Introduction to classical Metropolis Monte Carlo

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Where is Kiel?

Figure: Kiel

Where is Kiel?

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What is Kiel?

Figure: Picture of the Kieler Woche 2008

What is Kiel?

Figure: Dominik Klein from the Handball club *THW Kiel*

Outline

Introduction

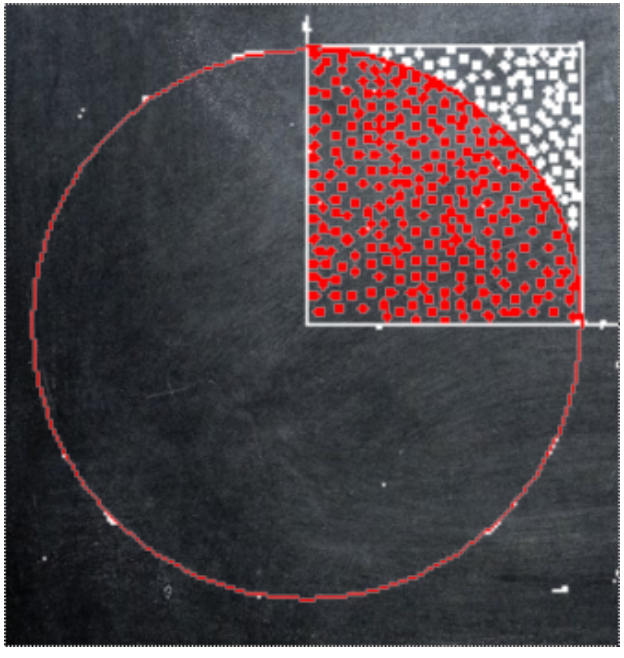
The term *Monte Carlo simulation* denotes any simulation which utilizes random numbers in the simulation algorithm.

Figure: Picture of the Casino in Monte-Carlo

Advantages to use computer simulations

- Simulations provide detailed information on model systems.
- Possibility to measure quantities with better statistical accuracy than in an experiment.
- Check for analytical theories without approximations.
- MC methods have a very broad field of applications in physics, chemistry, biology, economy, stock market studies, etc.

Hit-or-Miss Monte Carlo: Calculation of π



One of the possibilities to calculate the value of π is based on the geometrical representation:

$$\pi = \frac{4 \times \pi R^2}{(2R)^2} = \frac{4 \times \text{Area of a circle}}{\text{Area of enclosing square}}.$$

Choose points randomly inside the square. Then to compute π use:

$$\frac{4 \times \text{Area of a circle}}{\text{Area of enclosing square}} \simeq \frac{4 \times \text{Number of points inside the circle}}{\text{Total number of points}}.$$

Volume of the m-dimensional hypersphere

m	Exact
2	3.1415
3	4.1887
4	4.9348
5	5.2637
6	5.1677
7	4.7247
8	4.0587

Exact result:

$$V^{md} = \pi^{m/2} r^m / \Gamma(m/2 + 1)$$

Volume of the m-dimensional hypersphere

m	Exact	quad. time	result
2	3.1415	0.00	3.1296
3	4.1887	$1.0 \cdot 10^{-4}$	4.2071
4	4.9348	$1.2 \cdot 10^{-3}$	4.9657
5	5.2637	0.03	5.2863
6	5.1677	0.62	5.2012
7	4.7247	14.9	4.7650
8	4.0587	369	4.0919

Exact result:

$$V^{md} = \pi^{m/2} r^m / \Gamma(m/2+1)$$

$$V^{3d} = 2 \int_{x^2+y^2 \le r^2} dx\, dy\, z(x,y)$$

Integral presentation: sum of the volumes of parallelepipeds with the base $dx\,dy$ and height

$$r^2 = x^2 + y^2 + z^2$$

$$\rightarrow z(x,y) = \sqrt{r^2 - (x^2+y^2)}$$

Volume of the m-dimensional hypersphere

m	Exact	quad. time	result	MC time	result
2	3.1415	0.00	3.1296	0.07	3.1406
3	4.1887	$1.0 \cdot 10^{-4}$	4.2071	0.09	4.1907
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7	4.7247	14.9	4.7650	0.19	4.7182
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Exact result:

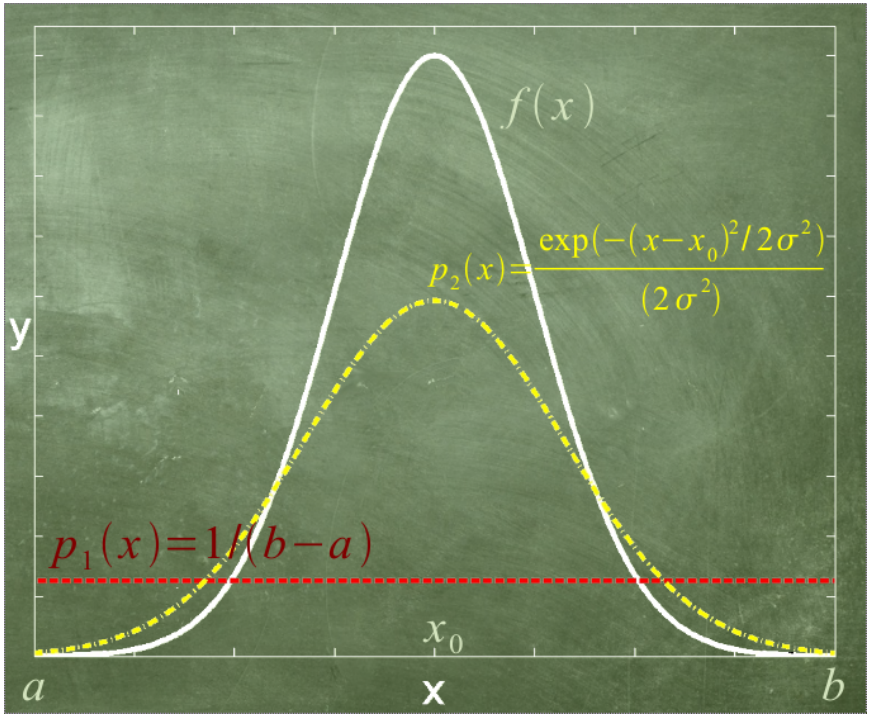
$$V^{md} = \pi^{m/2} r^m / \Gamma(m/2+1)$$

Monte-Carlo integration
m-dimensional vectors
$\mathbf{x} = (x_1, x_2, \ldots, x_m)$ are sampled in volume $V = (2r)^m$,

$$V^{m \cdot d} \approx \frac{V}{K} \sum_{i=1}^{K} f(\mathbf{x}_i)\Theta(\mathbf{x}_i),$$

$\Theta(\mathbf{x}) = 1$ if $(\mathbf{x} \cdot \mathbf{x}) \leq r^2$.

