

Imagine **ensemble** of huge number of states in equilibrium

Number of states A is $N_0(A)$, proportional to $P(A)$

We now make some random change in each state (e.g., flip spins)

Possible transitions: $A \rightarrow B, C, \dots$

Number of states A after the “update”

$$N_1(A) = N_0(A) + \sum_{B \neq A} N_0(B)P(B \rightarrow A) - N_0(A)P(A \rightarrow B)$$

This is the **master equation** for the stochastic process

If we want the distribution to remain $P(A)$ after the update

$$\sum_{B \neq A} N_0(B)P(B \rightarrow A) - N_0(A)P(A \rightarrow B) = 0$$

$$\sum_{B \neq A} P(B)P(B \rightarrow A) - P(A)P(A \rightarrow B) = 0$$

Many possible solutions; an obvious solution, called the **detailed-balance** solution (condition): For every A, B

$$P(B)P(B \rightarrow A) = P(A)P(A \rightarrow B)$$

Time evolution of a single configuration; **Markov process**

Time average of a Markov process same as ensemble average

If we make random updates on a single configuration, and satisfy detailed balance, $P(B)P(B \rightarrow A) = P(A)P(A \rightarrow B)$, and if the updates are such that any configuration can be reached in a series of updates (ergodicity).

Then, the time distribution of configurations A will approach the distribution P(A) independently of the initial configuration

Alternative form of the detailed-balance condition

With $P(A) = \exp[-E(A)/T]/Z = W(A)/Z$

$$\frac{P(B \rightarrow A)}{P(A \rightarrow B)} = \frac{W(A)}{W(B)}$$

We have to construct transition probabilities satisfying this

The transition probability can typically be written as

$$P(A \rightarrow B) = P_{\text{attempt}}^A(B) P_{\text{accept}}^A(B)$$

where the two factors have the following meaning:

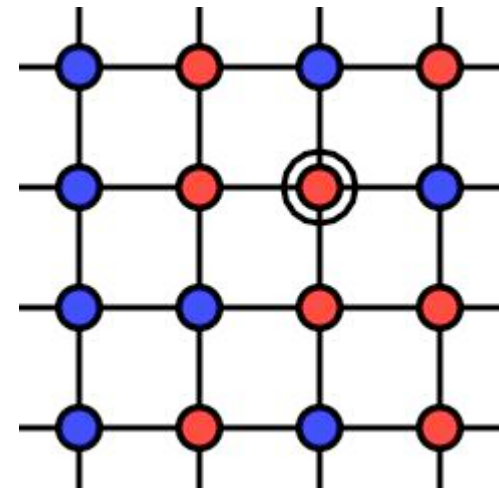
$P_{\text{attempt}}^A(B)$ - The probability of selecting B as a candidate among a number of possible new configurations

$P_{\text{accept}}^A(B)$ - The probability of actually making the transition to B after the selection of B has been done

If B has been selected but is not accepted (rejected); stay with A

For an Ising model

- Select a spin at random as a candidate to be flipped (attempt)
- Actually flip the spin with a probability to be determined (accept)
- Stay in the old configuration if the flip is not done (reject)



$P_{\text{attempt}}^A(B) = 1/N_{\text{spin}}$ uniform, independent of A, B

$P_{\text{accept}}^A(B)$ constructed to satisfy detailed balance condition

$$\frac{P_{\text{accept}}^A(B)}{P_{\text{accept}}^B(A)} = \frac{W(B)}{W(A)}$$

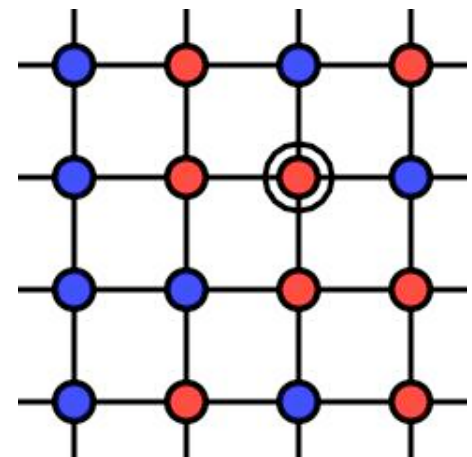
Two commonly used acceptance probabilities

Metropolis: $P_{\text{accept}}^A(B) = \min \left[\frac{W(B)}{W(A)}, 1 \right]$

Heat bath: $P_{\text{accept}}^A(B) = \frac{W(B)}{W(A) + W(B)}$

Easy to see that these satisfy detailed balance

The ratios involve the change in energy when a spin has been flipped (or, more generally, when the state has been updated in some way)



Metropolis algorithm for the Ising model

Spin update

- Select a spin at random
- Calculate the change in energy if the spin is flipped
- Use the energy change to calculate the acceptance probability P
- Flip the spin with probability P ; stay in old state with $1-P$
- Repeat from spin selection

