Exercise 06

The Boltzmann distribution

Deadline: Please, hand in your solutions by **Thursday, 19 June, 2.15 p.m.**

6.1 Microstates in a 5-level system (16 P)

Consider a system with N particles and five energy levels. The energy levels of the particles are equidistant, i.e $\epsilon_1 = 0$, $\epsilon_2 = 1$, $\epsilon_3 = 2$, $\epsilon_4 = 3$, $\epsilon_5 = 4$. Let us write the configuration of the system , i.e. the energies of the individual particles, at time t=0 as a vector, e.g

$$\mathbf{c}^\top(0) = (0, 4, 2, 1, 0, 3)$$

for a system with $N = 6$ particles. ($\mathbf{c}^\top$ denotes the transpose of $\mathbf{c}$.) You can change the configuration of the system by making the following energy-conserving move

- Raise the energy of a randomly chosen particle i by 1
- lower the energy of a randomly chosen particle j by 1.

E.g , for $i = 4$ and $j = 2$ in the above example this yields

$$\mathbf{c}^\top(0) = (0, \mathbf{4}, 2, \mathbf{1}, 0, 3)$$

$$\mathbf{c}^\top(1) = (0, \mathbf{3}, 2, \mathbf{2}, 0, 3)\,.$$

$i = j$, which has no net effect on the configuration, is an allowed move. However, you cannot increase the energy of a particle which is in the highest energy level, and you cannot decrease the energy of a particle which is the in the lowest energy level.

(a) Write a program which generates a series of configurations according to this algorithm. In the initial state, all particles are in energy level $\epsilon_2 = 1$. Simulate systems with $N = 10$, 100, and 1000 particles for 10'000 steps. (6 P)

To analyze your simulations,

(c) plot the total an energy as a function of time. (2 P)

(d) plot the populations of the five energy levels as a function of time. (2 P)

(e) calculate the average population in each energy level and the standard deviation (Discard the equilibration time from the trajectory.) (2 P)

(f) Assuming that the particles are distributed according to the Boltzmann distribution, estimate β from the simulation with $N = 1000$. (2 P)

(g) Discuss your results (about one paragraph). (2 P)

Hand in the code for the simulation program as well as for the analysis program. If you do not succeed in implementing the simulation program in (a), you can obtain trajectories from us and only do the analysis. Part (a) will then of course be graded with 0 points.

Hints:

- You can use the MatLab function `find()` to identify the positions of each element in an array which satisfies a certain criterion. E.g. `find(X>2)` returns the positions of all elements in the array `X` which are greater than 2.
- The MatLab command `datasample(Y,1)` returns one randomly chosen element from the array `Y`.
- If the simulations take longer than a few minutes, then there is probably something wrong in the your code.