Monte Carlo integration



Straightforward sampling

Random points $\{x_i\}$ are choosen uniformly

$$I = \int_a^b f(x)dx \approx \frac{b-a}{K} \sum_{i=1}^{K} f(x_i)$$

Importance sampling

$\{x_i\}$ are choosen with the probability $p(x)$

$$I = \int_a^b \frac{f(x)}{p(x)} p(x)dx \approx \frac{1}{K} \sum_{i=1}^{K} \frac{f(x_i)}{p(x_i)}$$

Optimal importance sampling

How to choose $p(x)$ to minimize the error of the integral

$$I \approx \frac{1}{K}\sum_{i=1}^{K}\frac{f(x_i)}{p(x_i)} \pm \sqrt{\frac{\sigma^2[f/p]}{K}} \qquad \sigma^2(x) = \frac{1}{K}\sum_{i=1}^{K}(x_i - \bar{x})^2$$

Solve optimization problem:

$$\min\left[\left(\frac{f(x)}{p(x)}\right)^2\right] = \int_Q \frac{f(x)^2}{p(x)^2}\,p(x)dx = \int_Q \frac{f(x)^2}{p(x)}\,dx = \min, \quad \int_Q p(x)dx = 1.$$

Extremum conditions:

$$\int_Q \frac{f(x)^2}{p(x)^2}\,\delta p(x)dx = 0 \qquad \text{and} \qquad \int_Q \delta p(x)dx = 0.$$

$\Rightarrow$ Sampling probability should reproduce peculiarities of $|f(x)|$. Solution: $p(x) = c \cdot f(x)$.

Statistical Mechanics

Consider an average of observable $\hat{A}$ in the canonical ensemble (fixed (N, V, T)). The probability that a system can be found in an energy eigenstate E_i is given by a Boltzmann factor (in thermal equilibrium)

$$\bar{A} = \langle A \rangle (N, V, \beta) = \frac{\sum_i e^{-E_i/k_B T} \langle i|\hat{A}|i\rangle}{\sum_i e^{-E_i/k_B T}} \tag{1}$$

where $\langle i|\hat{A}|i\rangle$ – expectation value in N-particle quantum state $|i\rangle$.

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Direct way to proceed:

- Solve the Schrödinger equation for a many-body systems.
- Calculate for all states with non-negligible statistical weight $e^{-E_i/k_B T}$ the matrix elements $\langle i|\hat{A}|i\rangle$.

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We need another approach! Equation (1) can be simplified in classical limit.

Problem statement

- Obtain exact thermodynamic equilibrium configuration

$$\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

of interacting particles at given temperature T, particle number, N, external fields etc.

- Evaluate measurable quantities, such as total energy E, potential energy V, pressure P, pair distribution function $g(r)$, etc.

$$\langle A \rangle (N, \beta) = \frac{1}{Z} \int d\mathbf{R}\, A(\mathbf{R})\, e^{-\beta V(\mathbf{R})}, \qquad \beta = 1/k_B T.$$

Monte Carlo approach

- Approximate a continuous integral by a sum over set of configurations $\{ x_i \}$ sampled with the probability distribution $p(x)$.

$$\int f(x) \cdot p(x)\, dx = \lim_{M \to \infty} \frac{1}{M} \sum_{i=1}^{M} f(x_i)_p = \lim_{M \to \infty} \langle f(x) \rangle_p$$

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- We need to sample with the given Boltzmann probability, $p_B(\mathbf{R}_i) = e^{-\beta V(\mathbf{R}_i)} / Z$,

$$\langle A \rangle = \lim_{M \to \infty} \frac{1}{M} \sum_{i} A(\mathbf{R}_i)\, p_B(\mathbf{R}_i) = \lim_{M \to \infty} \langle A(\mathbf{R}) \rangle_{p_B} .$$

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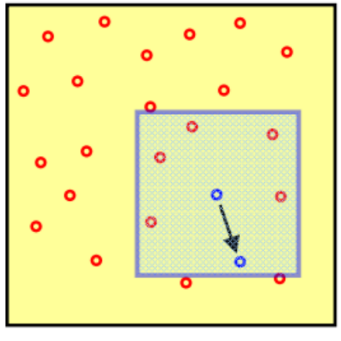
- Direct sampling with p_B is not possible due to the *unknown* normalization Z.
- Solution: Construct Markov chain using the Metropolis algorithm.
  - Use Metropolis Monte Carlo procedure (Markov process) to sample all possible configurations by moving individual particles.
  - Compute averages from fluctuating microstates. ▸ more

Metropolis sampling method (1953)



1. Start from initial (random) configuration R_0.
2. Randomly displace one (or more) of the particles.
3. Compute energy difference between two states: $\Delta E = V(R_{i+1}) - V(R_i)$.
4. Evaluate the transition probability which satisfies the detailed balance:

$$\upsilon(\mathbf{R}_i, \mathbf{R}_{i+1}) = \frac{p_B(\mathbf{R}_{i+1})}{p_B(\mathbf{R}_i)} = \min\left[1, e^{-\beta\Delta E}\right]$$

   - $\Delta E \leq 0$: always accept new configuration.
   - $\Delta E > 0$: accept with prob. $p = e^{-\beta\Delta E}$

5. Repeat steps (2)–(4) to obtain a final estimation: $\bar{A} = \langle A \rangle \pm \delta A$, with the error: $\delta A = \sqrt{\tau_A \sigma_A^2 / M}$.

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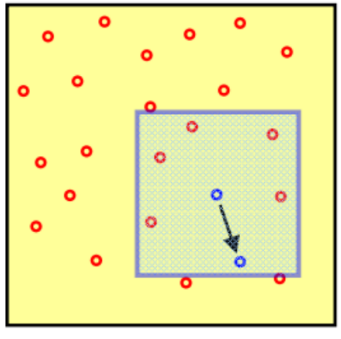

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- We reduce a number sampled configurations to $M \sim 10^6 \ldots 10^8$.
- We account only for configurations with non-vanishing weights: $e^{-\beta V(\mathbf{R}_i)}$.

