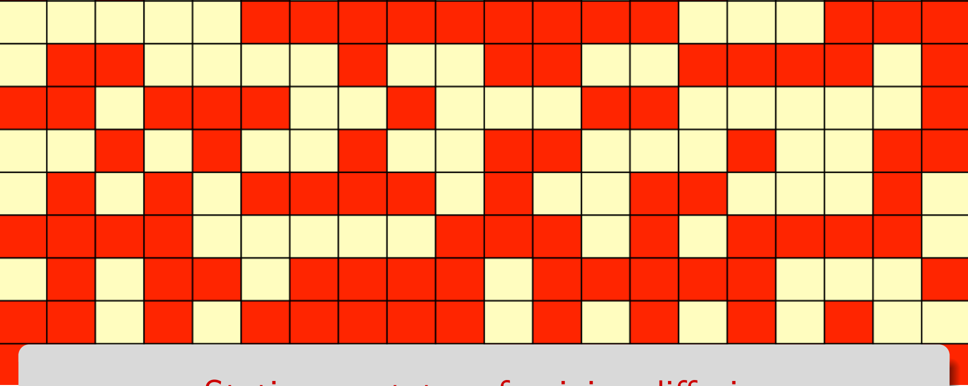


Stationary states of opinion diffusion

Project for the exam: AMS (DSE)

Paola Serra and Marzio De Corato

January 9, 2022

Theoretical Framework

Statistical Mechanics

"Ludwig Boltzmann, who spent much of his life studying statistical mechanics, died in 1906, by his own hand. Paul Ehrenfest, carrying on the work, died similarly in 1933. Now it is our turn to study statistical mechanics." States of Matter (1975), by David L. Goodstein

Concepts of statistical mechanics: aim [5]

Aim To predict the macroscopic properties of systems on the basis of their microscopic structure. This connection between these two scales is performed with statistical methods

Concepts of statistical mechanics: entropy [5]

Central problem of thermodynamics: characterize the actual state of equilibrium among all virtual states
Entropy postulate: there exist a function S of the extensive variables $(X_0, X_1 ... X_r)$ called entropy, that assumes the maximum value for a state of equilibrium among all vritual states and that possesses the following properties:

- Extensivity $S^{(1 \cup 2)} = S^1 + S^2$
- Convexity $S((1-\alpha)X^1 + \alpha X^2) \geq (1-\alpha)S(x^1) + \alpha S(X^2)$
- Monotonicity $\frac{\partial S}{\partial E}|_{X_1 ... X_r} = \frac{1}{T} > 0$

The equilibrium state corresponds to the maximum entropy compatible with the constrains

- **Fundamental postulate of statistical mechanics** $S = k_b \ln |\Gamma|$
  Where S is the thermodynamic entropy, k_b is Boltzmann constant and $|\Gamma|$ the volume in the phase space

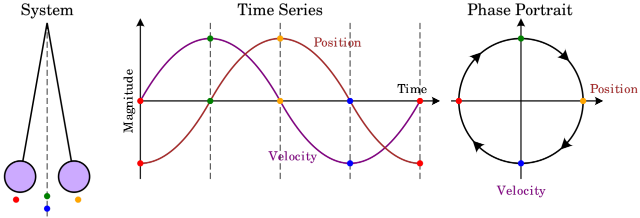


Image taken from [1]

Concepts of statistical mechanics: ensemble [5]

- **Statistical ensemble**: a large number of virtual copies of a system ; each of them is a possible state of the real system (epistemic probability) . It is the formalization of a repeated experiment proposed by Gibbs (empirical probability)
- **Microcanical ensamble:** $p = 1/W$ W is the number of microstates
- **Canonical ensamble:** $p = \frac{1}{Z}\exp\left(-\frac{E}{kT}\right)$ where $Z = \sum_i \exp\left(\frac{-E_i}{k_b T}\right)$

$$\langle A(x)\rangle = \frac{1}{Z}\int dx_s A(x_s) exp\left[-\frac{H^{(S)}(x_s)}{k_b T}\right] \quad (1)$$

$$Z = \int dx_s exp\left[-\frac{H^{S}(x_s)}{k_b T}\right] \quad (2)$$

$$\left\langle H(x)^2\right\rangle - \langle H(x)\rangle^2 = k_b T^2 C \quad (3)$$

Ising Model

Ising model [4, 3]

- An array of atoms that can take states ± 1. The energy of the system is given by $E(\mathbf{x}, J, H) = -\left[\frac{1}{2}\sum_{m,n} J_{mn}x_m x_n + \sum_n Hx_n\right]$ where J is the coupling constant between two neighbour sites, and H is an external field.
- The probability of the system to be in the state x is given by $p(x|\beta, J, H) = \frac{1}{Z(\beta,J,H)}\exp[-\beta E(x, J, H)]$ (canonical ensemble) where $\beta = 1/k_b T \quad Z(\beta, J, H) = \sum_x exp\left[-\beta E(x, J, H)\right]$
- It is useful to characterize the order level of a lattice (macroscopic) with the (spatial) correlation functions (whose input are microscopic quantities). In particular, for the Ising model, these are given by the following expression (with $H = 0$)

$$g(m) = \frac{\langle \sigma_i \sigma_{i+m} \rangle - \langle \sigma_i \rangle \langle \sigma_{i+m} \rangle}{1 - \langle \sigma_i \rangle \langle \sigma_{i+m} \rangle} = \langle \sigma_i \sigma_{i+m} \rangle$$

Numerical simulations

"Never make a calculation until you know the answer. Make an estimate before every calculation, try a simple physical argument (symmetry! invariance! conservation!) before every derivation, guess the answer to every paradox and puzzle. Courage: No one else needs to know what the guess is. Therefore make it quickly, by instinct. A right guess reinforces this instinct. A wrong guess brings the refreshment of surprise. In either case life as a spacetime expert, however long, is more fun!" John Archibald Wheeler

Numerical simulation [5]

- **Molecular dynamics:** the equation of motion are solved numerically PROS: information of both the dynamical and static properties of the system are explored
- **Monte Carlo:** a fictitious evolution process of the system is solved in order to get the equilibrium distribution PROS 1) also the systems whose dynamics is not defined can be explored 2) a fictitious dynamics can be considered in order to reach the equilibrium faster

Monte Carlo method [2]

