Title: Quantum Spin Simulations (PHYS 7380) - Lecture 5

Date: Apr 09, 2010 11:00 AM

URL: http://pirsa.org/10040047

Abstract:

Aore general finite-size scaling hypothesis

has been justified using the renormalization-group theory

$$Q(t, L) = L^{\sigma} f(\xi/L),$$

Jsing $\xi \sim |t|^{-1/\nu} \rightarrow$

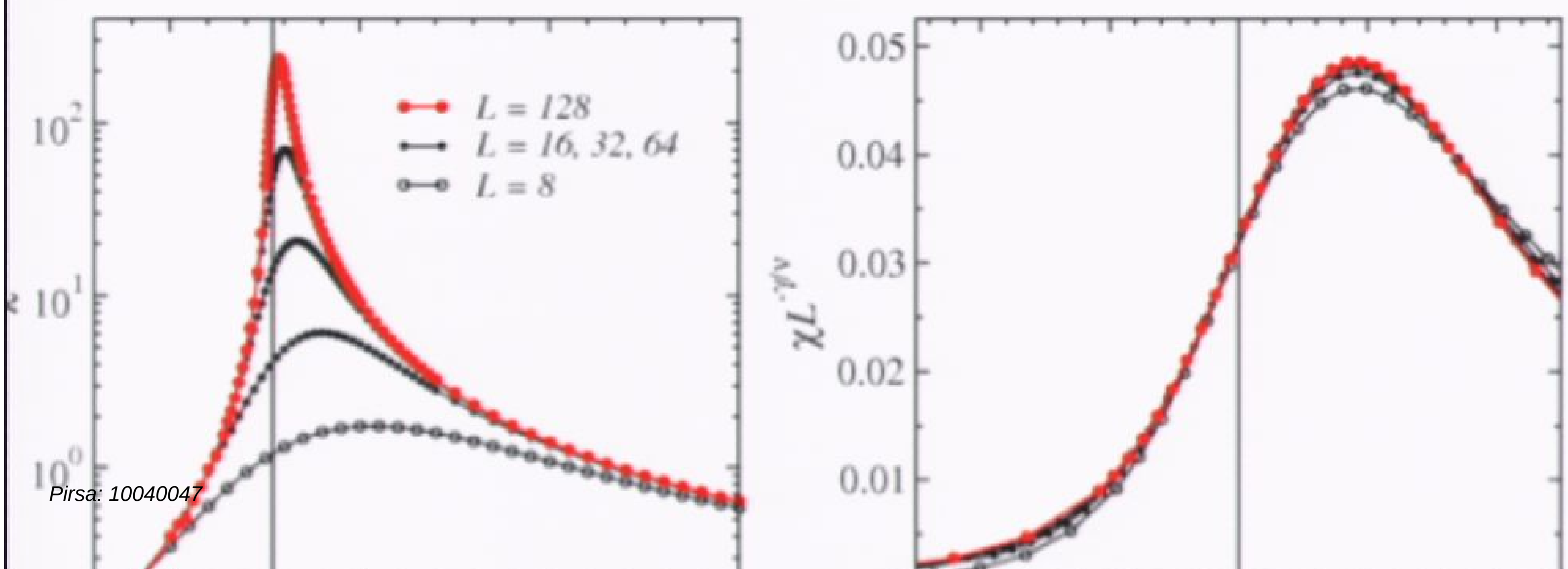
$$Q(t, L) = L^{\sigma} g(tL^{1/\nu})$$

From this we must be able to reproduce infinite-size form:

$$Q(t, L \rightarrow \infty) \sim |t|^{-\kappa}$$

vhich is the case if $g(x) \sim x^{-\kappa}$ and $\sigma = \kappa/\nu$

Test: susceptibility of 2D Ising model (Monte Carlo)



$T_c = 2/\ln(1 + \sqrt{2})$

$\nu = 1, \gamma = 7/4$

Normally: adjust Tc and exponents so that the data "collapse"

Monte Caro simulations

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Monte Carlo methods - based on random numbers

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

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Random (pseudo random) number generator on the computer

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

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Monte Carlo simulations in statistical physics
- normally refers to **importance sampling** of configurations (e.g., spins)

Monte Carlo simulation of the Ising model

The Metropolis algorithm

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

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- C_{n+1} obtained by modifying (updating) C_n

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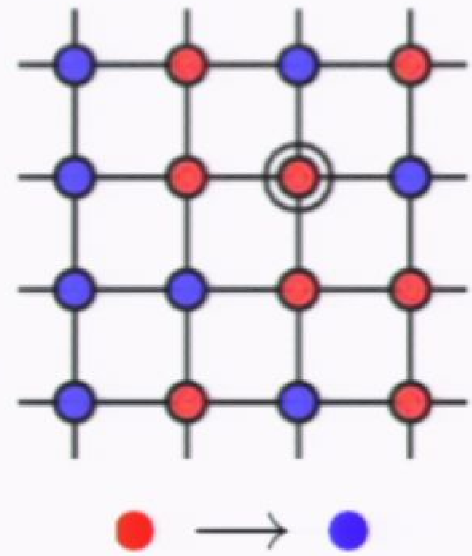

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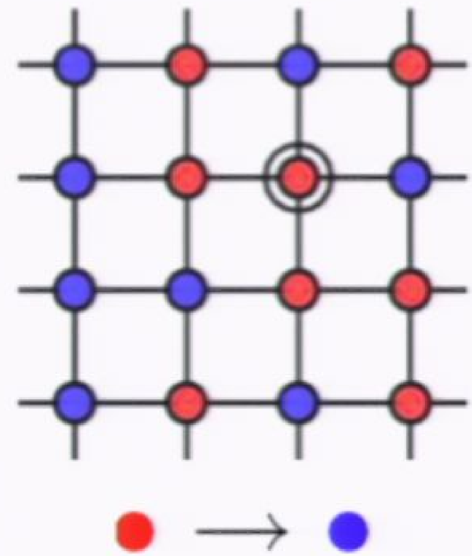
$$\frac{P_{\text{change}}(A \to B)}{P_{\text{change}}(B \to A)} = \frac{W(B)}{W(A)} \qquad W(A) = \mathrm{e}^{-E(A)/T}$$



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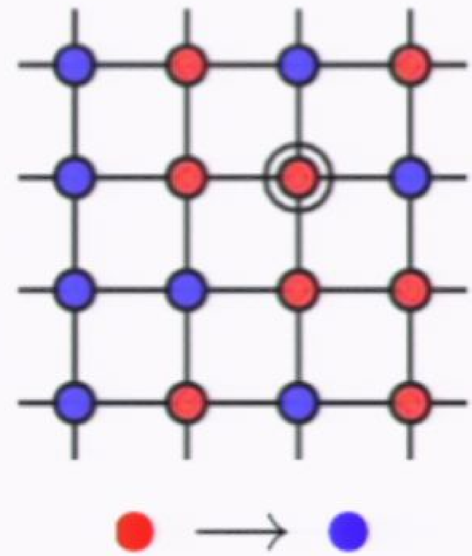

