Monte Caro simulations

Monte Carlo methods - based on random numbers

- Stanislav Ulam's terminology
  - his uncle frequented the Casino in Monte Carlo

Random (pseudo random) number generator on the computer

- Less glamorous than roulette tables or cards, but faster...
- $>10^9$ random numbers per second

Monte Carlo simulations in statistical physics

- normally refers to **importance sampling** of configurations (e.g., spins)
- generating configurations with probability equal to the Boltzmann probability
- MC simulations show clearly **how phase transitions can happen when $N \to \infty$**

Monte Carlo simulation of the Ising model

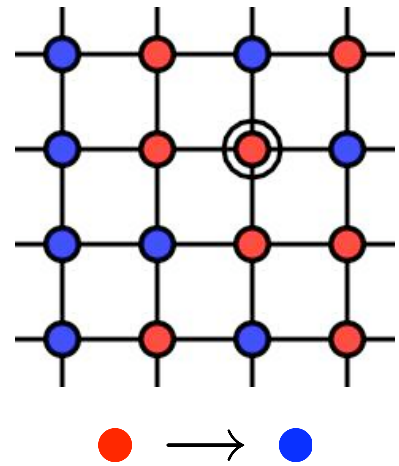
The Metropolis algorithm

[Metropolis, Rusenbluth, Rosenbluth, Teller, and Teller, Phys. Rev. 1953]

Generate a series of configurations (Markov chain); $C_1 \to C_2 \to C_3 \to C_4 \to \ldots$

- C_{n+1} obtained by modifying (updating) C_n
- changes satisfy the **detailed-balance principle**

$$\frac{P_{\rm change}(A \to B)}{P_{\rm change}(B \to A)} = \frac{W(B)}{W(A)} \qquad W(A) = \mathrm{e}^{-E(A)/T}$$



Starting from any configuration, such a stochastic process leads to configurations distributed according to W

- the process has to be **ergodic**
  - any configuration reachable in principle
- it takes some time to reach equilibrium

Metropolis algorithm for the Ising model. For each update perform:

- select a spin i at random; consider flipping it $\sigma_i \to -\sigma_i$
- compute the ratio $R=W(\sigma_1,\ldots-\sigma_i,\ldots,\sigma_N)/W(\sigma_1,\ldots\sigma_i,\ldots,\sigma_N)$
  - for this we need only the spins neighboring i
- generate **random number $0<r\leq 1$; accept flip if $r<R$** (go back to old config else)

$$P_{\rm change}(A \to B) = P_{\rm select}(B|A)P_{\rm accept}(B|A)$$

$$P_{\rm select} = 1/N, \quad P_{\rm accept} = \min[W(B)/W(A), 1]$$

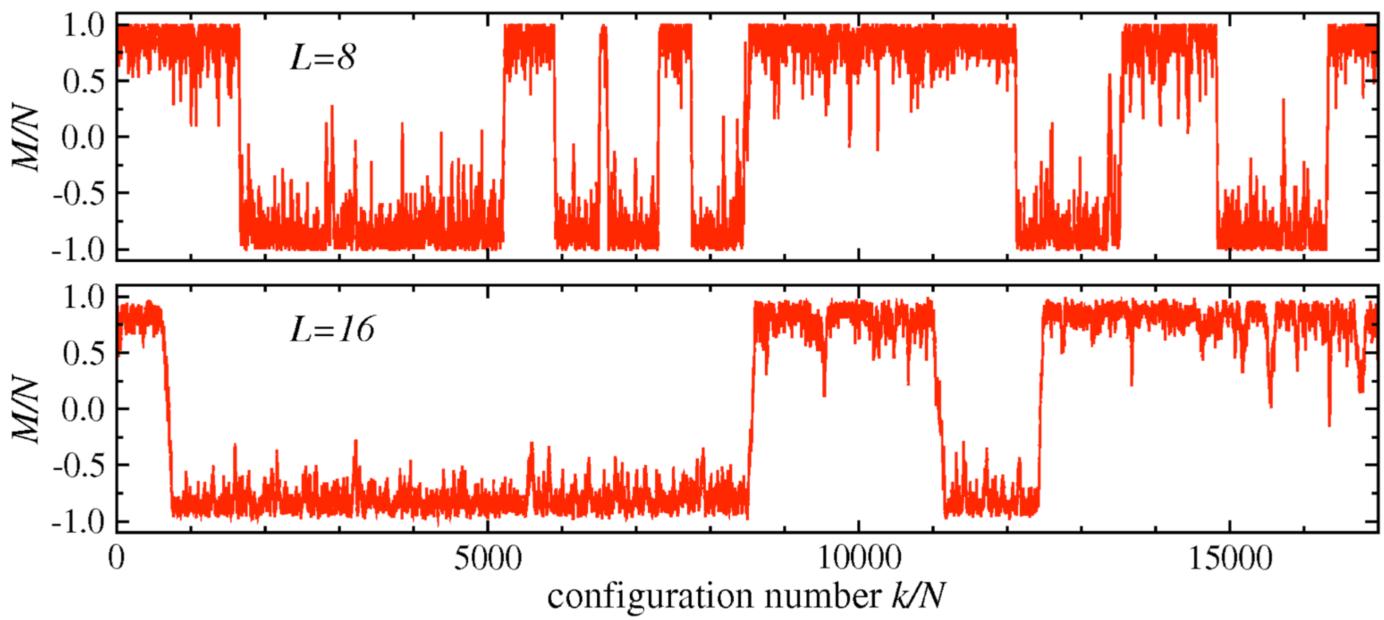
These probabilities satisfy detailed balance

