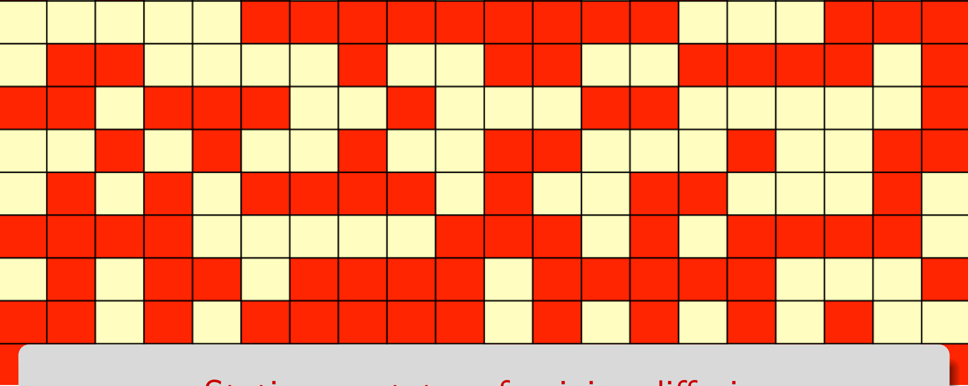


Stationary states of opinion diffusion

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 and temperature [2]

- Consider a system with total energy E that is composed by two subsystems (with energy E_1 and E_2 that can exchange only energy - canonical ensemble)
- There are many way in which the energy can distribute in the two systems with the constrain $E = E_1 + E_2$
- In particular given the energy E_1 the total number of degenerate states is $\Omega_1(E_1) \times \Omega_1(E_2)$
- We would have a measure of the degeneracy of the system that is additive, therefore

$$\ln \Omega(E_1, E - E_1) = \ln \Omega_1(E_1) + \ln \Omega_2(E - E_1)$$

- Every energy state of the total system is equal likely. Therefore the most probable state is the one that maximizes $\ln \Omega(E_1, E - E_1)$

$$\left(\frac{\partial \ln \Omega(E_1, E - E_1)}{\partial E_1} \right)_{N,V,E} = 0$$

Concepts of statistical mechanics: entropy and temperature [2]

- The previous statement is equal to the following one
$$\left(\frac{\partial \ln \Omega(E_1)}{\partial E_1}\right)_{N1,V1} = \left(\frac{\partial \ln \Omega(E_2)}{\partial E_2}\right)_{N2,V2}$$

- Introducing the following notation
$$\beta \equiv \left(\frac{\partial \ln \Omega(E_1)}{\partial E_1}\right)_{N1,V1}$$

- And introducing the concept of entropy
$$S(N,V,E) \equiv k_b ln\Omega(N,V,E)$$

We have the definition of thermodynamic temperature

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{V,N}$$
$$\equiv \frac{1}{k_b T}$$

Concepts of statistical mechanics: entropy and temperature [2]

- So we have proof the at the equilibrium, the configuration with maximum entropy, the temperature of the two sub-systems is equal

$$T_1 = T_2$$

Concepts of statistical mechanics: entropy and temperature [2]

- Given that the system 1 is in the state E_1 the second system have energy $E - E_i$. Therefore the degeneracy of the second system is equal to $\Omega(E - E_i)$
- Thus the probability of 1 to be in the state i will be

$$P_i = \frac{\Omega(E - E_i)}{\sum_j \Omega(E - E_j)}$$

- Expanding around $E_i = 0$

$$\ln \Omega_B(E - E_i) = \ln \Omega_B(E) - E_i \frac{\partial \log \Omega_B(E)}{\partial E} + O(1/E)$$

$$\ln \Omega_B(E - E_i) = \ln \Omega_B(E) - \frac{E_i}{k_b T} + O(1/E)$$

$$P_i = \frac{\exp(-E_i/k_b T)}{\sum_j \exp(-E_j/k_b T)}$$

Concepts of statistical mechanics: phase portrait [5]

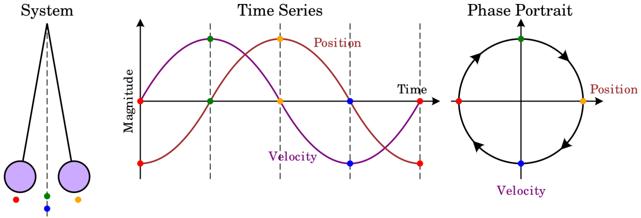


Image taken from [1]

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 $Z = \sum_i \exp\left(\frac{-E_i}{k_b T}\right)$

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

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

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

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]

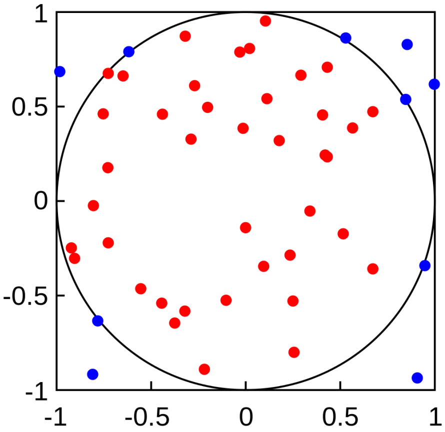


Image taken from [1]

