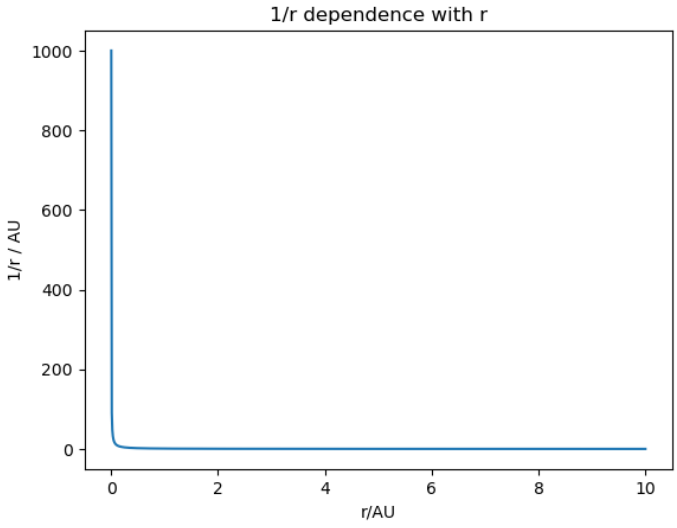

Figure 1 A plot of 1/r against r where r denotes the distance between two charges.

Figure 1 shows the relation of 1/r with the distance increasing between two charges, I have chosen the temperature to accept higher energy changes where the

energy increases by 3 standard deviations from the mean of multiple initial setups of the system as when a charge reaches a state around the global minimum the charge will be distributed further away from the charges, giving a reduction in the energy, and a small movement of the charge will create a much smaller change in the overall energy. When the charges are in high energy, unstable states the system will be explored with high probability, as the energy change from a charge moving from these states will be of a higher magnitude but will allow charges close to a minimum position to be more likely to stay in that position. I arbitrarily chose a sample size of 10^7 replicas of the system to draw the standard deviation from. The number of replicas of the system needs to be high as the energy can essentially range from the global minimum energy configuration to infinity, when the charges are all distributed incredibly close to each other. This means that to draw a stable standard deviation of the average energy many random replicas need to be generated or the standard deviation will fluctuate dramatically with each run of the simulation, which will affect the quality of all the simulations run with that chosen standard deviation. Unfortunately, due to the limitations of the computer, running sample sizes of more than 10^5 was not possible as the computer did not have enough RAM to store arrays of size $(> 10^4, N, N-1)$ for N > 13, where N is the number of charges. Splitting the array into chunks still lead to massive RAM overload and a significant slowing of the total system. For a low number of charges, the standard deviation was still fluctuating up to a sample size of 10^7.

	Sample size		
Rerun number	10^3	10^4	10^5
1	0.09003879	0.08550865	0.0932196
2	0.07375397	0.29035835	0.0932196
3	0.0634563	0.0730751	0.0932196
4	0.08853412	0.12918158	0.14660622
5	0.05823464	0.11698606	0.09663736
Rerun number	10^6	10^7	
1	0.12158712	0.13367278	
2	0.12382879	0.15236886	
3	0.22495922	0.16067839	
4	0.11737186	0.13081903	
5	0.10712902	0.14524350	

Table 1 A table of the derived σ values for 3 charges with increasing sample size to estimate the error on the determination of the sigma value for each charge configuration.

Table 1 shows the variation for 3 charges and shows that there is some stability but the resolution permitted for only a very small number of charges is ± 0.05 for the sigma value, which with a sample size of 10^7 is very high. The standard deviation for sigma is ± 0.011 and this gives an estimate on the possible error in the initial conditions. For N = 12 the standard deviation of sigma was ± 0.023. For N= 20 and with a sample size of 10^7, despite attempts to stabilise the program by array splitting and for loops, my computer system did not have enough power to calculate this stably.

A sample size of 10^4 maintains computer system stability whilst running the calculation for higher charges. This can possibly be stretched to 10^6 for low N.

Temperature reduction

The temperature was reduced geometrically and required tweaking; smaller geometric decreases increase the computation time but allows the charges to explore more possible energy states.

In order to get a good balance, the number of steps per temperature and the reduction in temperature need to be calculated together. The charges that are chosen each time are chosen using a uniform distribution, hence will be 'chosen' on average N times equal to the number of movements per each temperature iteration divided by the number of charges. Accepting this, the temperature reduction can be tempered with the number of charge movements per iteration to make sure that the system is initially accepting random movements.

In order to calculate the temperature reduction, I first needed to calculate the number of total 'steps' that the system needs to make to allow the charges to diffuse across the radius of the disk. I made use of a random walk algorithm. The algorithm makes N walkers take M steps each in random directions where the movement is scaled according to the delta chosen for the charge movements. I.e., a value is drawn from a uniform distribution between -1 to 1 for the x and y coordinate and this is then multiplied by the chosen δ to get the 'step' that a charge moves to mimic the movements of the charges in the simulation.

I then calculated the cumulative distance from the starting point and each walker that surpasses the desired radius is counted. The fraction of the total walkers that surpass this threshold gives the probability that a charge will have diffused across the radius of the disk.

The program calculates how many steps are needed by first moving the walkers $10 \cdot N$ steps where N is the number of charges in the system. The fraction of walkers reaching the radius is calculated and the number of steps is increased by 10% until 95% of the walkers reach the desired radius.

95% was chosen arbitrarily however this represents the probability that each walker will reach the desired radius in the given number of steps. As the system is random the chance cannot be 100% and the number of steps needed to reach higher probabilities will be geometric, meaning a much longer computation time in the limit that the probability tends to 1.

Once the total steps needed are calculated the temperature reduction can be calculated from the probability formula after n iterations

$$P(\Delta E, T, n, R) = e^{-\frac{\Delta E}{T \cdot R^n}}$$

Equation 3, n represents the number of iterations of temperature reduction and R represents the reduction of the temperature with each iteration.

I decided that the charges should have explored at least the radius of the disk by the time the probability of accepting a change in energy a single standard deviation from the average reaches 50%. This allows high energy movements to still be very likely and maintains a random system. Subbing in the value of T from Equation 2 and assuming $\Delta E \cong \sigma$ gives,

$$P(P_{initial}, n, R) = e^{\frac{\ln(\mathrm{P_{initial}})}{3 \cdot R^n}} = \frac{1}{2}$$

Solving for n,

$$n = \frac{\ln\left(-\frac{\ln(P_{initial})}{3 \cdot \ln(2)}\right)}{\ln(R)}$$

Equation 4, equation representing the n iterations with a reduction value of R to get the probability of accepting an energy change of σ to be 0.5.