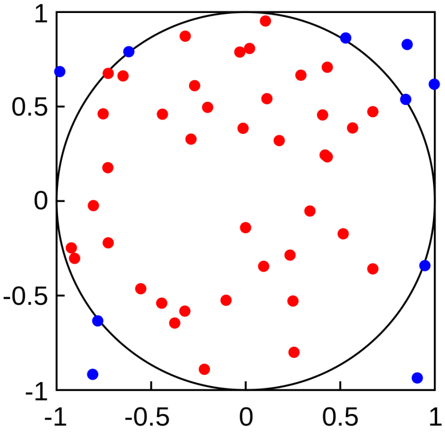


Image taken from [1]

Monte Carlo method [2]

- Lets consider the generic integral $I = \int_a^b dx\ f(x)$
- This can be recast in the following form $I = \int_0^1 dx\ w(x)\frac{f(x)}{w(x)}$
- If w(x) is the derivative of u(x) (non-decreasing,non negative) we have $I = \int_0^1 du\ \frac{f[x(u)]}{w[x(u)]}$
- If one considers L random values of u uniformely distributed in the interval [0,1] we have $I \approx \frac{1}{L}\sum_{i=1}^{L} \frac{f[x(u)}{w[x(x)]}$
- The choice of w is crucial since $\sigma = \frac{1}{L}\left[\left\langle \left(\frac{f}{w}\right)^2 \right\rangle - \left\langle \frac{f}{w} \right\rangle^2\right]$
- Brute Force $f = 10^{-260}$ and $\sigma = \frac{1}{Lf}$...is not a good idea
- PROBLEM: we do not know the form of the denominator (if we know it we do not need the Monte Carlo method)

Monte Carlo method [5]

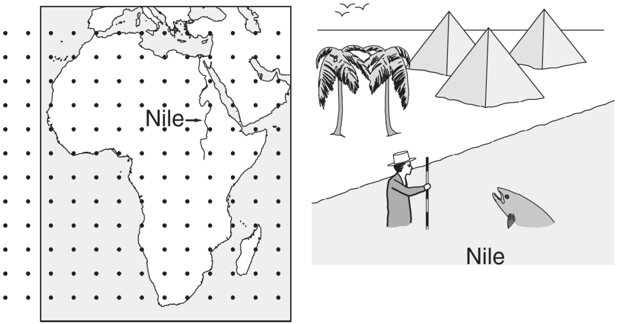


Image taken from [2]

Monte Carlo method: Metropolis idea [2]

$$\langle A \rangle = \frac{\int d\mathbf{r}^N \exp\left[-\beta E(\mathbf{r}^N)\right] A(r^N)}{\int d\mathbf{r}^N \exp\left[-\beta E(\mathbf{r}^N)\right]} \tag{4}$$

- We have a ratio between two integrals, therefore what we need to sample is the ratio and not the integrals alone
- The probability density is $N(r^N) = \exp\left[-\beta E(\mathbf{r}^N)\right]/Z$
- Metropolis idea: randomly generate points with this last probability distribution. In this case we have $\langle A \rangle \approx 1/L \sum_{i=1}^{L} n_i A(\mathbf{r}_i^N)$

Monte Carlo method: Metropolis idea [2]

- How the points are generated ? With a Boltzmann weighted Markov chain
- $\pi(old \rightarrow new) = \alpha(old \rightarrow new) \times acc(old \rightarrow new)$ where π is the transition probability element from the old state to the new state, α is the matrix element of Markov Chain and acc is the acceptance ratio.
- Detailed balance condition at the equilibrium $N(old)\pi(old \rightarrow new) = N(new)\pi(new \rightarrow old)$
- With a symmetric Markov transition matrix we have $N(old) \times acc(old \rightarrow new) = N(new) \times acc(new \rightarrow old)$
- Therefore we have

$$\frac{acc(old \rightarrow new)}{acc(new \rightarrow old)} = \frac{N(n)}{N(o)} = \exp\left[-\beta\left(E(new) - E(old)\right)\right] \tag{5}$$

- THE Z TERM IS NO MORE PRESENT ! We have only the difference between the two energies !!!

Monte Carlo method: Metropolis idea [2]

$$acc(old \to new) = \begin{cases} N(new)/N(old) & N(new) < N(old) \\ 1 & N(new) \geq N(old) \end{cases}$$

Therefore the overall transition probabilities are given by

$$\pi(old \to new) = \begin{cases} \alpha(old \to new) & N(new) \geq N(old) \\ \alpha(old \to new)\left[N(new)/N(old)\right] & N(new) < N(old) \end{cases}$$

$$\pi(old \to new) = 1 - \sum_{new \neq old} \pi(old \to new)$$

- In practice for each move a random number is generated from the uniform distribution between the interval $[0, 1]$, since $acc(old \to new) = \exp\left[-\beta\left(E(new) - E(old)\right)\right] < 1$. The move is accepted if the random number is lower than $acc(old \to new)$
- $\pi(old \to new)$ should be ergodic

Goals and methods

Goals and methods

- Reproduce the main result for a 2D anti ferromagnetic lattice ($J = -1$) with no external magnetic field ($H = 0$) with the montecarlo-metropolis
- Once checked that the script provide the correct results apply it to a lattice ($J = +1$). In this case the spins represent an opinion and the sites people. The goal is to find the stationary states (at $T = 0$ and $T \neq 0$)
- Introduce in the lattice some blocks that never change their status. These islands represent groups that never change mind and only diffuse their ideas. (at $T = 0$ and $T \neq 0$)

Results

Simulation features

- 10x10 lattice
- Periodic boundary conditions $\rightarrow$ the topology of a torus (genus equal to 1)
- 6000 steps

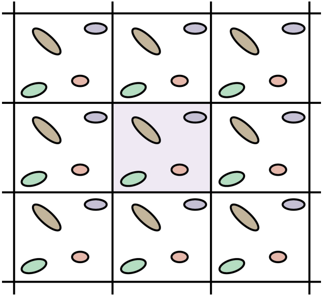


Image taken from [1]

