Practice 4

Annealing method to find global minimum of 2D Thompson model

The objective of this practice is to simulate a system composed of Coulomb charges in a two-dimensional trap (Thompson atomic model) by the classical Monte Carlo method and to use the annealing method to find the minimal energy configuration.

Methodology

The main steps to proceed are the following:

1. Write a Metropolis Monte Carlo code to simulate a system consisting of N Coulomb charges in a two-dimensional harmonic trap. The energy of the configuration is given by

$$E_{pot} = \sum_{i=1}^{N} \frac{1}{2} m\omega^2 r_i^2 + \sum_{i<j}^{N} \frac{q^2}{|\vec{r}_i - \vec{r}_j|}$$

   We can choose a convenient combination of unitless units to simplify this expression into the dimensionless energy:

$$\tilde{E}_{pot} = \sum_{i=1}^{N} \hat{r}_i^2 + \sum_{i<j}^{N} \frac{1}{|\hat{r}_i - \hat{r}_j|}$$

2. From there we generate a random initial configuration. In my case, I will start with a normal distribution of the N charges centered around the origin, with a standard deviation of 1 in dimensionless units.

3. Use Metropolis algorithm to simulate system properties at a fixed temperature $\tilde{T}$, that is, to define the probability of a given configuration with the expression

$$p(\hat{r}) = e^{-\tilde{E}(\hat{r})/\tilde{T}}$$

4. Use global moves (displace all particles at once) by randomly moving each coordinate $x' = x + \xi$ where ξ is drawn from a Gaussian distribution $p(\xi) = \exp(-\frac{1}{2}\frac{\xi^2}{(\Delta t)^2})$ or $\xi = (2u-1)\Delta t$ with $0 < u < 1$ being a uniformly distributed random variable.

5. Adjust the amplitude of the displacement Δt in such a way that the acceptance probability lies between $(0.1, 0.9)$.

6. Verify that after an initial transient regime, potential energy converges to a certain value and fluctuates around it.

7. Implement the annealing procedure in which the temperature is lowered by a tiny fraction at each iteration (e.g., $T := T \times 0.999$), starting from a high temperature (compared to the typical system energy) and ending with a low temperature.

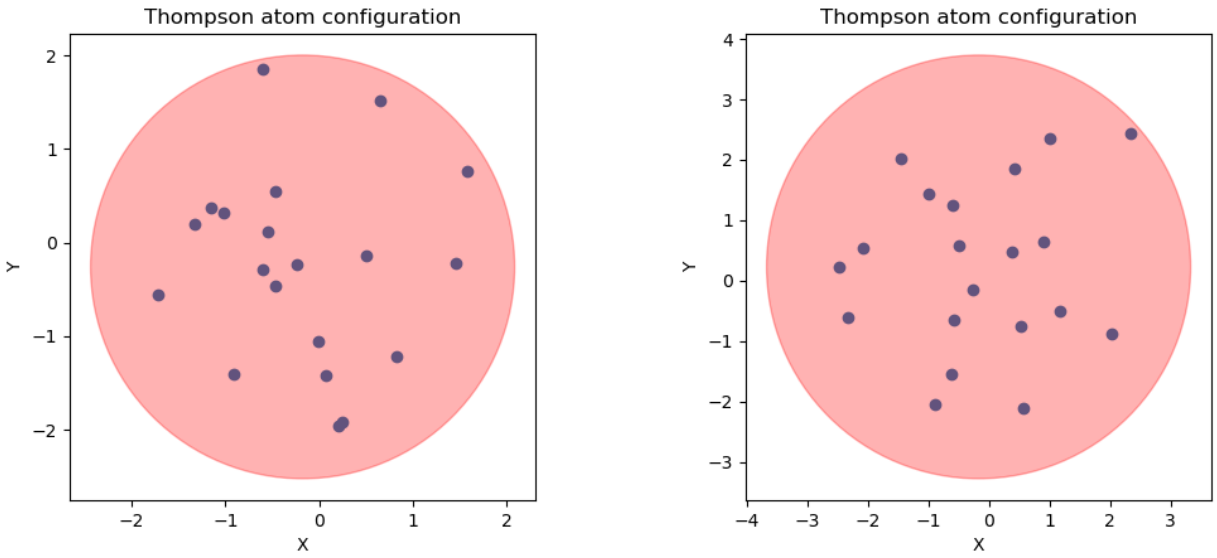
8. Repeat the annealing procedure a number of times to verify that the optimal configuration has been found and in the case when different final configurations are realized, take the one which has the lowest energy.

