2.2.3 Ising paramagnet

Dynamics and relaxation time for $H=0$

time t: discreate, measured in the number of spin-flips.

$$P_n(t+1) = \underbrace{\frac{n+1}{N}}_{\substack{\text{probability that}\\ \text{one of the } (n+1) \oplus \\ \text{turns into } \ominus}} P_{n+1}(t) + \underbrace{\frac{N-(n-1)}{N}}_{\substack{\text{prob. that one of}\\ \text{the } \ominus \text{ spins turns into } \oplus}} P_{n-1}(t)$$

For $N \gg 1$ the $P_n(t)$ changes slowly and we can replace:

$$P_n(t+1) - P_n(t) \simeq \frac{\partial}{\partial t} P_n(t)$$

$$\boxed{\frac{\partial P_n(t)}{\partial t} = \frac{n+1}{N} P_{n+1}(t) + \frac{N-n+1}{N} P_{n-1}(t) - P_n(t)}$$

Master equation

Equation of motion for $\langle n \rangle$

$$\frac{d}{dt}\langle n \rangle = \frac{d}{dt}\sum_n n P_n(t) = \sum_n n \frac{d}{dt} P_n(t)$$

$$= \underbrace{\sum_n n \frac{(n+1)}{N} P_{n+1}(t)}_{n \to n-1} + \underbrace{\sum_n n \frac{N-n+1}{N} P_{n-1}(t)}_{n \to n+1} - \sum_n n P_n(t)$$

$$= \sum_n \left[(n-1)\frac{n}{N} + \frac{(n+1)(N-n)}{N} - n\right] P_n(t) = \sum_n \left(1 - \frac{2n}{N}\right) P_n(t)$$

$$= 1 - \frac{2}{N}\langle n \rangle$$

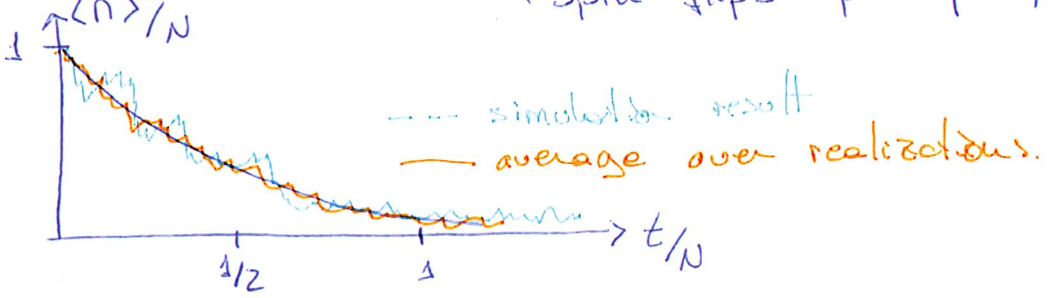
For the initial condition $n(t=0) = N$

$$\longrightarrow n(t) = \frac{N}{2}\left[1 + \exp\left(-\frac{2}{N}t\right)\right]$$

Conclusions:

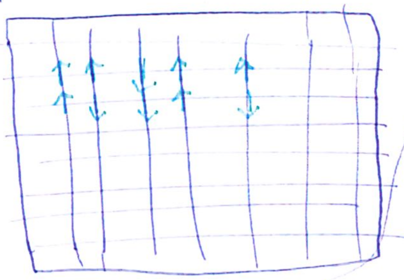
- Exponential relaxation
- Relaxation time $\tau = N/2$
- To eliminate the dependence of the relaxation time, time is usually expressed in MCS units

  MCS - Monte Carlo step per spin $\sim \tilde{\tau} = 1/2$
  (spin-flips per spin)



2.2.4. - Ising ferromagnet

Consider a d-dimensional cubic lattice with a spin in every node $s_i \in \{+1, -1\}$



- There is an interaction between next neighbours which favours the parallel orientation of the spins.

$$\mathcal{H}(\underline{s}) = -H \sum_i s_i - J \sum_{\langle i,j \rangle} s_i s_j$$

J>0 - coupling constant

	$\uparrow\uparrow$	$\uparrow\downarrow$	$\downarrow\uparrow$	$\downarrow\downarrow$
s_i	+	+	−	−
s_j	+	−	+	−
$-Js_is_j$	−	+	+	−

Monte Carlo procedure (Metropolis

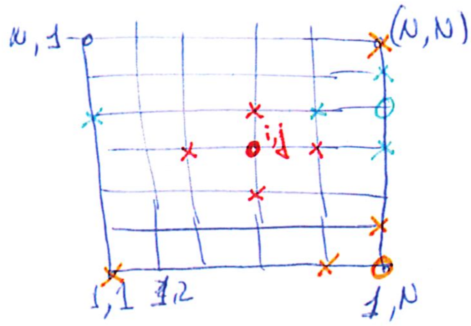
(i) Choose an initial ordered configuration (or unordered)