P is initially set at 0.9 to give an initial probability of 90% to accept an energy change of 3σ. I could have solved for R. Instead, I tested values of R ranging from $0.95 \leq R < 1$ in steps of magnitude 10^{-6} and found the lowest value of R that gave the n steps needed derived from the random walk simulation. Either method works to give an estimate on a suitable temperature reduction value.

If, for the derived value of R, the number of iterations is above the iterations needed, calculated from the random walk, the error estimate does not impact the results sufficiently for a calculation as it only increases the computation time and reduces the cooling speed which could improve the simulation results.

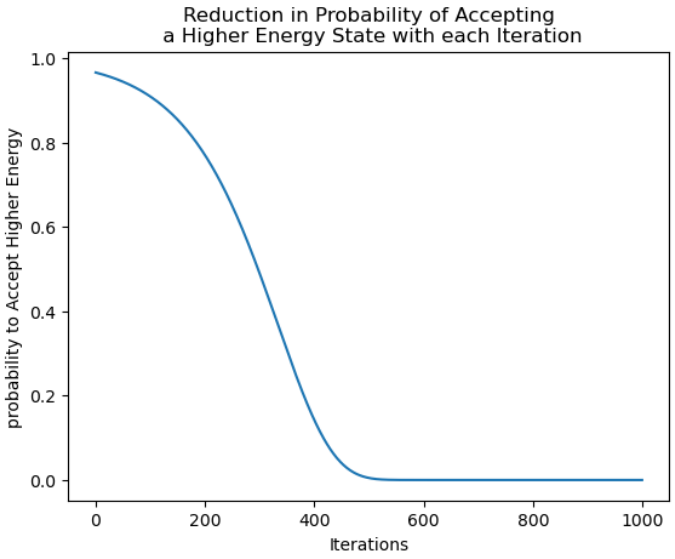

Figure 2 A plot showing the probability of accepting a higher energy state of 3σ with each reduction in the temperature value. The reduction in temperature was geometric and reduced by 1% each iteration.

Figure 2 shows the shape of the probability function as the temperature is reduced each iteration giving an idea of how the system will relax into a minimum energy state.

With these values derived from the number of charges, the chosen value of delta and the chosen number of steps that the program will make per temperature reduction, the simulations can be run self-sufficiently and the δ value can be balanced with the number of steps per iteration and the disk radius. On running the random walk with varying values of δ, a value of 3 was chosen to allow sufficiently small movements of the system to be more likely. 3 reduces the number of iterations that the simulation needs to run to get diffusion of charges across the radius, which would increase the computation time.

The number of steps per iteration was set at 100. This is a computational choice over a physical choice. As the program uses the number of steps per iteration to reduce the speed that the system cools, the number of steps per iteration can be chosen somewhat arbitrarily. It should not impact the exploration of the system too much within the desired criteria drawn from the random walks and calculation of iteration number, which are calculated from the chosen number of steps per iteration. The way the program deals with charges moving outside of the disk is to loop through randomly choosing a charge and moving it a random distance until a charge and move is found where the charge does not move outside the radius of the disk. As this is done with each step the system takes, when the system is relaxed into the global minimum state some charges will be distributed around the edge and this loop will take longer to run. Increasing the number of steps taken per each temperature iteration will increase the

computation time massively as the loop can theoretically run infinitely to find a suitable move.

Simulation termination

The criteria I chose for stopping a simulation was to compare the energy of the system after 100 iterations of temperature reduction to the energy of the system 100 iterations previous and round the value to a chosen degree of accuracy. I chose 8 decimal places. If the energy has not changed then the simulation is complete. Two possible reasons can arise for the negligible change in energy. Either the temperature is so low that in 100 iterations of temperature reduction the system rejects all the changes in energy as they lead to higher energy states and thus the system is saturated and cannot find lower energy states or the moves across 100 iterations of further temperature reduction are sufficiently small that to the degree of accuracy chosen the energy change is negligible and the system is in a stable state.

Simulation optimisation

The random nature of the simulations can lead to the program falling into local minima even with advanced tweaking of the initial conditions, especially if the local minimum is very close to the energy of the global minimum. This means that a singular simulation is not necessarily going to give the global minimum energy configuration. After running multiple simulations of the system and choosing the simulation that gives the lowest energy, this gives some reasonable estimation that the minimum found is the global minimum.

Multiple reruns of a simulation are independent of each other which is very useful in how the algorithm can be implemented in Python. Initial implementations ran a singular simulation repetitively to find the minimum energy configuration however this increases the computation time linearly with the number of simulations that are run, as it uses a sequential for loop. By vectorising the algorithm with use of NumPy, multiple simulations can be run in parallel using NumPy's vector algebra library. This was implemented in Python by increasing the dimensions of the simulation array to include an added dimension for the number of simulations and then vectorising each step of the algorithm such that each step is performed over all the simulations at once. E.g., M replicas of the system are generated, and a charge is chosen randomly and moved randomly across all M simulations, the energy change of all M replicas is calculated and each one tested whether to accept or reject the change in energy. The termination of the overall program is then complete when all the M simulations have reached the required criteria discussed above.

With this change, it made it computationally feasible to run many simulations for each charge configuration and choose the simulation that gives the lowest energy state. In testing I could run >40 simulations without a significant increase in computation time.

The average runtime for a singular simulation would be around 3-20minutes for low charge numbers and with the initial implementation the time to do M simulations would be roughly $M \cdot (time\ \ for\ one\ simulation)$ which was not feasible to run for multiple different configurations. With the new implementation, the longest time was roughly 1 hour and 30 minutes for 400 simulations of 16 charges. Which would have taken around 3-5 days to complete with the previous implementation of the algorithm.

This significantly improves the probability that in the M replicas the true global minimum is found, as the number of replicas M can be increased significantly more than previously, even if there are many local minima found in multiple of the M replicas of the system.

Stability testing of results

Whilst improvement in the number of simulations that can be run increases the confidence that the minimum energy configuration has been obtained it is useful to test the final configurations for stability.

If the final state is the global minimum, then the state is very stable to perturbations to the system. If the final state is a local minimum, then slight perturbations to the system will cause the collapse of the system into more lower energy states.

In order to explore the stability of each charge configuration I chose to take the final state of a configuration after the simulated annealing algorithm had been run, chose a charge randomly within that configuration and moved the charge to a random point on the disk. I then reran a simulated annealing algorithm on this perturbed state. This algorithm was run multiple times. Then the number of final configurations after the perturbation that stayed the same as the original final configuration before the perturbation were counted. This gives an estimate as to the likelihood that the original final configuration from the simulated annealing algorithm is the global minimum as opposed to a local minimum.

