Importance sampling Monte Carlo

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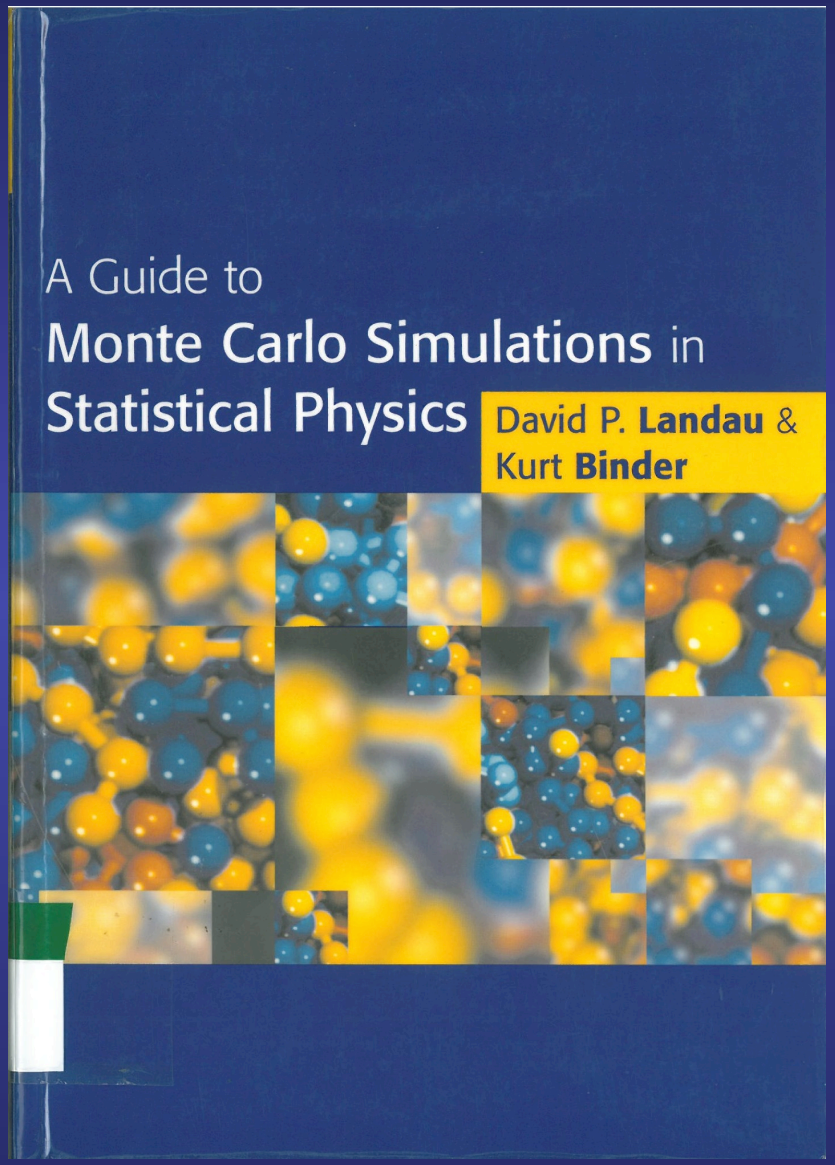
Bibliography



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The simple Ising model

Spins which are confined to the sites of a lattice and which might have only the values +1 or -1

The spins interact with the nearest neighbours on the lattice with interaction constant $\mathcal{J}$

$$\hat{\mathcal{H}} = -\mathcal{J}\sum_{i,j}\vec{S}_i\cdot\vec{S}_j - H\sum_i \vec{S}_i$$