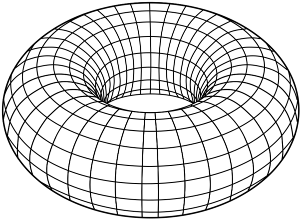
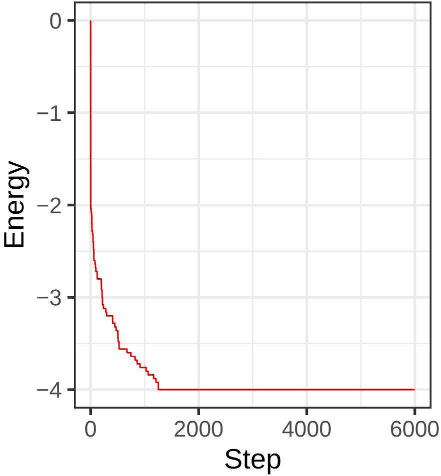
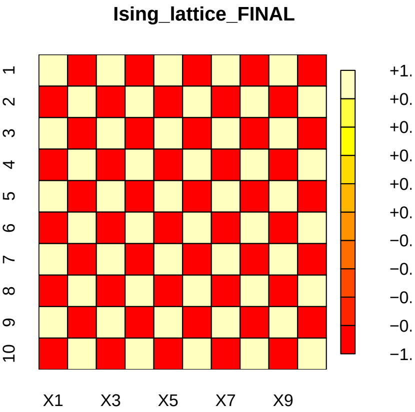


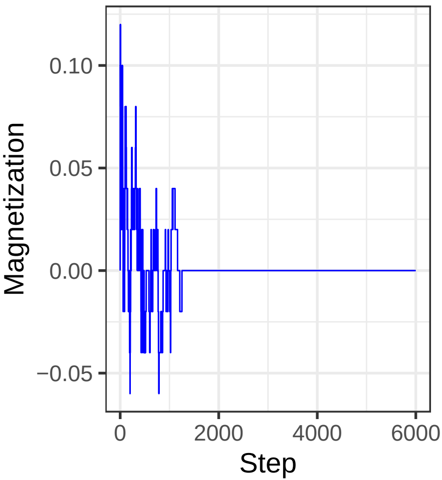
Image taken from [1]