I then chose to run a second stability testing model which moves all the charges a small movement γ in a random direction, by generating a uniform distribution between -1 and 1 and then normalising the result, then multiplying by a random value between 0 and some limit α. This perturbs the system around the minimum energy

configuration randomly and spreads the system out whilst maintaining the position of the lower energy states. The simulated annealing method is then rerun on these perturbed systems.

The final stability testing algorithm that I explored differed only in that the standard deviations were drawn from the perturbed system itself rather than drawn from randomised distribution of charges across the disk.

Results

Part 1 – General Trend of Charge Configurations

The first set of results were running simulations to look at the general trend of the minimum energy configuration for the point charges. The configurations are compared qualitatively to papers looking at the same problem comparing the energy values obtained. The units of energy are q^2/L where q is a unit of charge and L is an arbitrary unit of length.

The overall results showed that the charges distributed themselves into a regular polygon with sides equal to the number of charges up to 11 charges. When 12 charges are distributed it is more energetically stable to have 11 charges distributed around the edge and a singular charge sat at the centre of the disk. This trend went up to 17 charges, one charge at the centre and the rest distributed into a regular polygon of sides equal to the number of charges -1, at 17 charges it was then more energetically beneficial to have two charges distributed about the centre point and the rest distributed around the edge of the disk. With increasing charges, a number are distributed around the edge and a regular polygon of the other charges are then distributed closer to the centre of the disk forming concentric rings. The energy values obtained are rounded to 6 decimal places to match the accuracy of the referenced papers that the configurations are compared to. The simulation is run until the energy change after 100 iterations of temperature reduction didn't change to 8 decimal places which increases the confidence that the energy values to 6 decimal places are accurate.

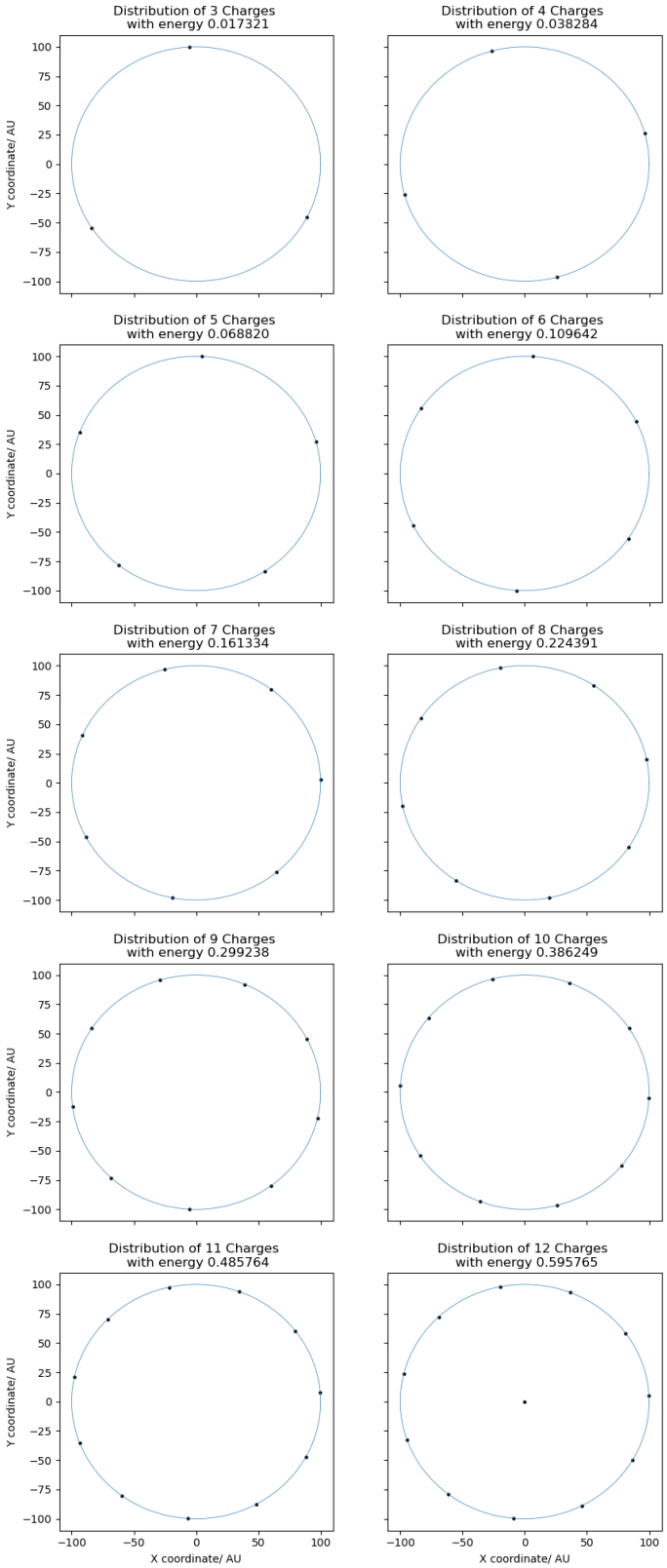

Figure 3 the minimum energy configuration of charges on a disk of arbitrary size 100 units radius, showing the distribution from 3 to 12 charges highlighting the change to the configuration at 12 charges.

Figure 3 shows all the minimum energy configurations up to 12 charges and agrees with (Berezin, 1985) where for 12 charges Berezin obtained a minimum energy configuration that gave a value of 59.57568, the magnitude of the energy is different, but this difference is due to the choice of the radius of the disk, in Berezin's paper the disk radius was 1 unit whereas I arbitrarily chose

a disk radius of 100 units which gives difference in magnitude of the energy as 10^2, if the energy was quoted in units q^2/R where R is the radius of the disk the values would be increased in magnitude by 10^2. I generated a configuration for 12 charges where the charges were all distributed in a regular polygon at the edge of the disk and the energy of the system was 0.5980736 which is the same as (Berezin, 1985) apart from the magnitude and shows that the singular charge at the centre is a lower minimum energy configuration.

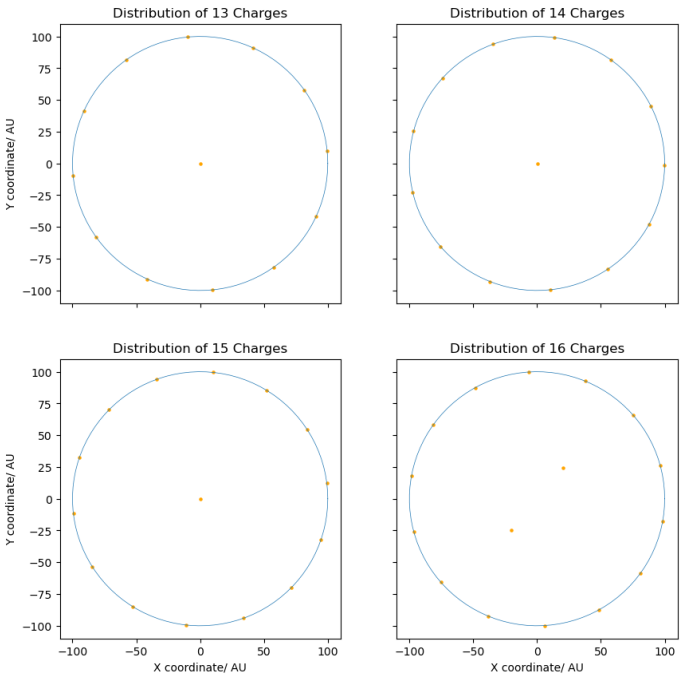

Figure 4 distribution of charges ranging from 13 to 16 charges marking the change in the configuration at 16 charges. 50 simulations were run for each charge number.