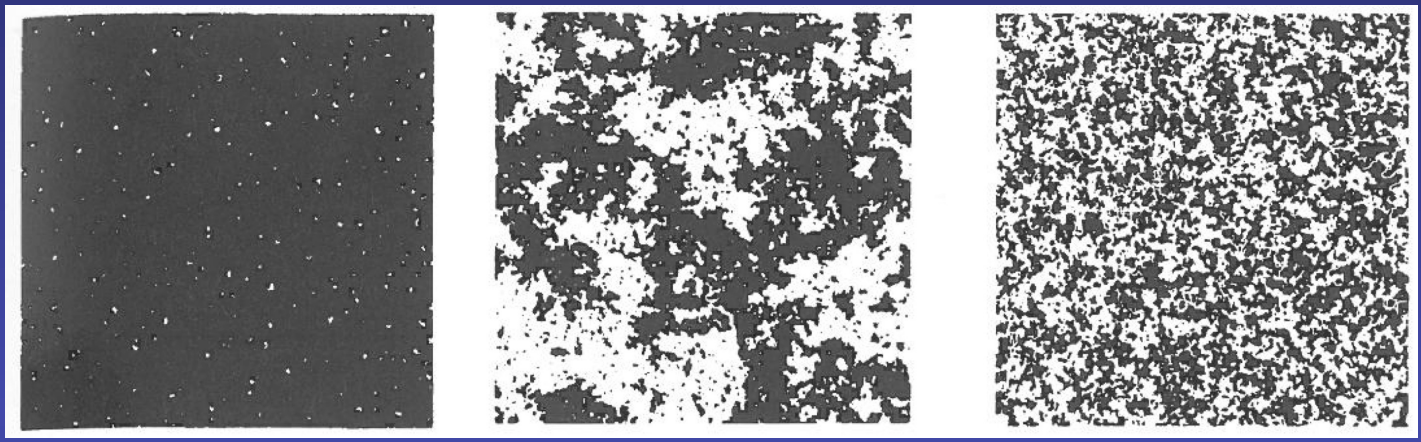
Spin-spin interaction

Interaction with an external magnetic field

This model has been solved exactly in one-dimension:
No phase transition

Onsager solved exactly in two-dimension with periodic boundary conditions and no-field
Second-order phase transitions
Divergence in the specific heat, susceptibility and correlation length

Configurations of the 2D Ising model at zero-field

$T << T_c$	$T \sim T_c$	$T >> T_c$
		
Almost at the ground state	**Close to the phase transition**	**High-temperature (no correlation between spins).**
Single large cluster of ordered spins and small clusters of oppositely oriented spins	**Broad distribution of clusters**	**All clusters of like spins are small**

Sampling algorithm

In the classic Metropolis method configurations are generated from a previous state using a transition probability which depends on the energy difference between the initial and final states

$$\frac{\partial P_n(t)}{\partial t} = -\sum_{n \neq m} [P_n(t) W_{n \to m} - P_m(t) W_{m \to n}]$$

$P_n(t)$ **probability of the system being in state** n **at time** t

$W_{n \to m}$ **is the transition rate from** n **to** m

In equilibrium $\frac{\partial P_n(t)}{\partial t} = 0 \Longrightarrow$ **The two terms of the right hand side must be equal ("detailed balance")**

$$P_n(t) W_{n \to m} = P_m(t) W_{m \to n}$$

Sampling algorithm

In the classic Metropolis method configurations are generated from a previous state using a transition probability which depends on the energy difference between the initial and final states

In equilibrium $$P_n(t)W_{n\to m} = P_m(t)W_{m\to n}$$

The probability of the n-th state occurring in a classical system is given by

$$P_n(t) = \frac{e^{-E_n/k_{\mathrm{B}}T}}{Z}$$

where Z is the partition function

This probability is usually not exactly known due to the denominator

Sampling algorithm

If we generate the n -th state from the m-th state in a Markov chain, the relative probability is the ratio of the individual probabilities, because the denominator cancels

