Exercise 07

The Boltzmann distribution

Deadline: Please hand in your protocol as a single pdf file to **stevan.aleksic@fu-berlin.de** by **Thursday, 29**^{t}h **June, 10.15 a.m.**. Protocol should contain Python code, plots, and comments.

7.1 Microstates in a 5-level system (100 P)

Consider a system with N particles and five different and equidistant energy levels (e.g.: $\epsilon_1 = 0$, $\epsilon_2 = 1$, $\epsilon_3 = 2$, $\epsilon_4 = 3$, $\epsilon_5 = 4$). The configuration of the system at time t is defined by the energy levels of the individual particles. We can represent it as a vector, for example:

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

for a system with $N = 6$ particles where $\mathbf{c}^\top$ denotes the transpose of $\mathbf{c}$. We can change the configuration of the system, imposing the energy conservation, by making the following transitions

- 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

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

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

If $i = j$, the configuration does not change. However, we cannot increase the energy of a particle which is in the highest energy level, and we cannot decrease the energy of a particle which is the in the lowest energy level.

(a) Implement a program which generates a series of configurations according to this algorithm. In the initial state, all particles are in energy level $\epsilon_2 = 1$. (50 P)

To analyze your simulations,

(c) Plot the total energy as a function of time. (10 P)

(d) Plot the populations of the five energy levels as a function of time. (10 P)

(e) Calculate the average population in each energy level and the standard deviation discarding the equilibration time from the trajectory. Plot them using the errobar(x,y,err) function. (10 P)

(f) Assuming that the particles are distributed according to the Boltzmann distribution, estimate β. (10 P)

(g) Repeat the analysis with $N = 10, 100, 1000, 10000$ particles for 10000 timesteps and discuss your results. (10 P)