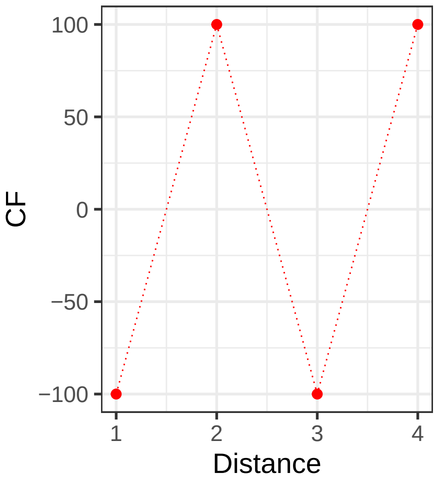
Antiferromagnetic J=-1, T=0



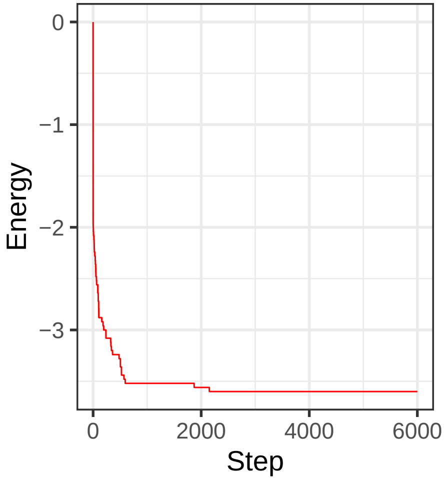


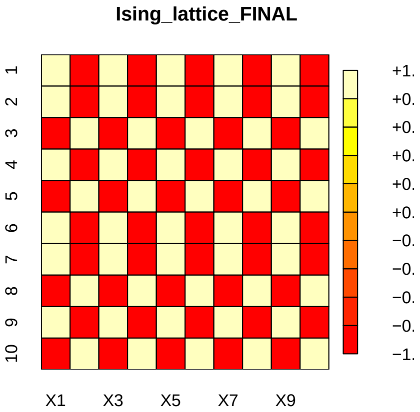
Antiferromagnetic J=-1, T=0



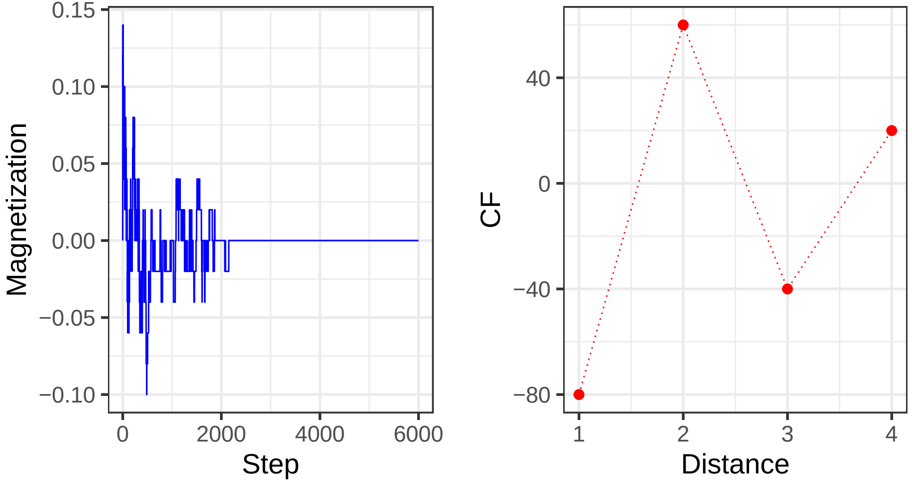


Antiferromagnetic J=-1, T=1.5

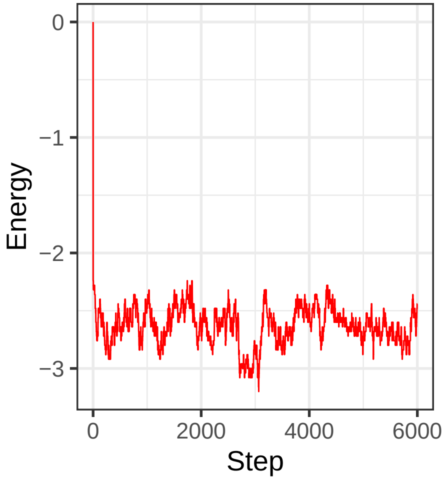


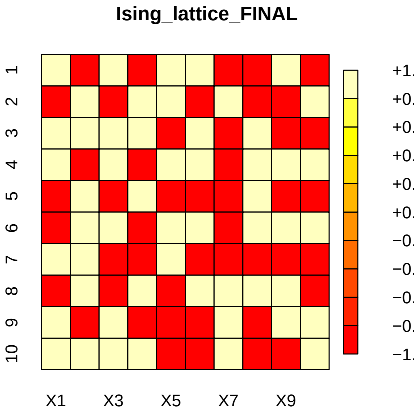


Antiferromagnetic J=-1, T=1.5

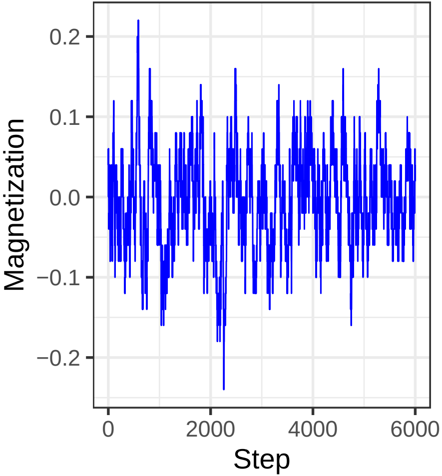


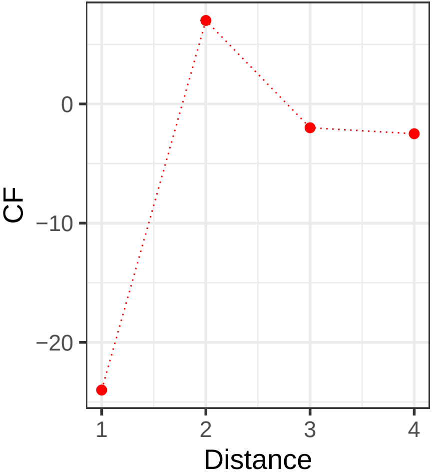
Antiferromagnetic J=-1, T=4



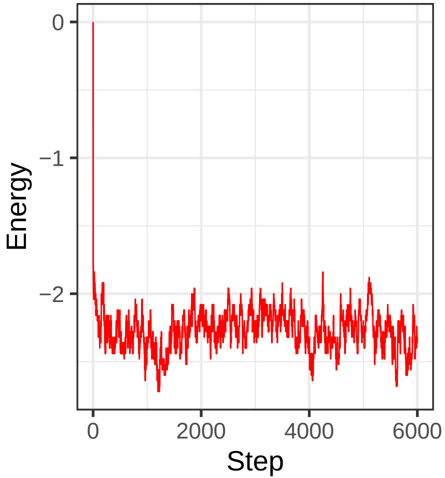


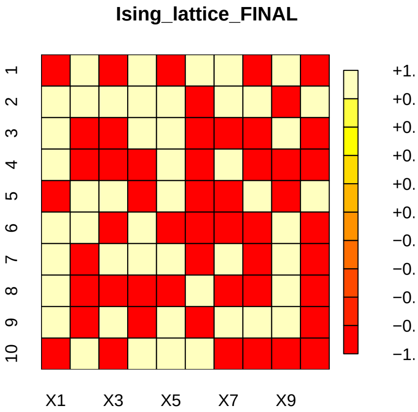
Antiferromagnetic J=-1, T=4



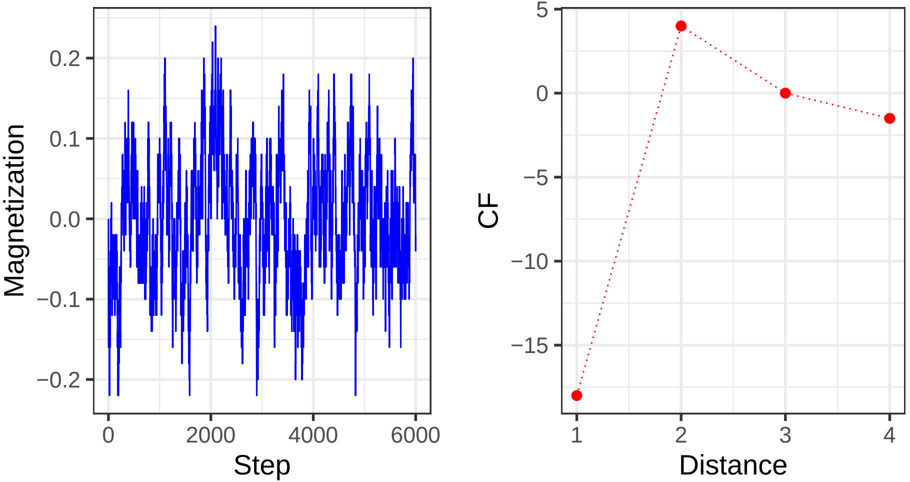


Antiferromagnetic J=-1, T=8