Simulations of 2D Ising model

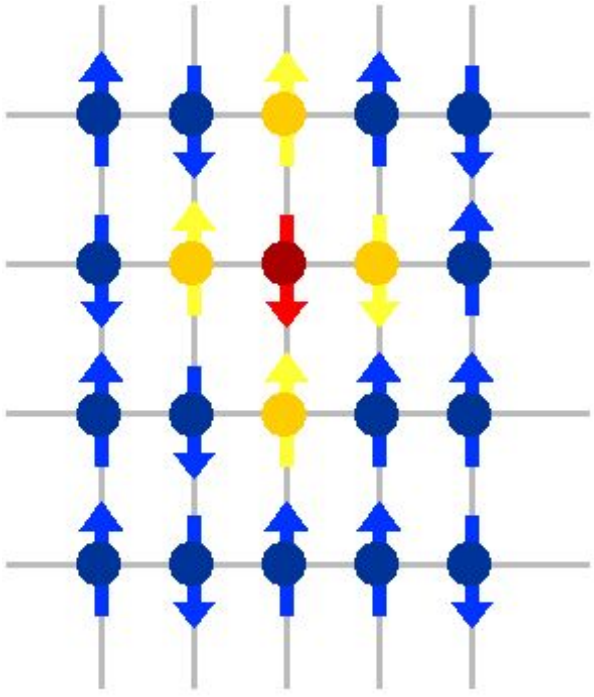


Figure: Lattice spin model with nearest neighbor interaction. The red site interacts only with the 4 adjacent yellow sites.

- We use the Ising model to demonstrate the studies of phase transitions.
- The Ising model considers the interaction of elementary objects called *spins* which are located at sites in a simple, 2-dimensional lattice,

$$\hat{H} = -J \sum_{i,j=nn(i)}^{N} \hat{S}_i \hat{S}_j - \mu_0 B \sum_{i=1}^{N} \hat{S}_i.$$

- Magnetic ordering:
  - $J > 0$: lowest energy state is *ferromagnetic*,
  - $J < 0$: lowest energy state is *antiferromagnetic*.

Equibrium properties

Mean energy $$\langle E \rangle = \mathrm{Tr}\, \hat{H}\hat{\rho},$$

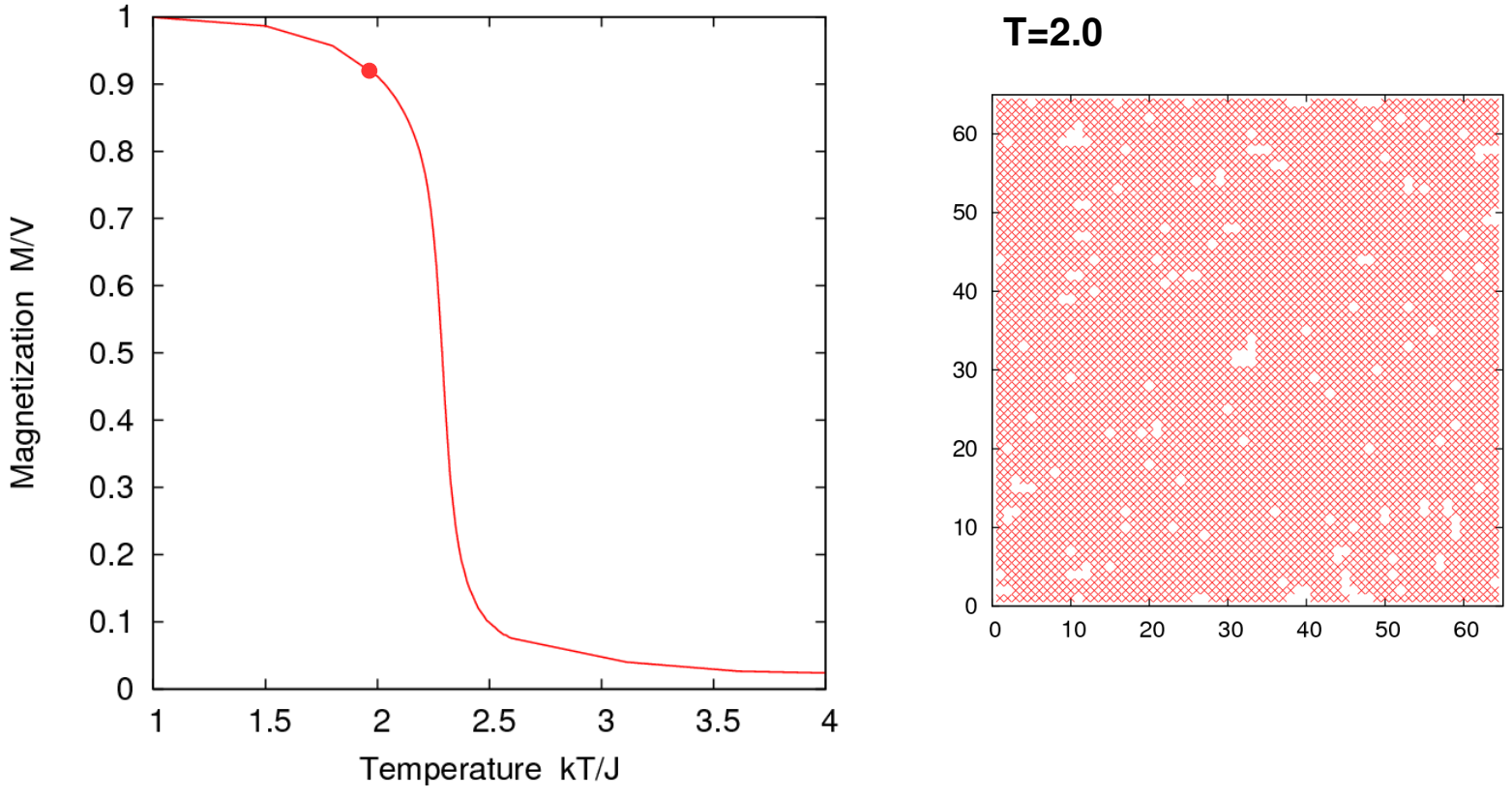
Heat capacity $$C = \frac{\partial \langle E \rangle}{\partial T} = \frac{1}{k_\mathrm{B} T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right),$$

Mean magnetization $$\langle M \rangle = \left\langle \left| \sum_{i=1}^{N} S_i \right| \right\rangle,$$

Linear magnetic susceptibility $$\chi = \frac{1}{k_\mathrm{B} T} \left(\langle M^2 \rangle - \langle M \rangle^2 \right),$$

where $\langle M \rangle$ and $\langle M^2 \rangle$ are evaluated at zero magnetic field ($B = 0$).

