Simulations in Statistical Physics

Course for MSc physics students

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Lecture 6

MC simulation of Hamiltonian systems

Elementary steps: Detailed balance and ergodicity

Having the space of configurations, MC starts with a proper definition of elementary MC steps, which enable an ergodic walk in that space. Fix the temperature. Then – after defining the BC and the initial conditions – a MC simulation consists of the following steps.

i) Choose elementary step Q → Q'
ii) Calculate ΔE
iii) Calculate $W(Q \rightarrow Q')$
iv) Generate a random number $r \in (0,1)$
v) If $r < W(Q \rightarrow Q')$ the new state is Q', otherwise it remains Q
vi) Count time increment
vii) Do the necessary measurements (! Relaxation time)
viii) go to i) until max # of steps

ii) Ising model

$$\mathcal{H}_{\text{Ising}} = -J \sum_{<i,j>} s_i s_j - h \sum_i s_i$$

Ergodic elementary step: Pick a spin at random and flip it.
Calculate the energy before (E_i) and after (E_f) the flip.

$$\Delta E = E_f - E_i$$

Note that due to the local interaction there are only few possible values of ΔE depending on the number of (anti) parallel neighboring sping and the existence of the external field.
Let us take the square n.n. lattice and $h = 0$.

# of ↑↓ spins	0	1	2	3	4
$\Delta E/J$	8	4	0	-4	-8
$\ln[w(Q \to Q')]$	-8β	-4β	0	0	0

If $h \neq 0$, we have 10 different values instead of 5, because the direction of the spin relative to h has to be considered

At criticality we the correlation length ξ diverges: We need as large samples as possible. “How much does it cost?”

The trivial dependence of the requested CPU time $t_{CPU} \sim L^d$.

But we have to equilibrate the system! How much time is needed for a system with diverging ξ to get to equilibrium?

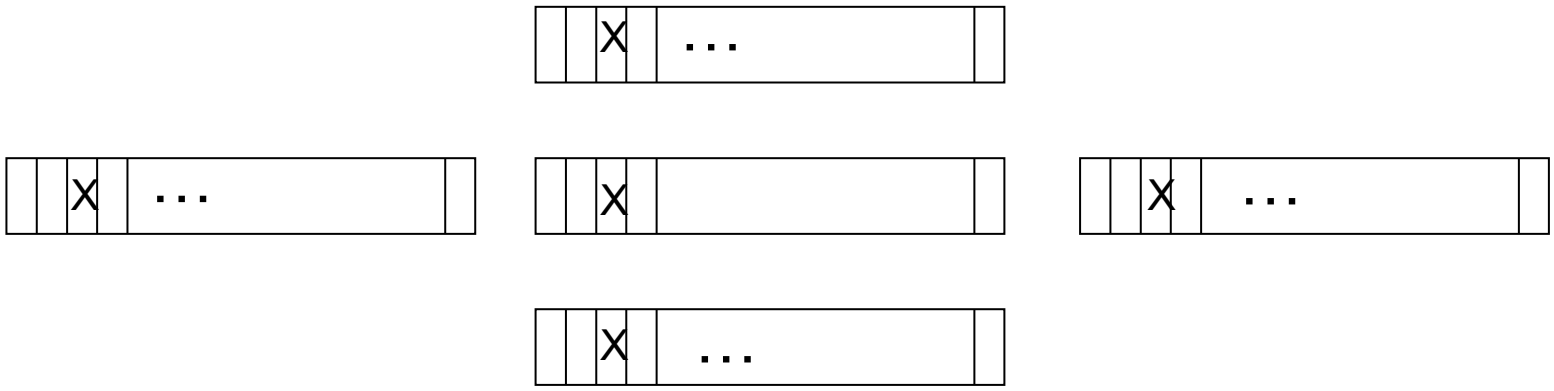
ξ is the size of the correlated regions. If the rearrangement propageted ballistically, we would need time proportional to ξ. At the critical point this would mean an addititional factor L

Even worse: The characteristic time goes as $\tau \sim \xi^z$ with $z \approx 2$. Exponent 2 would mean a diffusive propagation of (dis)order.

Thus at the critical point we have $t_{CPU} \sim L^{z+d}$

Serious problem! We need fast algorithms or change in z!