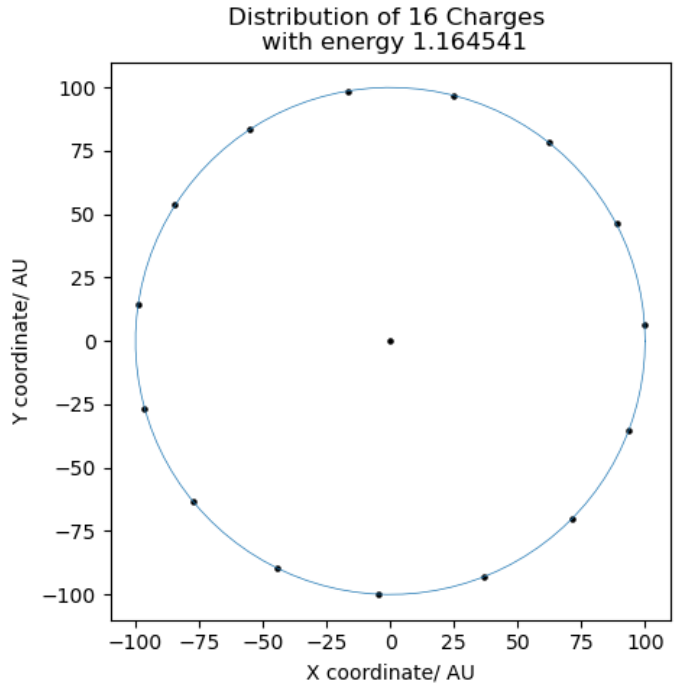

Figure 5 A plot of the charge configuration for 16 charges after running 600 simulations.

In the case of a charge numbers from 13 to 16, (Rees, 1985), says that the minimum energy configuration will be N-1 charges distributed in a regular polygon around the edge of the disk with one charge at the centre. I ran 50 simulations for each number of charges and chose the minimum energy configuration across the 50 simulations. In those initial 50 simulations all the configurations agreed apart from for 16 charges, Figure 4, where the minimum energy configuration had two charges distributed closer to the centre. On running a hypothetical configuration with one charge at the centre, the energy obtained was 1.16452 which indicates that the simulation run has not given the correct minimum energy configuration. On rerunning the simulation with a much higher number of simulations I found the correct minimum energy configuration.

Figure 5 shows that the lower energy final configuration can be reached and required a multitude more simulations run in order to obtain the global minimum. The change in configuration after many more simulations gives an indication that I have found the global minimum with this configuration. However, more rigorous analysis can be run to see if the final configuration obtained is a local minimum or the global minimum. This was discussed in Stability testing of results and the results are in Part 2 – Stability Testing Final Configurations.

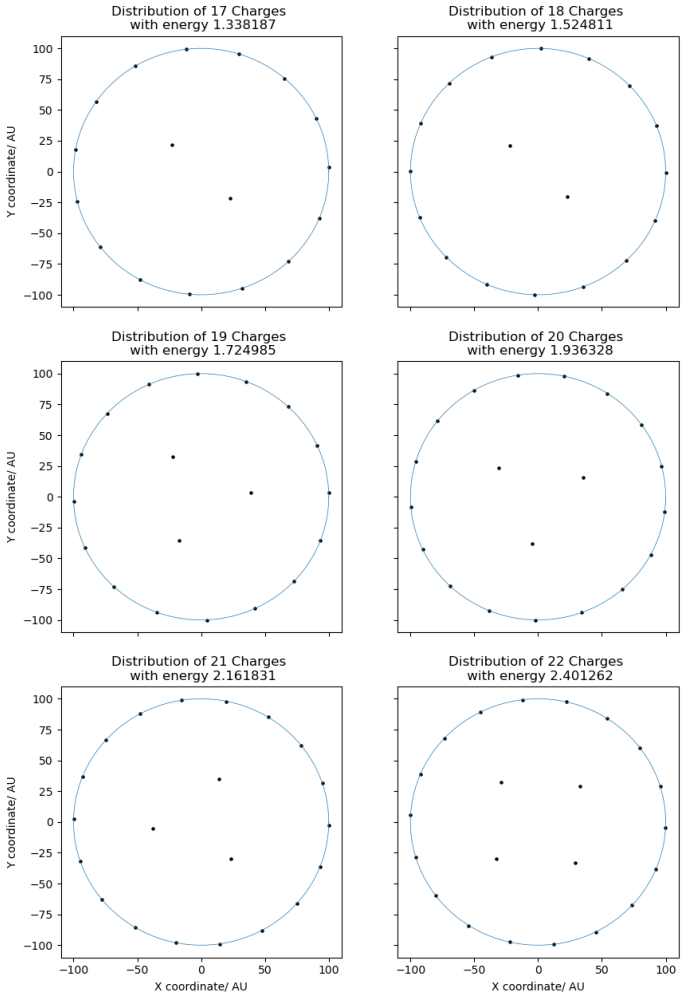

Figure 6 distribution of 17 to 22 charges showing the trend in the configuration, the charges are distributing themselves about the edge and then filling a space closer to the centre with a regular polygon.

Figure 6 shows the generation of an inner ring as the number of charges increases. There is no specific formula for how N charges should be distributed exactly, however the trend is to form inner concentric rings.

