Monte Carlo - application to the Ising model

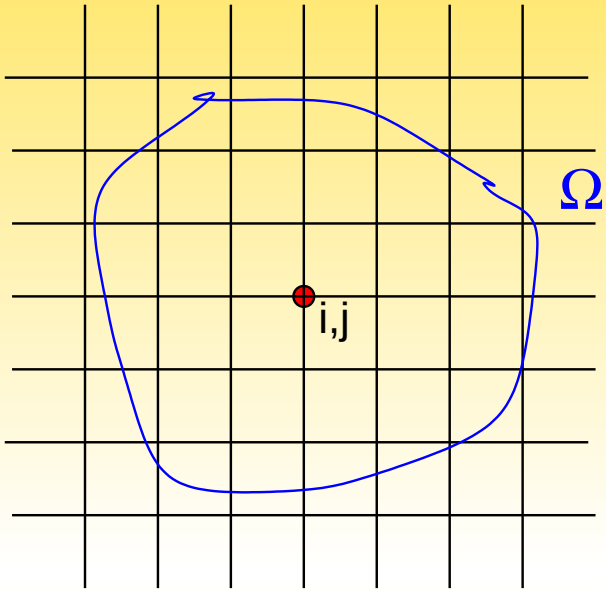
Computational Physics

4. október 2010

1 The two-dimensional Ising model

- The Ising model has been a great success in describing the rudimentary traits of collective phenomena and phase transitions in a large variety of systems.
- The Ising model is a collection of classical spins $s = \pm 1$ placed rigidly on a regular lattice. The total number of spins is

$$\boxed{N = N_x \cdot N_y}$$



- Spin i, j interacts with all spins within the region Ω.

  Commonly only nearest neighbors interactions are considered, we do so here.

Phase transitions are caused by collective behavior of the entities in the system. We assume it is favorable for the energy if neighboring spins are parallel.

The Hamiltonian of the system is, (the energy of each configuration α is described by)

$$\boxed{E_\alpha = -\frac{1}{2}\sum_{\langle i,j\rangle} JS_iS_j - \sum_i HS_i.}$$

Here is clear that,

1. Single spins parallel to H $(S_i = 1)$ are favored.
2. Parallel neighboring spins, $(S_iS_j = 1)$, are favored.

The minimization of the energy should concentrate on finding the E_α that have the lowest values.

1.1 Boundary conditions

What do the spins at the edge of the system influence the properties of the system?

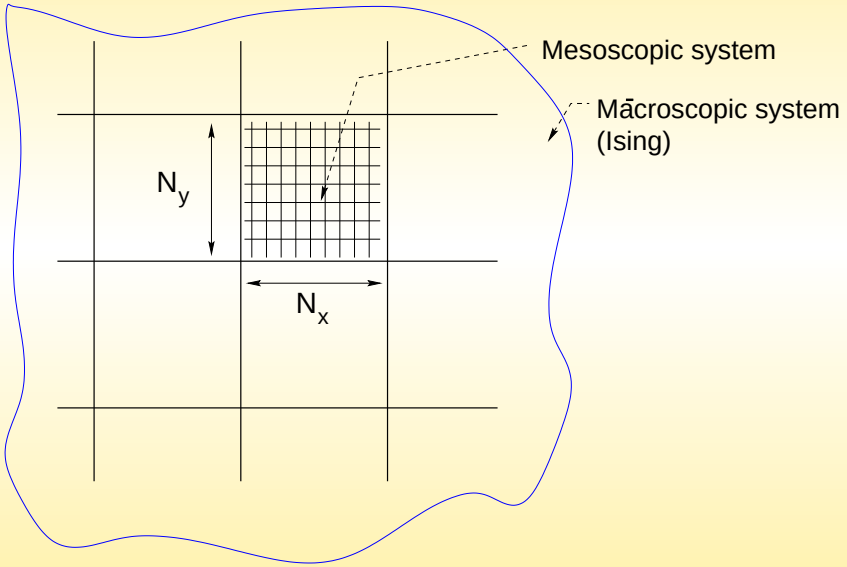
- Spins at the edge have fewer nn.
- The ratio of edge spins to the total number of spins

$$\frac{2\left(N_x + N_y\right) - 4}{N_x N_y} = 0.36 \quad (10 \times 10 \text{ lattice}).$$