Monte Carlo method [2]

- Lets consider the generic integral $I = \int_a^b dx\ f(x)$
- This can be recast in the following form $I = \int_0^1 dx\ w(x)\dfrac{f(x)}{w(x)}$
- If w(x) is the derivative of u(x) (non-decreasing,non negative) we have $I = \int_0^1 du\ \dfrac{f[x(u)]}{w[x(u)]}$
- If one considers L random values of u uniformely distributed in the interval [0,1] we have $I \approx \dfrac{1}{L}\sum_{i=1}^{L} \dfrac{f[x(u)]}{w[x(x)]}$
- The choice of w is crucial since $\sigma = \dfrac{1}{L}\left[\left\langle\left(\dfrac{f}{w}\right)^2\right\rangle - \left\langle\dfrac{f}{w}\right\rangle^2\right]$
- Brute Force $f = 10^{-260}$ and $\sigma = \dfrac{1}{Lf}$...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]

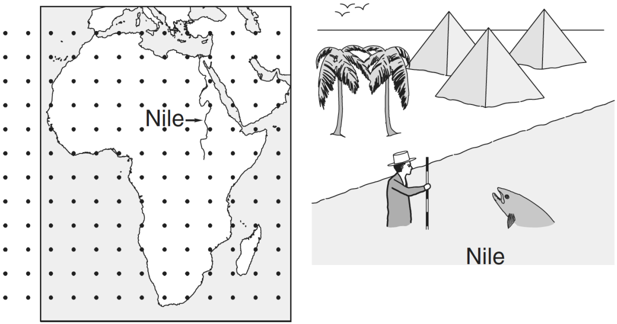


Image taken from [2]

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
- $\pi(old \to new) = \alpha(old \to new) \times acc(old \to new)$ 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 $N(old)\pi(old \to new) = N(new)\pi(new \to old)$
- With a symmetric Markov transition matrix we have $N(old) \times acc(old \to new) = N(new) \times acc(new \to old)$
- Therefore we have

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

- 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

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

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

- 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

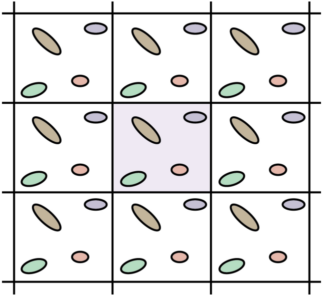


Image taken from [1]

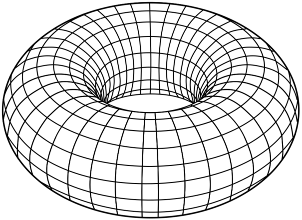
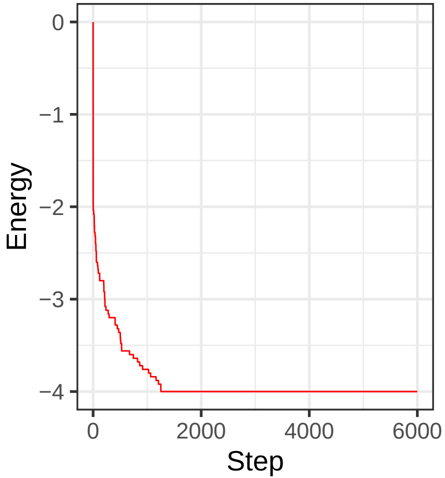
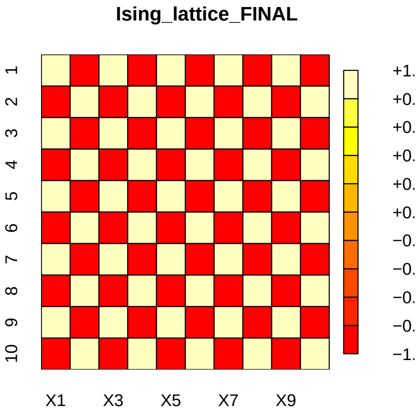


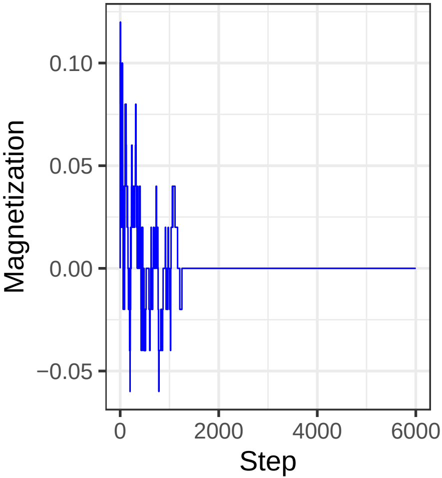
Image taken from [1]