Magnetization in 2D Ising model ($J > 0$, $L^2 = 64^2$)



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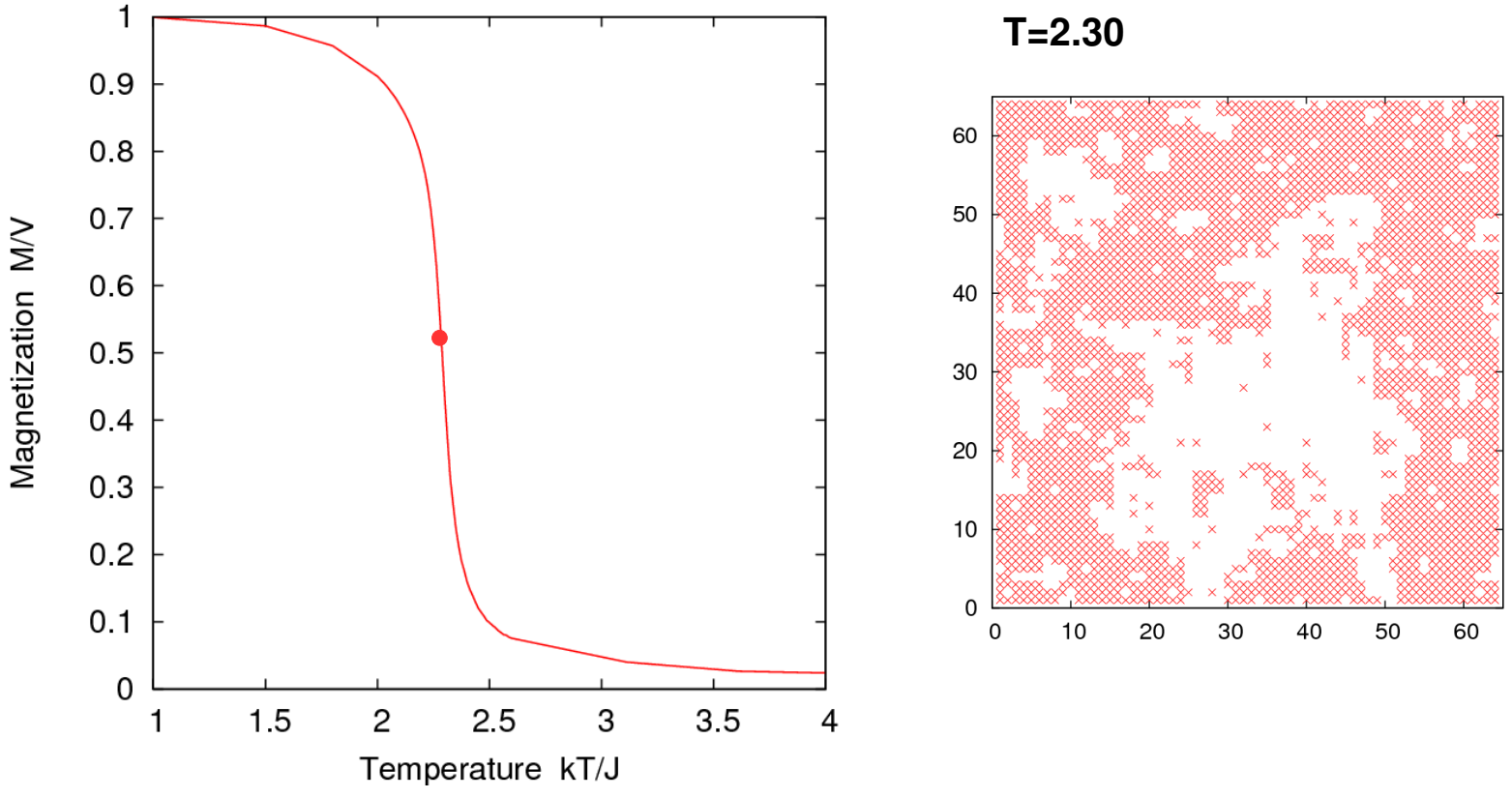

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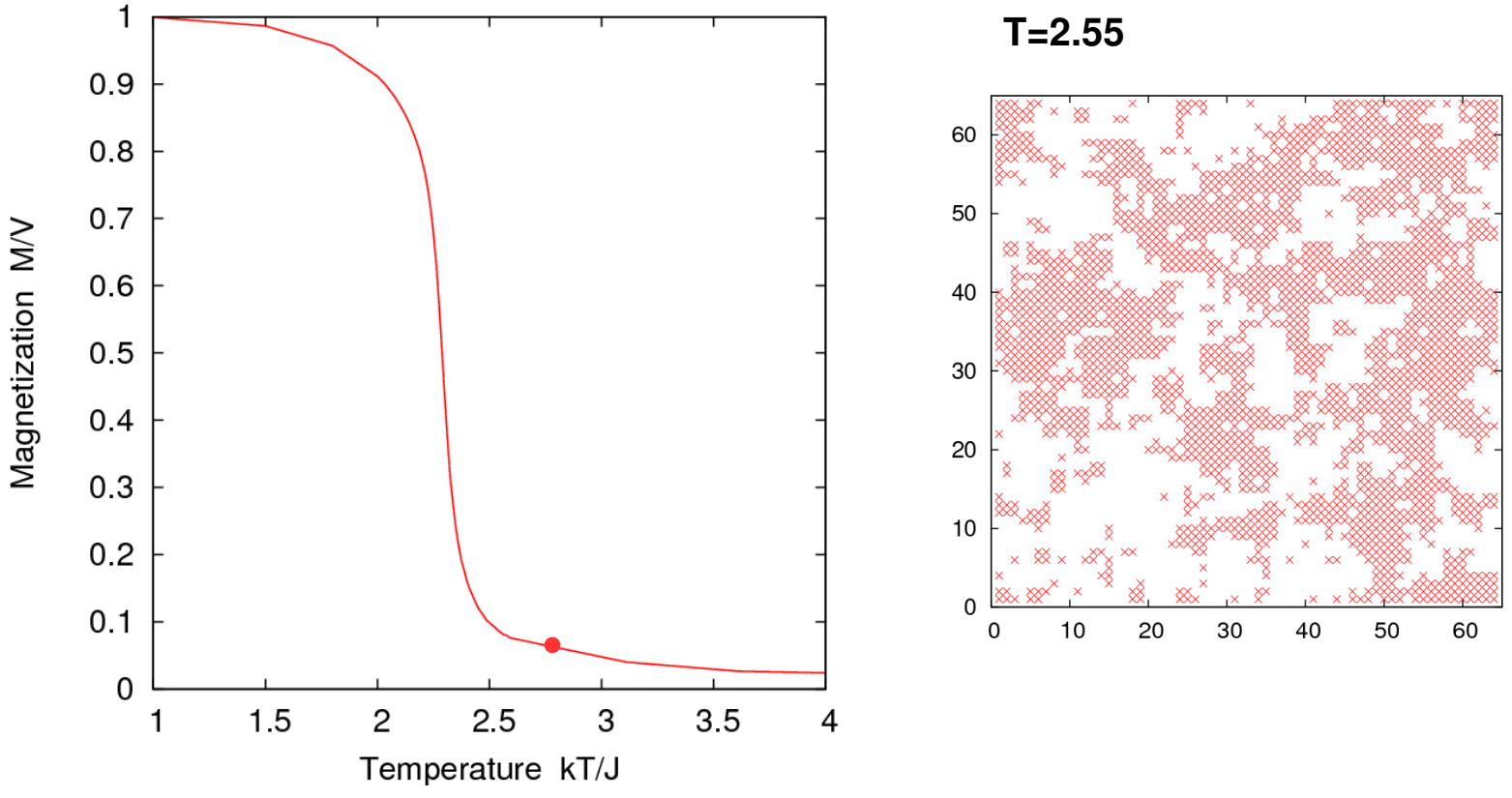