Symmetry breaking (magnetic phase transition) for h=0

A magnetized state, <m>≠0, breaks a symmetry (E invariant under all $\sigma_i \to -\sigma_i$)

- strictly, mathematically we must have <m>=0
- symmetry breaking (phase transition) can take place when N→∞
- how can we understand the symmetry breaking for N large but finite?

Time series of simulation data; **magnetization vs simulation "time" for $T<T_c$**



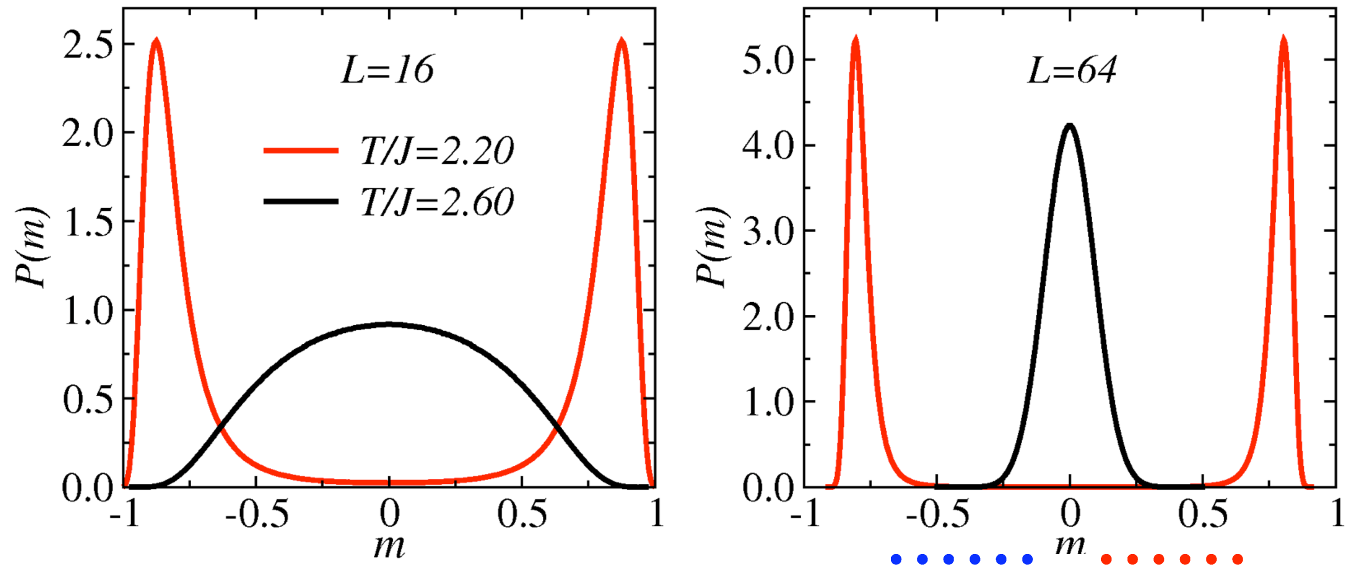
$$\frac{M}{N} = m = \frac{1}{N}\sum_{i=1}^{N}\sigma_i$$

There is a characteristic "reversal" time between m>0 and m<0 configurations

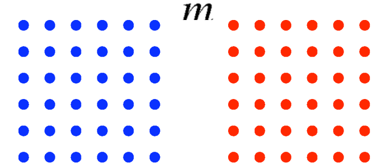
- reversal time diverges for N→∞
- the symmetry can be broken on practical time scales for finite (large) N
- also mechanism of phase transitions in real magnets (and other systems)

