MONTE CARLO METHODS (1)

Objectives:

- Implement a Markov-Chain Monte Carlo method whose description is given;
- Apply the Metropolis criterion;
- Sample a probability distribution using a Markov-Chain Monte Carlo method;
- Analyse the time series of an observable to determine the length of the burn-in phase;
- Sample the probability distribution of an observable using a Markov-Chain Monte Carlo method;
- Compute the mean of an observable.

No list manipulation is allowed in this tutorial!

I. Quantum ideal gas

We consider an ideal quantum gas in a three-dimensional box of linear size L at temperature T. The gas consists of N atoms of mass m, and each atom i is characterised by three quantum numbers $n_{x,i}$, $n_{y,i}$, $n_{z,i} = 1, 2, 3, 4 \ldots \infty$. The kinetic energy of atom i is

$$E_i = \frac{\pi^2 \hbar^2}{2mL^2} \left(n_{x,i}^2 + n_{y,i}^2 + n_{z,i}^2 \right). \tag{1}$$

Since the atoms do not interact, the total energy of the system E is the sum of the kinetic energies of all atoms. We assume that atoms are distinguishable.

Question 1: Show that, if one of the atoms changes one of its quantum numbers by one unit (say $n_{x,i} \to n_{x,i} \pm 1$), then the total energy E of the system changes by

$$\Delta E = \frac{\pi^2 \hbar^2}{2mL^2} \left(\pm 2 n_{x,i} + 1 \right). \tag{2}$$

We assume that the system is at equilibrium at temperature T. The probability distribution of a microstate $\ell = \{n_{x,1}, n_{y,1}, n_{z,1}, n_{x,2}, \ldots, n_{z,N}\}$ characterized by the $3N$ quantum numbers is

$$\mathcal{P}_\ell = \frac{e^{-\beta E_\ell}}{Z}, \quad \beta = \frac{1}{k_\mathrm{B} T}, \tag{3}$$

with Z the normalization constant (partition function), and

$$E_\ell = \frac{\pi^2 \hbar^2}{2mL^2} \sum_{i=1}^{N} \left(n_{x,i}^2 + n_{y,i}^2 + n_{z,i}^2 \right). \tag{4}$$

To simulate the system, we propose to implement the following Markov chain:

- At each step, randomly choose one of the atoms (say atom i) and one of its quantum numbers $n_{x,i}$, $n_{y,i}$ or $n_{z,i}$ (say $n_{\alpha,i}$). Propose a new configuration with the change $n_{\alpha,i} \to n_{\alpha,i} \pm 1$ (with the sign chosen randomly).
- If the proposed value of $n_{\alpha,i}$ is zero, reject this new configuration.

- Otherwise, compute the energy difference and accept or reject the new configuration according to the Metropolis rule.

It is convenient to use units where $\hbar = 1$, $L = 1$, $m = 1$, $k_\mathrm{B} = 1$.

Question 2: Define a function `MC_step(n, E, T)` which takes as input an array `n` of shape $(N, 3)$ containing the quantum numbers of all particles, the total energy E of the system, and the temperature T, implements the Markov chain described above, modifies in place the array `n` if the trial move is accepted and returns the new energy of the system E.
Hint: look at the function `numpy.random.randint`.

Question 3: For $N = 1000$ atoms and $T = 10$, compute and plot the energy of the system for $M = 200000$ steps, starting with all atoms in their ground state, $n_{x,i} = n_{y,i} = n_{z,i} = 1$. How many steps $M_\mathrm{b-i}$ does it roughly take for the Markov chain to find the region of thermal equilibrium (burn-in phase)? How does $M_\mathrm{b-i}$ changes with N?

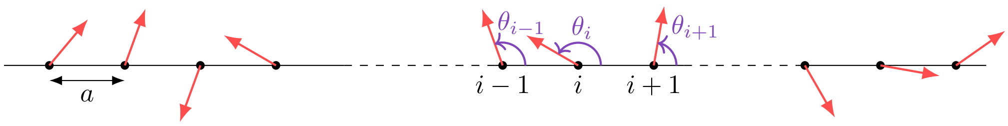
Question 4: For $N = 1000$ atoms, compute the mean energy $\langle E \rangle$ of the system at equilibrium for $T = 0, 2, 4, \ldots, 20$. Plot $\langle E \rangle / N$ as a function of T. Comment the evolution of the mean energy with temperature.
Hint: be careful that you should compute the average value of the energy in the equilibrium phase only, i.e., after removing points from the burn-in phase.

