1   Ergocity breaking

Sequential algorithm consists of choosing particles in a increasing order (and restarting to 1 when the last particle is reached). It is not considered as an efficient simulation method and is sometimes non ergodic. The non-ergodicity is associated with the fact that the dynamics cannot explore the entire phase space, which appears as a set of disconnected parts. To highlight this point, consider a one-dimensional Ising model.

1. Starting from a staggered configuration of a line of 4 spins, using a sequential algorithm with a Metropolis rule and by considering the system at an infinite temperature, draw the sequence of configurations until the system goes back to the initial configuration.

2. Give an example of a configuration unreachable by using the sequential algorithm when one starts from the stagerred configuration. Consider all available configurations of the system and determine the number of independent trajectories. (A trajectory corresponds to a complete sequence of spin flips of the system where the system goes back to the initial configuration).

3. Modify the previous algorithm as follows : at each step, one has a probability α of flipping the spin i and a probability $(1 - \alpha)$ of keeping the same configuration. Show that the new algorithm is ergodic if $\alpha \neq 1$.

2   Unit vectors

1. By using the spherical coordinates, and the inverse transformation method, show how to obtain a set of unit vectors randomy and uniformly distributed on the sphere.

2. Write a Python script which gives a 3D configuration of unit vectors uniformly distributed on the sphere in order to obtain a figure similar to Fig.1

3   Glauber Dynamics

Let us consider the one-dimensional Ising model described by the Hamilonian

$$H = -J \sum_i \sigma_i \sigma_{i+1} \tag{9}$$

where σ_i is a Ising variable and i an integer index running the one-dimensional lattice.

To perform tractable calculations, one often uses the Glauber dynamics. That is a stochastic process where the transition rate between two configurations which differs by a spin flip at site i is given by

$$\Pi(\sigma_i \to -\sigma_i) = \frac{1}{2}(1 - \sigma_i \tanh(\beta h_i)) \tag{10}$$

where $h_i = J(\sigma_{i-1} + \sigma_{i+1})$ is the local field of the spin σ_i.
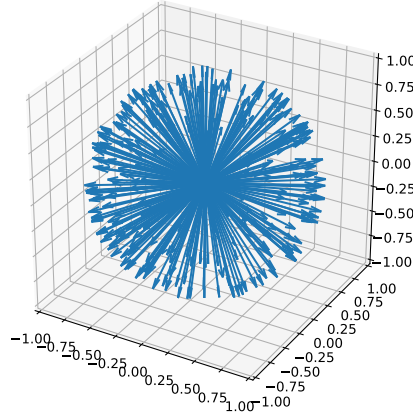
1. Show that the dynamics satisfies the detailed balance.

FIGURE 1 – Unit vectors

2. Justify that the dynamics converges to equilibrium.

3. By using the master equation, show that the mean value of σ_i evolves as

$$\frac{d < \sigma_i >}{dt} = - < \sigma_i > + < \tanh(\beta h_i) > \qquad (13)$$

4. Show that $\tanh(\beta h_i) = \gamma(\sigma_{i-1} + \sigma_{i+1})$ where γ is a function of βJ to be determined.

5. The mean values of all spins being identical, by using the fluctuation-dissipation theorem, the dynamic susceptibility $\chi(t)$ of the system is proportional to $\sum_i < \sigma_i(t) >$. Infer that the total susceptibility satisfies the differential equation

$$\frac{d\chi(t)}{dt} = -(1 - 2\gamma)\chi(t) \qquad (15)$$

6. From the above equation and the expression of γ, show that the characteristic relaxation time of the susceptibility behaves as $\frac{1}{1 - \tanh(2\beta J)}$.

Références

[1] Roy J. Glauber, *Time-Dependent Statistics of the Ising Model* J. Math. Phys.**4**, 294 (1963).