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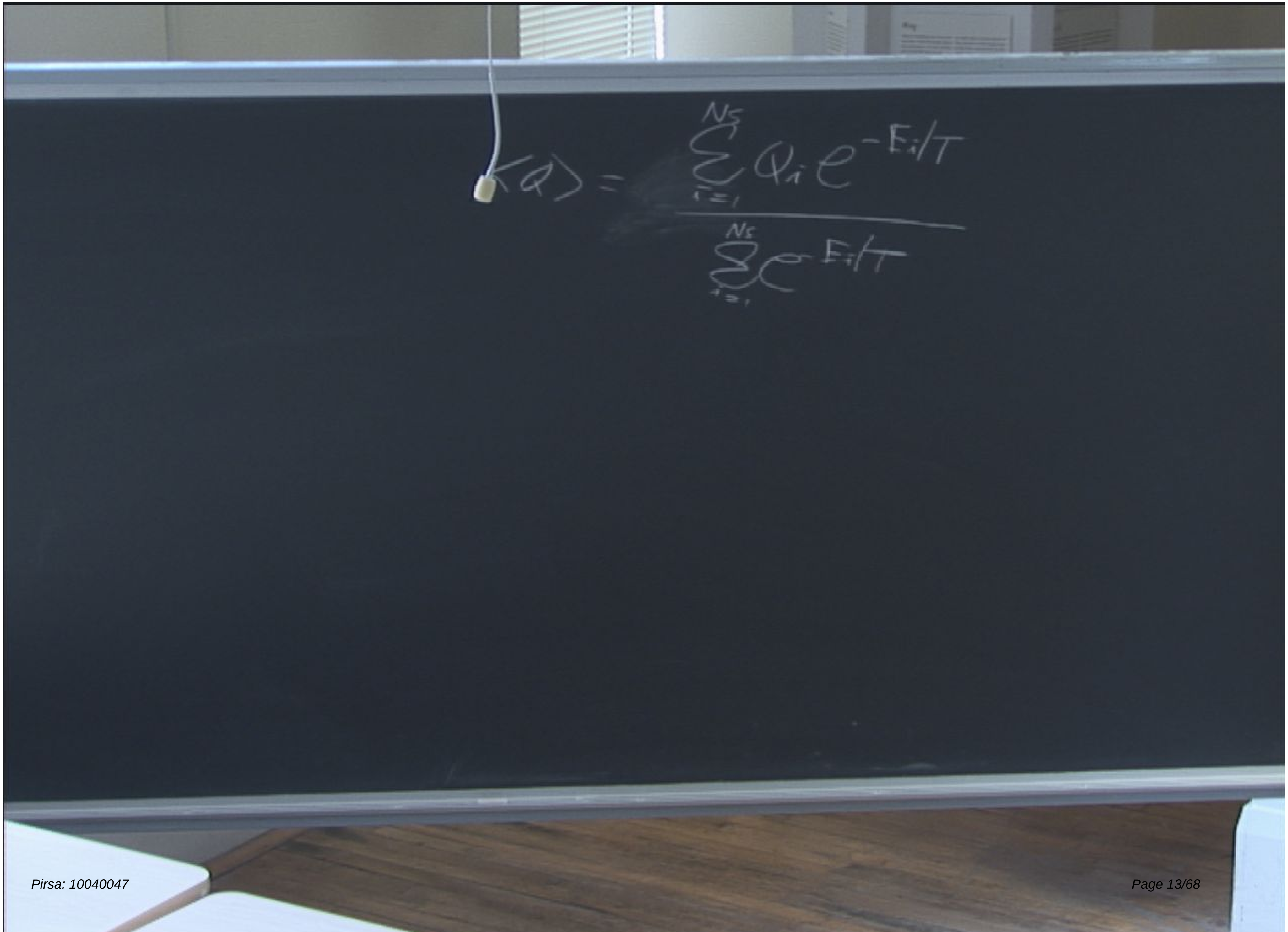
- the process has to be **ergodic**
  - any configuration reachable in principle
- it takes some time to reach equilibrium


$\langle Q \rangle = \frac{\sum_{i=1}^{N_s} Q_i e^{-E_i/T}}{\sum_{i=1}^{N_s} e^{-E_i/T}}$

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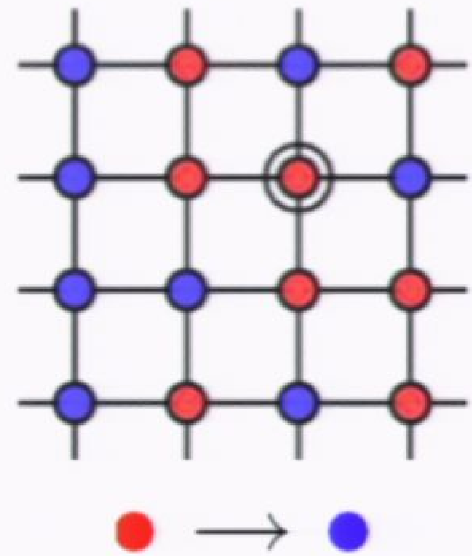

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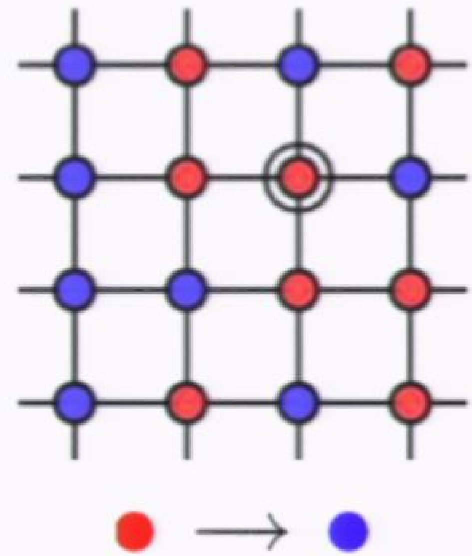

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- select a spin i at random; consider flipping it $\sigma_i \to -\sigma_i$
- compute the ratio $R=W(\sigma_1,\ldots-\sigma_i,\ldots,\sigma_N)/W(\sigma_1,\ldots\sigma_i,\ldots,\sigma_N)$
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- generate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

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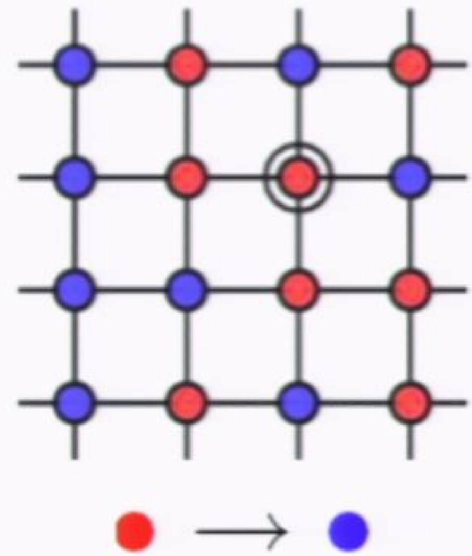