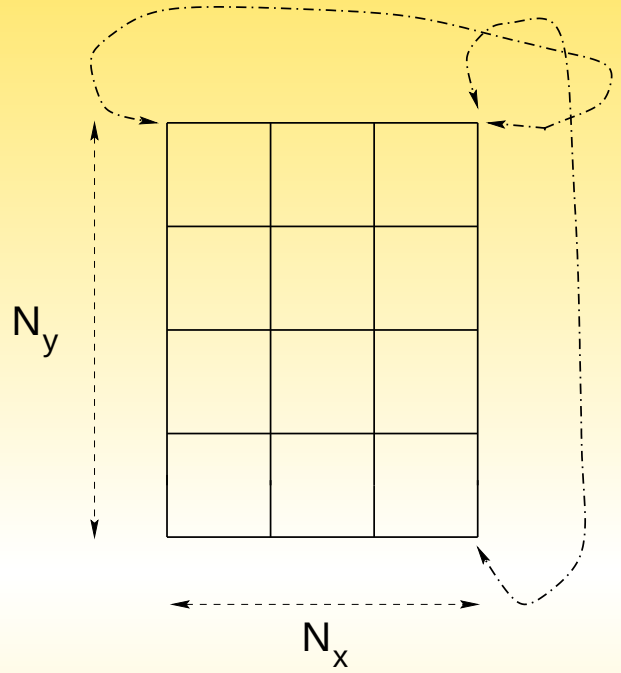
The contribution of edge spins vanishes when $N_x, N_y \to \infty$, but how large a system can we simulate?

Periodic boundary conditions

Example:



Is anything lost?



Implementation of periodic boundary conditions.

Modulus calculus can be used

if $i, j > N_x, N_y$ then the index of the lattice (matrix) moves to the origin, i.e. $i = 1$ of $j = 1$.

1.2 The Metropolis algorithm

To calculate the mean energy $\overline{E}$ and mean magnetization $\overline{M}$ in the Ising system we need the partition function Z: in the probability distribution

$$\boxed{P(E_\alpha) = \frac{1}{Z} e^{-\beta E_\alpha}.}$$

In Z we have a sum over **all states** of the system. Each spin has two values.

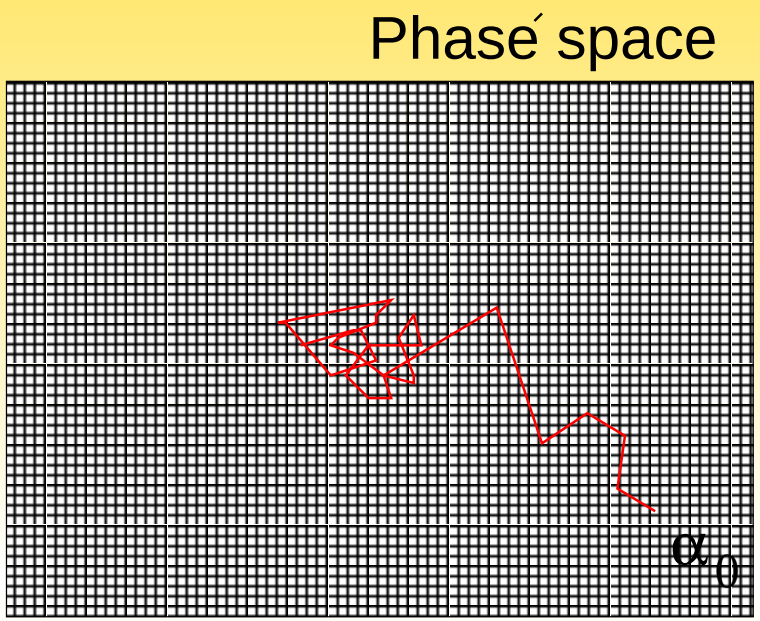
The number of states is:

$$2^N = 10^{N \log(2)} \simeq 10^{72} \quad (16 \times 16 \text{ lattice}).$$

How can we find the states with highest weights in the probability distribution?

