Exercise 4. Annealing method applied to find the global minimum of a two-dimensional Thompson atomic model

Objective: to simulate a system composed of Coulomb charges in a two-dimensional trap (Thomson atomic model) by the classical Monte Carlo method and to use the annealing method to find the minimal energy configuration.

Outline

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

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

   Dimensionless units of length r_0 and energy E_0 can be conveniently chosen in such a way that $E_0 = \frac{1}{2} m\omega^2 r^0 = \frac{q^2}{r_0}$. The dimensionless variables are positions, $\tilde{r} = r/r_0$, energy $\tilde{E} = E/E_0$, temperature $\tilde{T} = k_B T/E_0$. Using these units, the potential energy reads

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

   .

2. Generate a random initial configuration.

3. Use Metropolis algorithm to simulate system properties at a fixed temperature $\tilde{T}$.

4. Use global moves (all particles are moved) either local moves (single particle is moved at a time), by displacing each coordinate randomly $x' = x + \xi$ 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 in $(0.1, 0.9)$ range

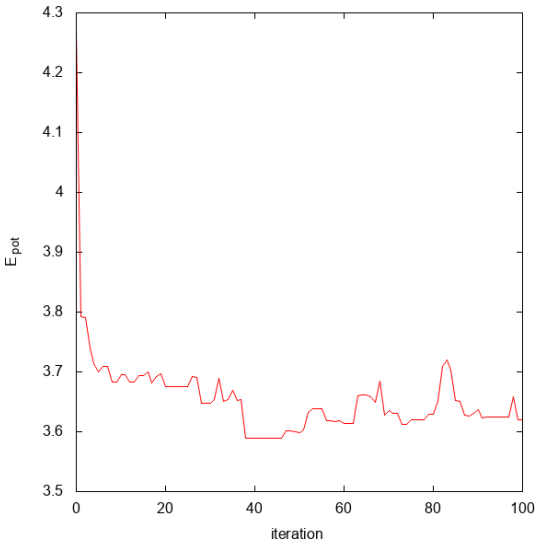
6. Verify that after an initial transient regime, potential energy converges to a certain value and fluctuates around it.

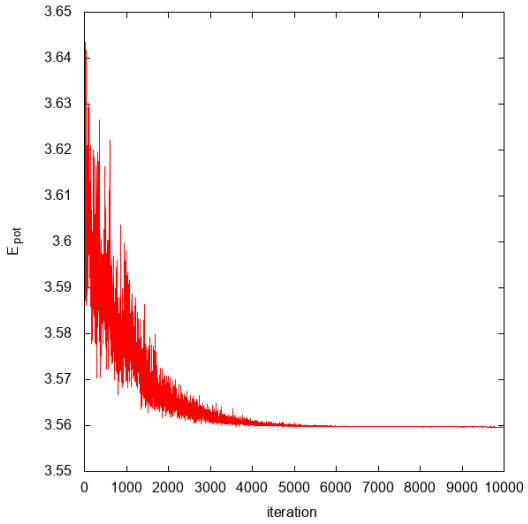
7. Implement the annealing procedure in which the temperature is lowered by a tiny fraction at each iteration (for example $T := T \times 0.999$), starting from a high temperature (large compared to the typical system energy) and ending with a low temperature.

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. Is it a shell structure? Is there a nucleation of a Wigner crystal visible in the center? What is the type of lattice which is visible in the center (square, hexagonal, etc.)?





Report

1. figure with a characteristic example of the energy dependence on the iteration number, show both the energy per particle and the temperature

2. snapshots of optimal configurations for $N = 5; 20; 26$ charges

3. occupations of the shells $(N_1, N_2, ...)$ as well as the energy per particle E/N for $N = 5; 20; 26$ charges. Report both the obtained numbers as well as the numbers provided in literature [PRB **49**, 2667 (19974)]

Some results to compare with:

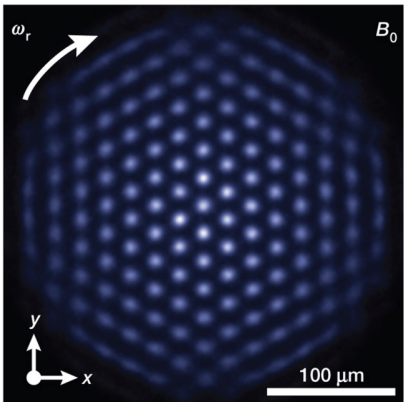


Figure 1: An image of an ion Coulomb crystal consisting of a single plane of Be + ions in a Penning trap. The crystal is rotating but the image is reconstructed using timing information from a position-sensitive photomultiplier. [Nature 484, 489 (2012)].