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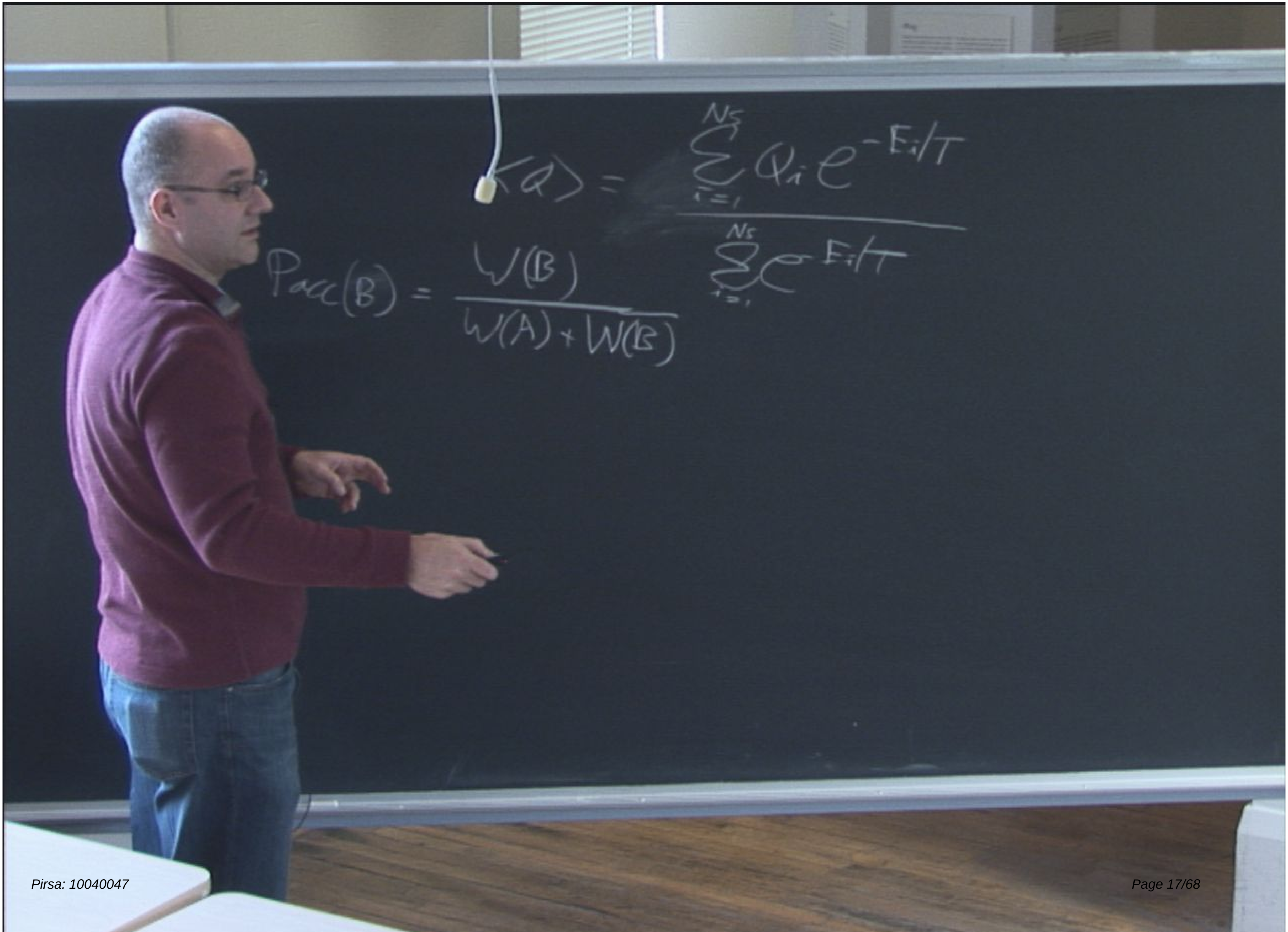
$$P_{\text{change}}(A \to B) = P_{\text{select}}(B|A)P_{\text{accept}}(B|A)$$ These probabilities



$\langle Q \rangle = \frac{\sum_{i=1}^{N_s} Q_i e^{-E_i/T}}{\sum_{i=1}^{N_s} e^{-E_i/T}}$
$P_{acc}(B) = \frac{W(B)}{W(A) + W(B)}$

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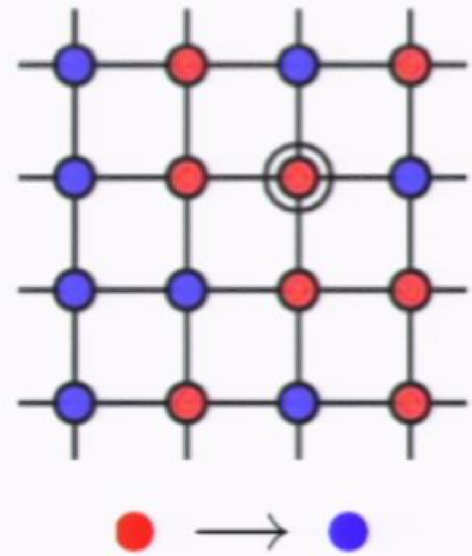

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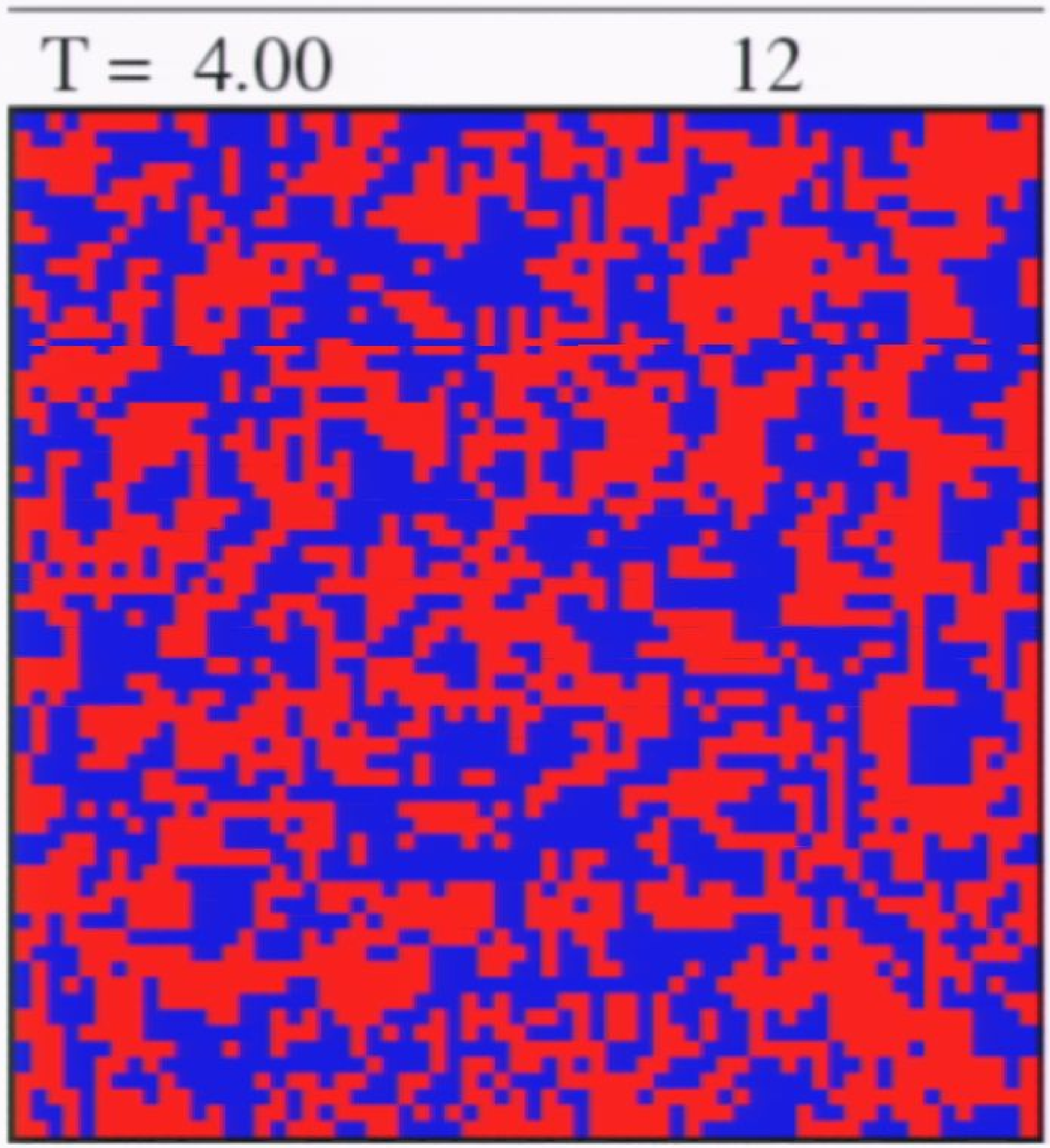
=0 simulations