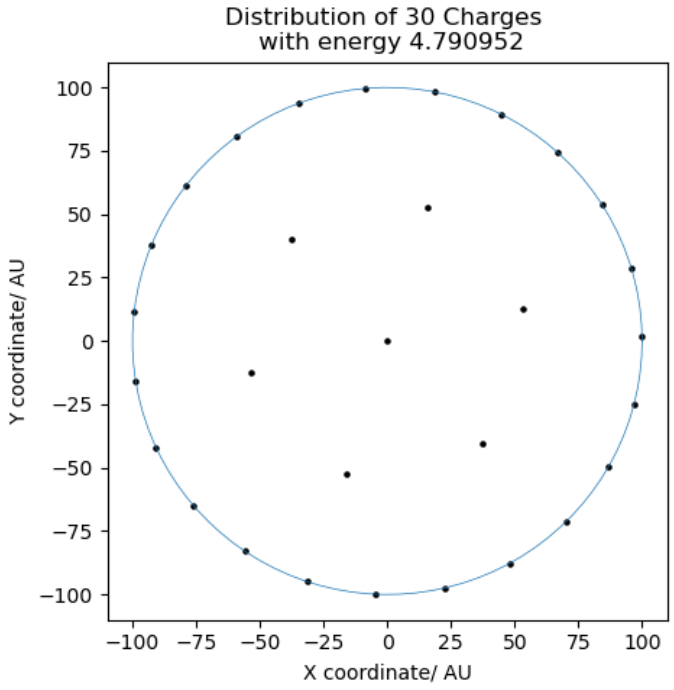

Figure 7 A plot of the minimum energy configuration for 30 charges after 70 simulations, a third concentric ring starts to form at the centre.

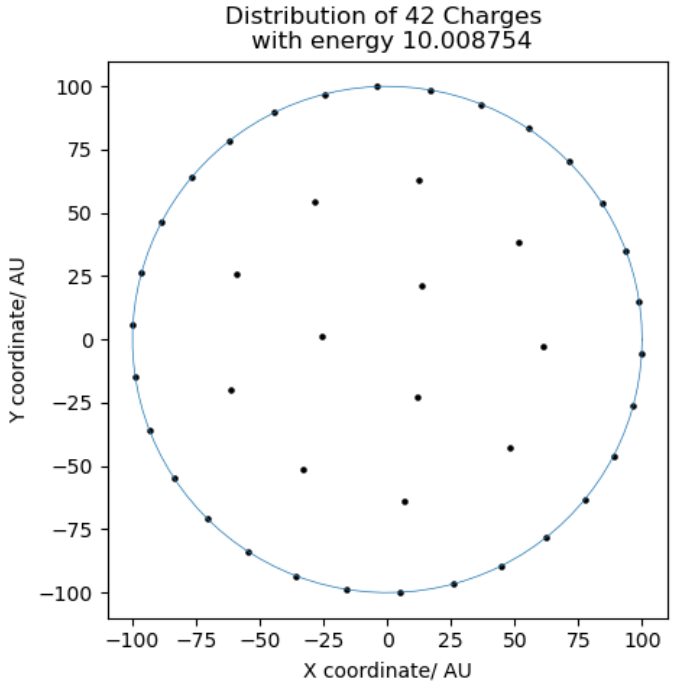

Figure 8 Plot of the minimum energy configuration of 40 charges after 40 simulations were run. The third concentric ring is fully formed with the triangular distribution.

The next most interesting result is when the charge number reaches 30 where a third concentric ring starts to form with one charge at the centre. Figure 7 and Figure 8 agree with (Nurmela, 1998) with the final configurations and the third concentric ring was fully formed by 42 charges where a triangular distribution forms at the centre. I ran the simulation for charge configurations from 3 charges to 56 charges and all the obtained final configurations can be found in the Appendix.

Part 2 – Stability Testing Final Configurations

The second set of results aimed to improve the confidence in the final configurations obtained that they are a global minimum and not a local minimum.

Each stability tested simulation was run for 40 simulations and the charge configurations from 11 to 24 charges were tested.

Number of charges	*No. simulations with same energy as original simulation energy*	*No. simulations with energy lower than original simulation energy*
11	5	0
12	37	0
13	24	0
14	6	0
15	2	0
16	0	0
17	12	0
18	4	0
19	19	0
20	3	0
21	0	0
22	13	0
23	7	0
24	2	0

Table 2 A table showing the number of perturbed systems that relaxed back into the same state as the original simulation. The energy values were rounded to 4 decimal places as otherwise the energies would differ slightly whilst still being the same energy configuration.

Table 2 shows that in the 40 simulations for each charge configuration there were no lower energy configurations found. However, due to the limitation on the accuracy of the energy comparison it highlights that this basic method doesn't necessarily give valuable information about the stability of the results. By further comparison of the figures after stability testing, for the systems that had zero states that were the same as originally found, the stability testing had pushed the charges into a higher energy configuration. Comparing the configurations to (Nurmela, 1998) the configurations obtained with the initial simulations from Part 1 – General Trend of Charge

Configurations are the same as Nurmela, for charge configurations ranging from 11 to 24 charges, and this could indicate that perturbing the configurations in the lower energy states pushes the configurations only into higher energy states.

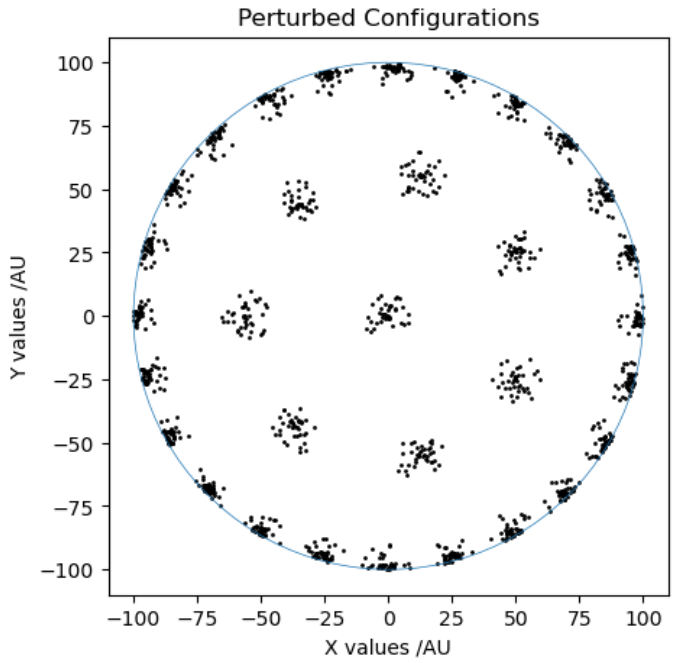

Figure 9 A plot of what the perturbed coordinates looked like across the 40 run simulations showing the distribution of the charges around the original minimum configuration. The upper limit of distance moved was $10\ units$.