Another way to look at it: **magnetization distribution**

- probability distrubution (histogram) of m during the simulation



$$\mathbf{m} = \frac{1}{N}\sum_{i=1}^{N} \sigma_i$$



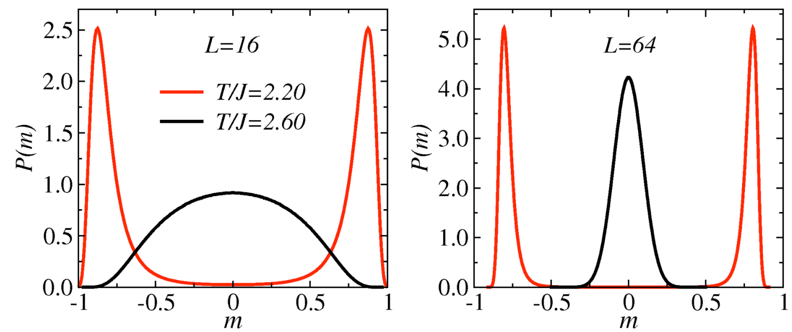
- single-peak distribution for $T>T_c$
- double-peak distribution for $T<T_c$
- peaks become sharper for increasing N
- no probability to fluctuate between m<0 and m>0 peaks for $N\rightarrow\infty$
  - have to go through low-probability m≈0 configurations

Why this peak structure? balance between

- large number of m≈0 configurations with high energy
- small number of |m|≈1 configuration with low energy
- entropy dominates at hight T, internal energy at low T

$$F = E - ST$$

Binder ratios and cumulants



Consider the dimensionless ratio

$$R_2 = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}$$

We can compute R_2 exactly for $N \to \infty$

- **for T<T$_c$:** $P(m) \to \delta(m-m^*)+\delta(m+m^*)$
  m^*=|peak m-value|

  $R_2 \to 1$

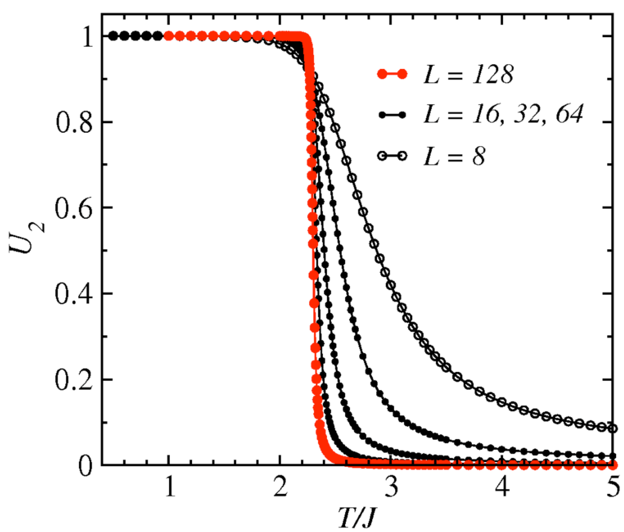
- **for T>T$_c$:** $P(m) \to \exp[-m^2/a(N)]$
  $a(N) \sim N^{-1}$

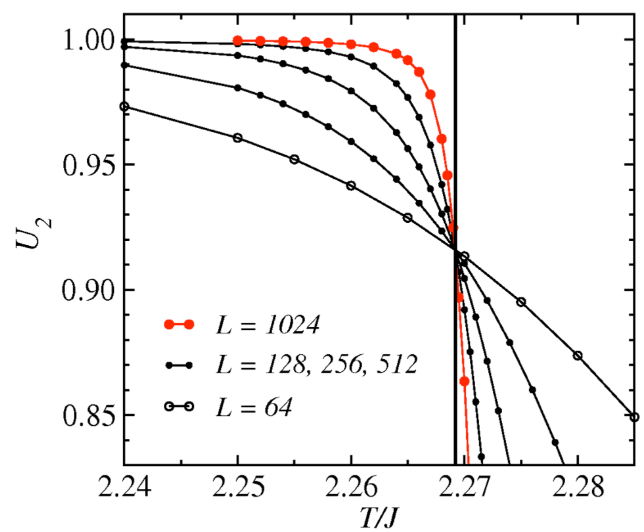
  $R_2 \to 3$ (properties of Gaussian integrals)

The **Binder cumulant** is defined as (n-component order parameter; n=1 for Ising)

$$U_2 = \frac{3}{2}\left(\frac{n+1}{3} - \frac{n}{3}R_2\right) \to \begin{cases} 1, & T < T_c \\ 0, & T > T_c \end{cases}$$

2D Ising model; MC results





Curves for different L normally cross each other close to T$_c$

Extrapolate crossing for sizes L and 2L to infinite size

- converges faster than single-size T$_c$ defs.