Current configuration: S

Configuration after flipping spin j : \tilde{S}_j

Acceptance probability: $P(S \rightarrow \tilde{S}_j) = \min \left[\frac{W(\tilde{S}_j)}{W(S)}, 1 \right]$

$$W(S) = e^{-E(S)/T} = e^{-\frac{J}{T} \sum \sigma_i \sigma_j} = \prod e^{-\frac{J}{T} \sigma_i \sigma_j}$$

Only terms (factors) containing spin j survive in W-ratio

$$\frac{W(\tilde{S}_j)}{W(S)} = \exp \left[-\frac{2J}{T} \sigma_j \sum_{\delta(j)} \sigma_{\delta(j)} \right], \quad \delta(j) = \text{neighbor of } j$$

We want a **simulation “time” unit** which is normalized by the system size N (probability of a given spin having been selected after a time unit should be N independent).

1 Monte Carlo step (MC steps): N random spin-flip attempts

Measurements of physical observables done after **equilibration**

➤ the correct Boltzmann distribution is approached after some time that depends on the initial configuration

Binning: Accumulate data over bins consisting of M MC steps

➤ Averages and statistical errors calculated from bin averages

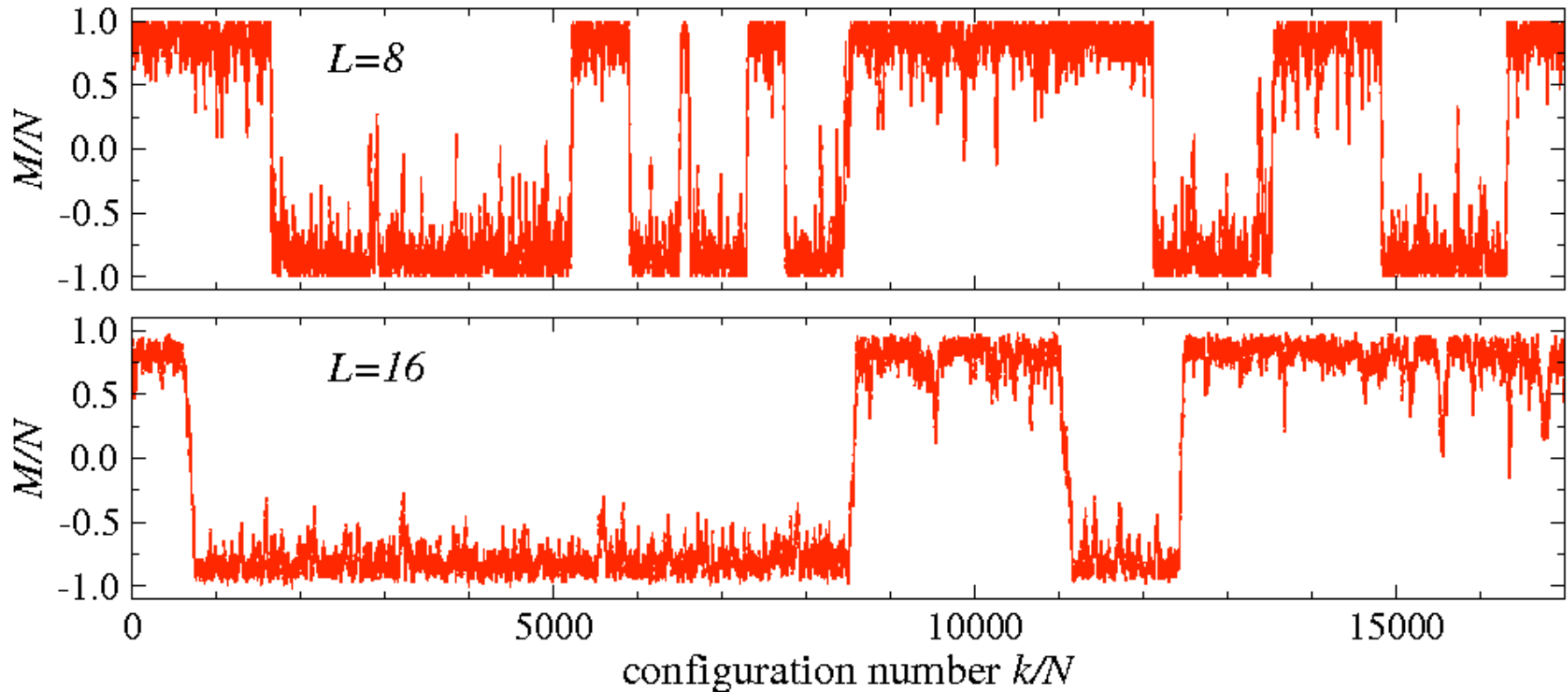
Flow of a complete simulation

- Generate arbitrary starting state
- Carry out a number of MC steps for equilibration
- Carry out a number of bins
 - each bin consists of M MC steps
 - measurements done after every (or every few) MC step
 - save bin averages in a file after each bin (or save internally in program)
- Calculate averages and statistical errors