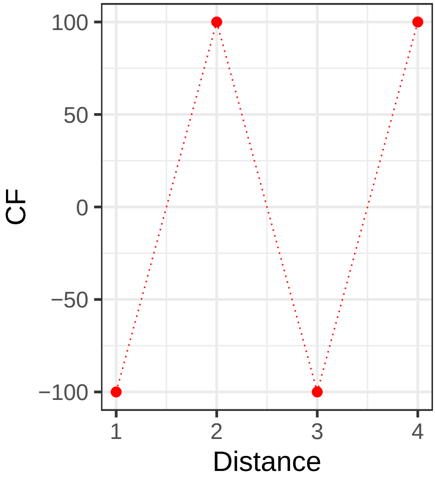
Antiferromagnetic J=-1, T=0



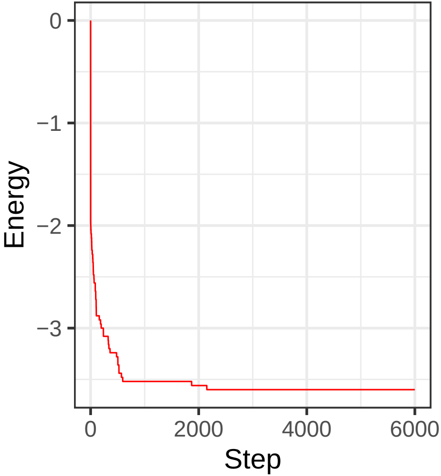


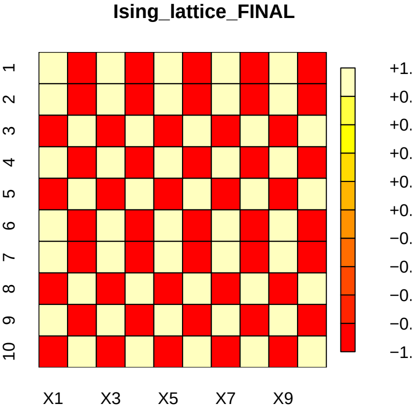
Antiferromagnetic J=-1, T=0



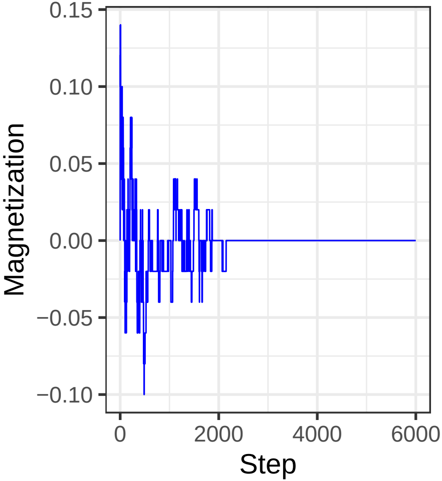


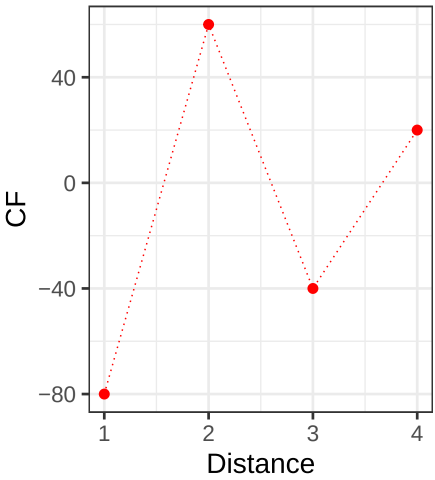
Antiferromagnetic J=-1, T=1.5



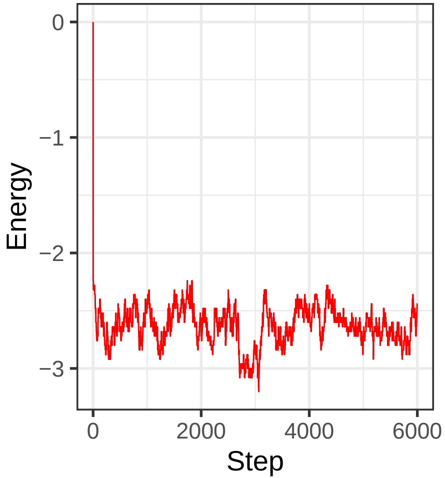