9. Find and plot the optimal configurations for $N = 5, 20, 26$ charges.

10. Observe the structure of the global minimum. Look for shell structures, formation of Wigner crystals in the center, and state the type of lattice visible in the center region (square, hexagonal, etc.).

4.1 First Part: Metropolis algorithm

In this first part we want the system to evolve from a transient regime and observe the fluctuations around the final state for a given temperature.

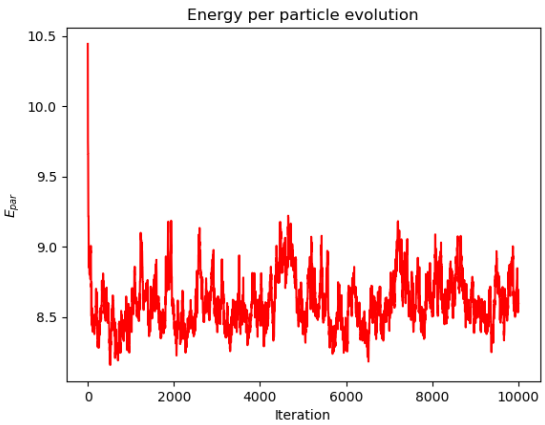


(a) Initial atom configuration

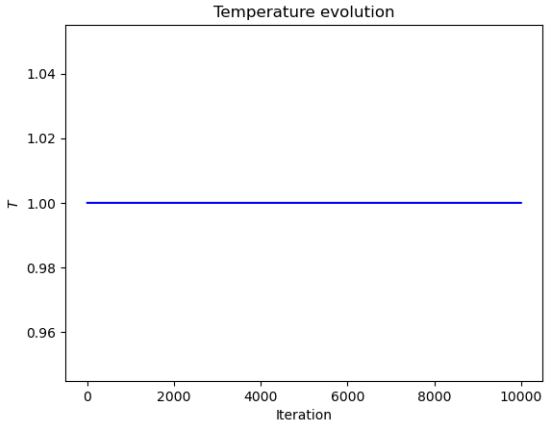
(b) Final atom configuration

Figure 4.1: Atom configuration for after Metropolis algorithm for $N = 20$ particles.

Even if this state is not the optimal configuration, we can see that the final configuration is less energetic than the first one by looking at the energy evolution throughout the iterations:



(a) Energy.



(b) Temperature.

Figure 4.2: Energy and temperature evolution for $N_{\text{iter}} = 10.000$ iterations.

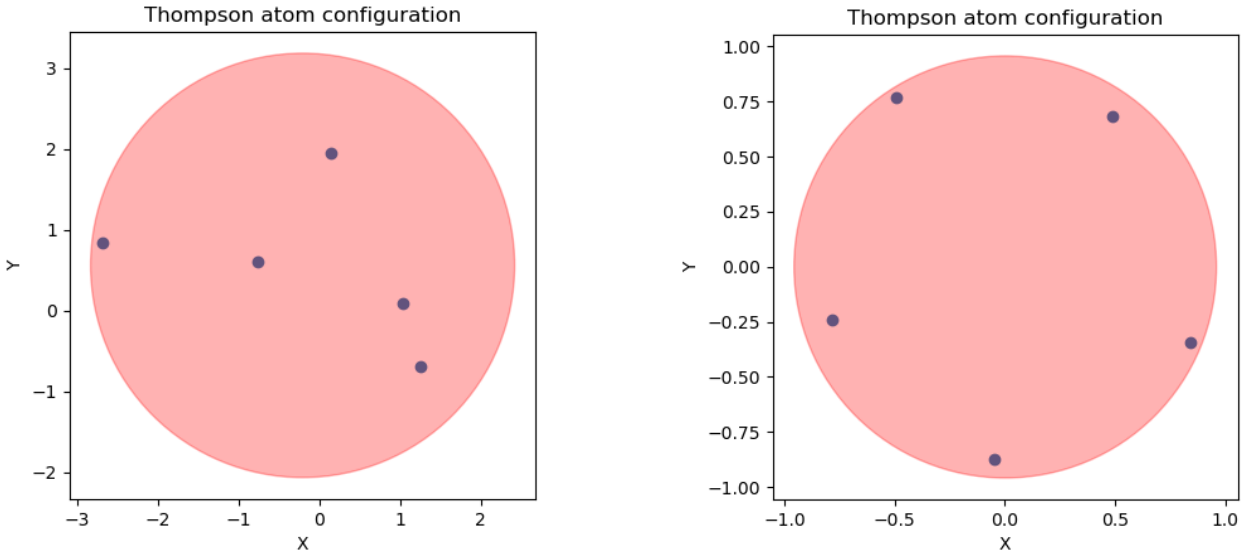
Notice that in this case, we kept the temperature constant, which led to an acceptance rate of $p_{\text{acc}} = 0.4587$ and caused the algorithm to oscillate around a certain configuration.