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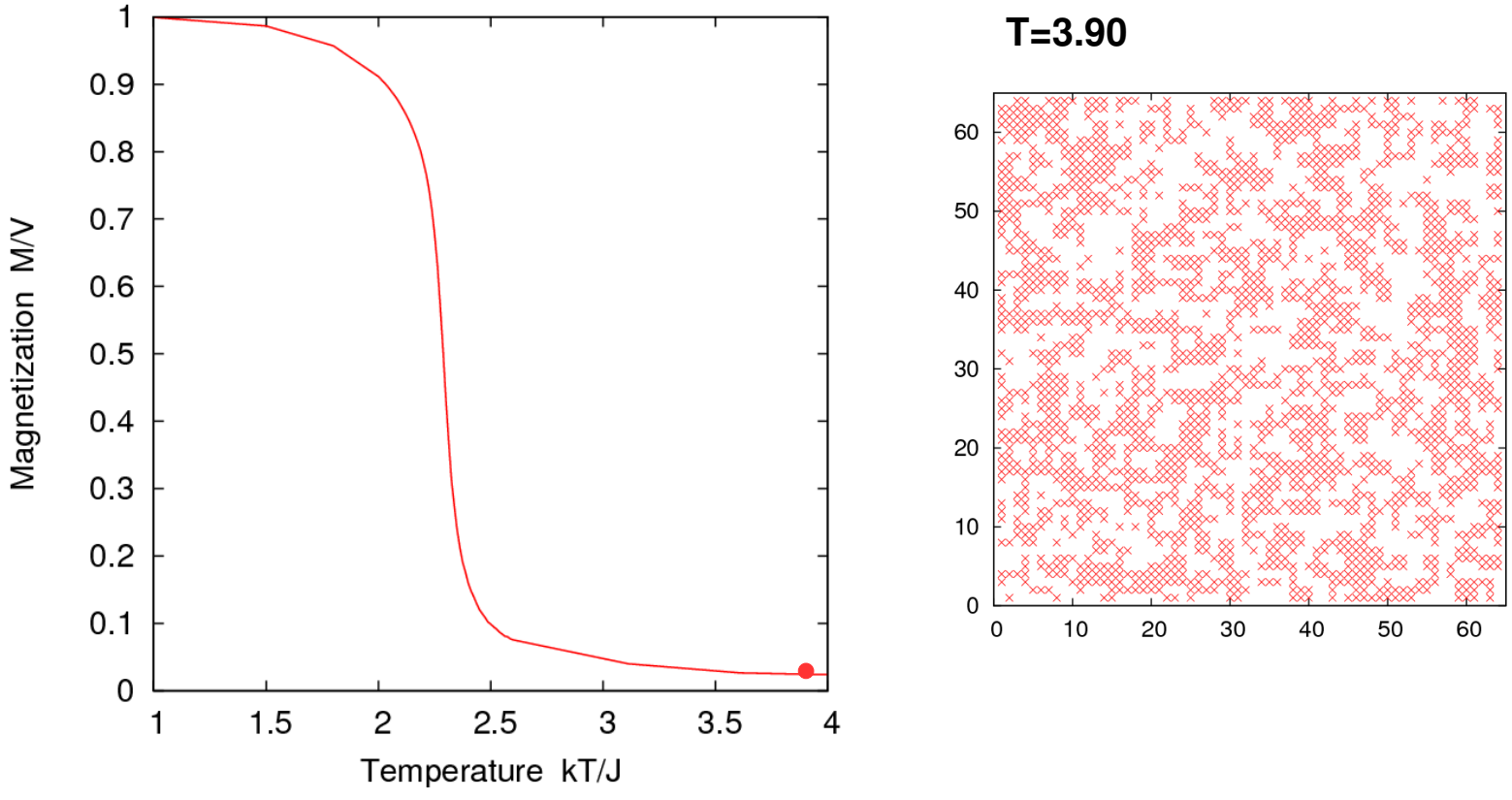


Straightforward implementation

In each step we propose to flip a single spin, $S_i \to -S_i$, and use the original Metropolis algorithm to accept or reject.

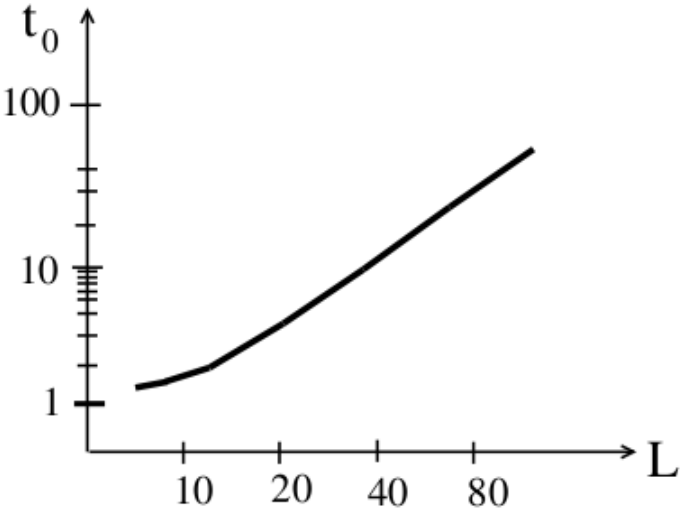
Phase-odering kinetics if we start from completely disordered state.

- $T > T_c$ Equilibration will be fast.
- $T < T_c$ Initial configuration is far from typical equilibrium state. Parallel spins form domains of clusters. To minimize their surface energy, the domains grow and straighten their surface.

For $T < T_c$ it is improbable to switch from one magnetization to the other, since acceptance probability to flip a single spin in a domain is low $e^{-4J\Delta\sigma}$, $\Delta\sigma = \pm 2$.

We need to work out more efficient algorithm.