The Metropolis algorithm makes a new state α' from α, we get a row of states that from a Markov-chain.

We "travel around" in the phase space and select the states that are most probable, i.e. low energy and high probability. The heat fluctuations at finite temperature are simulated with random numbers.



In the "middle" are states with high probability.

Since the "new state" only depends on the "last one" the "random walker" stays within the "middle region".

$\rightarrow$ We only select states with a high probability in

$$\boxed{\overline{E} = \sum_{\alpha} P(E_\alpha) E_\alpha .}$$

1.3 Further details on the application of MP

1. We initialize the lattice in the state α_1.

$$\boxed{\text{Calculate } E_{\alpha_1} \text{ and } M_{\alpha_1}.}$$

2. Make a test state α_t by turning one spin $S_{ij} \to -S_{ij}$.

$$\boxed{\text{Calculate } r = \frac{P(E_{\alpha_t})}{P(E_\alpha)}.}$$

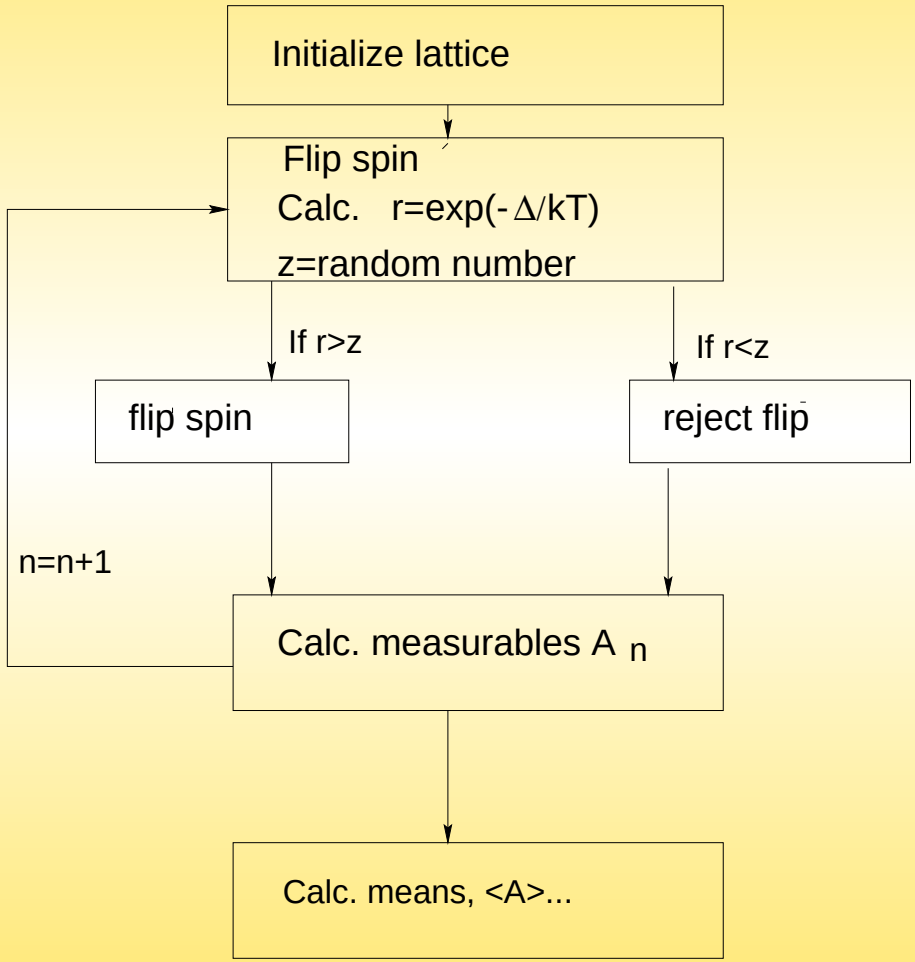
3. We use α_t as a new state if r fulfills certain condition, otherwise $\alpha' = \alpha$.