28×128 lattice N=16384)

ne MC sweep is N random flip ttempts

$_c$/J ≈ 2.27



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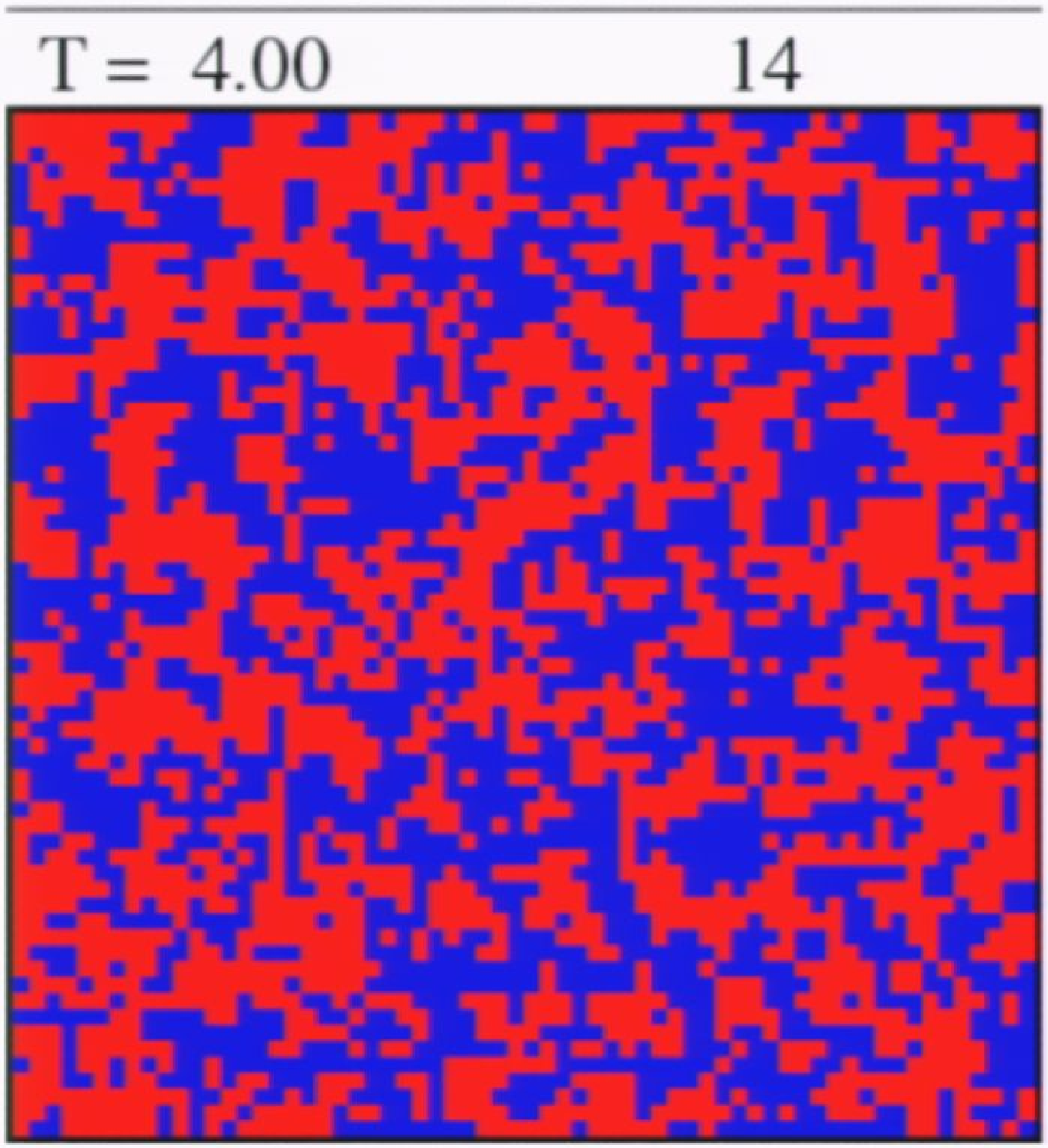

