Spin-1/2 Ising model: MC simulation

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Spin-1/2 Ising Model

A classical spin variable s_i, which takes $+1$ or -1 values corresponding to the states up or down, placed on each lattice site. Usually, the interaction among the spins is limited (however, not restricted) to the nearest neighbor spins only. The interaction energy or the exchange energy among two spins is given by J. The Hamiltonian for such an interacting system is given by

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i \, s_j - \mu B \sum_i s_i$$

where μ is the magnetic moment and B is external magnetic field and $\langle \cdots \rangle$ represents the nearest neighbor interaction. The first term in the Hamiltonian is responsible for the cooperative behavior. For *J*=0, the Hamiltonian corresponds to a paramagnetic system.

Ground state configuration

First we set the external field B=0 and then the Hamiltonian is given by

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i \, s_j$$

Consider two spins only along a one dimensional chain. Since the spins have two states each, there are total 2^2= 4 configurations possible

There are two parallel configurations, both up spins and both down spins and two anti-parallel configurations, one up and another down. The Hamiltonian for the parallel and anti-parallel configurations are then given by

$$\mathcal{H}_{\mathrm{P}} = -J \quad \text{and} \quad \mathcal{H}_{\mathrm{A}} = J$$

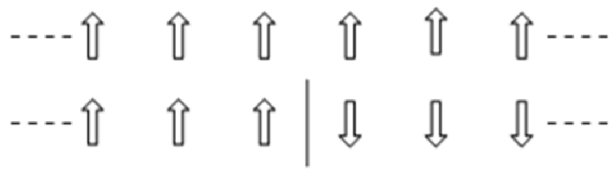
The free energy for N parallel and anti-parallel configurations can be calculated as

$$F_{\mathrm{P}} = -Nk_BT \ln Z = -NJ$$

$$F_{\mathrm{A}} = -Nk_BT \ln Z = +NJ$$

Since the free energy corresponding to parallel configuration is lowest, the ground state configurations are:

Ising Model in One dimension



Consider a chain of N spins with one domain wall as shown above.

The change in free energy is given by $\Delta F = \Delta E - T\Delta S = 2J - k_B T \ln N$

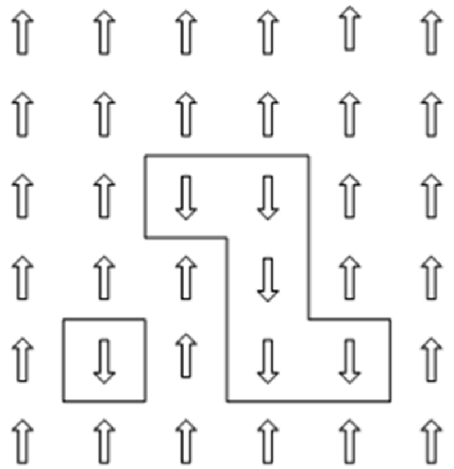
Since N is large, for $T \neq 0$, the second term in the free energy will dominate which corresponds to the presence of domain wall. Since $\Delta F < 0$, the fluctuation in spin orientation will be cost free. No long range order in the spin orientation will appear and thus there will be no spontaneous magnetization. On the other hand, for $T = 0$, the first term in the free energy will survive and the ground state configuration is either all spins up or all spins down. A long range order state is then possible only at $T = 0$. Therefore, in one dimensional spin-1/2 Ising model on phase transition will occur at any finite temperature except at $T = 0$.

Exact result: $$\langle \mathcal{M}/N \rangle = \frac{sinh(\beta \mathcal{B})}{(sinh^2(\beta \mathcal{B}) + e^{-2\beta J})^{1/2})}.$$

For B=0 the magnetzation is zero. This means that for a one-dimensional Ising mode there is no spontaneous magnetization.

Ising Model in Two dimensions

For the configuration given, the number of anti-parallel spins is 16 and the length of the domain wall for both the domains is 16. Since each anti-parallel spins costs $2J$ amount of energy, the internal energy change for a domain wall of length L would be $\Delta E = 2JL$.



The maximum entropy is given by $S = k_B \ln \omega$ where ω is the number of all possible domain configurations for the same number of anti-parallel spins. The domain walls can be constructed by making a walk along the boundary. For each step of walk there are three possibilities and thus $\omega = 3^L$. Therefore the change in entropy would be $\Delta S = k_B L \ln 3$.

The change in free energy is then given by

$$\Delta F = \Delta E - T\Delta S = 2JL - k_B T L \ln 3$$

Now, there may exist a critical temperature T_c above which the second term in the free energy will dominate. The second term is the entropy term and hence there will be large number of domain walls. No long range order can be established and no spontaneous magnetization can exists. On the other hand, Below T_c, the term coming from the interaction of the spins will dominate. There will be less number of domain walls and long range order would be possible. Also, spontaneous magnetization can exist. Therefore phase transition is possible to explain with spin-1/2 Ising Hamiltonian at any finite temperature in the space dimension two or above.

Order-disorder transition and Ising Model

Order-disorder transition of Beta brass: Beta-brass is a binary alloy consists of equal number of Cu and Zn atoms. Each sub-lattice has simple cubic structure and they inter-penetrate into each other and form a body centre cubic structure. At room temperature, neither of the sub-lattices contains atoms of other type and it is called a ordered state. However, above a critical temperature $T_c = 733K$ both the sub-lattices are occupied by both the atoms and it is called a disordered state. The order parameter of the transition can be defined as the difference between the concentration of Cu and Zn atoms on a chosen sub-lattice. For the Cu sub-lattice, it can be defined as

$$\Delta c = \frac{c_{Cu} - c_{Zn}}{c_{Cu}}$$

At room temperature, Δc is equal to one whereas at above T_c it is going to be zero. Thus there is a continuous phase transition at $T = T_c$ from a order to a disordered state. In order to study such a phase transition, we introduce a two states variable $s_i = \pm 1$, $s_i = 1$ if a site is occupied with Cu and $s_i = -1$ if a site is occupied with Zn. The phase transition can be studied constructing a Hamiltonian including all the interactions among Cu and Zn atoms in the Beta brass. There could be three different types of interaction in this system, Cu-Cu, Zn-Zn and Cu-Zn (or Zn-Cu) and the corresponding interaction energies can be taken as J_{CuCu}, J_{ZnZn}, and J_{CuZn}.