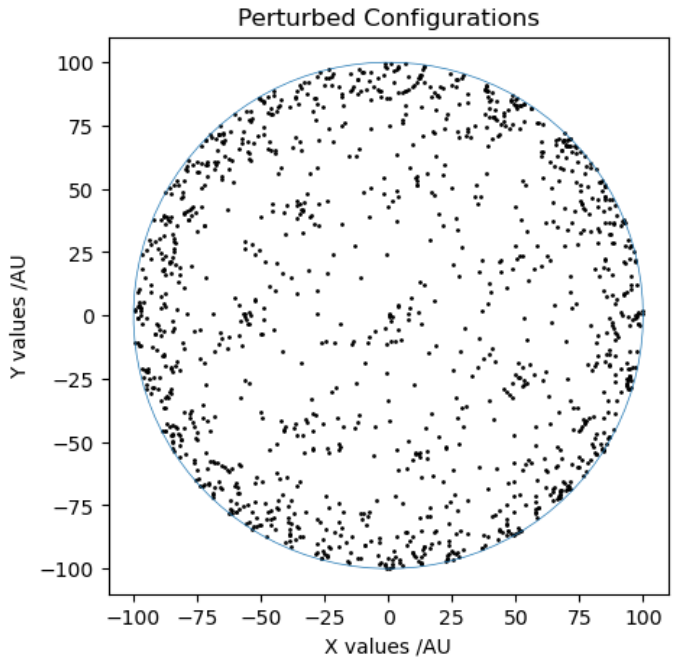

Figure 10 A plot of what the perturbed coordinates looked like across the 40 run simulations showing the distribution of the charges around the original minimum configuration. The upper limit of distance moved was $30\ units$.

The first configuration that differed from (Nurmela, 1998) was for 32 charges, which would indicate that my results have not given the global minimum when running the stability testing algorithm for 32 charges. However, after 40 perturbations the system could not find a lower energy state.

The second stability testing algorithm moved all the charges randomly by some distance $0 < distance < \alpha$, where α is the upper limit to the distanceD. I looked at the configuration for 32 charges as it had a different configuration to configurations found in papers.

The system still fell into energy configurations equal to or higher than the previously obtained minimum energy configuration. Figure 9 Shows that the perturbation isn't that large, and a larger perturbation could push the system out of the local minimum. Figure 10 had an increased upper limit of movement distance, but still failed to yield the lower energy configuration of (Nurmela, 1998). The system is at the point where increasing the upper limit on the movement distance will create a distribution like an initial simulation. By trying with a reduced temperature based upon the perturbed coordinates, no lower energy state was found.

Part 3 – Lattice Geometries

These results looked at the geometries of the final configurations. Looking first at each different configuration and the distances from the origin of the disk, then to numerically evaluate the geometry of the shapes formed close to the centre of the disk.

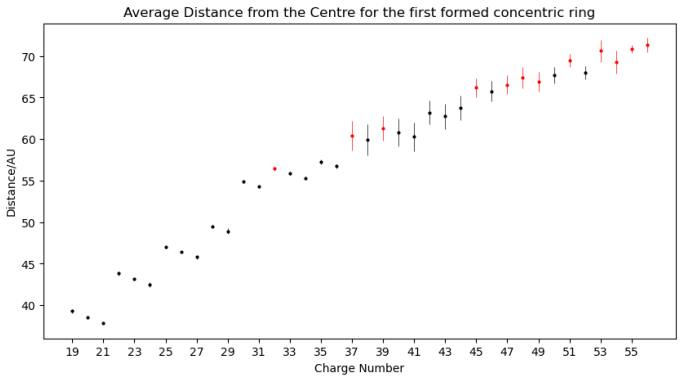

Figure 11 a plot of the average distance from the centre of the disk for the concentric ring forming closest to the edge of the disk, the red highlighted points are where the final configurations did not agree with (Nurmela, 1998)

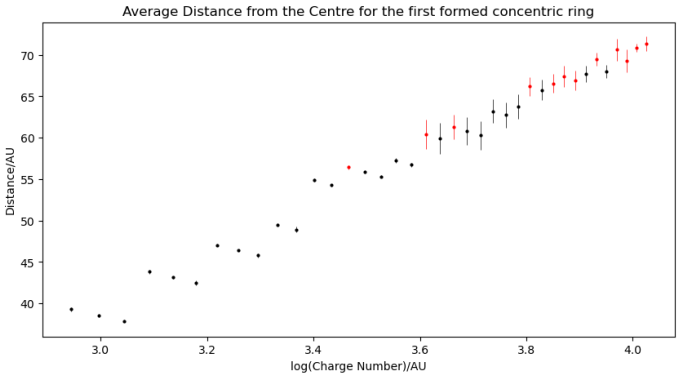

Figure 12 A plot of the logged number of charges against the average distance from the origin. For higher charge numbers the relationship appears linear, highlighting the asymptotic relation.

Figure 11 and Figure 12 A plot of the logged number of charges against the average distance from the origin. For higher charge numbers the relationship appears linear, highlighting the asymptotic relation. Figure 12 shows that there is a large difference in the distance of the inner ring for a low number of charges, as the charge number increases the distance seems to asymptote. There were not enough charge configurations calculated to look at the trend for more inner rings.

Looking at the specific geometries generated within the disk. For $19 \leq N \leq 21$ charges the geometry appeared to be an equilateral triangle, and this also was the same when the triangular pattern appeared again for $42 \leq N \leq 44$ charges, and the distances calculated between each of the charges seemed to confirm this,

Charge number	*Distance between the 3 centre charges, units arbitrary* *Error of* ± 0.5*units*		
19	68	68	68
20	67	67	67
21	66	66	66
42	44	44	44
43	44	44	44
44	43	43	43

Table 3 The distances of 3 charges in a triangular pattern at the centre of the disk, rounded to 1 decimal place.

The uncertainty in these values can be obtained from the effect that the different distances will have on the energy and the delta of the initial program. To increase the distance between the charges by 0.1 units the simulation would have to move a charge in the x and y direction by $5 \cdot 10^{-3}\ units$. The program is run with a scaling on the x and y changes of 3, this means that the probability of the program moving a charge less than or equal to this distance ≈ 0.00028, calculated from $3 \cdot 10^{8}$ samples to get stability at 5 decimal places, which then must be multiplied by the chance to choose that charge which is 1/N where N is the number of charges. Thus, giving a probability ranging between $6.36364 \cdot 10^{-6} < P(N) < 1.47368 \cdot 10^{-5}$ of making a move of that small a magnitude, which means the program would have to take steps between $67857 < steps(N) < 157142$ for a reasonable chance that the program will make this move at the point where the charges are in this equilibrium state. The program terminates after 100 iterations of temperature reduction and each temperature reduction consists of 100 total steps, which is a minimum of only 10000 steps. Therefore, the values are rounded to one integer as this means the program must make $683 < steps(N) < 1582$ to move this distance or less which is more likely with the simulation parameters.

This equilibrium geometry forming regular polygons continued when the configuration had a square and pentagon at the centre of the configuration.