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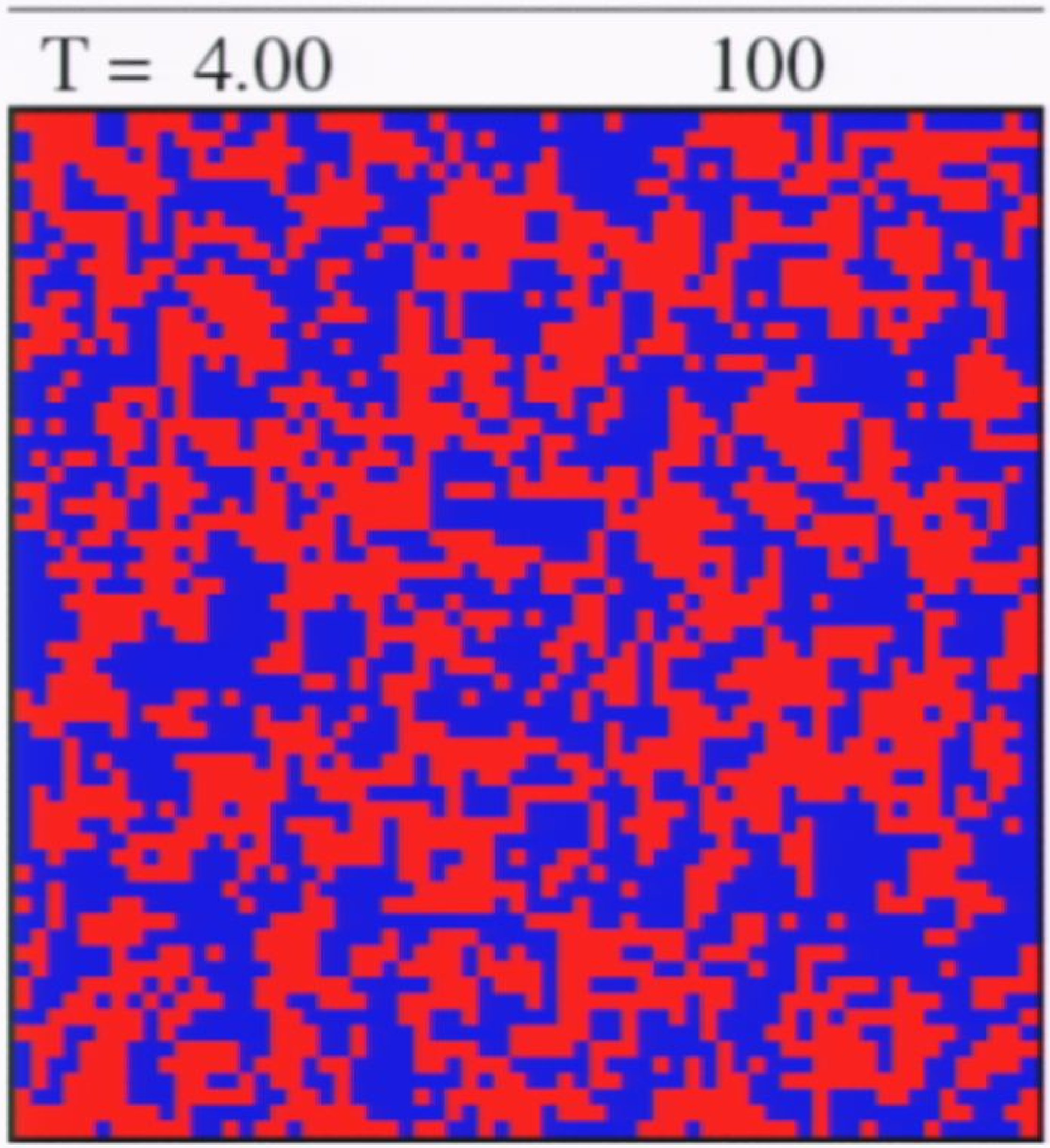
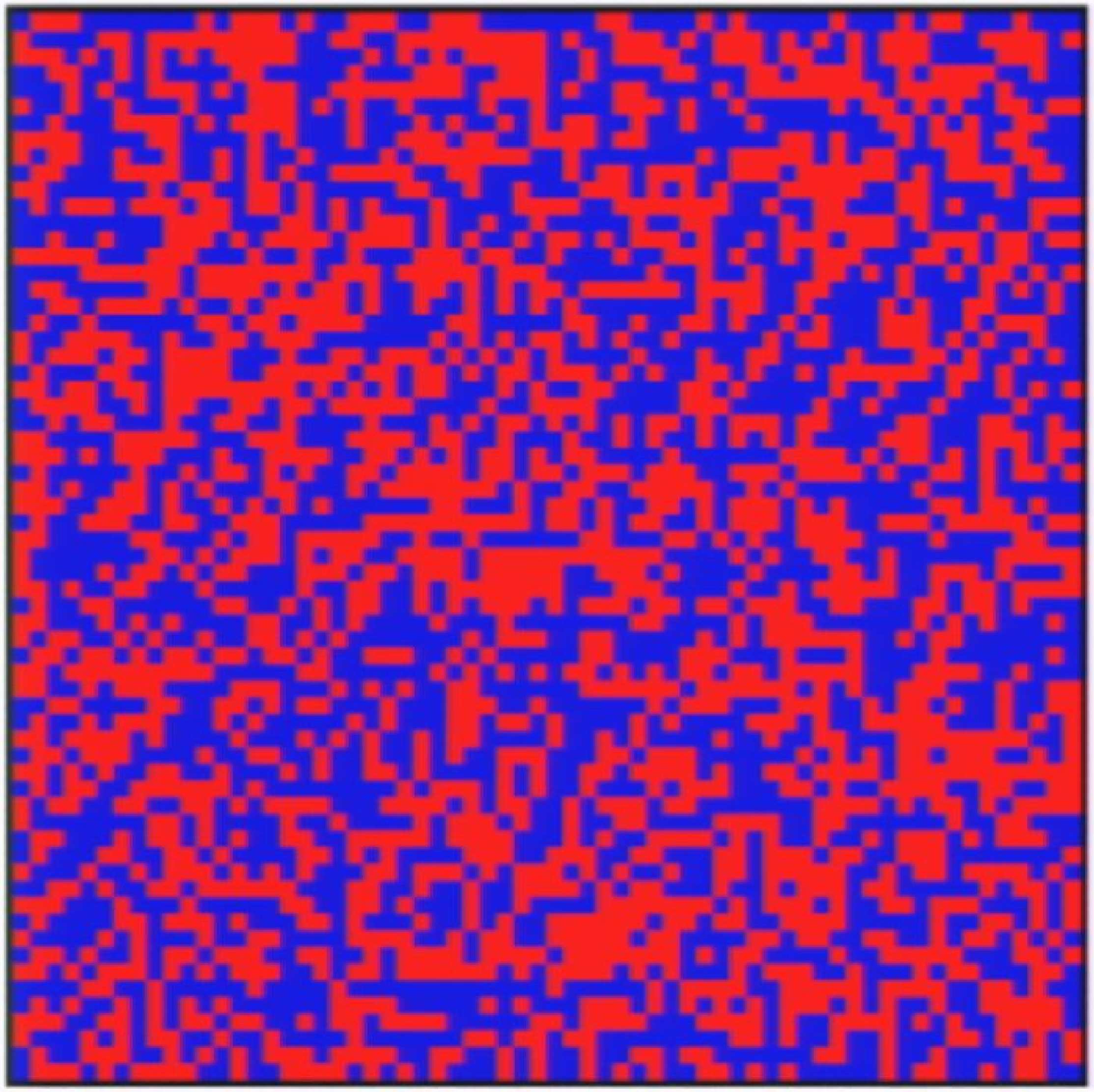
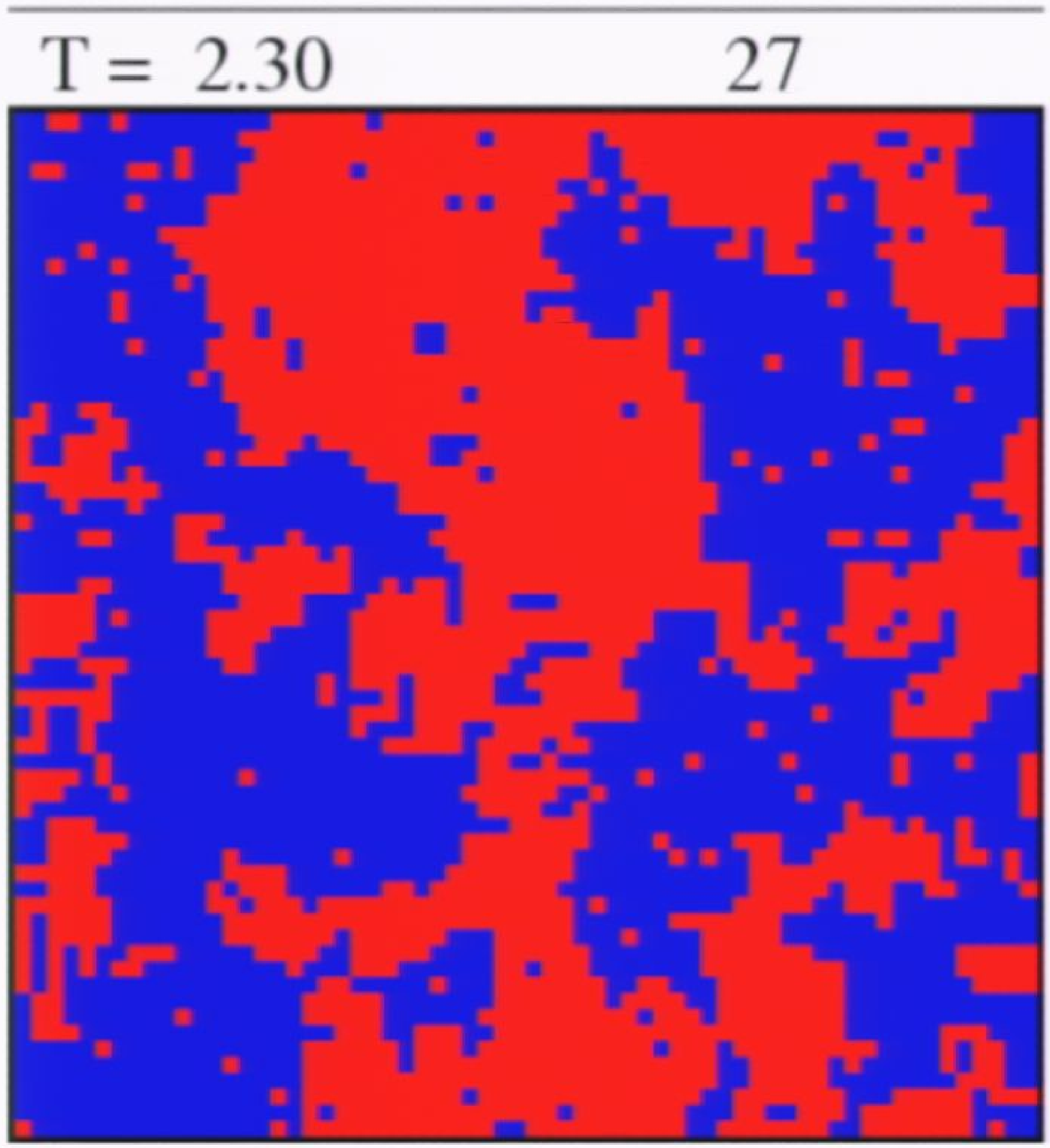