Ising Hamiltonian for beta brass:

$$\mathcal{H} = \frac{1}{4}\sum_{\langle \boldsymbol{ij} \rangle} \boldsymbol{J_{CuCu}}(\mathbf{1} + \boldsymbol{s_i})(\mathbf{1} + \boldsymbol{s_j}) + \frac{\mathbf{1}}{\mathbf{4}}\sum_{\langle ij \rangle} J_{ZnZn}(1 - s_i)(1 - s_j) + \frac{1}{4}\sum_{\langle ij \rangle} J_{CuZn}\{(1 + s_i)(1 - s_j) + (1 - s_i)(1 + s_j)\}$$

Ising Model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - \mu B \sum_i s_i$$

Set B=0.

The critical temperature:

$$2 \tanh^2 \frac{2J}{k_B T_c} = 1, \qquad k_B T_c / J = 2.269185.$$

Scaling:

$$M \sim (-t)^{\beta} \qquad \chi \sim |t|^{-\gamma} \qquad C_B \sim |t|^{-\alpha} \qquad \xi \sim |t|^{-\nu}$$

Critical exponents:

$$\alpha = 0 \text{ (logarithmic)}, \beta = 1/8, \gamma = 7/4, \nu = 1.$$

$$\beta(\delta - 1) = \gamma \qquad \Rightarrow \qquad \delta = 15$$

Metropolis algorithm for spin-1/2 Ising model

1. Choice of initial state: Take a (L × L) square lattice. A random spin configuration is taken as initial state assigning s = +1 (or −1) to the lattice sites randomly with probability 0.5 corresponding to up spin (or down spin) respectively.

2. Calculation of energy change: Choose a site j randomly from the sites with s = +1 or −1 which correspond to the initial state of the j spin. The final state is the state with the overturned spin at the jth site. The change in energy $\Delta E = E_f - E_i$ for the sing Hamiltonian without external field is given by

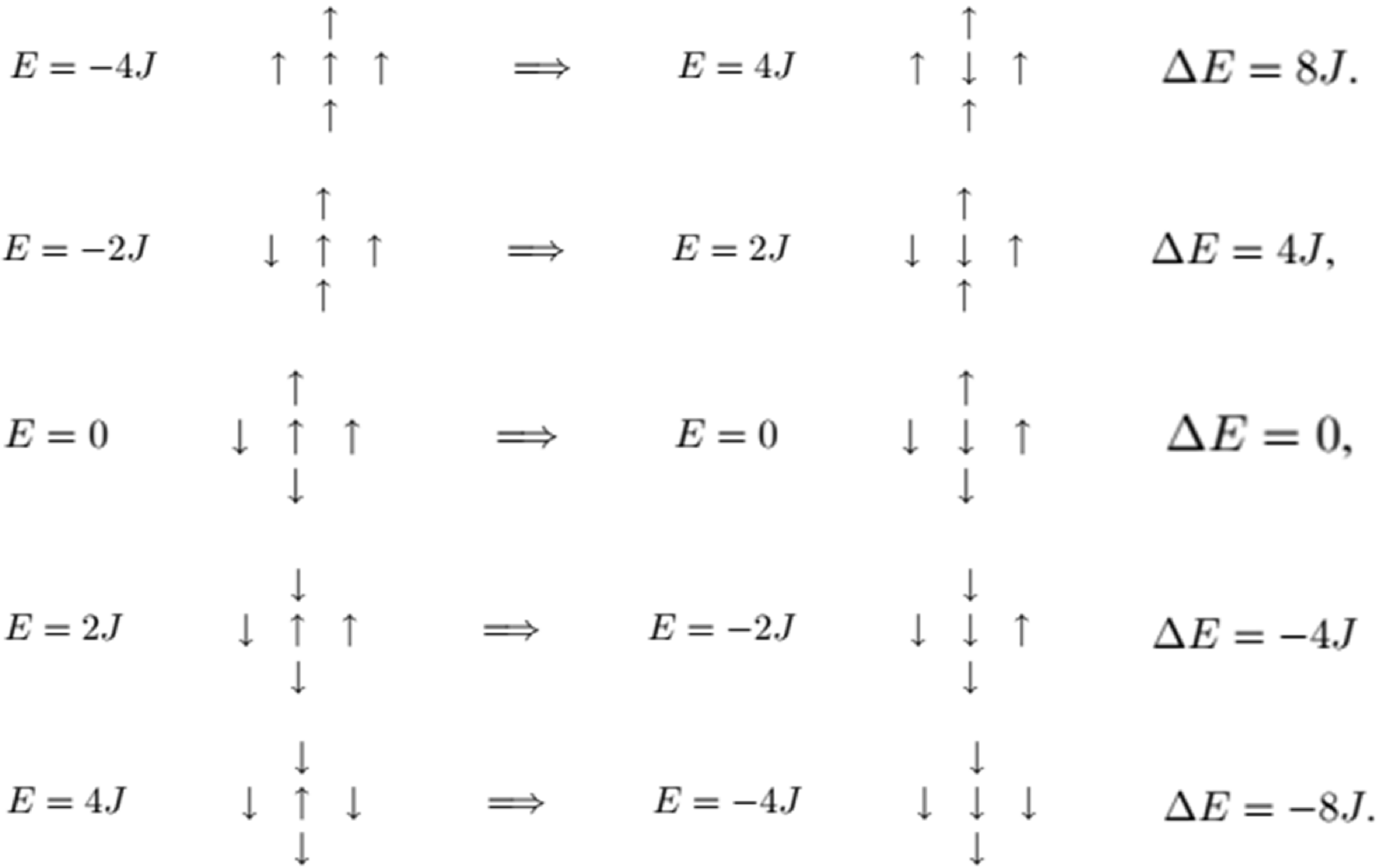
$$\Delta E = 2Js_j \sum_{k=1}^{4} s_k$$

where sj is the initial spin state and s_k s are the nearest neighbour spins.

3. Accept or reject the spin flip: If ΔE < 0 flip the spin, else call a random number r uniformly distributed between 0 and 1. If $r \leq \exp(-\Delta E/k_B T)$ flip the spin, otherwise do not flip it.

