Exercise 07

The Boltzmann distribution

Deadline: Please hand in your protocol in pdf format by Thursday, the 13th of June 2019, 10 am to jan.joswig@fu-berlin.de and marca.manni@fu-berlin.de.

8.1 Microstates in a 5-level system (100 points)

Consider a system of N-particles in five equidistant energy levels (e.g. $\varepsilon_1 = 0$, $\varepsilon_2 = 1$, $\varepsilon_3 = 2$, $\varepsilon_4 = 3$, $\varepsilon_5 = 4$). The configuration (microstate) of the system at time t is defined by the energies of the individual particles. This can be represented by a vector, for example:

$$c(t = x) = (0, 4, 2, 1, 0, 3) \tag{1}$$

for a system of $N = 6$ particles. The configuration of the system can be changed (while the total energy is conserved) by the following transition:

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

In the example above this could yield ($i = 4$, $j = 2$):

$$c(t = x + 1) = (0, \mathbf{3}, 2, \mathbf{2}, 0, 3) \tag{2}$$

If $i = j$, the configuration does not change. The energy of a particle in the highest level can not be increased (and the energy of a particle in the lowest level can not be lowered), which means, that such a transition is forbidden.

1. Write a Python-script that generates a series of configurations according to this scheme. In the initial state all particles should be in the second lowest energy level.
2. Plot the total energy of the system as a function of time.
3. Plot the population of the energy levels as function of time.
4. Calculate the average population of each energy level and the standard deviation after the equilibration period and plot the results with errorbars.
5. Assuming that the particles energy is distributed according to a Boltzmann distribution, estimate β.
6. Do the analysis with $N = 10, 100, 1000, 10000$ particles simulated for about 10000 timesteps and discuss the results.