T = 2.30 1

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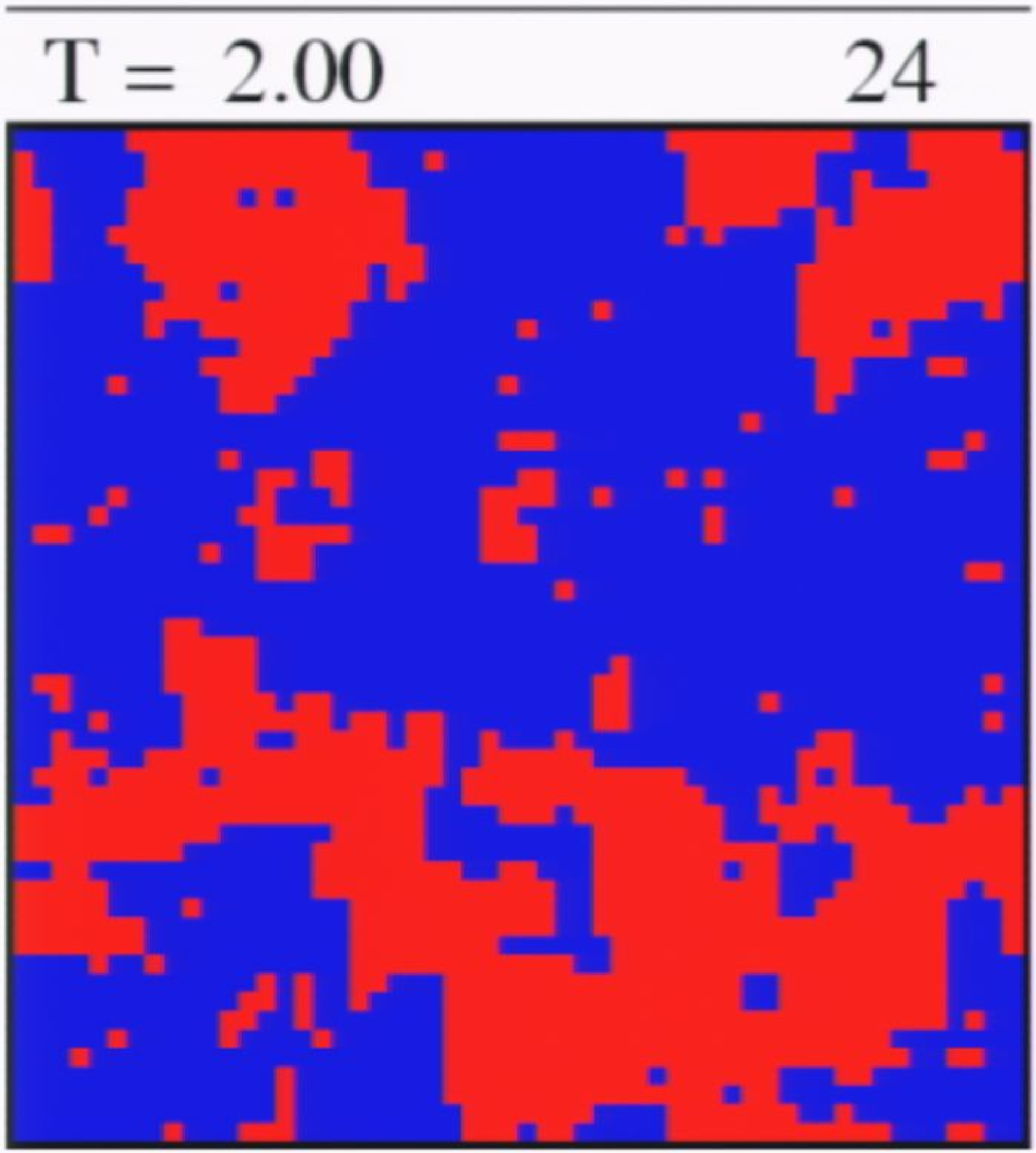
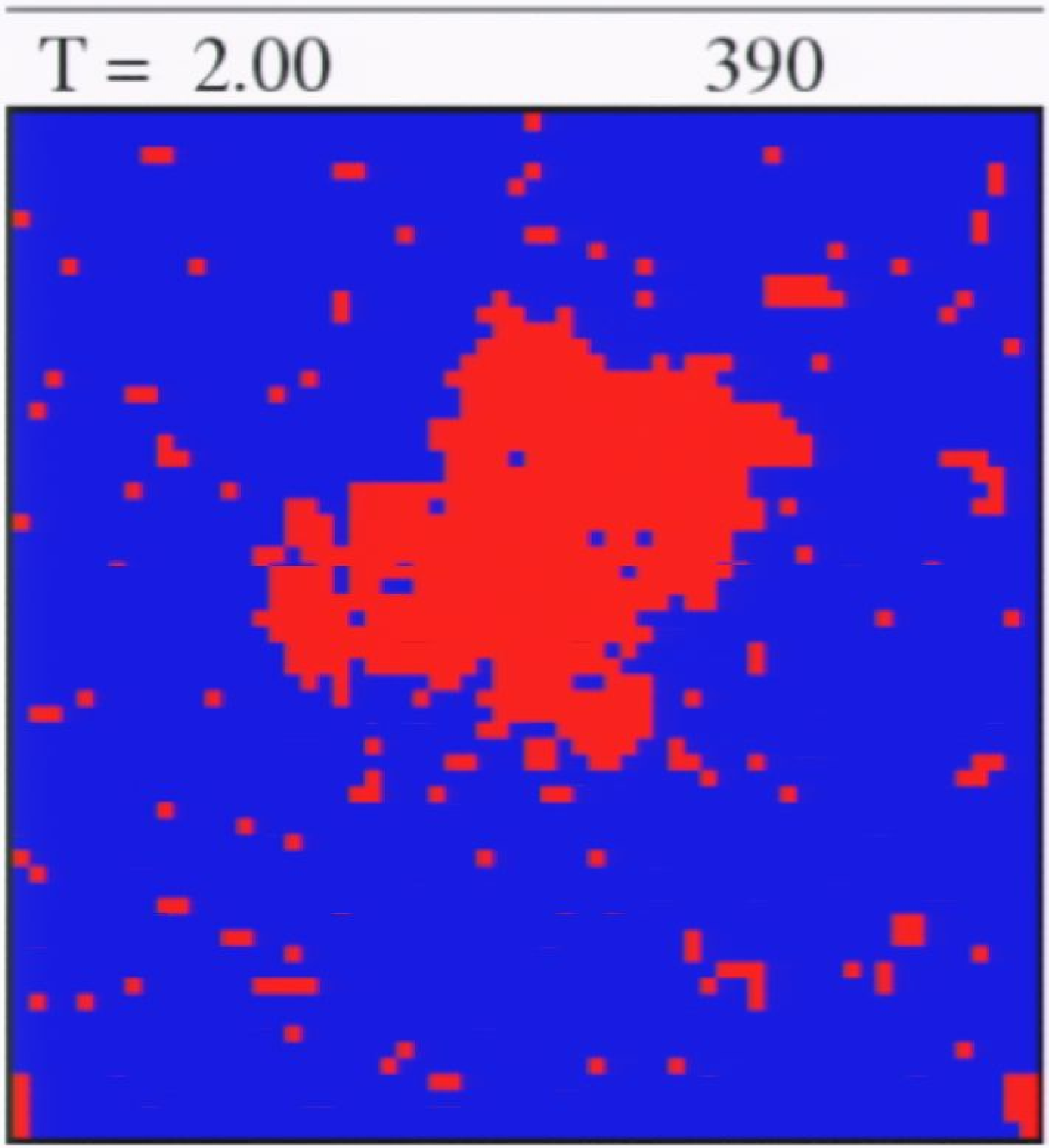
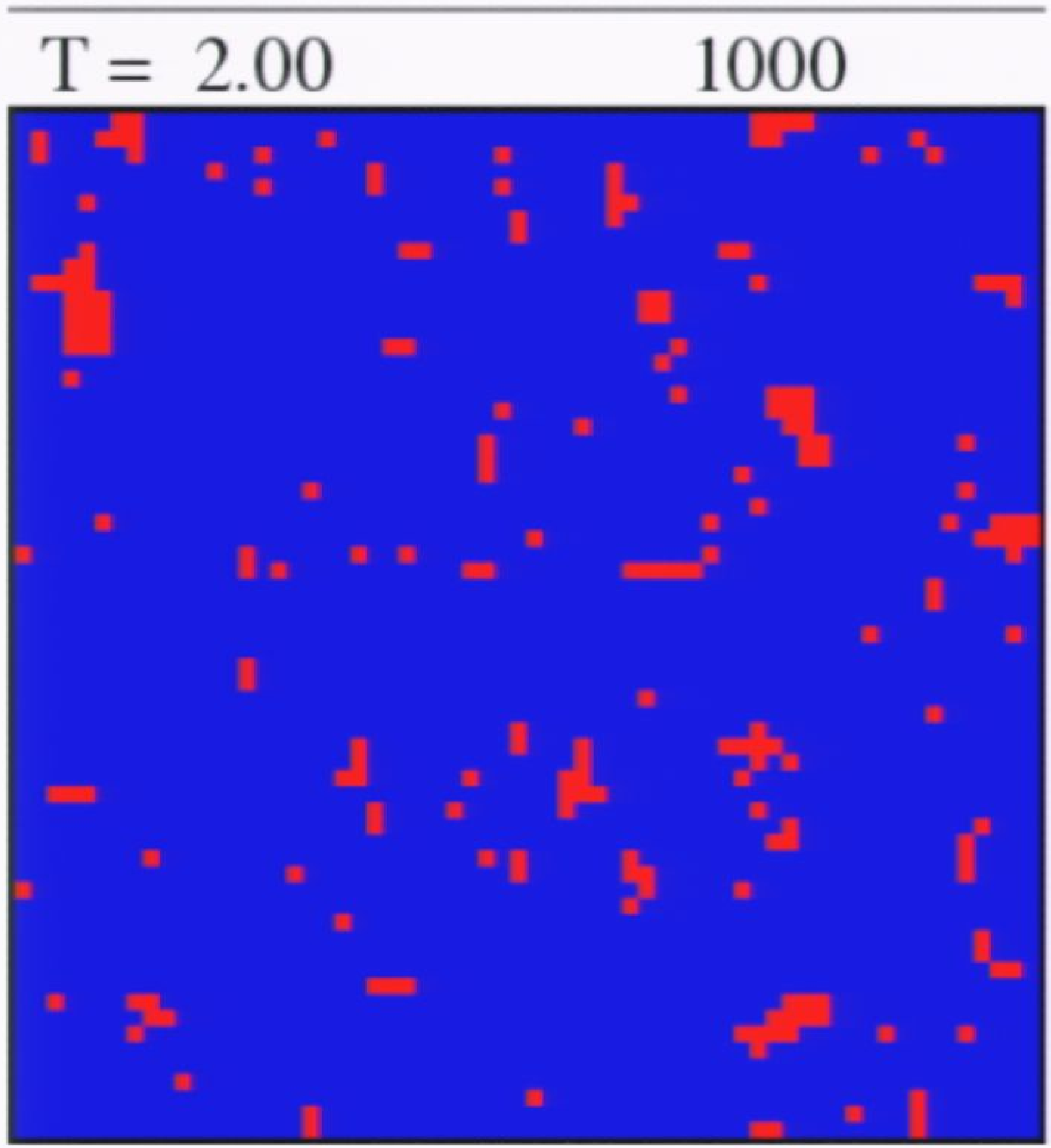
27