4.2 Second Part: Simulated Annealing

In this second part, we are interested in finding the optimal configuration for which the energy of the system is minimum. For that, we will start with a relatively high temperature value and reduce it after every iteration with the cooldown rate.

4.2.1 $N = 5$ charged particles

For 5 particles, the initial and final states look like this:

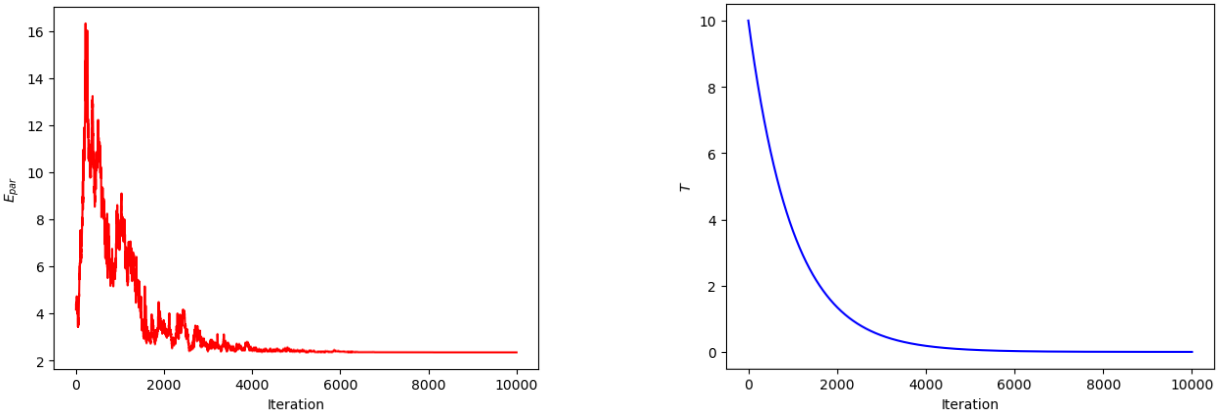


(a) Initial atom configuration

(b) Final atom configuration

Figure 4.3: Atom configuration for after Simulated Annealing for $N = 5$ particles.

We can see a single shell structure containing the 5 charged particles similarly spaced and, if we take a look at the energies



(a) Energy.

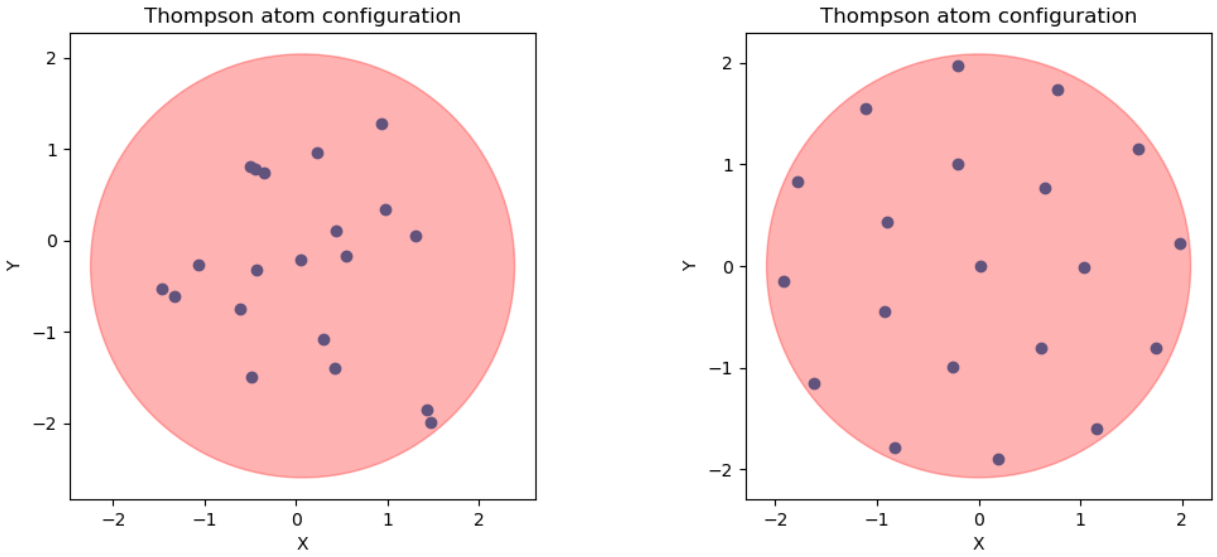
(b) Temperature.