Simulations in critical region



Autocorrelation function near critical temperature T_c:

$$A(i) \to A_0 \exp\left(-i/t_0\right)|_{i\to\infty}$$

"Critical slowing down"

$$t_0 \approx \tau_{O,\text{int}} \sim L^z$$

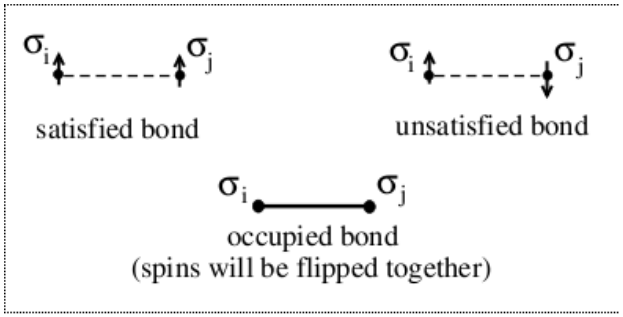
z – dynamical critical exponent of the algorithm. more

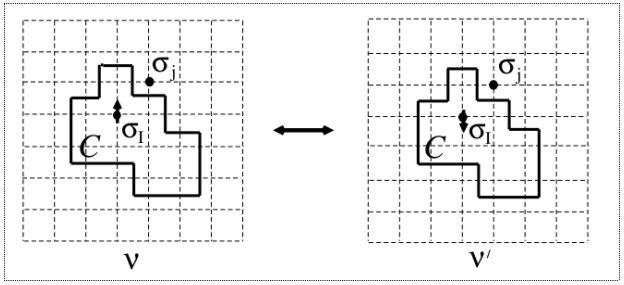
For the original *single spin-flip* alrogithm $z \approx 2$ in 2D.

$$L = 10^3 \Rightarrow \tau_{O,\text{int}} \sim 10^5 \ldots 10^6$$

Classical cluster algorithms

Original idea by Swendsen and Wang and later slightly modified by Niedermayer and Wolf. more



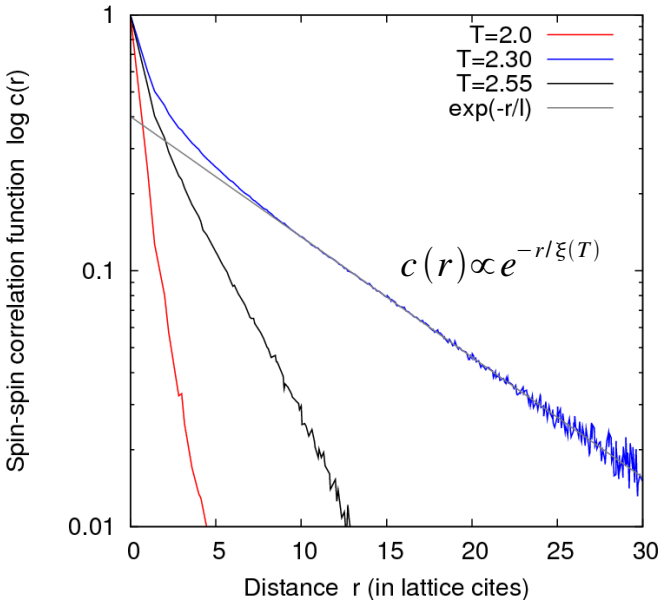


1. Look at all n.n. of spin σ_l and if they point in the same direction include them in the cluster C with the probability P_{add}.
2. For each new spin added to C repeat the same procedure.
3. Continue until the list of n.n is empty.
4. Flip all spins in C *simultaneously* with probability A.

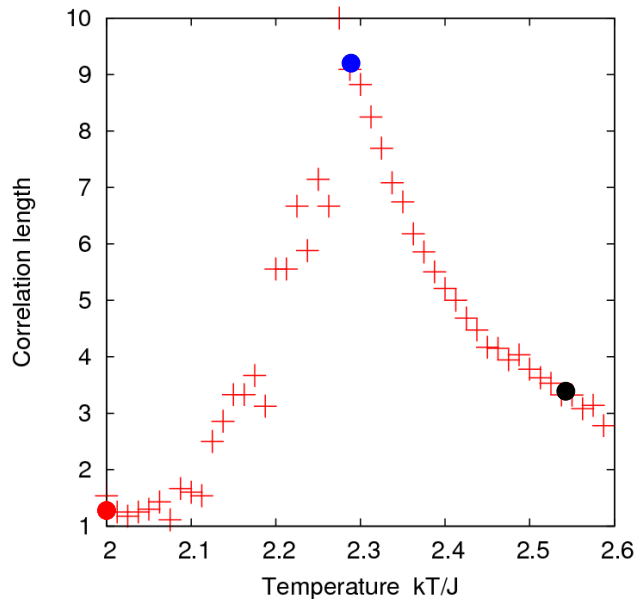
Spin-spin correlation.

Spin-spin correlation function.
Correlation length

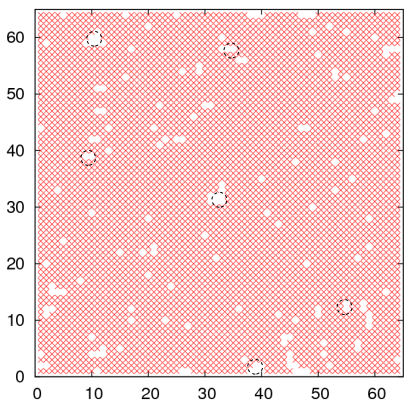
$$c(r)=(\langle s_i \cdot s_{i+r}\rangle-\langle s_i\rangle\langle s_{i+r}\rangle)/\langle s_i^2\rangle$$