Discussion

In results Part 1 – General Trend of Charge Configurations the results were promising, for low charge numbers the results agreed with referenced papers, and only at 32 charges was there a diversion from configurations found in other papers. If the number of simulations is increased the confidence in the final configuration obtained being the global minimum increases, but the exact confidence is difficult to calculate. Hence, rerunning the models with arbitrarily high simulation number can get more accurate configurations, especially as the number of charges increases as the number of local minima will increase with charge number.

The results for stability testing the final configurations were not as useful, the system still relaxed into the previously found minimum energy configuration or higher energy configurations and did not improve confidence in the final configurations obtained. Increasing the number of simulations run could yield improved results and increasing the magnitude of the perturbation. However, this tends towards a rerunning of the original simulation and the stability testing algorithm should not need to put the system back to a random state.

The results in Part 3 – Lattice Geometries showed an asymptotic relation with the first concentric ring, this would agree with the coulomb force being related to the inverse distance. Many more charges distributed at the centre would be needed to push the ring closer to the ring of charges at the edge of the disk. This will also be affected by the increasing number of charges distributed at the edge of the disk with increasing charge number.

The packing geometries generated at the centre of the ring were explored and the number of charges distributed on the disk did not appear to have an impact on the geometry. For low charge numbers the shape formed was a regular pattern, the same as for high charge numbers. The only difference was the edge length of the regular polygon which would be due to the increased influence of more charges further away from the centre. The overall lattice geometry was not calculated within this project, (Mughal & Moore, 2007) treat this problem in more detail. The geometries determined appear to agree with Mughal's shell-like ordering for small clusters, as the shells are regular polygons. Higher charge configurations N > 50 would have to be calculated to explore the change into hexagonal ordering.

In the section Initial conditions and parameter optimisation I discussed the possibility of calculating the error on sigma and make use of a random walk simulation for calculating initial parameters. Whilst the Uncertainty on those values can be useful to know, the transference to the uncertainty in obtaining the minimum energy configuration cannot be drawn directly from those values. As the exact path and probabilities is randomised across the simulation. The sample sizes in each case were mostly limited by the computing power of my computer and to keep my system stable whilst running simulations I couldn't push into higher sample sizes, especially with higher charge number as the array size grows rapidly with increased charge number. Which reduced the possibility of obtaining stable and accurate measurements of the uncertainty in the initial parameters for each simulation.

Careful array splitting for each simulation and charge number alongside more advanced array chunking algorithms to balance the time of the simulation with how much Ram is available in the system would not be worthwhile for accuracy of initial parameters that will not significantly impact the probability of getting correct configurations.

The reduced processing power to calculate the initial parameters could have an impact on the possibility of getting a good simulation however, looking at the charge configurations obtained and comparing them to the referenced papers, my algorithm seems quite stable at finding global minimum configurations. Instability increases with charge numbers $\approx N > 30$, however this could be counteracted by increasing the number of simulations run. In the case of determining sigma, from Equation 2, Table 1 shows that the calculated minimum resolution for stability gives variation in the initial values of the probability function for 3 charges ranging from $0.76 \rightarrow 0.81$, for energy changes of 3σ. This will affect the randomness of the initial system and could be larger as the number of charges increases.

There are trade-offs from my decisions with algorithm that runs the simulation. As discussed previously taking the movements to be approximately continuous rather than discretising the disk to some small delta lengths improves the accuracy of the simulation. The accuracy naturally increases with iterations as only smaller and smaller movements are allowed by the temperature equation. Whilst this can be mimicked by reducing the delta values over time, the reduction in the delta value would need to be tweaked very carefully otherwise the simulation would terminate before the desired level of accuracy is reached and the system could more easily fall into local minima. The limitation of this method is in the analysis of the confidence bands of the energy values and the positions of the charges, as the system is randomised rather than discretised the minimum energy configuration is not necessarily fixed as in the discrete case and can vary slightly with each simulation. Also, by the uniqueness of a true global minima, if an energy value is found that is lower than a previously found energy value, this value is more accurate than the previous value. I.e., by averaging across 'similar energy states' the accuracy of the true energy value decreases as there only exists one value that is correct and the average would be biased towards higher energy states. Which means averaging is not necessarily a useful way to improve the accuracy of the final energy.

The way that my results can then be interpreted is to put them into the context of an application, should the energy of a system of N charges on a disk need to be calculated then the accuracy to which the energy can be measured physically will determine the chosen degree of accuracy to run the simulation. In order to get reasonable configurations, I set the decimal to accuracy to 8 for the simulations, but this could be varied and rerun. Care needs to be taken when the energy is rounded such that the global minimum and local minimum energies coincide. This would start to give many wrong configurations that are at the same energy level. This can be avoided by running the simulation to any arbitrary degree of accuracy to explore the correct configuration, but then the energy value of this configuration could be rounded to whatever degree of accuracy is necessary for the application.

Overall, the most useful way to find global minima was to run multiple repeats of the simulated annealing algorithm for each charge number and choose the configuration from all the simulations that gave the lowest energy. The system is still a 'directed random' system that cannot deterministically give the correct results every time. The simulated annealing algorithm should have a temperature

at the start of essentially infinity and a final temperature of zero. This is mimicked but not achieved with a computer and without an infinite timeframe this is impossible. As such, quantity of simulations run with good initial parameters seemed to outperform careful over optimisation of initial parameters. From my results, the most likely states to fall into local minima were states just before a change in configuration, be it 11 to 12 charges where one charge gets expelled to the middle at 12, or 16 to 17 charges where at 17 two charges get expelled to the middle. By increasing the number of simulations runs around key changes the confidence in the configuration can improve.

Conclusion

The Paper aimed to explore the charge configurations for N charges confined to a disk, stability testing the minimum energy configurations and looking at the geometries formed within the minimum energy configurations.

Overall, stable minimum energy configurations up to 32 charges were found in agreement with referenced papers and the energy levels calculated by (Berezin, 1985) and (Rees, 1985). Beyond 32 charges the configurations become unstable with only a subset agreeing with (Nurmela, 1998). The trend showed that the charges arranged themselves into polygons on the surface of concentric rings forming inside the disk with increasing charge number.

With further numerical investigation of the geometries, the inner polygons closest to the origin of the disk formed regular polygons which agreed with (Mughal & Moore, 2007) and their description of shell-like ordering. The outer concentric rings were not numerically analysed.

The stability testing on found global minima did not improve the confidence in the minimum energy configuration and could not find the global minimum for N=32 charges to agree with (Nurmela, 1998). The running of stability testing led to the conclusion that it is more efficient to run multiple simulations on the same number of charges using the initial algorithm to find the global minimum. Exploration of the system around a local minimum configuration did not push the system into the global minimum consistently.