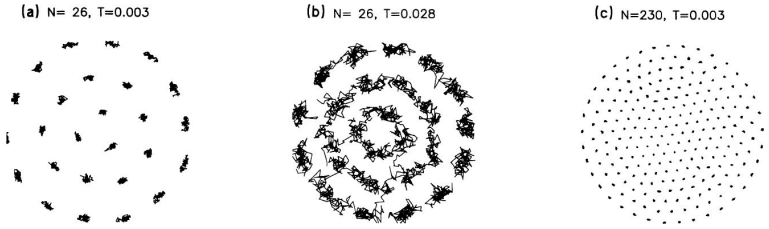


Figure 2: Electron trajectories during 1000 Monte Carlo steps for parabolic-confinement. Results are shown for different numbers of electrons and for different temperatures. [V. M. Bedanov and F. M. Peeters "Ordering and phase transitions of charged particles in a classical finite two-dimensional system" Phys. Rev. B **49**, 2667 (1994)]

TABLE I. Ground-state configurations for the system with parabolic-confinement potential. Shell structures ($N_1, N_2, ...$), energies (E/N), and percentage of sixfold-coordinated particles (P_6).

N	$N_1, N_2, ...$	E/N (reduced units)	P_6 (%)
1	1	0.0	
2	2	0.75000	
3	3	1.31037	
4	4	1.83545	
5	5	2.33845	
6	1, 5	2.80456	0
7	1, 6	3.23897	100
8	1, 7	3.66890	0
9	2, 7	4.08813	50
10	2, 8	4.48494	100
11	3, 8	4.86467	67
12	3, 9	5.23895	100
13	4, 9	5.60114	25
14	4, 10	5.95899	60
15	5, 10	6.30758	40
16	1, 5, 10	6.64990	83
17	1, 6, 10	6.98291	71
18	1, 6, 11	7.30814	86
19	1, 6, 12	7.63197	100
20	1, 7, 12	7.94961	62
21	1, 7, 13	8.26588	75
22	2, 8, 12	8.57418	80
23	2, 8, 13	8.87765	70
24	3, 8, 13	9.17590	91
25	3, 9, 13	9.47079	83
26	3, 9, 14	9.76273	75

Figure 3: [V. M. Bedanov and F. M. Peeters "Ordering and phase transitions of charged particles in a classical finite two-dimensional system" Phys. Rev. B **49**, 2667 (1994)]

Some ideas for debugging

1. The easiest way (but not the most efficient one) is to create a routine, that calculates the energy for a given set of particle coordinates, $E(\mathbf{r}_1, ..., \mathbf{r}_N)$. Metropolis algorithm can be implemented by calculating $\exp\{-[E(\mathbf{R}') - E(\mathbf{R})] \,/\, (k_B T)\}$.

2. For a single particle, $N = 1$, the optimal position is $x = y = 0$. At a finite temperature, the potential energy of a single particle is $E_{pot} = \frac{1}{2} m\omega^2(\langle x^2 \rangle + \langle y^2 \rangle) = k_B T$. In dimensionless units, $\tilde{E} = \tilde{T}$

3. For two particles, $N = 2$, the optimal configuration has to be symmetric $x_1 = -x_2 = r$, $y_1 = y_2 = 0$ (or any rotated configuration). The energy in this case is $E_{pot} = x_1^2 + x_2^2 + 1/|x_1 - x_2| = 2r^2 + 1/(2r)$ which reaches its minimal value $E_{pot} = 1.5$ for $r = 0.5$.

4. For N particles, the total energy can be approximated as $\tilde{E}/N = (N^{2/3} - 1)2^{1/3}$ and the system size grows slowly with the number of particles as $N^{1/3}$. In other words, the dependence on the number of particles is rather weak, so that in practice the initial coordinates can be generated randomly in the unit box ($-1 < x < 1$, $-1 < y < 1$) for any number of particles, and the algorithm will eventually converge to the optimal system size. Alternatively, one might adjust the