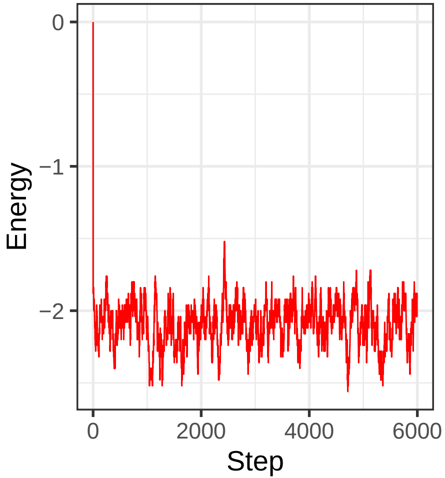


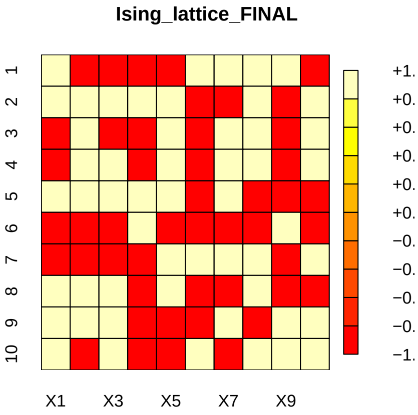


Antiferromagnetic J=-1, T=8

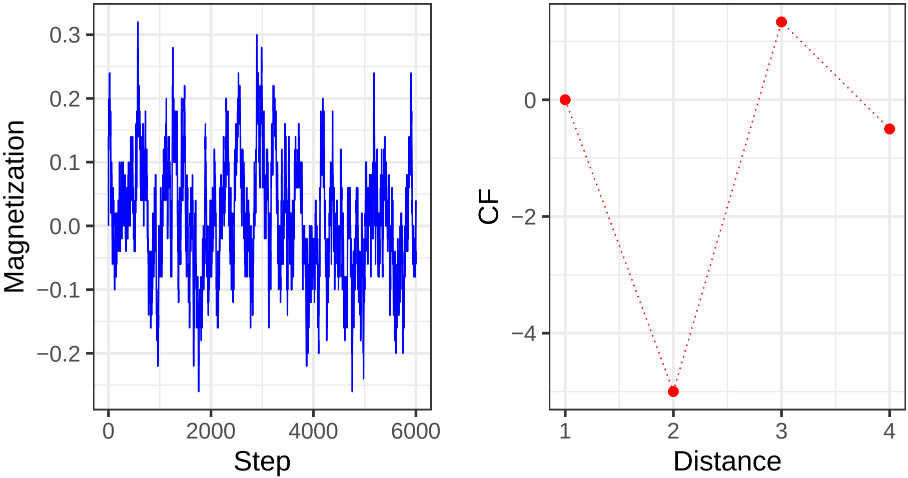


Ferromagnetic J=-1, T=30

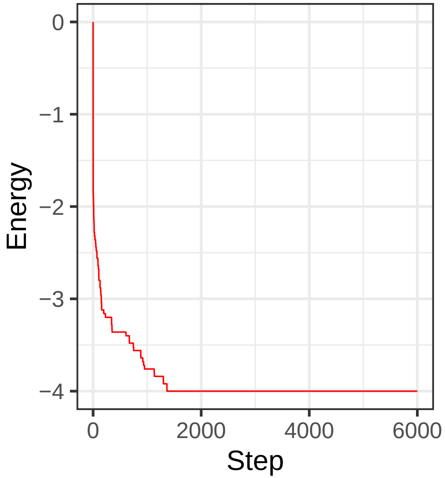


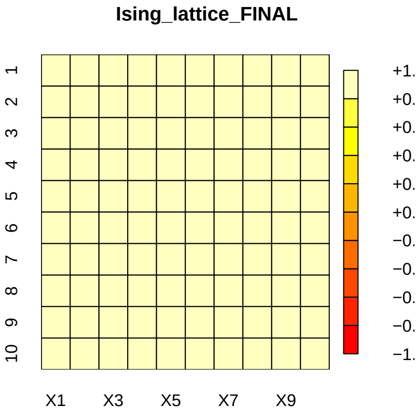


Ferromagnetic J=-1, T=30

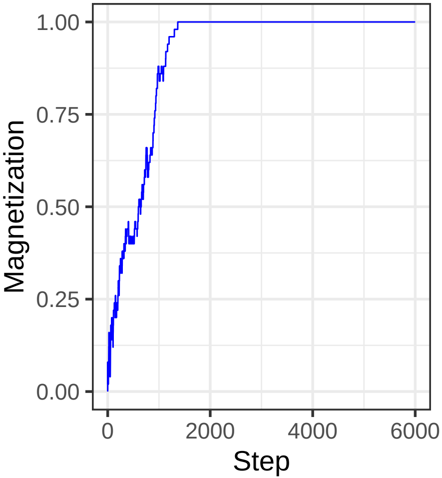


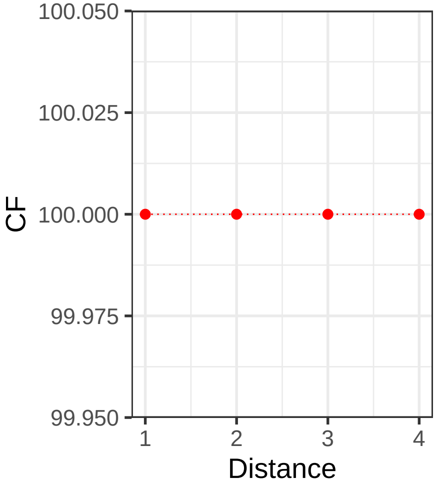
Ferromagnetic J=+1, T=0



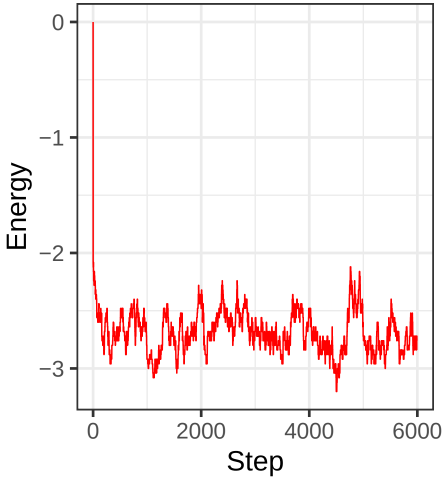


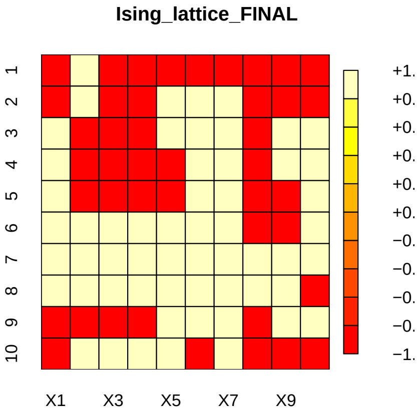
Ferromagnetic J=+1, T=0



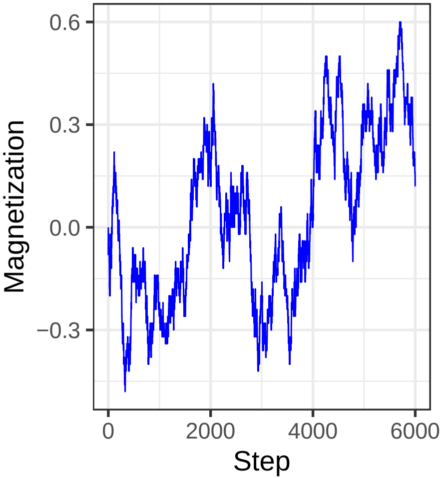


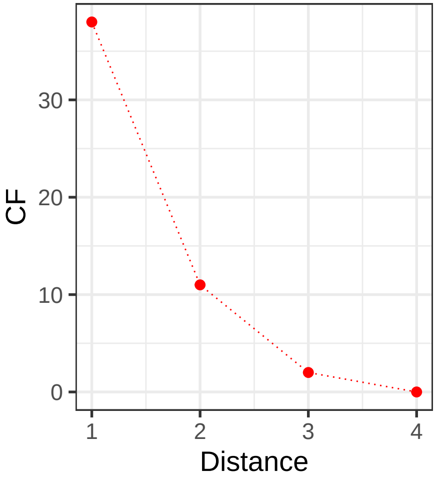
Ferromagnetic J=+1, T=8



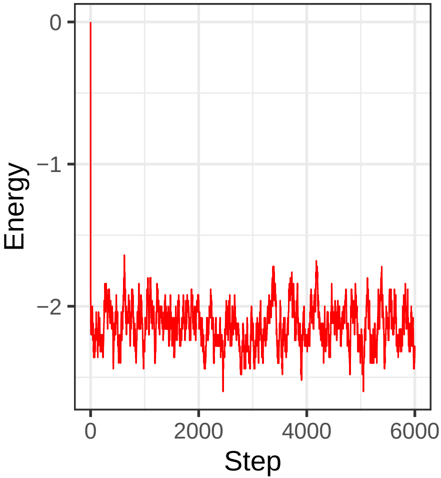