Figure 4.4: Energy and temperature evolution for $N_{\text{iter}} = 10.000$ iterations.

we obtain a final value of the energy (per particle) of $E/N = 2.342$, which is very close to the actual ground state energy $E_0 \simeq 2.338$ (0.137%). Notice that at the beginning, due to the high temperature, the system evolves to configurations with much higher energies. However, after some time has passed and the temperature drops down (to $T^* = 4.52 \times 10^{-4}$), we are able to (approximately) converge to the ground state.

4.2.2 $N = 20$ charged particles

Next, for 20 particles, we obtain

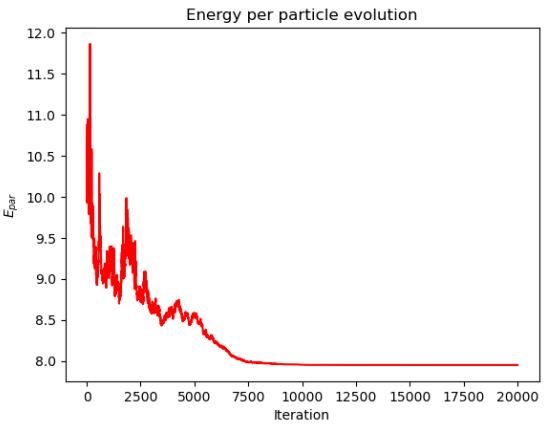


(a) Initial atom configuration

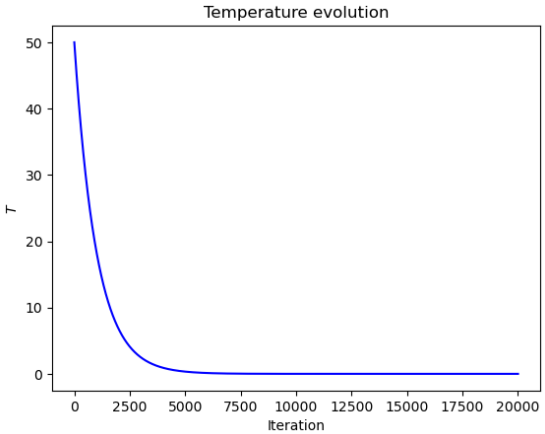
(b) Final atom configuration

Figure 4.5: Atom configuration for after Simulated Annealing for $N = 20$ particles.

In this case, since we have many particles, the optimal configuration now has 3 shells. The inner shell only contains 1 particle, while the middle and outer shells have 7 and 12 particles respectively. Plotting the energy evolution, we see the following:



(a) Energy.