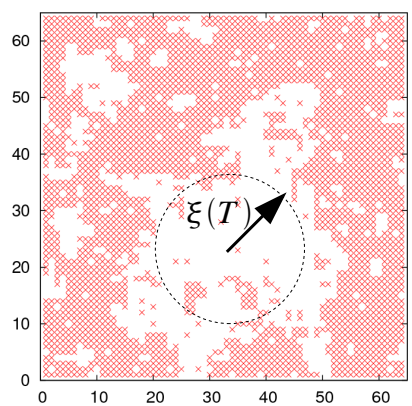
$$\xi(T,L)\propto|T-T_c|^{-1}\leq L/2$$



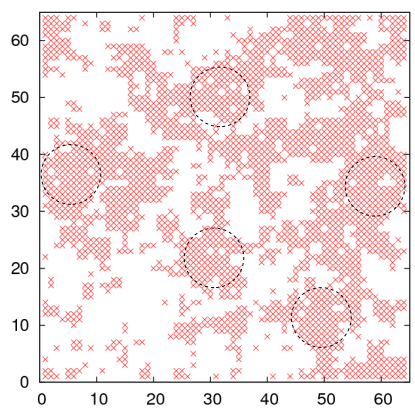
T=2.0



T=2.30

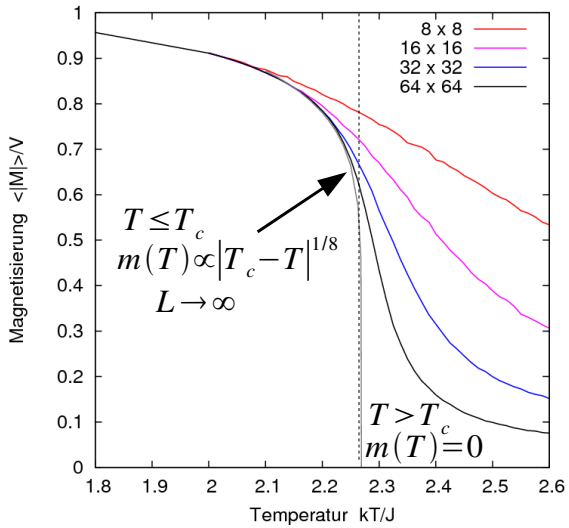


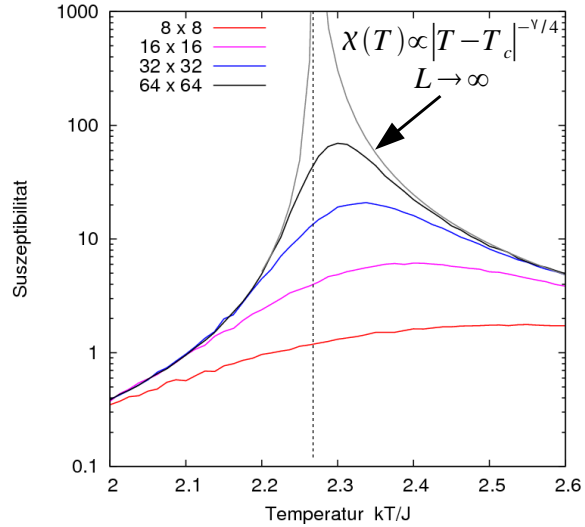
T=2.55

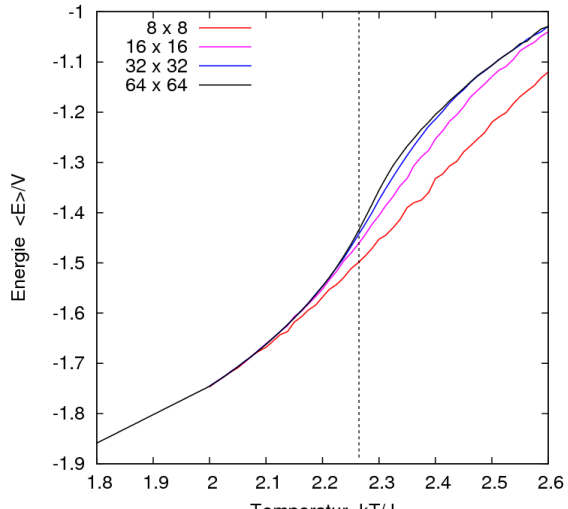


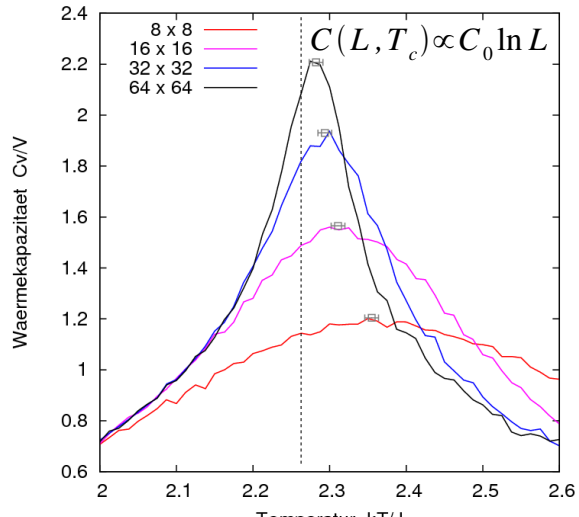
L dependence: Magnet., suscep., energy, spec. heat

System size L-dependence:
magnetization - susceptibility
energy - specific heat



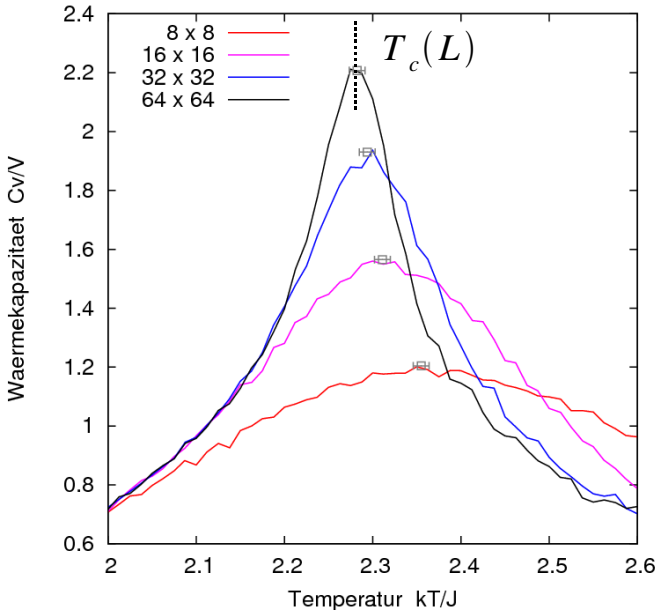




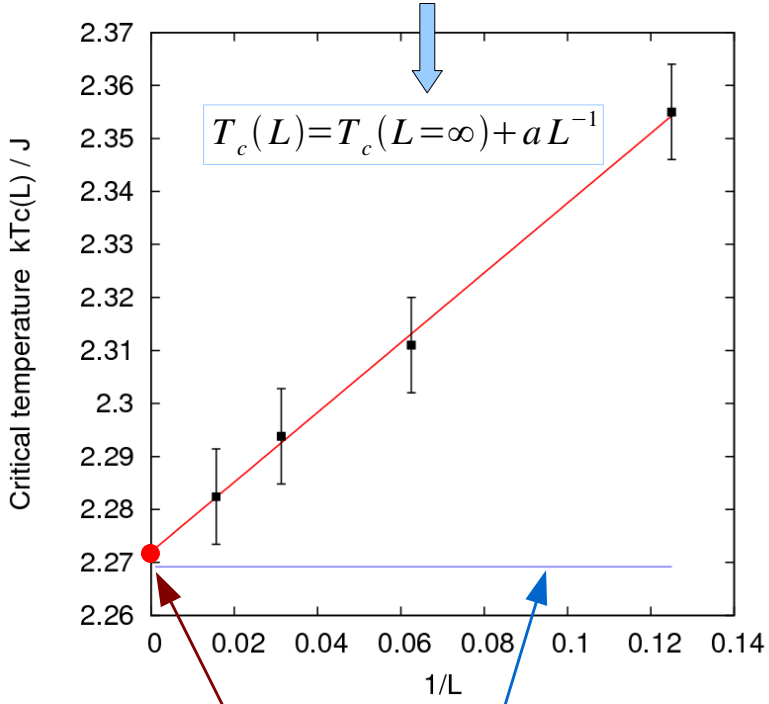


Finite size scaling and critical properties.