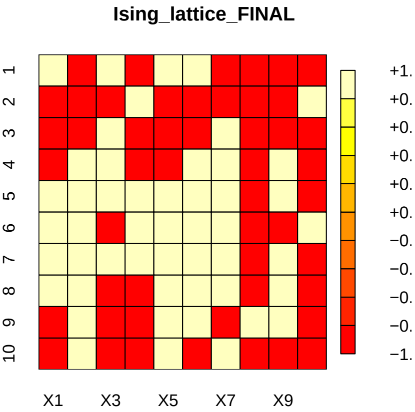
Ferromagnetic J=+1, T=8



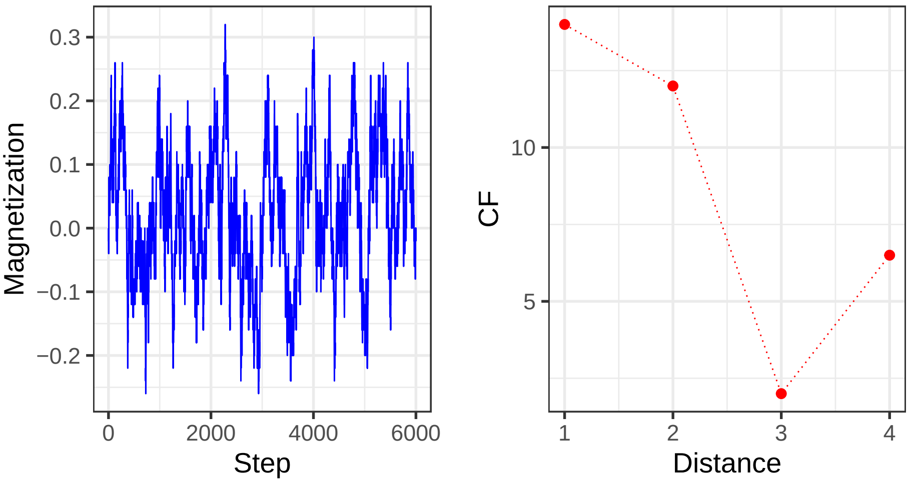


Ferromagnetic J=+1, T=16

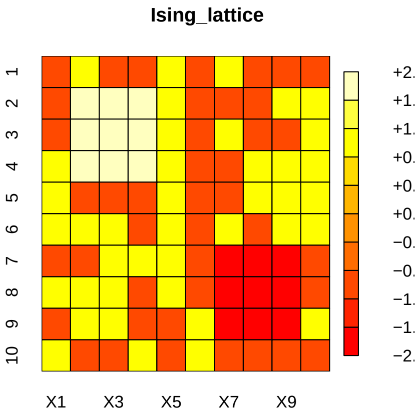




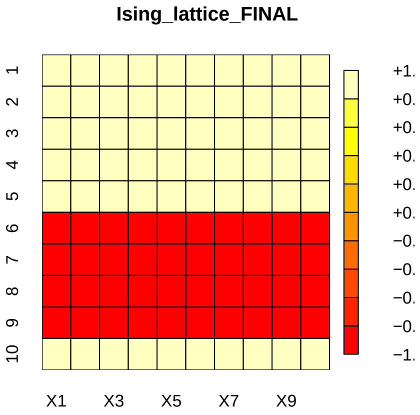
Ferromagnetic J=+1, T=16

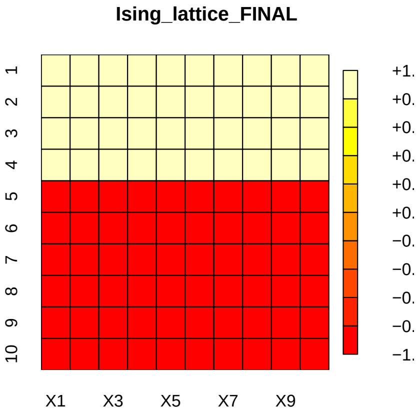


Ferromagnetic with two centers T=0

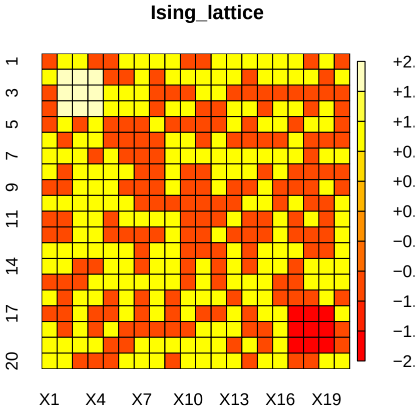


Ferromagnetic with two centers T=0

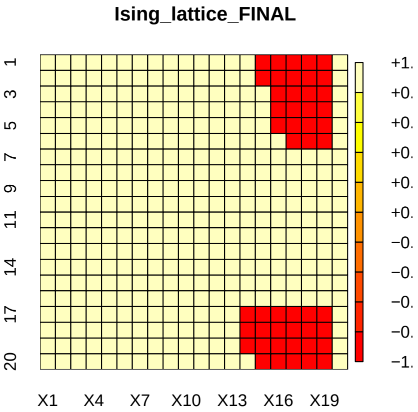


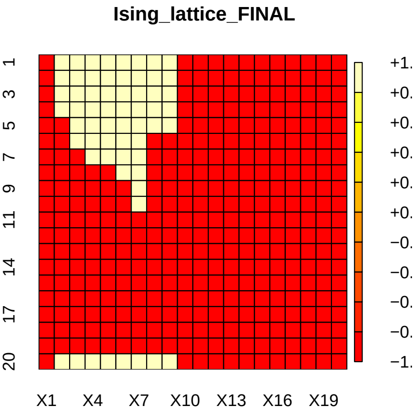


Ferromagnetic with two centers T=0, 20×20

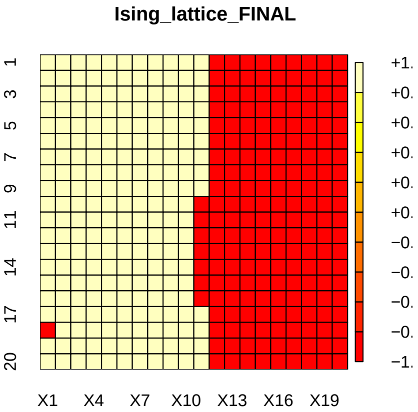


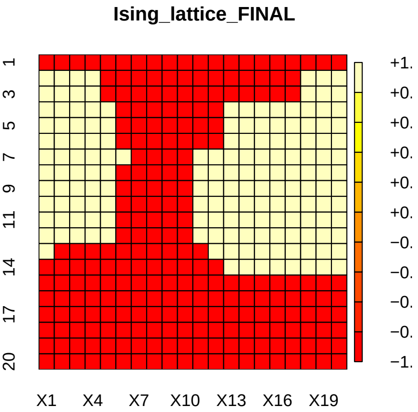
Ferromagnetic with two centers T=0, 20×20