Illustration of simulation

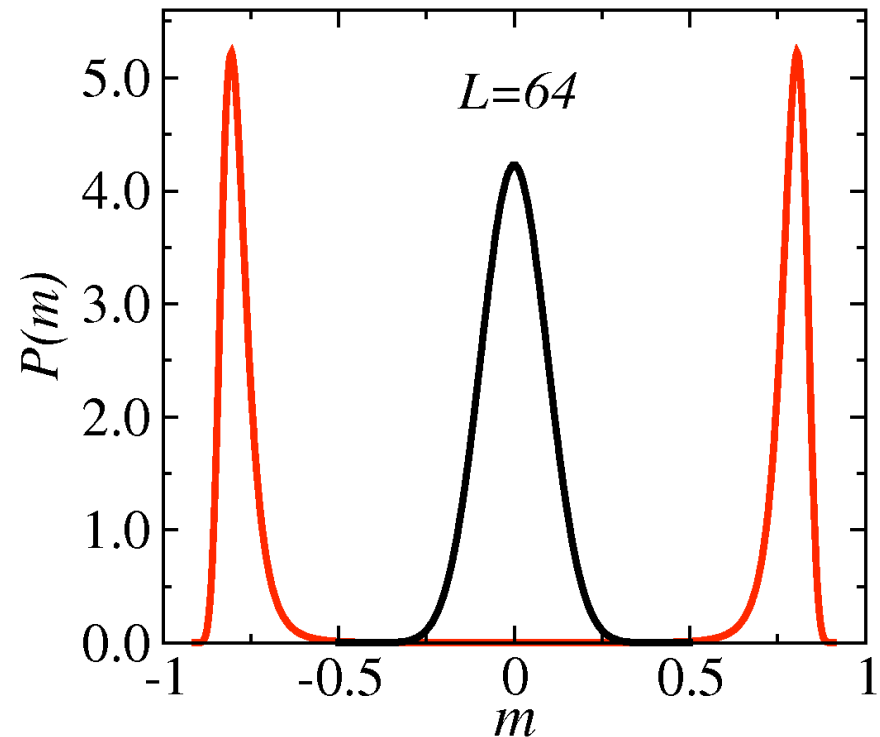
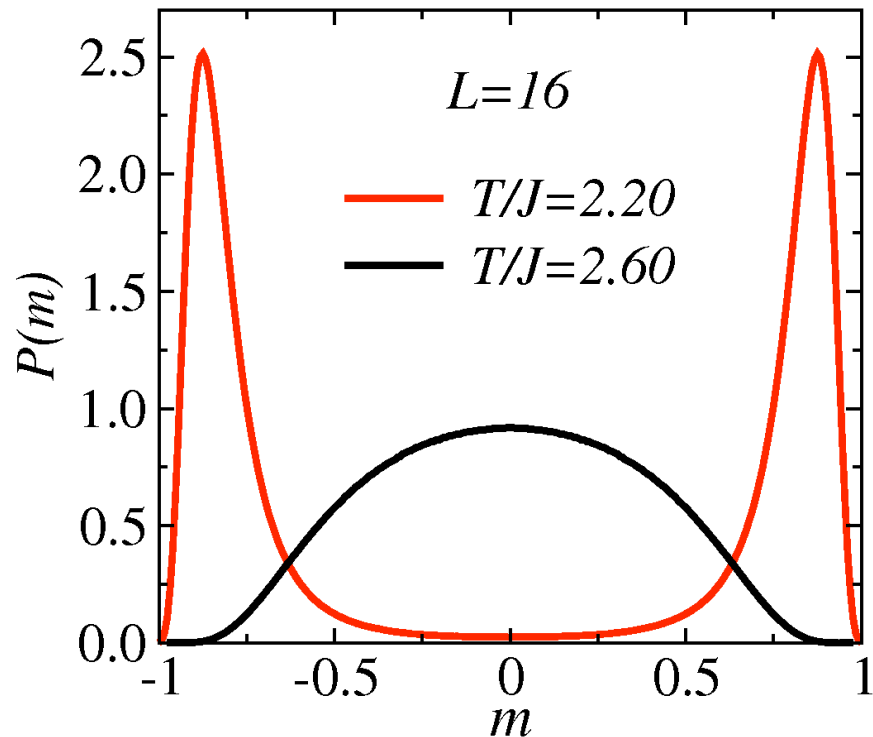
Evolution of the magnetization, 2D Ising model, $T/J=2.2$ (below T_c)

- $\langle M \rangle = 0$, but time scale for M-reversal increases with L
- Symmetry-breaking occurs in practice for large L



The magnetization distribution depends on T and L

- single peak around $m=0$ for $T > T_c$
- double peak around $+\langle m \rangle$ and $-\langle m \rangle$ for $T < T_c$



Symmetry breaking (sampling of only $m > 0$ or $m < 0$ states) occurs in practice for large L

- Because extremely small probability to go between them