Finite size scaling and critical properties



$$\xi(T, L) \propto |T - T_c|^{-1} \leq L/2$$



Numerical estimation for critical temperature: $kT_c^{est}(L=\infty)/J = 2.2719 \pm 0.008$

Exact value: $kT_c(L=\infty)/J = 2/\ln(1+\sqrt{2}) \approx 2.26918$

When/Why should one use classical Monte Carlo?

Advantages

1. Easy to implement.
2. Easy to run a fast code.
3. Easy to access equilibrium properties.

Disadvantages

1. Non-equilibrium properties are not accessible ($\rightarrow$ Dynamic Monte Carlo).
2. No real-time dynamics information ($\rightarrow$ Kinetic Monte Carlo).

Requirements

1. Good pseudo-random-number generator, e.g. Mersenne Twister (period $2^{19937} - 1$).
2. Efficient *ergodic* sampling.
3. Accurate estimations of autocorrelation times, statistical error, etc.

Fin

Thanks for your attention!

Next lecture: Monte Carlo algorithms for quantum systems

Markov chain (Markov process)

back

The *Markov chain* is the probabilistic analogue of a trajectory generated by the equations of motion in the classical molecular dynamics.

- We specify *transition probabilities* $\upsilon(\mathbf{R}_i, \mathbf{R}_{i+1})$ from one state $\mathbf{R}_i$ to a new state $\mathbf{R}_{i+1}$ (different degrees of freedom in the system).
- We put restrictions on $\upsilon(\mathbf{R}_i, \mathbf{R}_{i+1})$:
  1. *The conservation law* (the total probability that the system will reach some state $\mathbf{R}_i$ is unity): $\sum_{\mathbf{R}_{i+1}} \upsilon(\mathbf{R}_i, \mathbf{R}_{i+1}) = 1$, for all $\mathbf{R}_i$.
  2. The distribution of $\mathbf{R}_i$ converges to the *unique equilibrium state*: $\sum_{\mathbf{R}_i} p(\mathbf{R}_i)\upsilon(\mathbf{R}_i, \mathbf{R}_{i+1}) = p(\mathbf{R}_{i+1})$.
  3. *Ergodicity:* The transition is ergodic, i.e. one can move from any state to any other state in a finite number of steps with a nonzero probability.
  4. All transition probabilities are *non-negative:* $\upsilon(\mathbf{R}_i, \mathbf{R}_{i+1}) \geq 0$, for all $\mathbf{R}_i$.
- In thermodynamic equilibrium, $dp(\mathbf{R})/dt = 0$, we impose an additional condition – the *detailed balance*

$$p(\mathbf{R}_i)\upsilon(\mathbf{R}_i, \mathbf{R}_{i+1}) = p(\mathbf{R}_{i+1})\upsilon(\mathbf{R}_{i+1}, \mathbf{R}_i),$$

Ergodicity

- In simulations of classical systems we need to consider only *configuration integral*

$$Q_{NVT}^{\text{class}} = \text{Tr}\left[e^{-\beta\hat{H}}\right] = \frac{1}{N!}\left(\frac{2\pi m k_B T}{h^2}\right)^{3N/2}\int d\mathbf{r}^N\, e^{-\beta V(\mathbf{r}^N)}$$

- The average over all possible microstates $\{\mathbf{r}^N\}$ of a system is called *ensemble average*.
- This can differ from real experiment: we perform a series of measurements during a certain time interval and then determine average of these measurements.
  Example: Average particle density at spatial point $\mathbf{r}$

$$\bar{\rho}(\mathbf{r}) = lim_{t\to\infty}\frac{1}{t}\int_0^t dt'\,\rho(\mathbf{r}, t'; \mathbf{r}^N(0), \mathbf{p}^N(0))$$

Ergodicity

- System is *ergodic*: the time average does not depend on the initial conditions.
  $\rightarrow$ We can perform additional average over many different initial conditions $(\mathbf{r}^N(0), \mathbf{p}^N(0))$

$$\bar{\rho}(\mathbf{r}) = \frac{1}{N_0} \sum_{N_0} lim_{t\to\infty} \frac{1}{t} \int_0^t dt' \, \rho(\mathbf{r}, t'; \mathbf{r}^N(0), \mathbf{p}^N(0))$$

N_0 is a number of initial conditions: same NVT, different $\mathbf{r}^N(0), \mathbf{p}^N(0)$.

$$\bar{\rho}(\mathbf{r}) = \langle \rho(\mathbf{r}) \rangle_{NVE} \quad \text{time average} = \text{ensemble average}$$

Nonergodic systems: glasses, metastable states, etc.

Autocorrelations

back

Algorithm efficiency can be characterized by the integrated autocorrelation time τ_{int} and autocorrelation function $A(i)$:

$$\tau_{O,int} = 1/2 + \sum_{i=1}^{K} A(i)\,(1 - i/K), \quad A(i) = \frac{1}{\sigma_O^2}\langle O_1 O_{1+i}\rangle - \langle O_1\rangle\langle O_{1+i}\rangle.$$

Temporal correlations of measurements enhance the statistical error:

$$\epsilon_{\bar{O}} = \sqrt{\sigma^2_{\bar{O}}} = \sqrt{\frac{\langle O_i^2\rangle - \langle O_i\rangle^2}{K}}\sqrt{2\tau_{O,int}} = \sqrt{\frac{\sigma^2_{O_i}}{K_{eff}}}, \quad K_{eff} = K/2\tau_{O,int}.$$

Detailed balance for cluster algorithms

back

Detailed balance equation

$$(1 - P_{\text{add}})^{K_\nu} \, P_{\text{acc}}(\nu \to \nu') e^{-\beta E_\nu} = (1 - P_{add})^{K_{\nu'}} \, P_{acc}(\nu' \to \nu) e^{-\beta E_{\nu'}}$$

Probability to flip all spins in C:

$$A = \frac{P_{\text{acc}}(\nu \to \nu')}{P_{\text{acc}}(\nu' \to \nu)} = (1 - P_{\text{add}})^{K_{\nu'} - K_\nu} \, e^{2J\beta (K_{\nu'} - K_\nu)}$$

If we choose $P_{\text{add}} = 1 - e^{-2J\beta} \Rightarrow A = 1$, i.e every update is accepted.

- $T \gg T_c$: $P_{\text{add}} \to 0$, only few spins in C (efficiency is similar to the *single spin-flip*)
- $T \leq T_c$: $P_{\text{add}} \to 1$, we flip large spin domains per one step.

Wolf algorithm reduces the dynamical critical exponent to $z \leq 0.25$. Enormous efficiency gain over the *single spin-flip*!