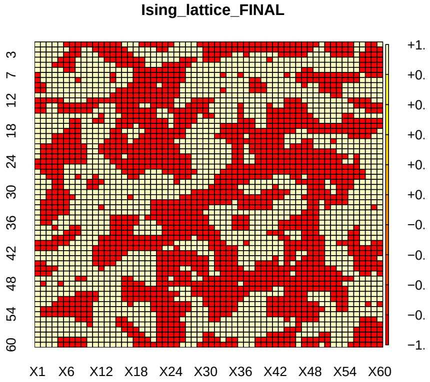


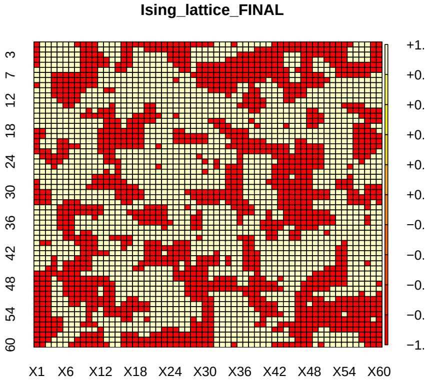
Ferromagnetic with two centers T=0.25, 20×20



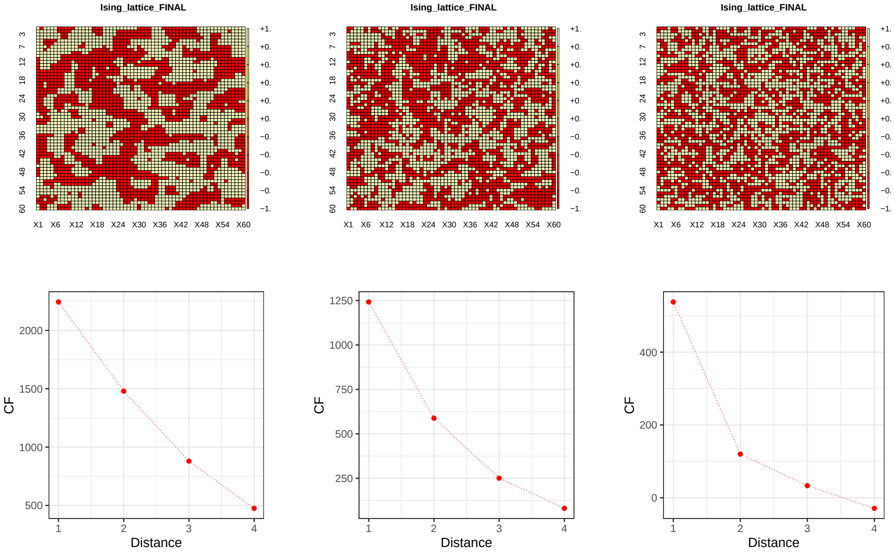


Ferromagnetic with two centers T=0, 60×60





Ferromagnetic with two centers $T > 0$, 60×60



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Concepts of statistical mechanics: entropy [5]

Central problem of thermodynamics: characterize the actual state of equilibrium among all virtual states

Entropy postulate: there exist a function S of the extensive variables $(X_0, X_1 ... X_r)$ called entropy, that assumes the maximum value for a state of equilibrium among all vritual states and that possesses the following properties:

- Extensivity $S^{(1\cup 2)} = S^1 + S^2$
- Convexity $S((1-\alpha)X^1 + \alpha X^2) \geq (1-\alpha)S(x^1) + \alpha S(X^2)$
- Monotonicity $\frac{\partial S}{\partial E}|_{X_1 ... X_r} = \frac{1}{T} > 0$

The equilibrium state corresponds to the maximum entropy compatible with the constrains

Concepts of statistical mechanics: entropy [5]

- **Fundamental postulate of statistical mechanics** $S = k_b \ln |\Gamma|$
- Where S is the thermodynamic entropy, k_b is Boltzmann constant and $|\Gamma|$ the volume in the phase space

$$
\begin{aligned}
S(X_0, ..., X_r) = k_b \ln \int_\Gamma dx = \\
k_b \int dx \prod_{i=0}^{r} [\theta(X_i(x) - (X_i - \Delta X_i))\theta(X_i - X_i(x))]
\end{aligned}
\tag{6}
$$

- $(X_0, ..., X_r)$ are the extensive variables
- The θ functions assures that the integrand is not null only in the interval $X_i - \Delta X_i \leq X_i(x) \leq X_i$

Concepts of statistical mechanics: micro-canonical ensamble

- Lets focus on a particular observable A (extensive)

$$S(X;a) = k_b \ln \int_\Gamma dx \delta(A(x) - a) \tag{7}$$

$$S(X) = S(X;a*) \geq S(X;a) \tag{8}$$

$$\begin{aligned} \frac{|\Gamma(a)|}{|\Gamma|} &= \frac{1}{|\Gamma|} \int_\Gamma dx \delta(A(x) - a)) \\ &= \exp\left\{ \frac{1}{k_b} \left[S(X;a) - S(X;a^*) \right] \right\} \\ &\simeq \exp\left\{ \frac{1}{k_b} \left[\frac{\partial^2 S}{\partial A^2}|_{a^*} (a - a^*)^2 \right] \right\} \end{aligned} \tag{9}$$

$$a^* = \langle A(x) \rangle = \frac{1}{|\Gamma|} \int_\Gamma dx A(x) \tag{10}$$

Concepts of statistical mechanics: canonical ensemble

$$a^* = \frac{1}{|\Gamma|} \int_\Gamma dx_s dx_R A(x_s) \tag{11}$$

$$\langle A(x) \rangle = \int dx_s dx_r A(x_S) \delta(H^{(s)}) \tag{12}$$

$$\langle A(x) \rangle = \frac{1}{|\Gamma|} \int dx_s dx_r A(x_s) \delta(H^S(x_s) + H^R(x_R) - H^S(x_S)) \tag{13}$$

$$\langle A(x) \rangle = \frac{1}{|\Gamma|} \int dx_s A(x_s) \times \int dx_r \delta(H^R(x_R) - (E - H^{(S)}(x_s))) \tag{14}$$

$$\int dx_r \delta(H^R(x_R) - (E - H^{(S)}(x_s))) \simeq \exp\left\{ \frac{1}{k_b} S^R(E - H^S) \right\} \tag{15}$$