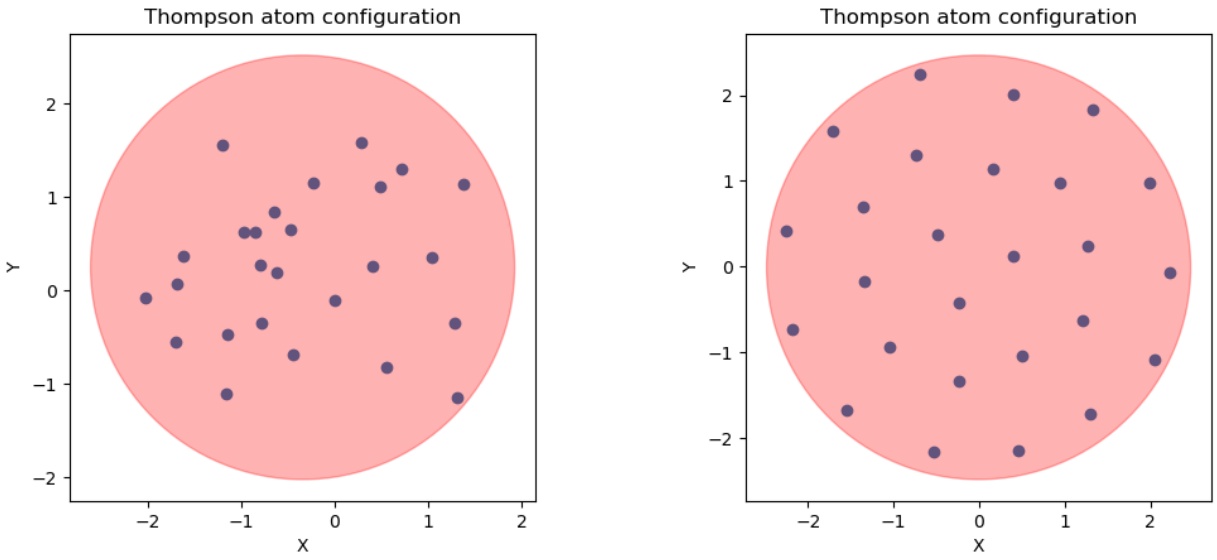
(b) Temperature. Acceptance probability $p_{\text{acc}} = 0.39515$

Figure 4.6: Energy and temperature evolution for $N_{\text{iter}} = 20.000$ iterations.

At the end of the simulated annealing, the temperature is $T^* = 1.02 \times 10^{-7}$ and the final value of the energy (per particle) is $E/N = 7.950$ which, compared to the ground state energy $E_0 \simeq 7.94961$, comes within 0.006% of error. We can safely say that we have managed to reach the ground state configuration.

4.2.3 $N = 26$ charged particles

Finally, let us try to find the optimal atom configuration for $N = 26$ particles:

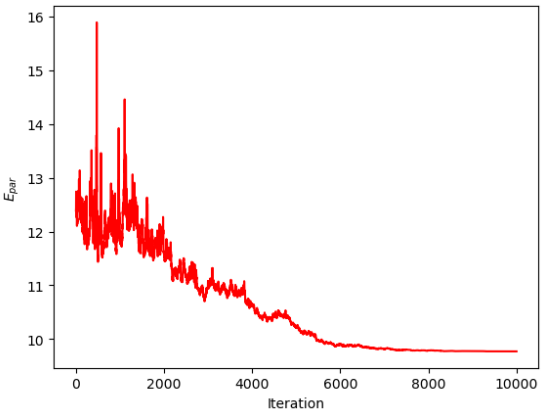


(a) Initial atom configuration

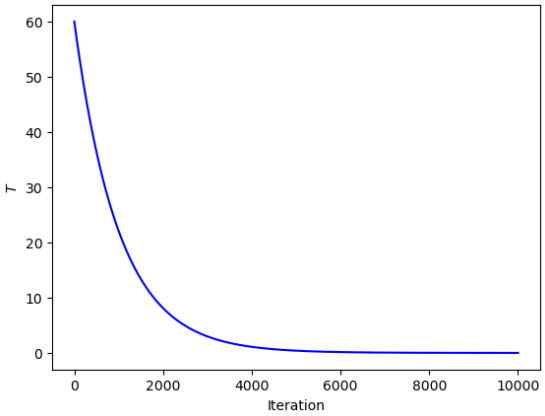
(b) Final atom configuration

Figure 4.7: Atom configuration for after Simulated Annealing for $N = 26$ particles.

Compared to the previous case, we notice that the number of shells has not changed, but the number of particles in each shell has increased. The inner shell now has 3 particles, and the middle and outer ones have 9 and 14 particles each.



(a) Energy.



(b) Temperature. Acceptance probability $p_{\text{acc}} = 0.6384$

Figure 4.8: Energy and temperature evolution for $N_{\text{iter}} = 10.000$ iterations.

For a final temperature of $T^* = 2.71 \times 10^{-3}$, the energy (per particle) is $E/N = 9.771$. The relative error compared to the actual value ($E_0 \simeq 9.762$) is 0.087%. Using more iterations and adjusting the parameters according to the resulting acceptance value, we can probably find a better solution if needed.