4. Iteration: Go to the next site and start from (2). Repeat the process for all spins.

Calculation of change in energy:



Spin configuration:

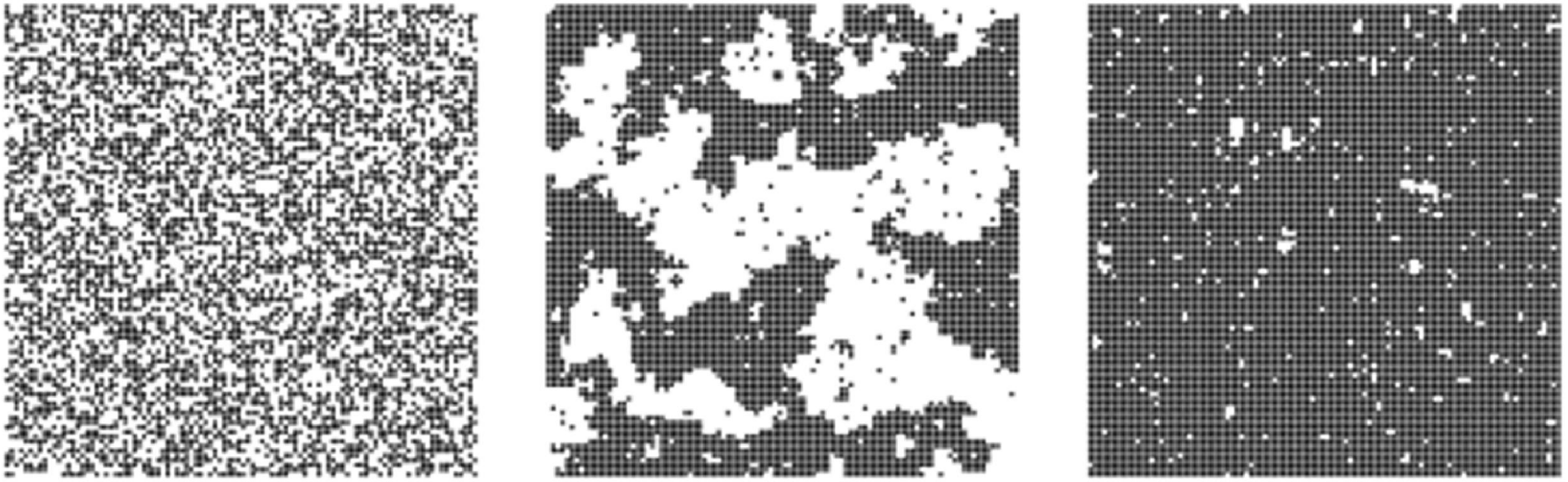


Figure 1.13: Spin configuration at temperature $k_B T/J = 2.0$, corresponds to $T < T_c$ ($k_B T_c/J \approx 2.27$). t is the MC time step per spin.

Spin configuration:

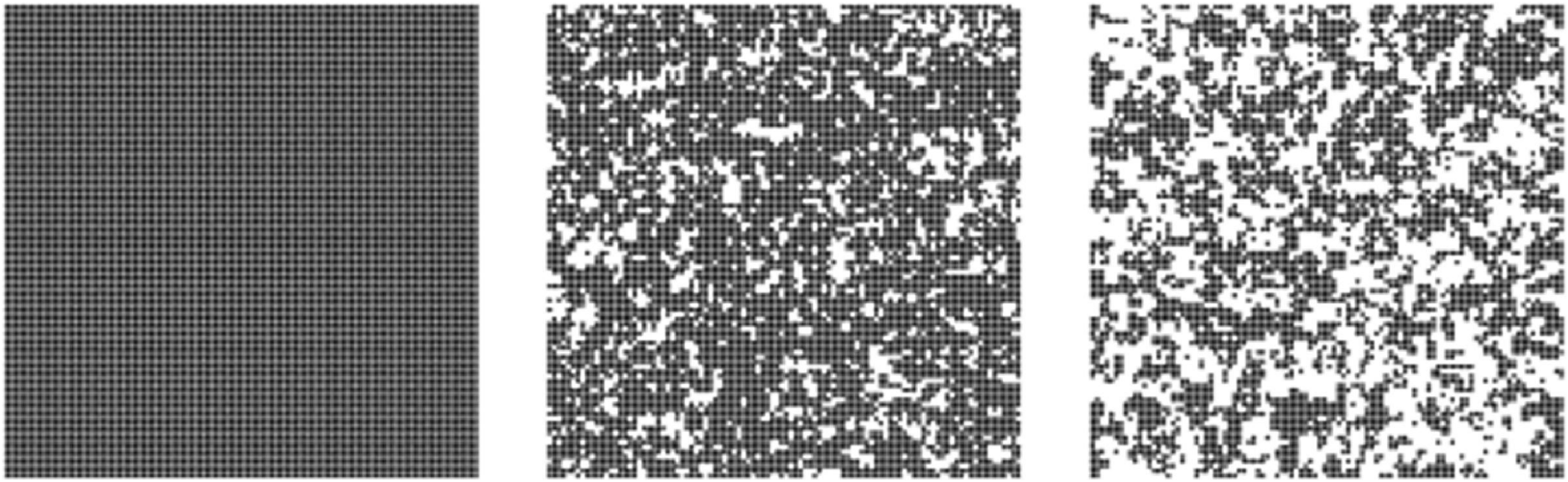
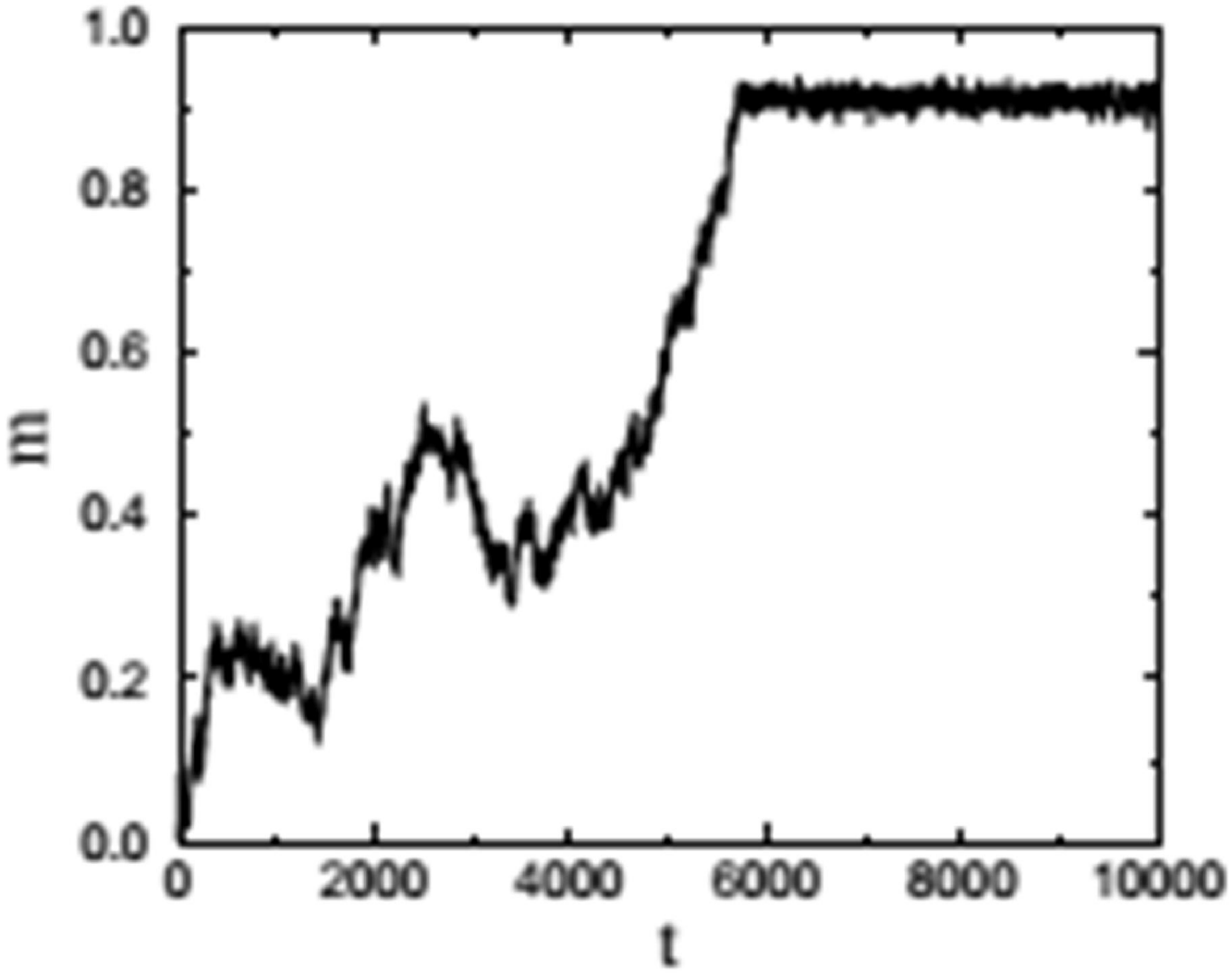