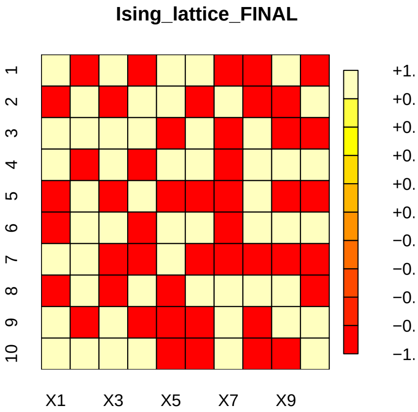
Antiferromagnetic J=-1, T=1.5



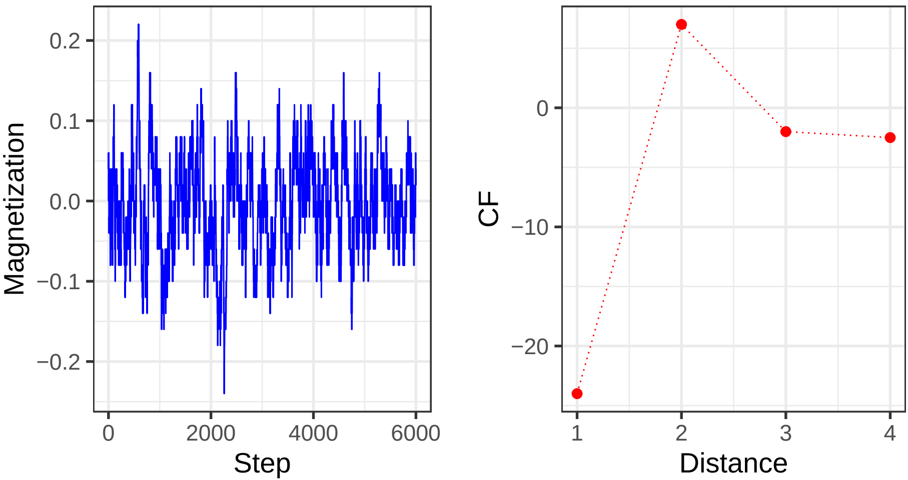


Antiferromagnetic J=-1, T=4

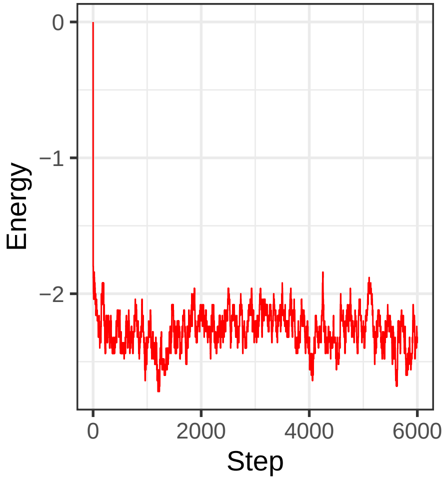


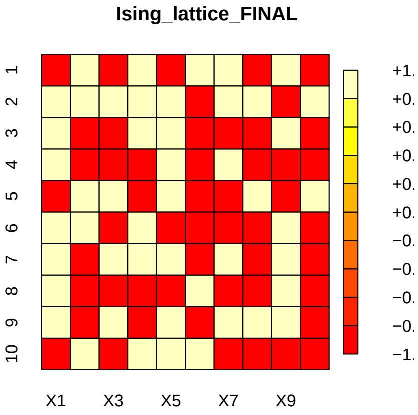


Antiferromagnetic J=-1, T=4

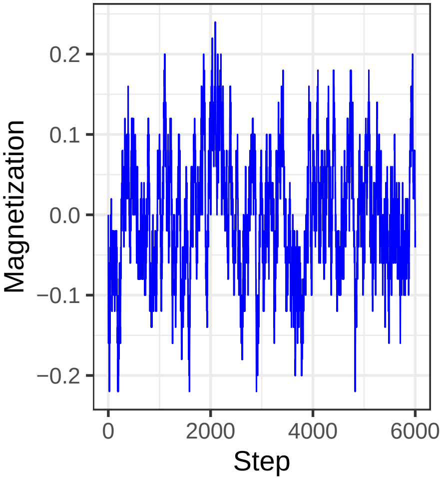


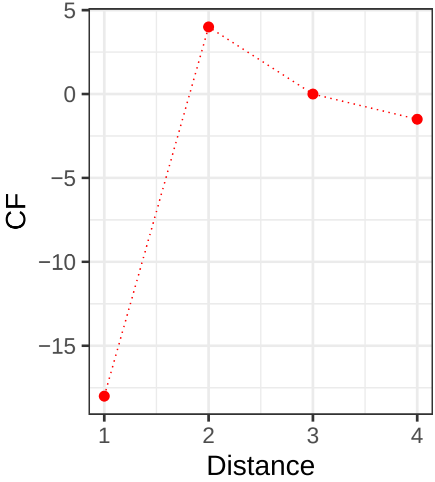
Antiferromagnetic J=-1, T=8