Consider the quantity r

$$r = \frac{P(E_{\alpha_t})}{P(E_\alpha)} = e^{-\beta(E_{\alpha_t} - E_\alpha)} = e^{2\beta S_{ij}(Jf_{ij}+H)}$$

where $f_{ij} = S_A + S_B + S_C + S_D$. ($S_A \ldots$ are next neighbors)

1.4 Flow diagram for MP



We repeat this procedure N_{MC} times obtaining an ensemble of energy and magnetization values.

$$E_{\alpha_1}, E_{\alpha_2}, \ldots, E_{\alpha_{N_{MC}}}$$
$$M_{\alpha_1}, M_{\alpha_2}, \ldots, M_{\alpha_{N_{MC}}}$$

which are used to evaluate $\overline{E}$ and $\overline{M}$.

Many variants exists.

1.5 Evaluation of mean values in MP

With the use of the MP algorithm to find states the definition of mean values changes:

$$\overline{E} = \sum_{\alpha} P(E_\alpha) E_\alpha \quad \rightarrow \quad \overline{E_m} = \sum_{\gamma} \frac{1}{N_m} E_\gamma$$

$$\overline{M} = \sum_{\alpha} P(E_\alpha) M_\alpha \quad \rightarrow \quad \overline{E_m} = \sum_{\gamma} \frac{1}{N_m} M_\gamma$$

where the sums on the left side are over all states α, but the sums on the right side are only over all states γ that have been selected by the MP algorithm.

2 Ising and Metropolis

Further details:

- **Spins and the lattice:**

  Max number of spins $N_x N_y$. Elements in the matrix (spins on a lattice) are written as

  $$S_{ij}: \quad i = 1, \ldots, N_x \quad j = 1, \ldots, N_y$$

  Sometimes a general designation is used

  $$S_i: \quad i = 1, \ldots, N_x N_y.$$

  Each spin has two states i.e. $\uparrow$ or $\downarrow$. The number of states the **system** can be in is thus

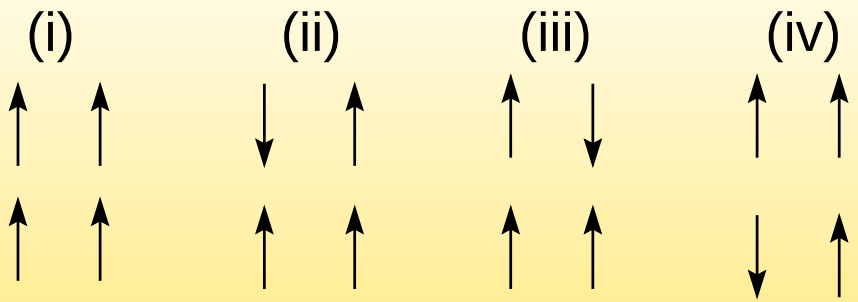
  $$\underbrace{2 \cdot 2 \cdot 2 \cdot \ldots \cdot 2}_{N_x N_y} = 2^{N_x N_y}.$$

- **Spin configurations of states:**

  States or spin configurations of the system are determined by the state of single spins.

  Example:

  2×2 lattice i.e. $N_x = N_y = 2$. The number of states is $2^{2 \cdot 2} = 16$.



- The energy and magnetization of the states at $B = 0$ is

$$E_{(i)} = -8J, \qquad E_{(ii)} = E_{(iii)} = E_{(iv)} = -2J,$$
$$M_{(i)} = 4, \qquad M_{(ii)} = M_{(iii)} = M_{(iv)} = 2.$$

  It is important not to mix the following quantities

  - N_x : The number spins in x direction.
  - N_y : The number spins in y direction.
  - N_{MP} : The number of states found by the Metropolis algorithm.