Figure 1.14: Spin configuration at $k_BT/J = 3.0$, corresponds to $T > T_c$ ($k_BT_c/J \approx 2.27$). t is the MC time step per spin.

Equilibrium:



Equilibrium configurations

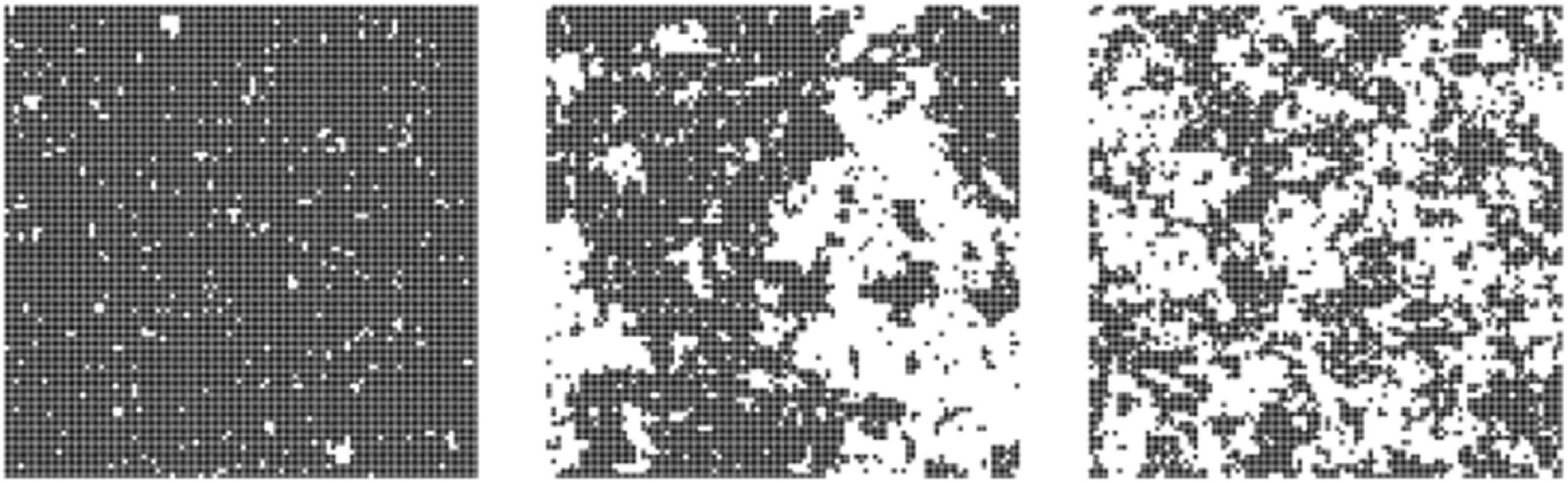


Figure 1.16: Equilibrium spin configuration at different temperatures around T_c after 8000 Monte Carlo time step per spin.

Magnetization and Susceptibility:

The magnetization *m* per spin in a state *n* is given by

$$M_n = \sum_{i=1}^{L^2} s_i^n$$

Since only one spin *k* flips at a time in the Metropolis algorithm, so the change in magnetization is given by

$$\Delta M = M_m - M_n = \sum_{i=1}^{L^2} s_i^m - \sum_{i=1}^{L^2} s_i^n = s_k^m - s_k^n = 2s_k^m \qquad s_k^n = -s_k^m$$

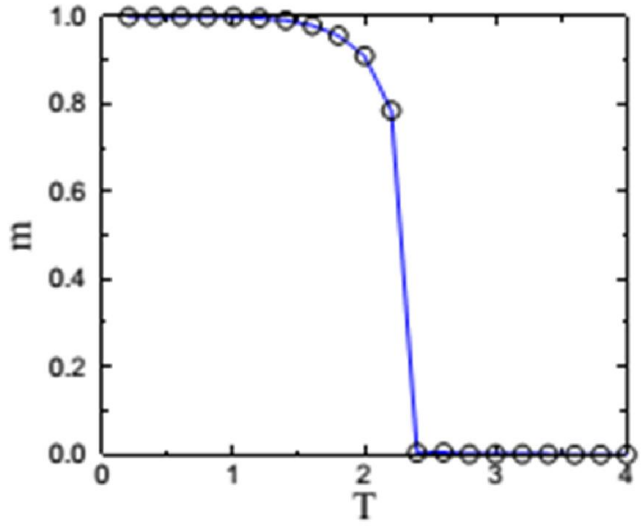
One can then calculate the magnetization at the beginning of the simulation and then use the following equation

$$M_m = M_n + \Delta M = M_n + 2s_k^m \qquad \langle m \rangle = \frac{1}{N_c \times L^2} \sum_{k=1}^{N_c} M_k$$