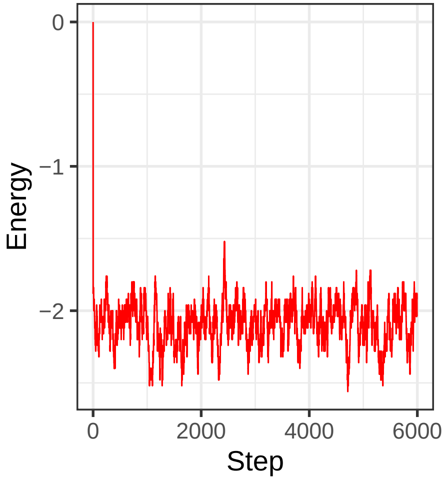


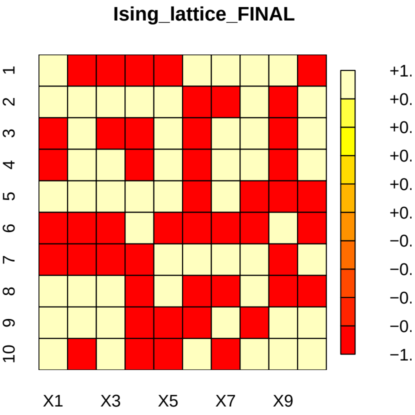
Antiferromagnetic J=-1, T=8





Ferromagnetic J=-1, T=30





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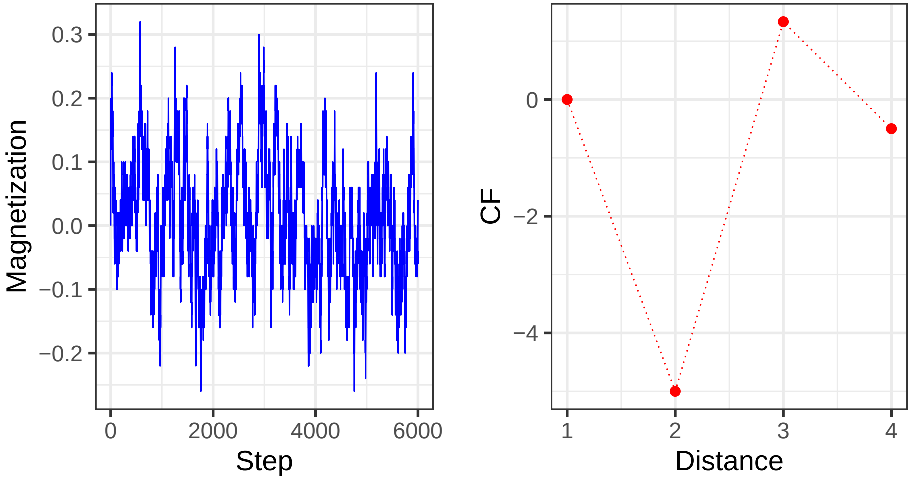
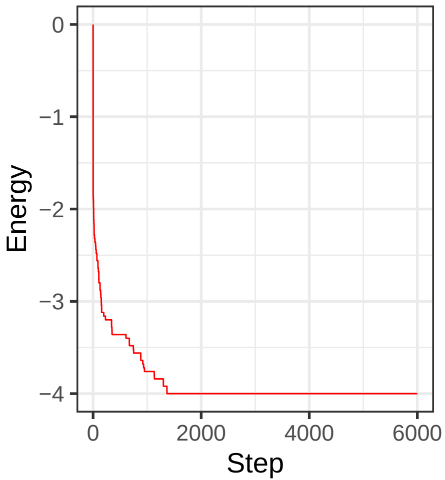
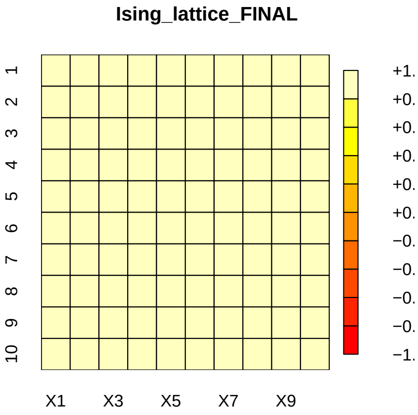
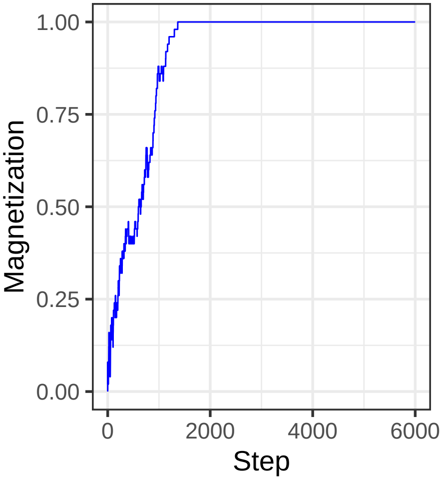