(ii) Choose a lattice node r

(iii) Calculate the energy difference of an hypothetical spin flop $s_r \to -s_r$

In a 2-d lattice

$s_r \sim s_{ij}$



→ the calculation of the energy difference is local, this is it is related only to the chosen lattice nodes, and the nearest-neighbours. All the other terms in the energy cancel in the difference

$$\mathcal{H}\{s_{11}, s_{12}, \dots, -s_{ij}, \dots s_{NN}\} - \mathcal{H}\{s_{11}, s_{12}, \dots, s_{ij}, \dots s_{NN}\}$$

$$= -J(-s_{ij})\{s_{i+1,j} + s_{i-1,j} + s_{i,j-1} + s_{i,j+1}\}$$

$$= (-J)(s_{ij})\{s_{i+1,j} + s_{i-1,j} + s_{i,j-1} + s_{i,j+1}\}$$

$$= 2J\{s_{i+1,j} + s_{i-1,j} + s_{i,j+1} + s_{i,j-1}\}$$

⇝ we consider periodic boundary conditions.
$(N+1 \to 1 \quad ; \quad 1-1 \to N)$

(iv) In case $\Delta E \leq 0$ ⇝ $s_{ij} \longrightarrow -s_{ij}$ (accepted)

(v) In case $\Delta E > 0$
Choose a random number ρ with equal probability in the interval $[0,1]$

- in case $\exp(-\beta \Delta E) > \rho$ ⇝ $s_{ij} \to -s_{ij}$
- in case $\exp(-\beta \Delta E) < \rho$ ⇝ no flip

(vi) Calculate the magnetization $M = \sum_i s_i$

2.2.5 Calculation of the mean values

(i) ₂The Markov process provides a path in the phase space that if long enough, covers a representative subset of the phase space.

1 ⟹ the number of configurations used in a simulation is always just a very small subset of all the points in the phase space

3 —> It does not make sense to calculate data for averaging too often because the configurations that follow each other in short succession are strongly correlated.

Rule of thumb: calculate averages every couple of MCS..

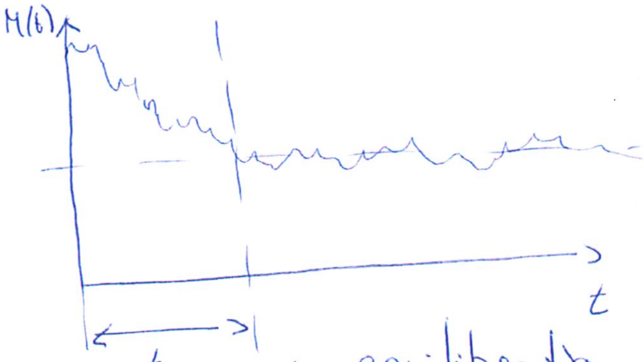
MCS = Monte Carlo step per spin

(ii) In section 2.1.2 we have seen that the information about the initial state is forgotten after some relaxation time τ

- For the Ising paramagnet $\tau = N/2$ some MCS are sufficient, increasing with N
- For other models, such as the Ising ferromagnet, τ can be much longer

therefore - we calculate an observable (such as the magnetization $M = \sum_i s_i$) at a time according to a MCS and write to a file.

then draw its ~~evo~~ time evolution



t_{eq} : equilibration time

For calculating the mean values the small times are typically <u>not</u> considered.

(iii) In thermodynamics, there are often quantities that are calculated by derivation according to intensive variables.

Examples:

magnetic susceptibility $\chi = -\left.\frac{\partial M}{\partial H}\right|_{H=0}$

specific heat: $C_{H=0} = T\frac{\partial S}{\partial T}$

these quantities should not be calculated via a (complex and inaccurate) discretization of the derivatives, but via the mean values of fluctuations.

Example: specific heat

from thermodynamics $TdS = du - HdM$

$$C_{H=0} = \left.\frac{\partial u}{\partial T}\right|_{H=0} = \left.\frac{\partial}{\partial T}\langle \mathcal{H} \rangle\right|_{H=0} = \frac{\partial}{\partial T}\frac{1}{Z}\left[\sum \mathcal{H} e^{-\beta \mathcal{H}}\right] =$$

$$\beta = \frac{1}{k_B T} \rightarrow = -\frac{1}{k_B T^2}\frac{\partial}{\partial \beta}\left[\frac{1}{Z}\sum \mathcal{H} e^{-\beta\mathcal{H}}\right]$$

$$= -\frac{1}{k_B T^2}\left[\frac{1}{Z}\sum(-\mathcal{H})^2 e^{-\beta\mathcal{H}} + \frac{1}{Z^2}\left(\sum \mathcal{H} e^{-\beta\mathcal{H}}\right)^2\right]$$

$$C_{H=0} = k_B\left[\langle(\beta\mathcal{H})^2\rangle - \langle\beta\mathcal{H}\rangle^2\right]$$

C_H can be calculated from the energy fluct. ☑