T = 2.00
24


T = 2.00
390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1000

Symmetry breaking (magnetic phase transition) for h=0

A magnetized state, $\langle m \rangle \neq 0$, breaks a symmetry (E invariant under all $\sigma_i \rightarrow -\sigma_i$)

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- symmetry breaking (phase transition) can take place when $N \rightarrow \infty$
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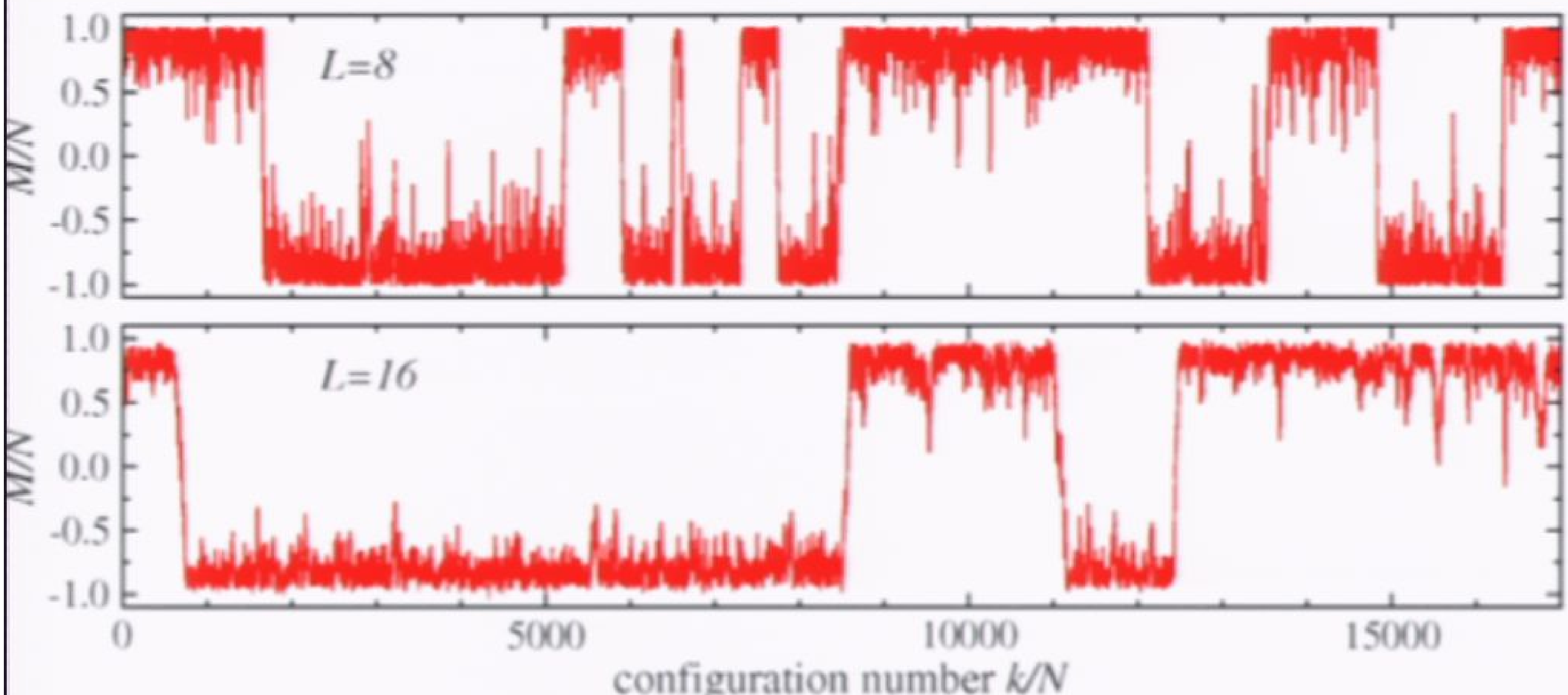
Time series of simulation data; **magnetization vs simulation "time" for $T<T_c$**