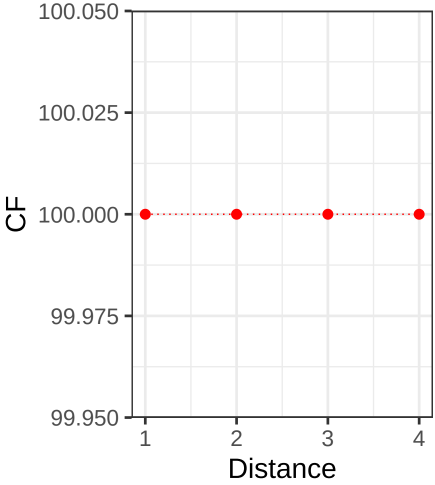
Ferromagnetic J=+1, T=0



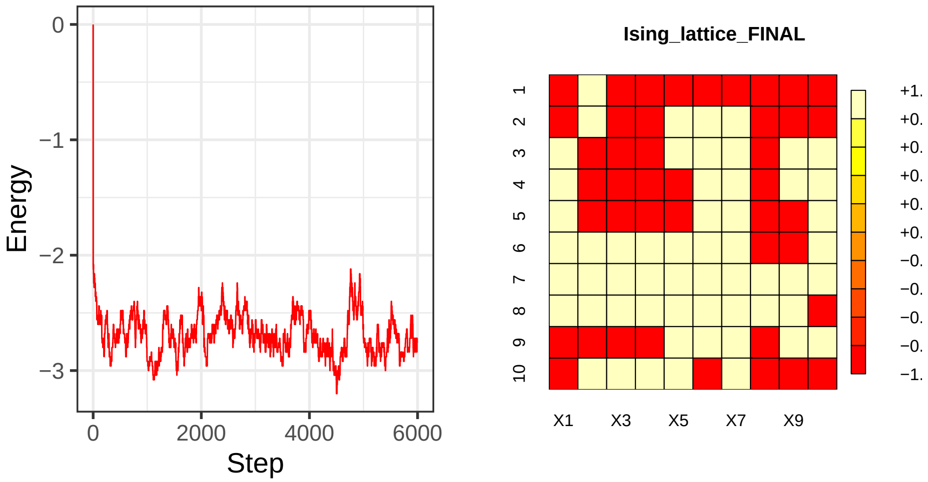


Ferromagnetic J=+1, T=0

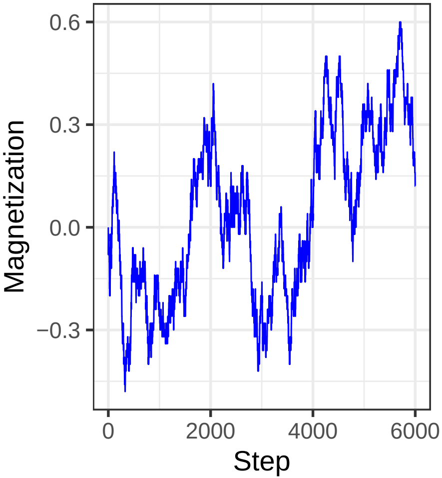


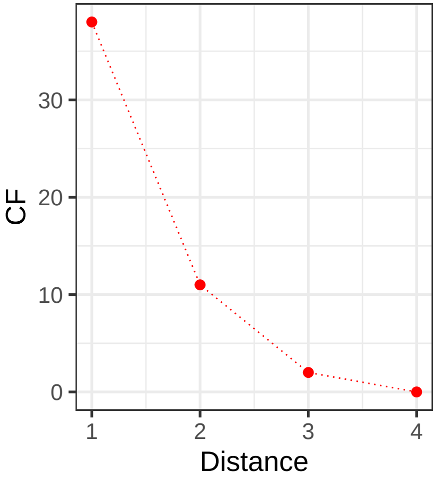


Ferromagnetic J=+1, T=8

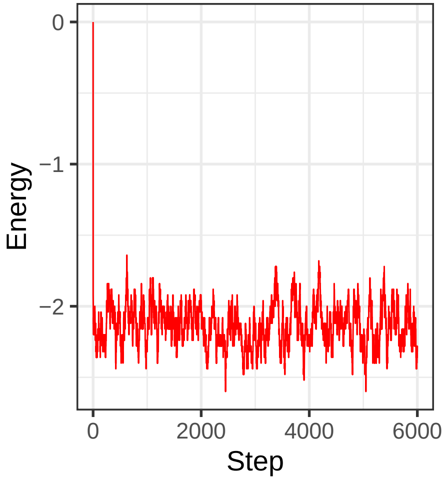


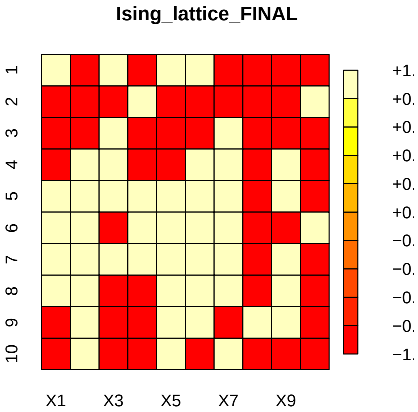
Ferromagnetic J=+1, T=8



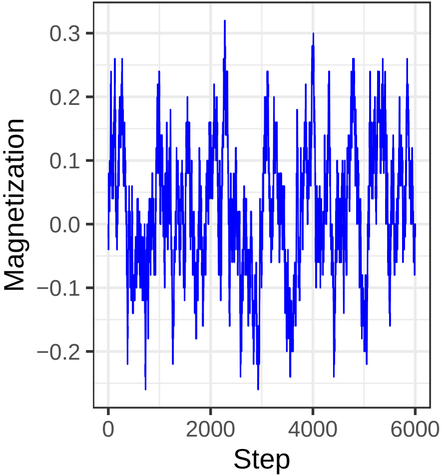


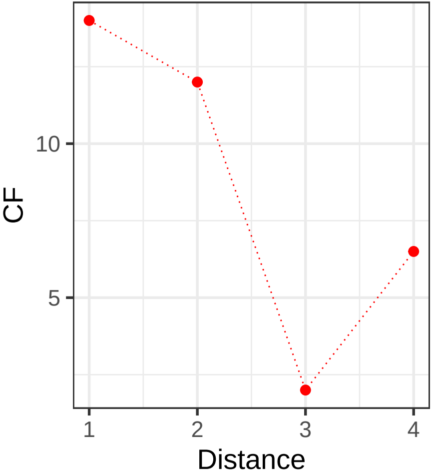
Ferromagnetic J=+1, T=16



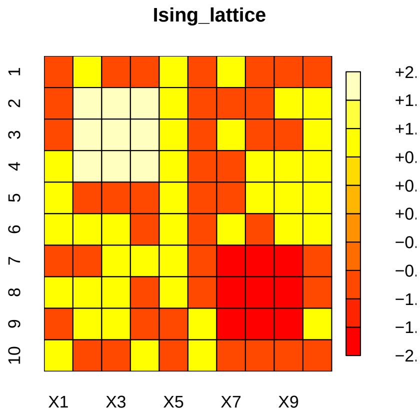