The outermost concentric ring was looking at the distance of the ring to the origin of the disk. The distance appeared to asymptote. This would be expected due to the electron-electron repulsion increasing as the charges on the outer concentric rings are pushed towards charges distributed on the edge of the disk. The overall trend across all the charges was analysed, as opposed to looking at the pattern of the distance when changes to the minimum energy configuration occurred.

Future work would look at configurations for a higher number of charges and the overall lattice structure, which would change in the limit of many charges. Exploration of other techniques for stability testing could be useful.

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Appendix

The simulated annealing algorithm is used widely for any optimisation problem that requires searching for a global minimum.

Outside academia, simulated annealing is used to find the optimum paths for the travelling salesman problem, the shortest route between N cities. This can be used in industry for Logistics as shown in (Grabusts, Musatovs, & Golenkov, 2019) where the researchers looked at finding the shortest route between 8 Belarusian milk and meat processing companies.

The method can also be applied more generally to minimisation costs for companies as shown in (Aydoğan & Cetek, 2023) where they look at minimising the fuel costs, ground delay costs and air delay costs by planning the best routes for all flights over the fixed route and free route airspace.

The method can also be applied to manufacturing systems where (Das, Lashkari, & Sengupta, 2006) look at using simulated annealing to improve the cellular manufacturing process. They explore minimising costs and system reliability by optimisation of inter cell material handling costs, cost of machine operation and minimising under utilisation of cells to minimise the costs. The algorithm is also applied to route planning along the assembly line for different part types, like the travelling salesman problem.

In academia, simulated annealing has a wide range of applications. The algorithm can be used for minimising the energy function in dimensions higher than 2D.

An example beyond physics where simulated annealing is used it in the study of protein structures as shown by (Chou & Carlacci, 1991) where simulated annealing is used to select optimal starting conformations for energy minimisation in protein structures replacing the previous use of personal intuition to find optimal energy configurations. The simulated annealing algorithm calculates the minimum energy configuration for very complex protein structures that contain many local minima.

Simulated annealing can also be used in designing optical waveguide grating structures to maximise reflection characteristics for photonic use. This is shown in (Wu & al, 1993) where they use simulated annealing to find the set of numbers required to optimise the Fourier function of the grating to within target parameters by introducing a cost function that calculates the energy difference between the current Fourier function and the target Fourier function.

A third example is in measuring sound velocity distribution in scattering media for the purpose of improvements to medical imaging. (Goto & al, 1995) Look at minimising the cost function between the measured sound field from small cancer or blood cells and the calculated sound field, this calculated sound field is then optimised via simulated annealing by minimising the cost function.

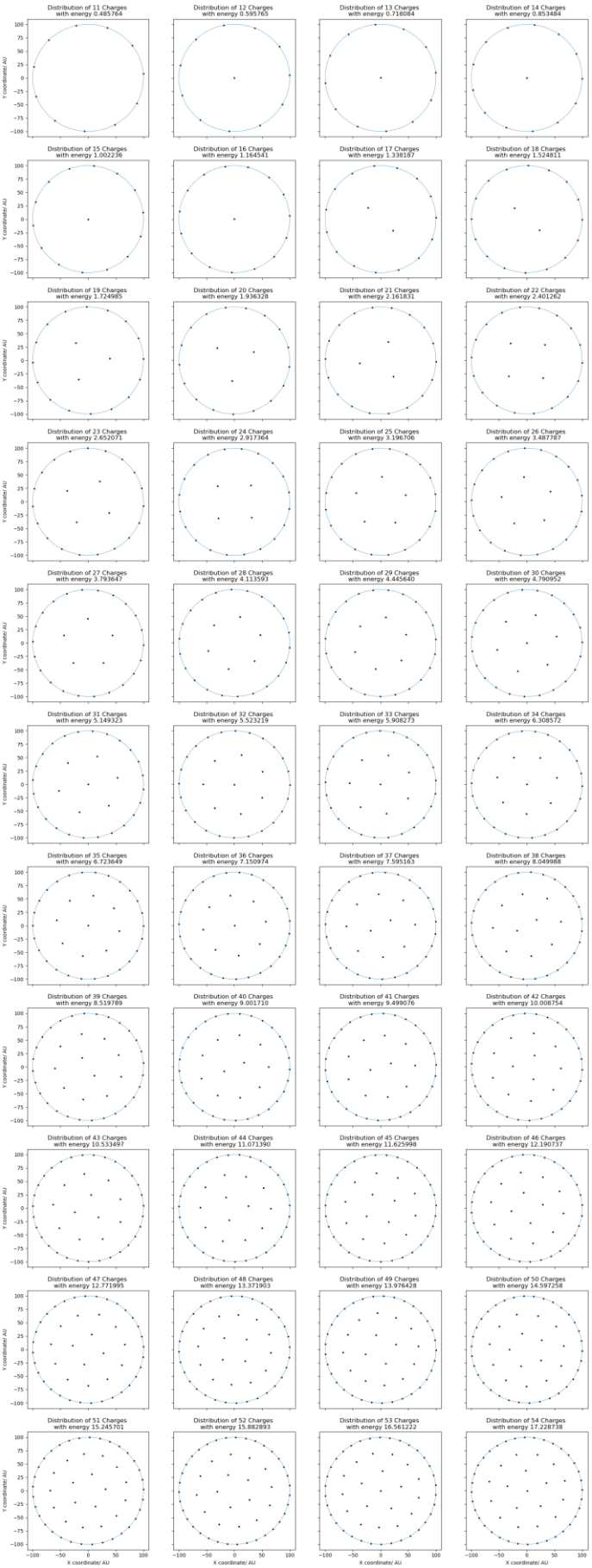

Figure 13 A figure for all the obtained minimum energy configurations up to 54 charges and the associated energy, each simulation was run more than 50 times, but lower charges were run more to focus on the accuracy.

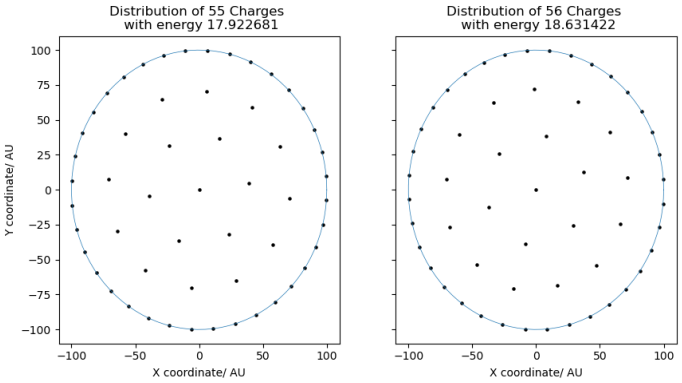

Figure 14 The plot of the minimum energy charge configurations for 55 and 56 charges.