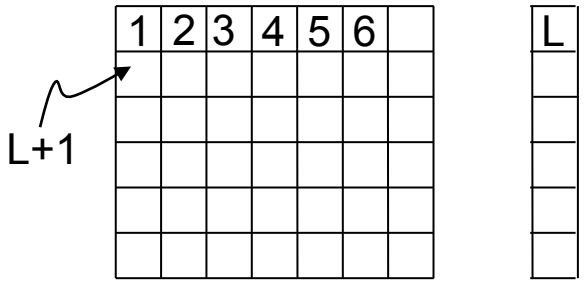
The information about a spin is binary, we can assign 1 to up and 0 to down spins. In principle, we could put 32 spins into a single 32-bit word. While this would save a lot of memory, the handling of the single spins becomes tedious.
We want to handle all the spins in a word simultaneously. Then (taking the square lattice as an example) the following problem arises:



The spins have to be put into the words such that the X-s represent neighbors in the lattice. Then simple XOR indicates the antiparallel spin pairs in a pair of words.

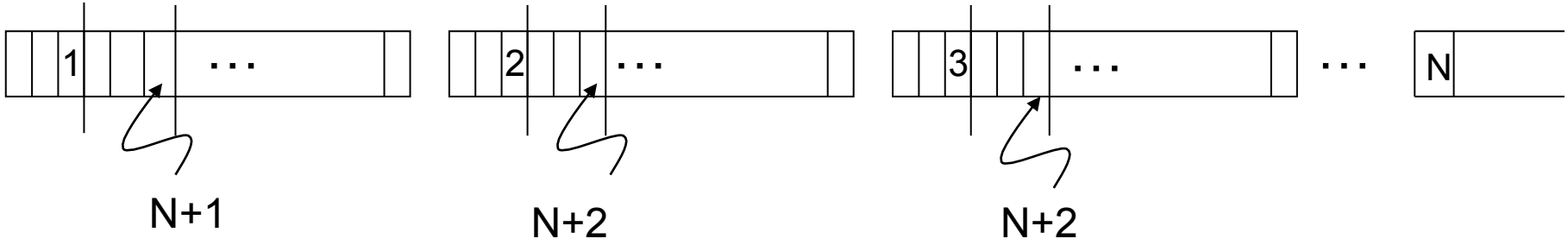
Another problem is that we need the sum of antiparallel neighbors, which can be up to 4. I.e., 3 bits are needed to store the information about the energy of a spin.

These two problems can be solved simultaneously.
We put a spin only into every 3-d bit. The words are filled up in a special way ensuring the proper neighborhods.



$N = L/10$ words/row used in

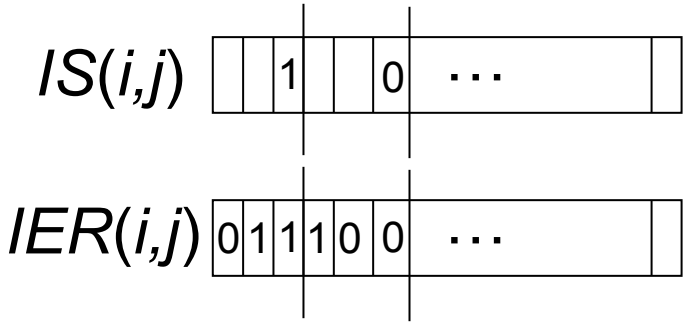
$IS(i,j)$, $i = 1,\ldots L/10$; $j = 1,\ldots L$



We define an array *IER*(*i,j*) for storing the number of antiarallel spins for the 10 spins in *IS*(*i,j*).

$$IER(i,j)=\mathrm{XOR}(IS(i,j),IS(i\text{-}1,j)+\mathrm{XOR}(IS(i,j),IS(i+1,j))+$$
$$\mathrm{XOR}(IS(i,j),IS(i,j\text{-}1))+\mathrm{XOR}(IS(i,j),IS(i,j+1))$$

Now we have for an index pair *i,j* the words *IS* and *IER*



So far we could handle 10 spins in parallel. The MC decision has to be made individually: Shift both the spin under consideration and the corresponding *IER* value to the right end of the words, mask out the *IER* value, calculate the transition probability and flip the spin with a negation if necessary. Special care needed at the end of the words and at BC-s!

The sequence of updates is deterministic, but this does not influence the equilibrium properties. Moreover, the value of the exponent *z* remains unaltered, thus we can only influence the prefactor in the relationship $t_{\mathrm{CPU}} \sim L^{d+z}$ (The gain is about a factor of 3-4.)

How to influence the exponent *z*? Physics helps.
Large *z* due to local („diffusive”) dynamics.
What if we flipped groups of spins together?

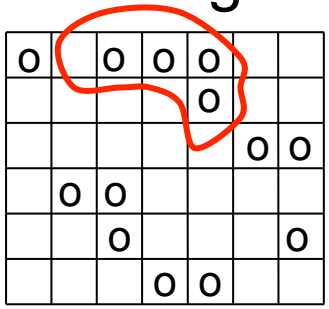
Cluster algorithms

Cluster algorithms

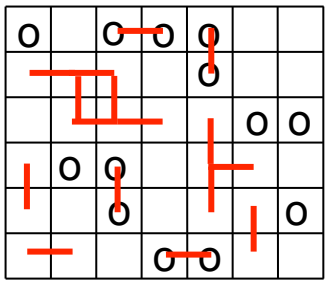
What is the optimal group of spins to be flipped tgether?
Detailed balance has to be fulfilled.