Concepts of statistical mechanics: canonical ensemble

$$\exp\left\{\frac{1}{k_b}S^R(E-H^S)\right\} \simeq \exp\left[\frac{1}{k_b}S^R(E)\right] \exp\left[-\frac{1}{k_b}\frac{\partial S^{(R)}}{\partial E}|_E H^{(S)}(x_S)\right] \tag{16}$$

$$\langle A(x)\rangle = \frac{1}{Z}\int dx_s A(x_s) exp\left[-\frac{H^{(S)}(x_s)}{k_b T}\right] \tag{17}$$

$$Z = \int dx_s exp\left[-\frac{H^S(x_s)}{k_b T}\right] \tag{18}$$

$$\langle A(x)\rangle = \frac{1}{Z}\int dE \int dx \delta(H(x)-E) A(x) exp(-\frac{E}{k_b T}) \tag{19}$$

$$\langle A(x)\rangle = \frac{1}{Z}\int dE' a^*(E') exp\left[-\frac{E'-TS(E')}{k_b T}\right] \tag{20}$$

Concepts of statistical mechanics: canonical ensemble[5]

$$Z \simeq \exp\left[-\frac{E^* - TS(E^*)}{k_b T}\right] = \exp\left(-\frac{F}{k_b T}\right) \tag{21}$$

$$\frac{\partial lnZ(\beta)}{\partial \beta} = -\frac{1}{Z}\int dxH(x)\exp\left[-\frac{H}{k_b T}\right] = -\left\langle H(x)\right\rangle = -E \tag{22}$$

$$\frac{\partial^2 lnZ(\beta)}{\partial \beta^2} = \left\langle H(x)^2\right\rangle - \left\langle H(x)\right\rangle^2 \tag{23}$$

$$\left\langle H(x)^2\right\rangle - \left\langle H(x)\right\rangle^2 = -\frac{\partial E}{\partial(1/k_b T)} = k_b T^2 \frac{\partial E}{\partial T} = k_b T^2 C \tag{24}$$

In this way a statistical quantity the variance has been connected to a thermodynamic quantity: the temperature.

Monte Carlo method: Metropolis idea [5]

- The true dynamics is replaced with a fictitious stochastic dynamics. The state at $t+1$ depends only from the state at t. $\rightarrow$ Markov Chain
- The evolution of probability is described by the **master equation** $\Delta p_a(t) = \sum'_{b \neq a} [W_{ab} p_b(t) - W_{ba} p_a(t)]$
- The stationary state is given by $\rightarrow$ $\sum'_{b \neq a} [W_{ab} p_b(t) - W_{ba} p_a(t) = 0 \quad \forall a$
- Detailed balance property $W_{ab} W_{bc} W_{ca} = W_{ac} W_{cb} W_{ba}$
- Therefore the statinary state is given by $W_{ab} p_b(t) - W_{ba} p_a(t) = 0 \quad \forall a, b$

Monte Carlo method: Metropolis idea [5]

- We would sample p_a^{eq}
- This can be performed as long as the W_{ab} is ergodic and the detailed balance property holds
- The transition between any two arbitrary states can take place as long as one waits for a sufficient amount of time

Application [5]

- $H(\sigma) = -\sum_{\langle ij \rangle} J\sigma_i\sigma_j - \sum_i h\sigma_i$
- $P_\sigma = \frac{e^{-H(\sigma)/k_b T}}{Z} \qquad Z = \sum_\sigma e^{-H(\sigma)/k_b T}$
- The observable are calculated as $E = \langle H \rangle = \sum_{sigma} H(\sigma) P^B_{\sigma'} \quad M = \sum_\sigma (\sigma_i \sigma)\, P^B_\sigma$
- The markov chain states should be the microstates σ and P_σ the stationary distribution
- $$W_{\sigma\sigma'} = W_{\sigma'\sigma}\ \frac{P_\sigma}{P_{\sigma'}} = W_{\sigma'\sigma} \exp - \frac{H(\sigma) - H(\sigma')}{k_b T}$$
- The Z term is no more present !!!

Application [5]

- $W_{\sigma'\sigma} = \begin{cases} \kappa H(\sigma') < H(\sigma) \\ \kappa \exp\left\{-\left[H(\sigma') - H(\sigma)\right]/k_b T\right\} \end{cases} \quad \{A\} \neq [A]_T = \frac{1}{T}$
- $A(\sigma) = \langle A \rangle \left[1 + O(N^{-1/2})\right] \forall \sigma \in \Gamma$
- $S = 0.5 N k_b ln 2 \quad \frac{|\Gamma|}{2^N} \approx 2^{-0.5N} \quad N = 100 \quad 10^{-15}$
- $\approx [A]_T = \frac{1}{T} \sum_{t=T_0}^{T\langle A \rangle_0 + T} A_{\sigma(t)}$
- $\left\langle \Delta A_T^2 \right\rangle \approx \frac{1}{T} \left(A_{\sigma(t)} - [A]_T\right)^2$
- σ_t and $\sigma_{t'}$ are indipendent if $|t - t'|$ is larger that a characteristic time τ_0
- $\left\langle \Delta A_T^2 \right\rangle \approx \frac{\tau_0}{T} \left(A_{\sigma(t)} - [A]_T\right)^2$

- We would calculate an integral of type $\langle A \rangle = \int_0^1 dx A(x)\rho(x)$ where ρ is the probability distribution.
- Evaluate the integrand in N+1 points uniformly arranged between 0 and 1 $\langle A \rangle \approx \frac{1}{N+1} \sum_{i=0}^{N} A(x_i)\rho(x_i)$
- A better convergence is reached if the x_i density is proportional to $\rho(x)$. In this case we have $\langle A \rangle = 1/N \sum_{i=1}^{N} A(\mathbf{x}_i)$.