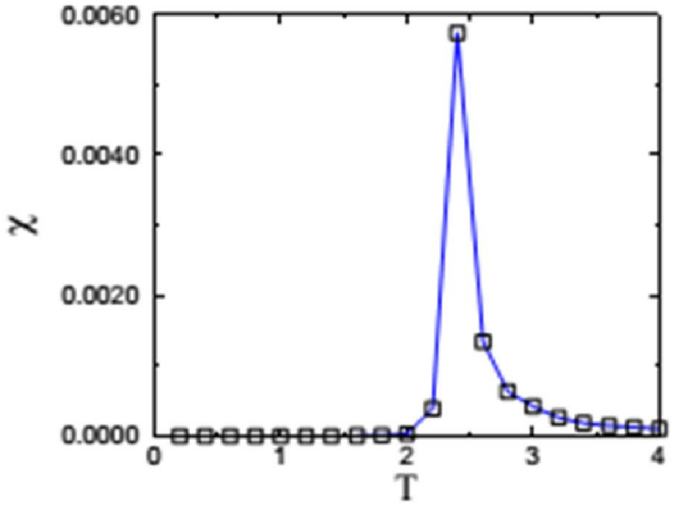
One could calculate the per spin susceptibility as

$$\chi_T = \frac{1}{k_B T} [\langle m^2 \rangle - \langle m \rangle^2]$$

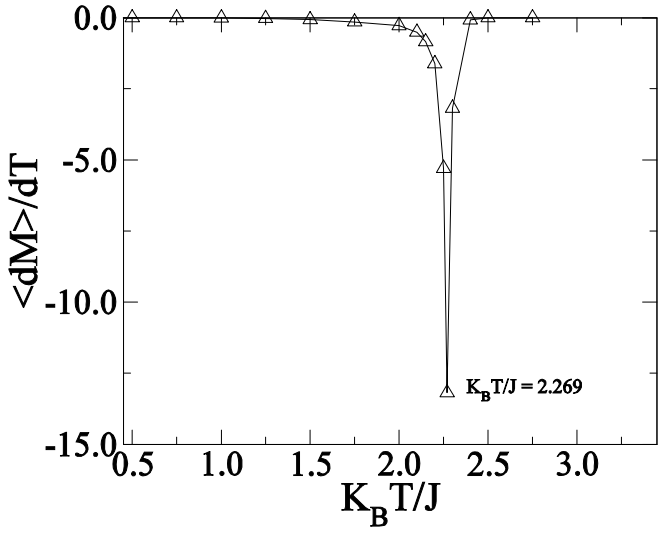
Magnetization and Susceptibility:



Magnetization M



Susceptibility χ



On a 2d square lattice of size 100 ×100.

Energy and specific heat:

$$E_n = -J \sum_{\langle ij \rangle} s_i^n \, s_j^n$$

Set *J*=1

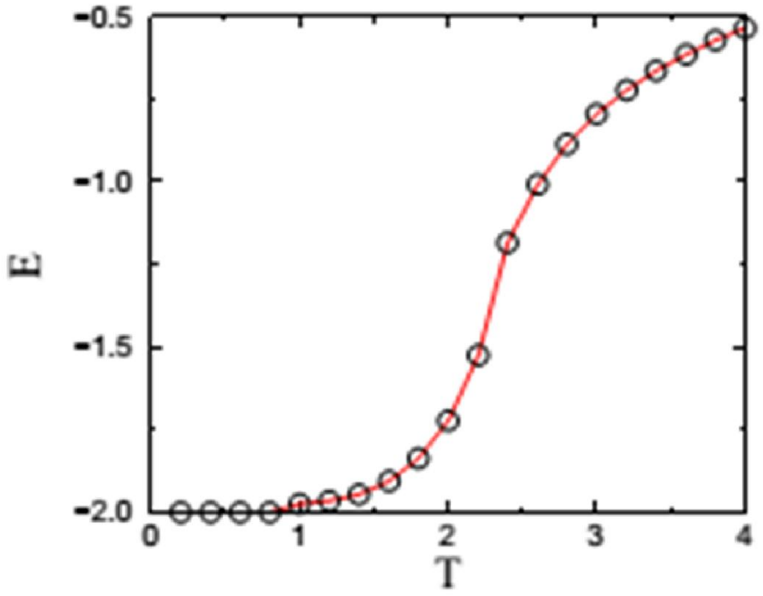
The energy difference in going from state n to state m is: $\Delta E = E_m - E_n$

$$E_m = E_n + \Delta E.$$

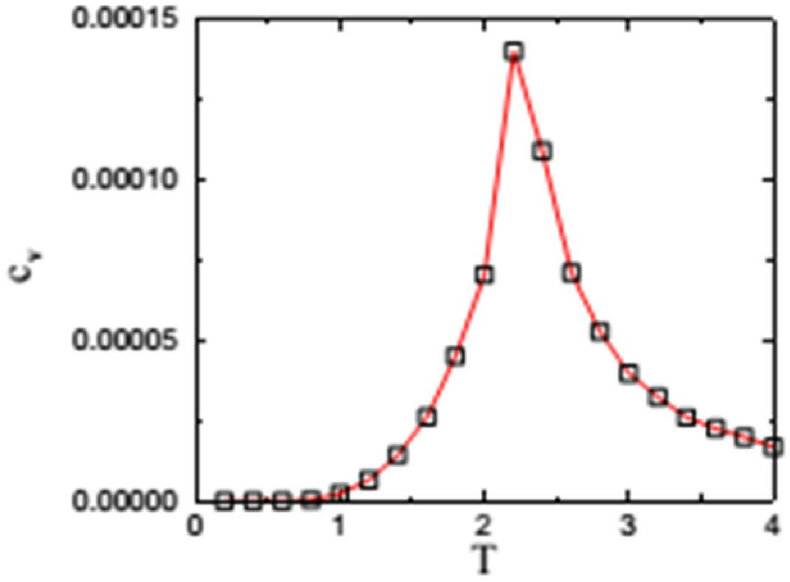
One may calculate the per spin specific heat as

$$c_V = \beta^2(\langle E^2 \rangle - \langle E \rangle^2)$$

Energy and specific heat:



Energy E



Specific Heat C_v

Time auto correlation

In order to take average of a physical quantity, we have presumed that the states over which the average has been made are independent. Thus to make sure that the states are independent, one needs to measure the "correlation time" τ of the simulation. The time auto correlation $C_m(t)$ of magnetization is defined as

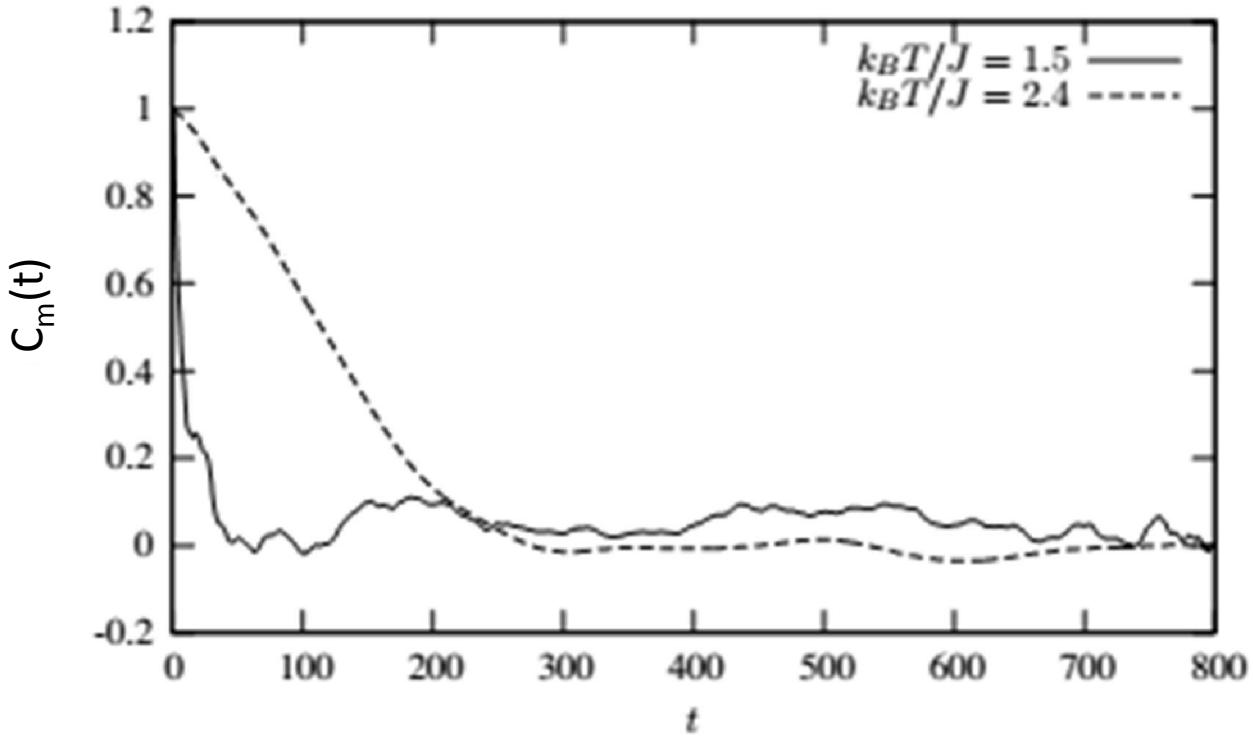
$$C_m(t) = \sum_{t'} [m(t') - \langle m \rangle][m(t'+t) - \langle m \rangle] = \sum_{t'} m(t')m(t'+t) - \langle m \rangle^2.$$

The auto correlation Cm(t) is expected to fall off exponentially at long time

$$C_m(t) \sim e^{-t/\tau}.$$

Thus, at t = τ , Cm(t) drops by a factor of 1/e from the maximum value at t = 0. For independent samples, one should draw them at an interval greater than τ . In most of the definitions of statistical independence, the interval turns out to be 2τ .

Time auto correlation



Cluster update algorithms

Cluster update algorithms are the most successful global update methods in use. These methods update the variables globally , in one step, whereas the standard local methods operate on one variable at a time

A global update can reduce the autocorrelation time of the update and thus greatly reduce the statistical errors.

Fortuin-Kasteleyn cluster decomposition

$$H = -J \sum_{\langle ij \rangle} (s_i s_j - 1),$$

where *J* is the interaction energy between any two nearest neighbor Ising spins s_i and s_j . If the spins s_i and s_j are aligned in the same direction, the energy for the bond connecting the two spin is 0 and if the two spins are antiparallel the energy is 2*J* .

$$H = 2J(N_E - B),$$

where N_E is the total number of bonds in the lattice and *B* is the number of bonds between similar spins.

The partition function of the system is:

$$Z = \sum e^{-\beta H} = \sum_B e^{-2J\beta(N_E - B)} = \sum_B q^{(N_E - B)} \qquad q = e^{-2J\beta}. \qquad p = 1 - q = 1 - e^{-2J\beta}.$$

Now, out of *B* satisfied bonds let *b* bonds are occupied with probability *p*. Number of ways *b* bonds can be arranged out of *B* number of bonds is