1. **Metropolis**

   If the test state α_t is accepted then the spin lattice changes:

$$S_{ij} \rightarrow -S_{ij}.$$

   This means a new state, a new spin configuration, with energy $E_{\alpha_{l+1}}$ and magnetization $M_{\alpha_{l+1}}$:

$$\begin{aligned} E_{\alpha_{l+1}} &= E_{\alpha_l} - 2\,S_{ij}\,(J f_{ij} + H), \\ M_{\alpha_{l+1}} &= M_{\alpha_l} + 2S_{ij}. \end{aligned}$$

   We make the new states by flipping the spins regularly or randomly and obtain a sequence of states:

$$\begin{aligned} &E_{\alpha_1}, E_{\alpha_2}, \ldots, E_{\alpha_{N_{MP}}} \\ &M_{\alpha_1}, M_{\alpha_2}, \ldots, M_{\alpha_{N_{MP}}}. \end{aligned}$$

3 The scaling of the calculation

We want to get rid of boring units by using dimensionless or scaled quantities.

Which quantities in the problem have a dimension?

(length, mass, energy, ...).

$$\begin{aligned} [J] &\equiv \text{energy}, \\ [k_B T] &\equiv \text{energy}, \\ [H] &\equiv \text{energy!} \end{aligned}$$

We measure the thermal energy and the external field in J:

$$E_\alpha \to \frac{E_\alpha}{J} = -\frac{1}{2} \sum_{<i,j>} S_i S_j - \sum_i \left(\frac{H}{J} \right) S_i$$

$$r = e^{2(\beta J)(f_{ij}+(\frac{H}{J}))S_{ij}}.$$

We use scaled variables

$$\beta J = \left(\frac{J}{k_B T}\right) \to \beta \quad : \quad \text{dimensionless}$$

$$\frac{H}{J} \to B \quad : \quad \text{dimensionless}$$

We thus use temperature on the "scale" $k_B T = 0, \ldots$

(in units of J**).**

Thus, we have no worries about units and dimension. We obtain the physics properties dimensionless. Natural scales...

$k_B T_c$ is measured in terms of J.

4 Normalization of quantities

In order to compare $\overline{E}$ and $\overline{M}$ for different lattice sizes we need to normalize the quantities in terms of $N_x N_y$.

Calculate per spin:

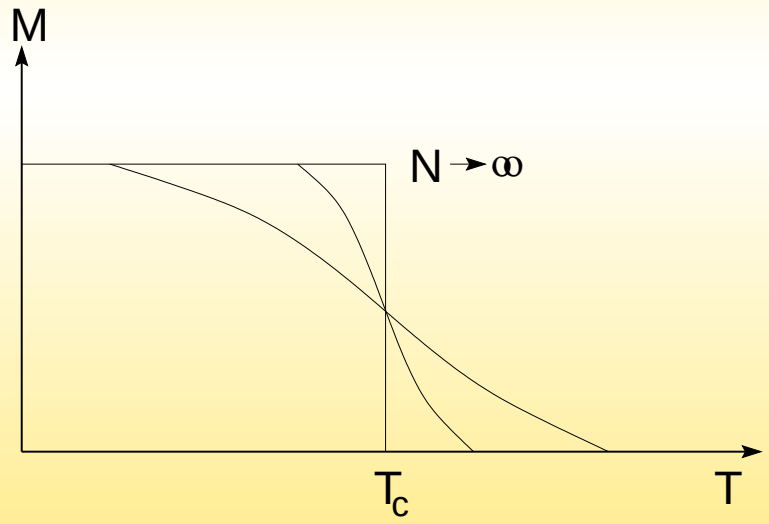
$$E_\alpha \to \frac{E_\alpha}{N_x N_y} \qquad \text{energy per spin,}$$

$$M_\alpha \to \frac{M_\alpha}{N_x N_y} \qquad \text{magnetization per spin.}$$

Example:

The magnetization varies with lattice size

$N_x = N_y = N$.