The solution – based on an old relationship between the percolation and the Potts model – is that we consider the spin configuration as a correlated site percolation problem, where up spins correspond to occupied and down spins to empty sites. In addition to that we define random bonds between parallel spins as „open" with a temperature-dependent probability: $p_B = 1 - e^{-2\beta J}$

Ising cluster



Ising configuration



Ising „droplets"

clusters ≥ droplets

(E.g., in 3d percolation transition temperature of clusters < T_c)

Two methods: **Swendsen-Wang:**

- 1 Take the Ising correlated site – random bond percolation configuration ($p_B = 1 - e^{-2\beta J}$)
- Identify the droplets by Hoshen-Kopelman algorithm
- Flip each droplet with probability: ½ (h=0)
- Go to 1

Wolff:

- 1 Define a droplet by picking a spin at random in a spin configuration
- 2 Identify all parallel spins, perimeter to the droplet
- 3 Check an unvisited bond to a parallel perimeter spin, and open it with $p_B = 1 - e^{-2\beta J}$, block it with 1-p_B, include spin into the droplet if there is an open bond leading to it
- Go to 3 for all unvisited bonds
- Go to 2 until no new spins can be included
- Flip the droplet and erase the bond information
- Go to 1

Detailed balance (for Wolff)

$$P^{\mathrm{eq}}(Q)W(Q \to Q') = P^{\mathrm{eq}}(Q')W(Q' \to Q)$$

Metropolis:

$$W(Q \to Q') = \min\left\{1, \frac{P^{\mathrm{eq}}(Q')}{P^{\mathrm{eq}}(Q)}\right\}$$

W can be splitted into two parts:

$$W(Q \to Q') = \Theta(Q \to Q')\, p(Q \to Q')$$

where

$$\Theta(Q \to Q') : \text{prob./unit time consider move } Q \to Q'$$

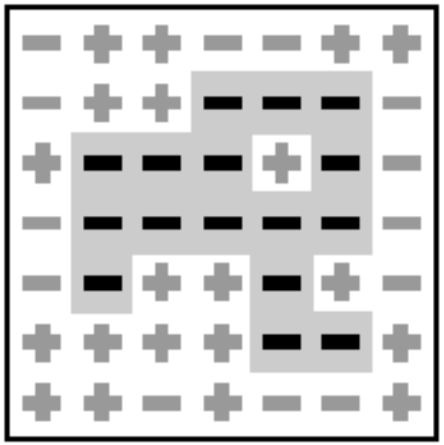
$$p(Q \to Q') : \text{prob. accept move } Q \to Q'$$

With this we have:

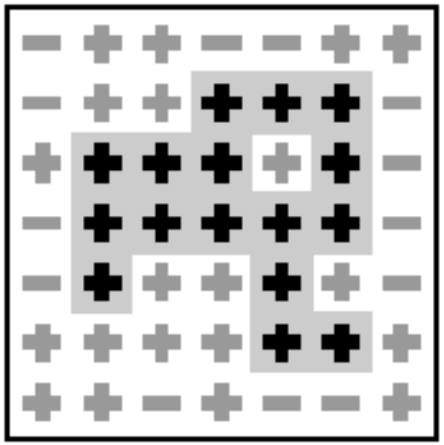
$$p(Q \to Q') = \min\left\{1, \frac{P^{\mathrm{eq}}(Q')\Theta(Q' \to Q)}{P^{\mathrm{eq}}(Q)\Theta(Q \to Q')}\right\}$$

The aim is to define the droplets such that the acceptance probability becomes independent of the configurations.

A Wolff droplet (gray) before flipping



a



b

The new configuration The droplet contour is still shown, though the bonds are eliminated after flipping

In a) there are 9 „-" perimeter sites not connected to the droplet, leading to a factor of $(1-p_B)^9$ in $\Theta(a \to b)$. In the opposite direction we have $(1-p_B)^{19}$.