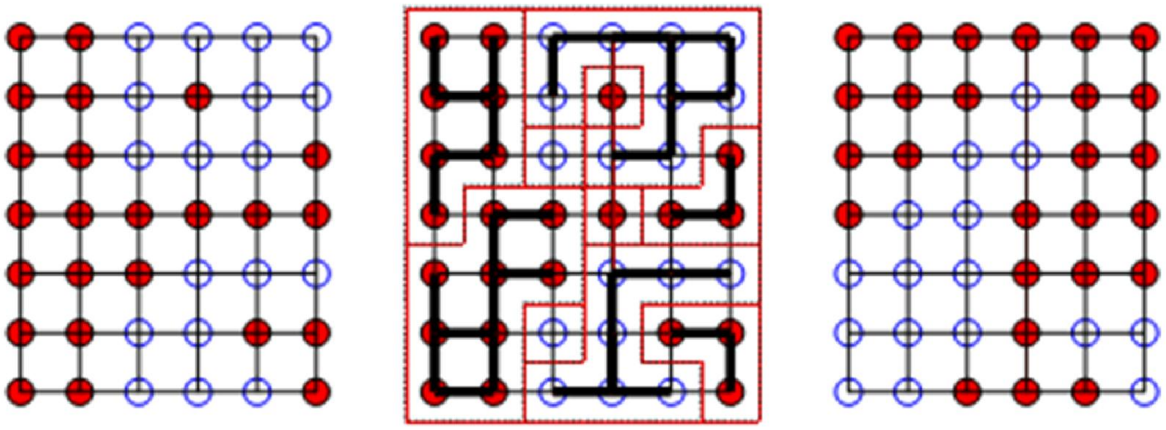
$$\Omega(B, b) = \frac{B!}{b!\,(B-b)!} \qquad P(B, b) = \Omega(B, b) p^b (1-p)^{B-b}. \qquad \sum_{b=0}^{B} P(b, b) = (p+q)^B = 1$$

$$Z = \sum_B q^{N_E - B} (p+q)^B = \sum_B q^{N_E - B} \sum_{b=0}^{B} \Omega(B, b) p^b (1-p)^{B-b} = \sum_B \sum_{b=0}^{B} \Omega(B, b) p^b q^{N_E - b}$$

Swendsen-Wang algorithm: PRL **58** (1987) 86.

Beginning with an arbitrary configuration s_i, one SW cluster update cycle is:

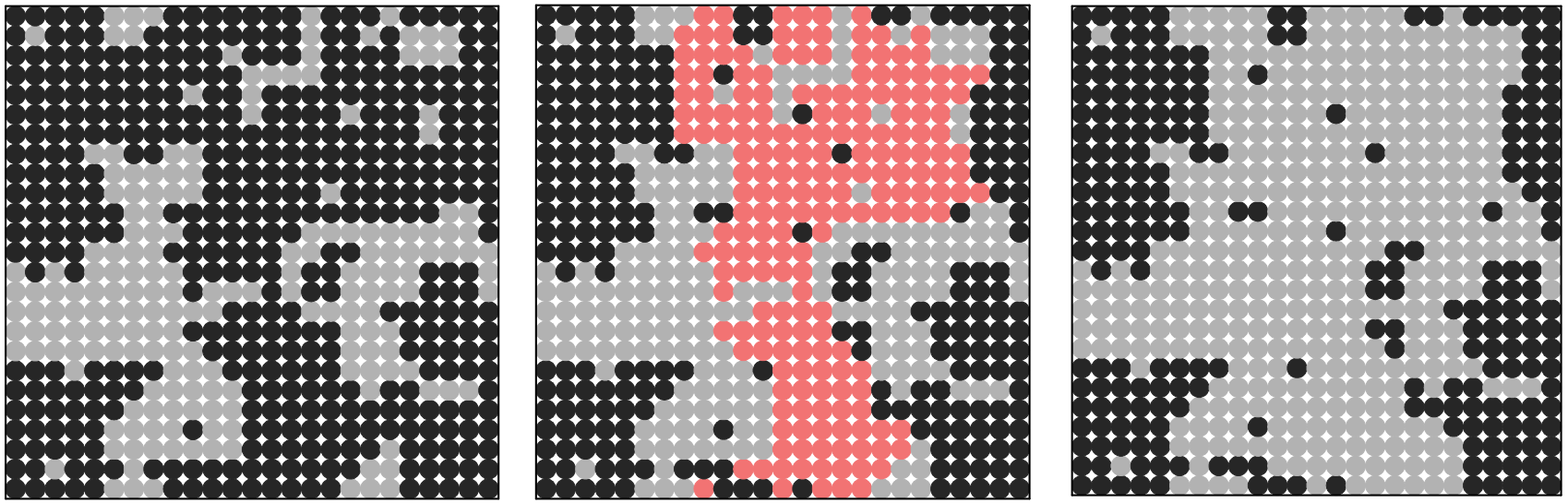
1. Inspect all nn-states s_i, s_j. If $s_i = s_j$, create a bond between sites i, j with probability $p = 1 - \exp(-2\beta)$ (otherwise no bond).
2. Construct clusters = sets of points connected by bonds.
3. Set each cluster to a *random* value ± 1.



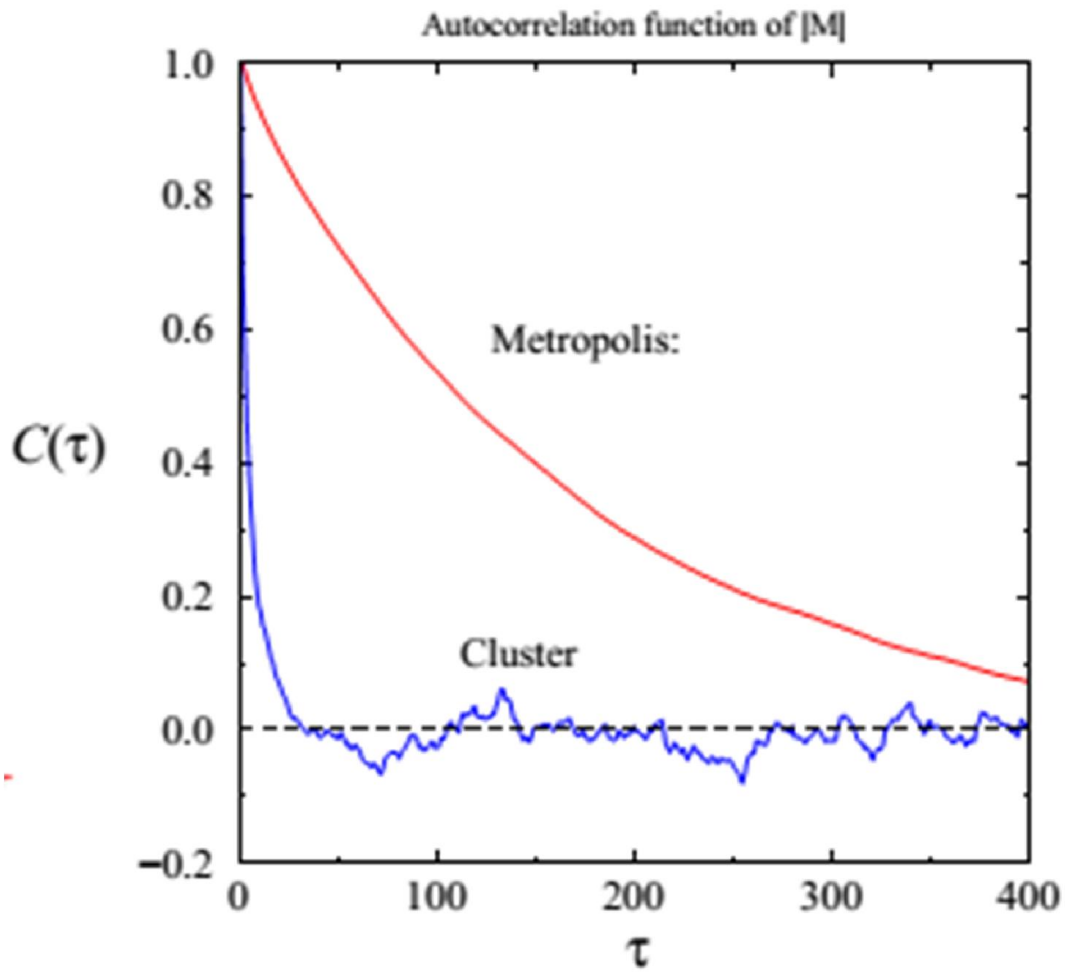
Wolff single cluster algorithm: PRL **62** (1989) 361