5 Further quantities of interest

We calculate the energy and the magnetization, but are also interested in their variation around the mean values:

The variation is defined by

$$\boxed{(\Delta E)^2 = \overline{E^2} - \overline{E}^2}$$

$$\boxed{(\Delta M)^2 = \overline{M^2} - \overline{M}^2}$$

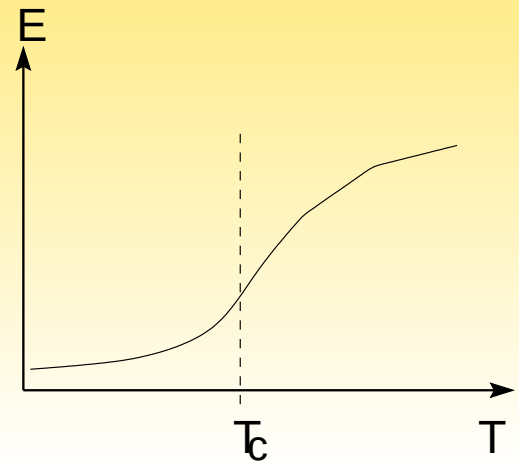
and is connected to the heat capacity C_B and the susceptibility χ_T:

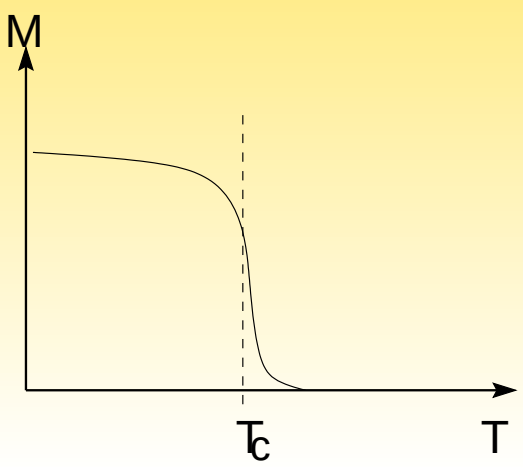
$$\boxed{C_B = \frac{(\Delta E)^2}{k_B T^2}}$$

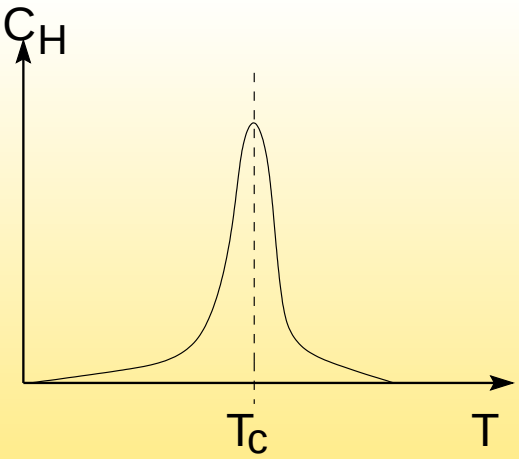
$$\boxed{\chi_T = \frac{(\Delta M)^2}{k_B T}}$$

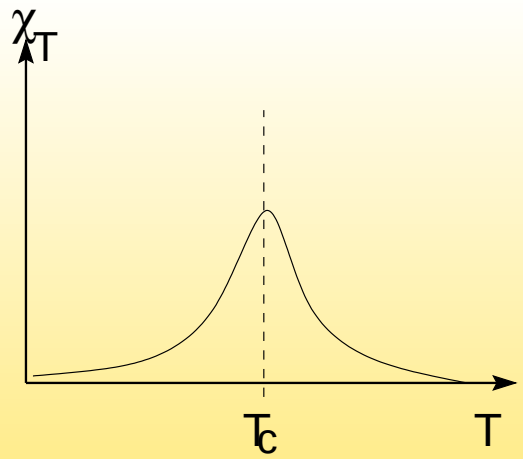
Special collective phenomena happen around the critical temperature $k_B T \simeq 2.27J$ where C_H of χ_T take a maximum.

In an infinite system we have a point of singularity, phase transition, where fluctuations happen at **all length scales**.


E
T_c
T


M
T_c
T


C_H
T_c
T


χ_T
T_c
T