Ferromagnetic J=+1, T=16

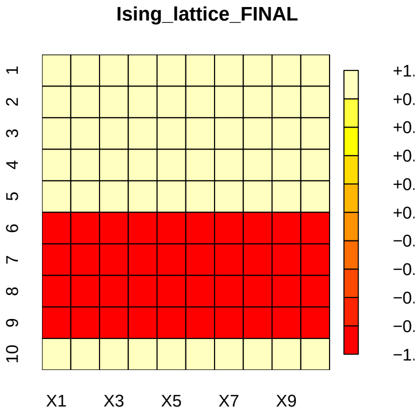


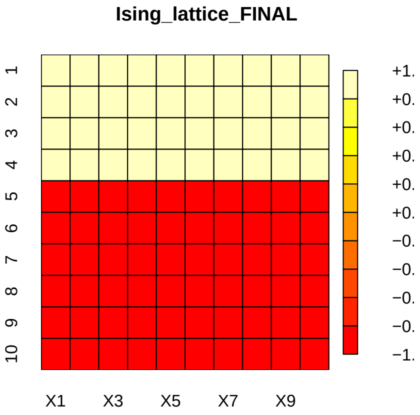


Ferromagnetic with two centers T=0

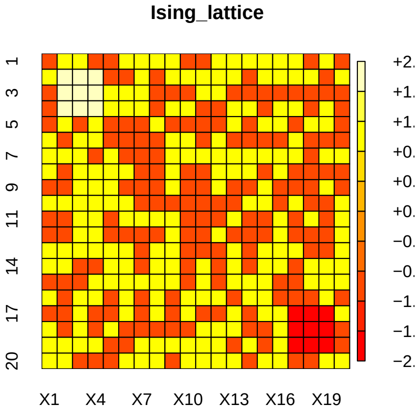


Ferromagnetic with two centers T=0

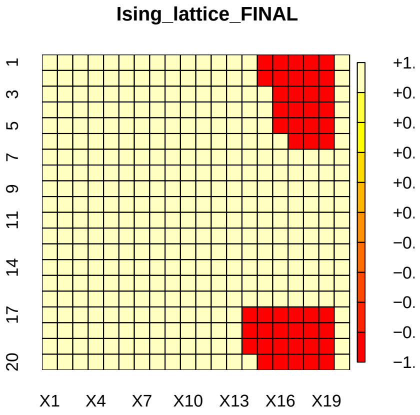


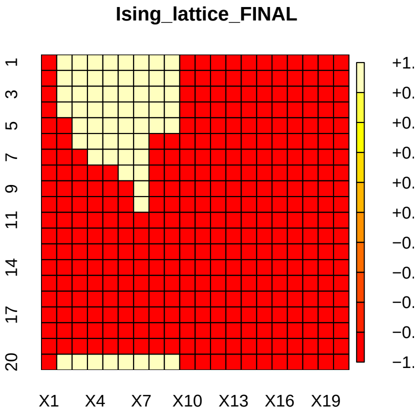


Ferromagnetic with two centers T=0, 20×20

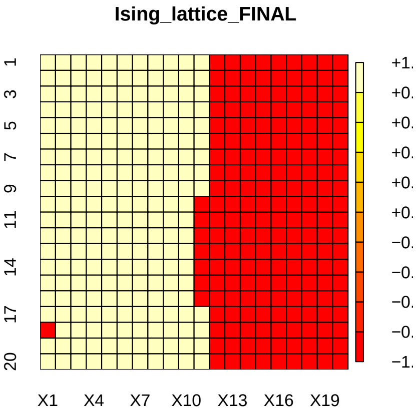


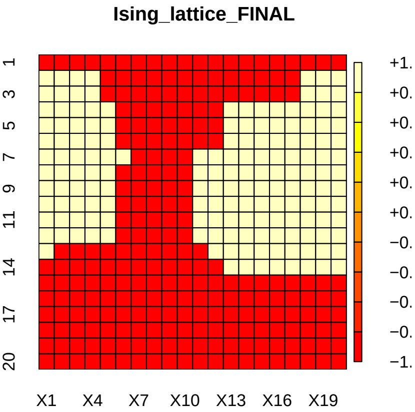
Ferromagnetic with two centers T=0, 20×20