II. Fully-connected XY model in one dimension

We consider a system of N spins on a one-dimensional chain of linear size L at temperature T. These spins are two-dimensional vectors and they occupy regularly spaced sites, the distance between two sites being a. One spin (say i) interacts with all other spins (long-range interacting system) and tends to align with them. The alignment interaction between spins i and j is captured by the following interaction energy:

$$E_{i,j} = -\frac{\mathcal{J}}{N}\cos(\theta_i - \theta_j), \tag{5}$$

where θ_i (resp. θ_j) stands for the angle made by spin i (resp. spin j) with the axis of the chain, and $\mathcal{J} > 0$ the coupling constant. The coupling constant is normalized by N so that the system has a well-defined thermodynamic limit (Kac prescription).



The Hamiltonian of the system $\mathcal{H}$ is the sum of all interaction energies, namely,

$$\mathcal{H}(\theta_1, \ldots, \theta_N) = \sum_{i=1}^{N}\sum_{j=i+1}^{N} E_{i,j} = -\frac{\mathcal{J}}{N}\sum_{i=1}^{N}\sum_{j=i+1}^{N}\cos(\theta_i - \theta_j). \tag{6}$$

We can always choose units such that $\mathcal{J} = 1$, $a = 1$ and $k_\mathrm{B} = 1$.

Question 1: Show that the change in the total energy of the system [given by Eq. (6)] if one of the spins changes its orientation, say $\theta_i \to \theta_i + \delta$, equals

$$\Delta E = \frac{2\mathcal{J}}{N}\sin\left(\frac{\delta}{2}\right)\left[\sum_{j=1}^{N}\sin\left(\theta_i - \theta_j + \frac{\delta}{2}\right) - \sin\left(\frac{\delta}{2}\right)\right]. \tag{7}$$

We assume that the system is at equilibrium at temperature T. The probability density of a microstate $\{\theta_1, \theta_2, \ldots, \theta_N\}$ characterized by the N values of angles is

$$\mathrm{d}\mathcal{P}(\theta_1, \ldots, \theta_N) = \frac{e^{-\beta\mathcal{H}(\theta_1, \ldots, \theta_N)}}{Z} \mathrm{d}\theta_1 \ldots \mathrm{d}\theta_N, \quad \beta = \frac{1}{k_\mathrm{B}T}, \tag{8}$$

with Z the normalization constant (partition function), and $\mathcal{H}$ given by Eq. (6). To simulate the system, we propose to implement the Markov chain described below. At each step of the Markov chain, we sweep the entire chain of spins, from left to right.

- Start with spin 1. Propose a new configuration with the change $\theta_1 \to \theta_1 + \delta_1$ with δ_1 uniformly distributed in the range $[-\epsilon, \epsilon]$.
- Compute the energy difference and accept or reject the new configuration according to the Metropolis rule.
- Start again with spin 2, then spin 3, etc. until you have swept the entire chain.

Question 2: Define a function `MC_sweep(theta, T, epsilon)` which takes as input an array `theta` of size N containing the angles made by all spins with the axis of the chain, the temperature T, and the maximum angular shift for trial moves ϵ, implements the Markov chain described above for one sweep of the chain and modifies in place the array `theta` each time a trial move is accepted.

We define an order parameter

$$S = \sqrt{\left\langle \left(\frac{1}{N} \sum_{i=1}^{N} \vec{s_i} \right)^2 \right\rangle}, \tag{9}$$

with $\vec{s_i} = (\cos\theta_i, \sin\theta_i)$ the orientation of spin i, and $\langle\cdot\rangle$ the equilibrium average. The order parameter is such that $S \to 1$ when all spins are aligned, while $S \to 0$ when all spins point to different directions.

Question 3: For $N = 100$ spins, $\epsilon = 1.0$, and for several values of temperature between $T = 0$ and $T = 1$, compute the mean order parameter S of the system at equilibrium. Plot S as a function of temperature, and comment its evolution.
Hint: be careful that you should compute the average value involved in the definition of the order parameter in the equilibrium phase only, i.e., after removing points from the burn-in phase whose length you have to estimate for each temperature by running short simulations.

Question 4: Repeat question 3 for $N = 20$ and $N = 200$ spins. Plot all the curves $S(T)$ for the three sizes $N = 20$, $N = 100$, and $N = 200$ on the same graph. What do you see?

Question 5 (bonus): In practice, the maximum angular shift ϵ should be chosen such that the acceptance rate (the fraction of accepted trial moves) is between 20% and 50%. For $N = 100$ and $T = 0.1$, compute and plot the acceptance rate for 10 values of ϵ regularly spaced between 0 and π. How should one choose ϵ?