$$\Theta(a \to b) = \Theta_{\text{interior}}(a \to b) \times (1 - p_B)^9$$

$$\Theta(b \to a) = \Theta_{\text{interior}}(b \to a) \times (1 - p_B)^{19}$$

$E_a = E_{\text{interior}} + E_{\text{exterior}} - 9XJ + 19XJ$

$E_b = E_{\text{interior}} + E_{\text{exterior}} - 19J + 9XJ$

$$\frac{P^{\text{eq}}(b)}{P^{\text{eq}}(a)} = \frac{e^{-\beta E_b}}{e^{-\beta E_a}}$$

http://physics.bnu.edu.cn/application/faculty/guowenan/ising/index.html

$n_{\text{same}} = 9,\ n_{\text{diff}} = 19$

$$p(a \to b) = \min\left\{1, \frac{e^{\beta J n_{\text{diff}}} e^{-\beta J n_{\text{same}}}}{(1-p_B)^{n_{\text{same}}}} \frac{(1-p_B)^{n_{\text{diff}}}}{e^{-\beta J n_{\text{diff}}} e^{\beta J n_{\text{same}}}}\right\} =$$

$$\min\left\{1, \frac{e^{-2\beta J n_{\text{same}}}}{(1-p_B)^{n_{\text{same}}}} \frac{(1-p_B)^{n_{\text{diff}}}}{e^{-2\beta J n_{\text{diff}}}}\right\}$$

In 2d z = 0 (log)!
3d ~0.1

Thus, with the choice $p_B = 1 - e^{-2\beta J}$ we have $p(a \to b)=1$

Wolff algorithm is strightforwardly generalized to Potts and XY- or Heisenberg-models.

($\mathscr{H}_{\text{Potts}} = -J_H \sum_{<i,j>} \delta_{s_i,s_j} - \sum_i \delta_{h,s_j}$ $\qquad s_i = 1,2,3...q$)

For continuous spin models define a random direction with unit vector $\hat{\mathbf{n}}$

$$p_B = 1 - e^{-2\beta J_H (\hat{\mathbf{n}}\mathbf{s}_i)(\hat{\mathbf{n}}\mathbf{s}_j)}$$

Flip spins $\perp$ to **n**

Parallelizable algorithms	The idea applicable to other systems as well.

Magnetic field breaks the symmetry and this is reflected in the acceptance probability.

There are different ways to take magnetic field into account. The simplest is to consider the droplet as a single superspin and make a usual MC decision. E.g., for the SW algorithm

$$W_{\text{droplet}}(\downarrow \to \uparrow) = \frac{e^{2Hs}}{e^{2Hs} + e^{-2Hs}} \text{ and } W_{\text{droplet}}(\uparrow \to \downarrow) = \frac{e^{-2Hs}}{e^{2Hs} + e^{-2Hs}}$$

in a field opinting upward (s is the size of the droplet).

Reweighting technique

What if we could calculate the distribution function at a given temperature? $Z(\beta) = \sum_i e^{-\beta E_i} = \int \omega(E) e^{-\beta E} dE$

The β-dependence is in the trivial Boltzmann factor, the information about the system is in the density of states, which is the same for all β-s.

$$P_E^{\mathrm{eq}}(\beta) = \frac{\omega(E) e^{-\beta E}}{Z(\beta)}$$

$$\omega(E) = P_E^{\mathrm{eq}}(\beta) Z(\beta) e^{\beta E} = P_E^{\mathrm{eq}}(\beta') Z(\beta') e^{\beta' E}$$

$$P_E^{\mathrm{eq}}(\beta) = P_E^{\mathrm{eq}}(\beta') \frac{e^{(\beta'-\beta)E}}{\sum_{E'} P_{E'}^{\mathrm{eq}}(\beta') e^{(\beta'-\beta)E'}}$$

Because:

$$\frac{Z(\beta)}{Z(\beta')} = \sum_{E'} P_{E'}^{\mathrm{eq}}(\beta') e^{(\beta'-\beta)E'}$$

If we can compute accurately at a given temperature (small system!) we have results for other (nearby) temperatures as well.

Other ensembles

Micorocanonical: Energy is conserved. We allow for the variation of the energy within a narrow band. This is maintained by a „bag” of a „daemon” (Santa Claus).

Creutz:
-1 Pick a site
- If the flip causes energy change too much for the tolerance bag, reject the flip and go to 1. Otherwise
- If energy is gained put the gain into the bag, if it is lost, extend it from the bag.
- Go to 1

Essentially deterministic, easy to parallelize.

General observation: In case of conservation the dynamic exponent *z* is larger. Dynamic universality classes within static ones

Conserved order parameter: Kawasaki dynamics

In fact, the ensemble we have dealt so far for the Ising model is the grand canonical one, as we have governed the system by the externel field, the intensive variable conjugate to the extensive magnetization (order parameter).

Canonical ensemble: The variables are *T* and *M,* fixed, i.e., the order parameter is conserved.

The elementary step is: Exchange up-down spin pairs
Otherwise usual Metropolis can be applied.
Diffusive dynamics is more physical (pick neighboring spins)
For proper avarages (detailed balance!) a time step elapses even if parallel spins are picked.

This method is able to simulate, e.g., an AB alloy.