Computing expectation values and their statistical errors

Definition: Monte Carlo sweep = N spin-flip attempts

- a natural unit of simulation "time"
- "measure" observables after every (or every n) sweep

Boltzmann probability accounted for at sampling stage →

$$\bar{Q} = \frac{1}{N_s} \sum_{i=1}^{N_s} Q_i, \qquad N_s = \text{number of samples}$$

is the estimate for the true expectation value;

$$\bar{Q} \to \langle Q \rangle, \qquad (N_s \to \infty)$$

Statistical errors (error bars): $\langle Q \rangle = \bar{Q} \pm \sigma_Q$

- the measurements are not statistically independent
- independent only after a number of sweeps >> autocorrelation time

Divide the simulation into B "bins", M sweeps in each bin; N_s=BM

- bin averages: $\bar{Q}_b, \; b = 1, \ldots, B$

$$\bar{Q} = \frac{1}{B} \sum_{b=1}^{B} \bar{Q}_b, \qquad \sigma_Q^2 = \frac{1}{B(B-1)} \sum_{b=1}^{B} (\bar{Q}_b - \bar{Q})^2$$

If M is sufficiently large (>> autocorrelation time) the average and error are statistically sounds (corresonding to independent Gaussian-distributed data)

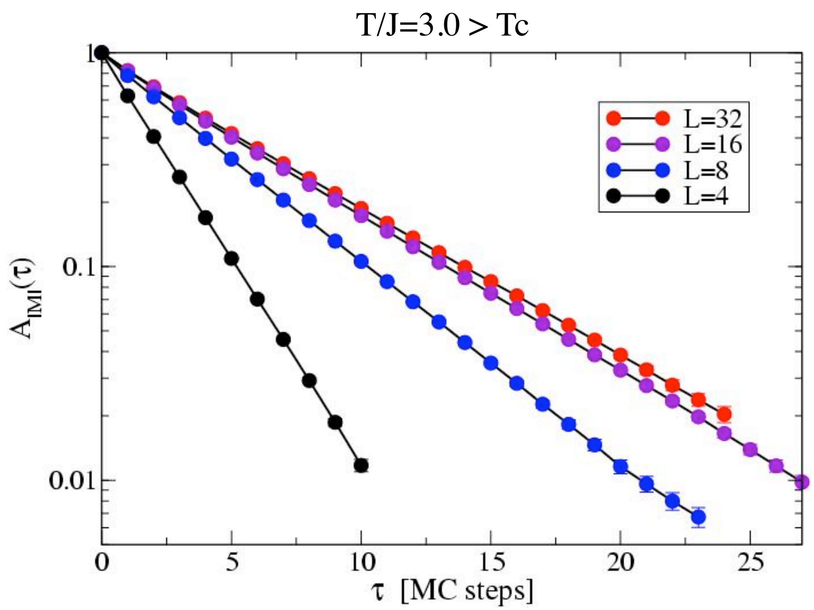
- probability of true value being "inside the error bars" ≈2/3

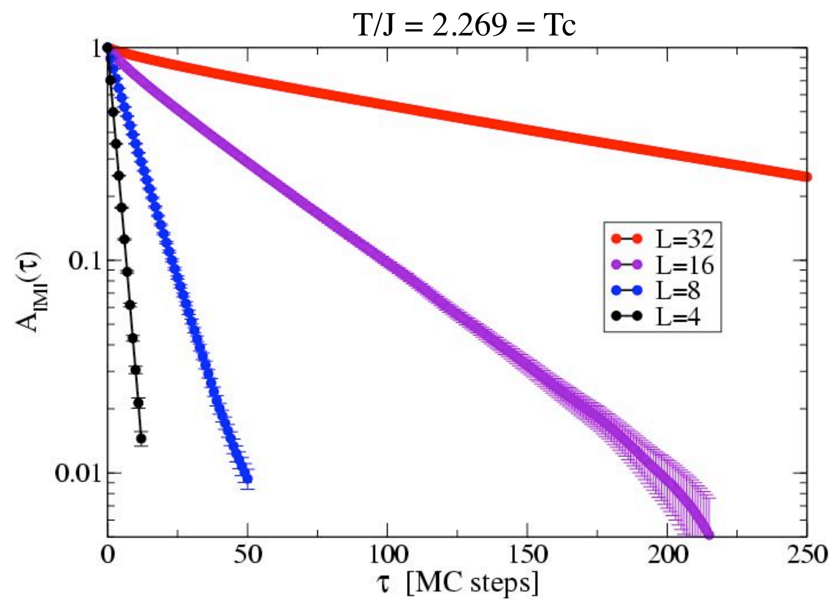
Autocorrelation functions

- characterization of how measurements become statistically independent

$$A_Q(t) = \frac{\langle Q(i+t)Q(i)\rangle - \langle Q\rangle^2}{\langle Q^2\rangle - \langle Q\rangle^2}, \quad (\rightarrow \mathrm{e}^{-t/\Theta},\ t \rightarrow \infty)$$

the autocorrelation time Θ grows as $T \rightarrow T_c$ (diverges for $N \rightarrow \infty$, $T \rightarrow T_c$)





This problem can be largely overcome by using **cluster algorithms**

- for standard Ising, XY, Heisenberg,...
- but not in all cases, e.g., in the presence of external fields, frustrated systems,...