Only the energy difference between the two states is needed

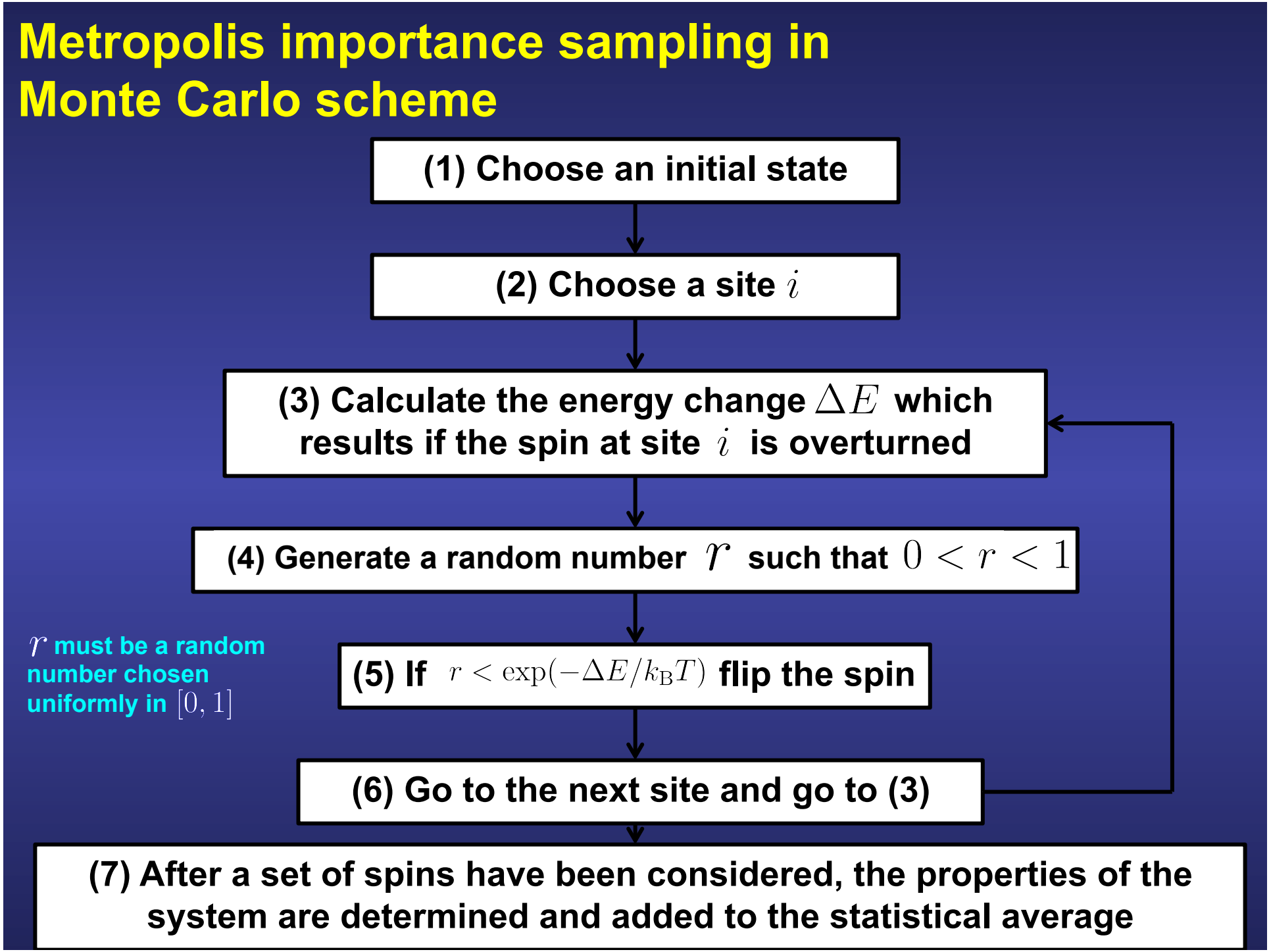
$$\Delta E = E_n - E_m$$

Any transition rate that satisfied detailed balance is acceptable

$$W_{n\to m} = \frac{1}{\tau_0}\exp^{-\Delta E/k_{\mathrm{B}}T} \quad \Delta E > 0$$
$$= \frac{1}{\tau_0} \quad \Delta E < 0$$

where τ_0 is the time required to attempt a spin-flip.
Often, this time unit is set equal to unity and suppressed from the equations

Metropolis importance sampling in Monte Carlo scheme



Metropolis importance sampling in Monte Carlo scheme

The standard measure of Monte Carlo time is the Monte Carlo step/size (MCS/site)
It corresponds to the consideration of every spin in the system once

Once the number of states is sufficiently large that the initial transients are negligeable, then the desired averages are computed

$$\langle A \rangle = \sum_n P_n A_n = \sum_n \frac{e^{-E_n/k_{\mathrm{B}}T}}{Z} A_n$$

Note that if an attempted flip is rejected, the old state is counted again for averaging

Some precautions to be taken

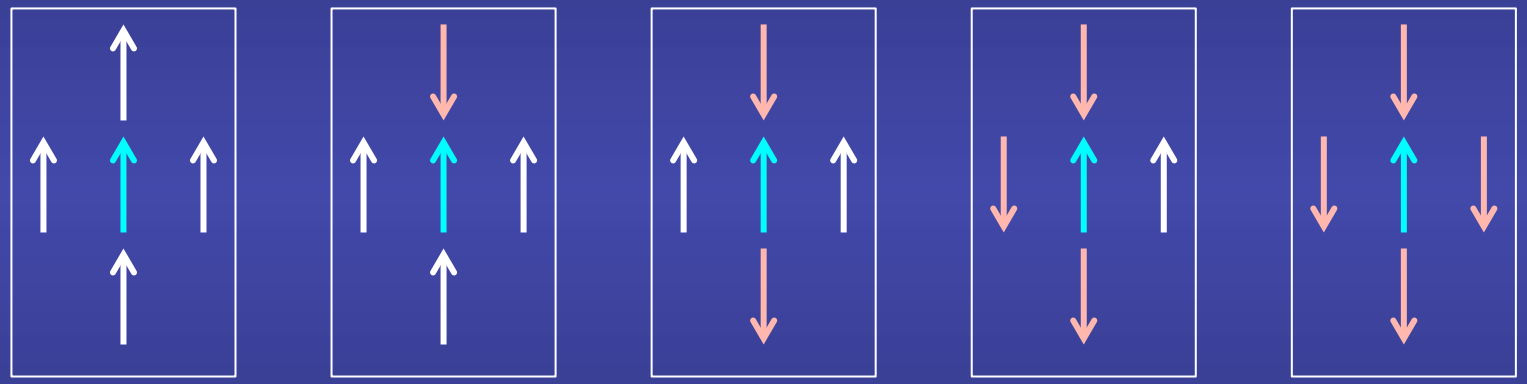
Repeat a given run with different initial states to see if the same equilibrium distribution is reached

Repeat runs with different random numbers

Simplifications of the Ising model

For each spin there are only a small number of different environments which are possible

For a square lattice with nearest neighbour interactions, each spin might have



nearest neighbour parallel to it

There are only 5 different energy changes associated with a succesful spin flip
They can be computed for each possibility and stored in a table.
Since the exponential then need not be computed for each spin-flip trial, a tremendous saving in cpu time results