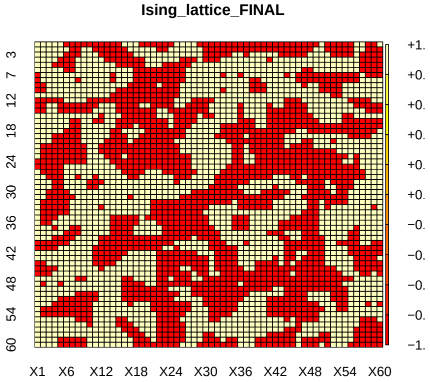


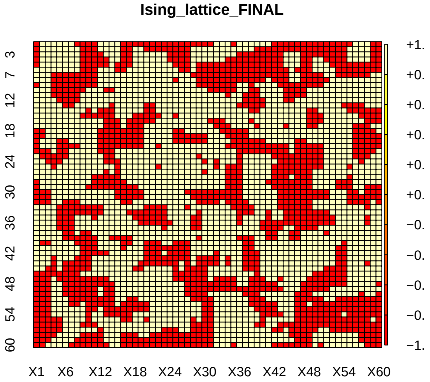
Ferromagnetic with two centers T=0.25, 20×20



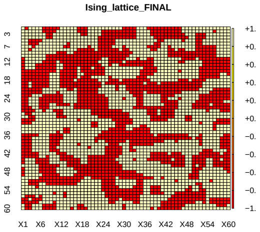


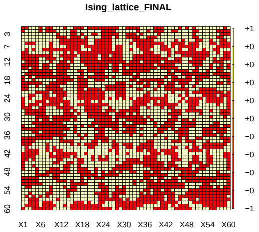
Ferromagnetic with two centers T=0, 60×60

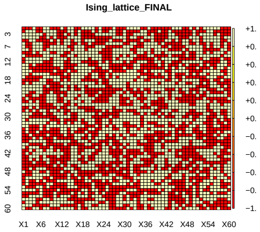


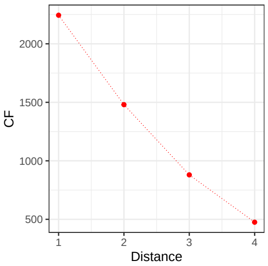


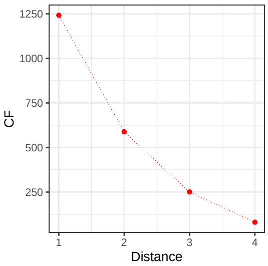
Ferromagnetic with two centers $T > 0$, 60×60

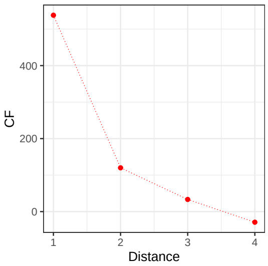




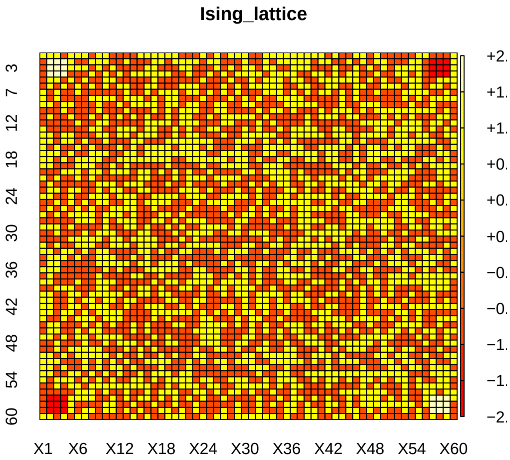




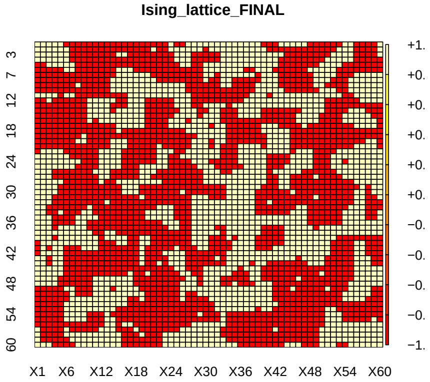


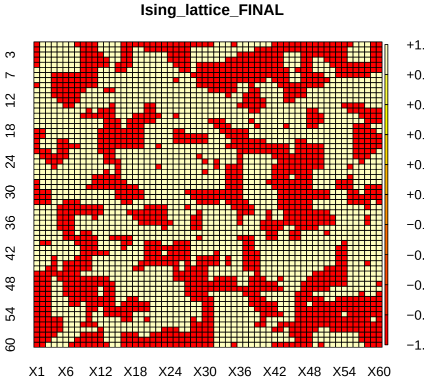


Ferromagnetic with four centers T=0, 60×60



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