Principle: do the cluster decomposition as in S-W , but invert ('flip') only one randomly chosen cluster! In practice:

1. Choose random site i.
2. Study neighbouring sites j. If $s_j = s_i$, join site j to cluster with probability $p = 1 - \exp(-2\beta)$.
3. Repeat step 2 for site j, if it was joined to the cluster. Keep on doing this as long as the cluster grows.
4. When the cluster is finished, invert the spins which belong to it.



Auto correlation in cluster algorithm



Ergodicity and detailed balance in cluster algorithm

Ergodicity: There is always a non-zero probability that the cluster will contain a single spin and by flipping a sequence of single spins any configurations can be reached.

Detailed balance:

Consider two spin configurations C and C’ in which the spins take the values s_i and s'_i which can be transformed into each other by reversing a single cluster of spins. The change in energy due to the flipping of the spins will come only from the spin interactions along the boundary of the cluster. The ratio of the transition probabilities in going from C to C’ and vice versa is:

$$\frac{P(C \to C')}{P(C' \to C)} = \exp[2\beta J \sum_{i,j} s_i s_j] = \exp[-\beta(E_{C'} - E_C)].$$

In the above expression the spin s_i belong to the cluster C or C’ and the neighboring spins s_j do not belong to the cluster.

Effect of finite size

Critical temperature:

$$T_c(L) = T_c + aL^{-1/\nu}$$

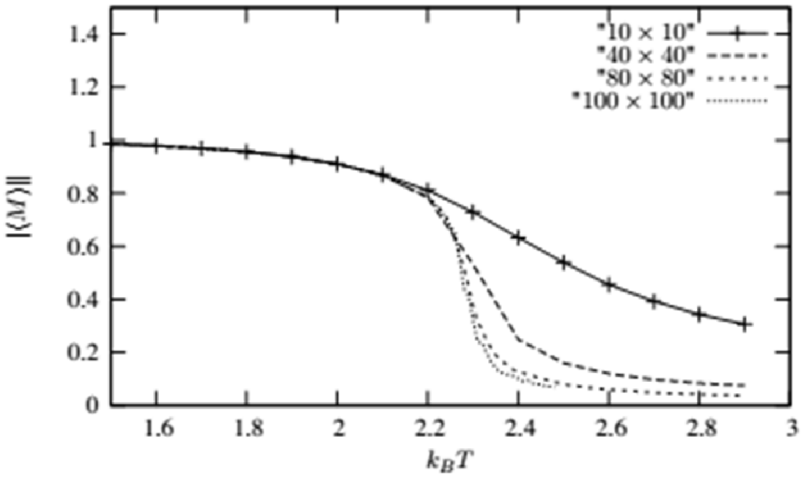
Thermodynamic quantities:

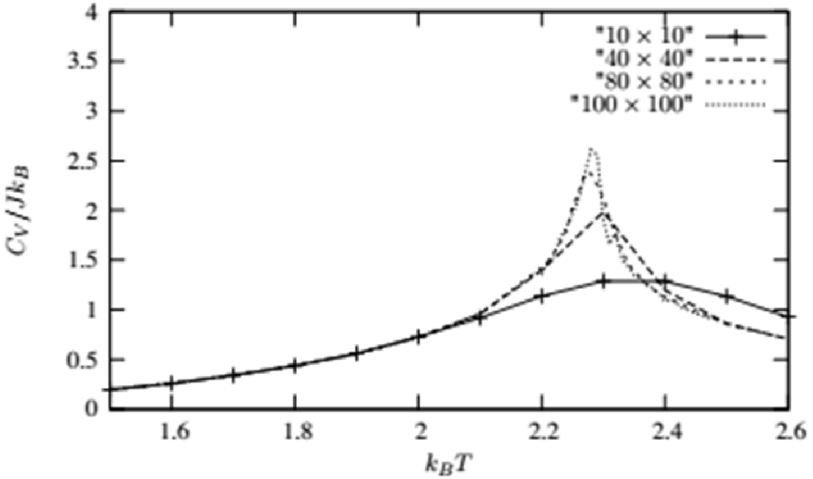
$$\begin{aligned} M &= L^{-\beta/\nu}\phi(\epsilon L^{1/\nu}) \\ \chi &= L^{\gamma/\nu}\tilde{\chi}(\epsilon L^{1/\nu}) \\ C_v &= L^{\alpha/\nu}\tilde{S}(\epsilon L^{1/\nu}) \end{aligned}$$

At $T = T_c$:

$$\begin{aligned} M &= L^{-\beta/\nu} \\ \chi &= L^{\gamma/\nu} \\ C_v &= L^{\alpha/\nu}. \end{aligned}$$

Finite size effect





Error analysis

Statistical error:

$$\text{error} = \sqrt{\frac{1}{N(N-1)} \sum_{i=1}^{N} (x_i - \langle x \rangle)^2}$$

Systematic error: Since the systematic errors do not appear in the fluctuations of the individual measurement, they are more difficult to estimate than statistical errors. The main source of systematic error in the Ising Model simulation is the choice of finite number of MC time steps to equilibrate the system. There is no good general method for estimating systematic errors. Each source of such error has to be considered separately and a strategy has to be identified