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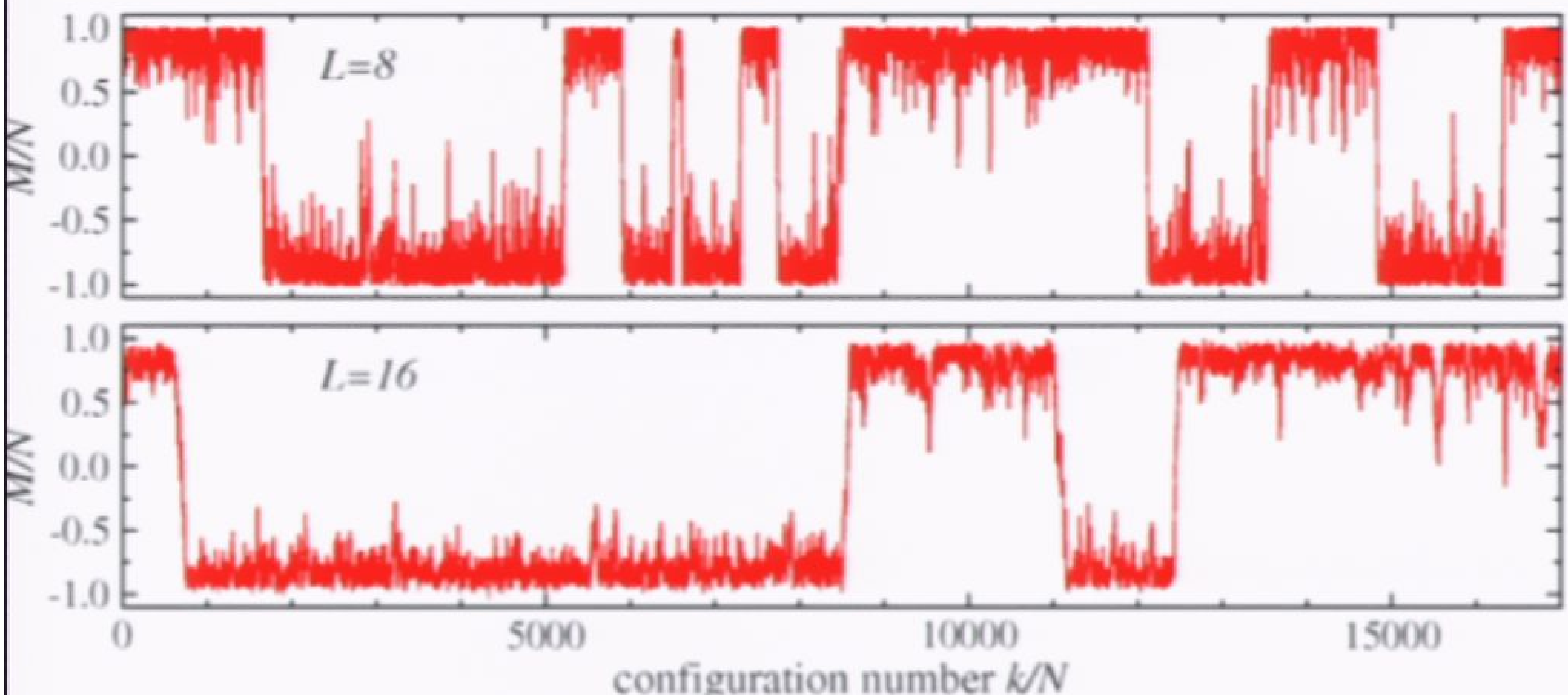

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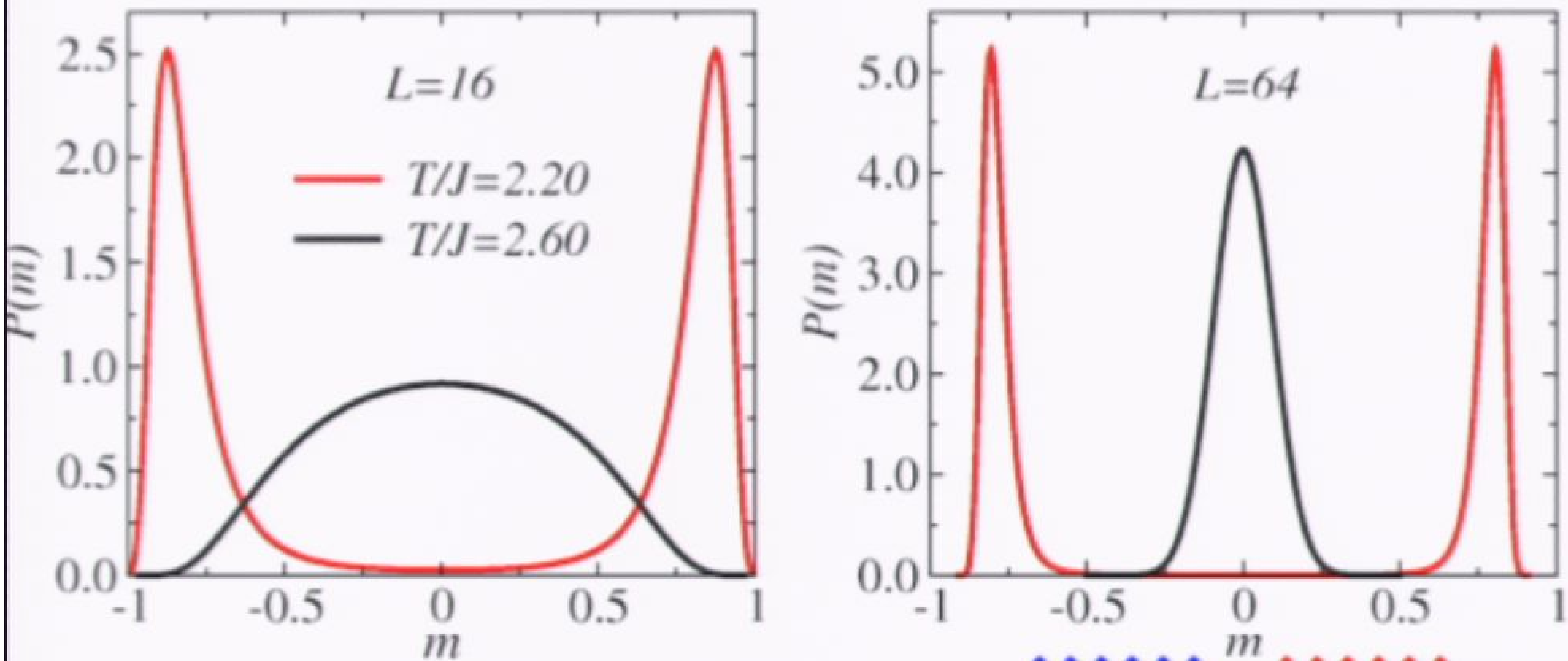

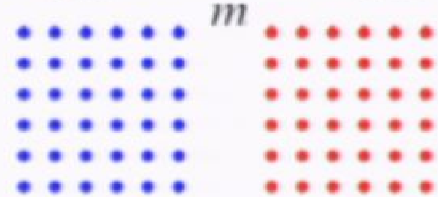

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- no probability to fluctuate between $m<0$ and $m>0$ peaks for $N\to\infty$
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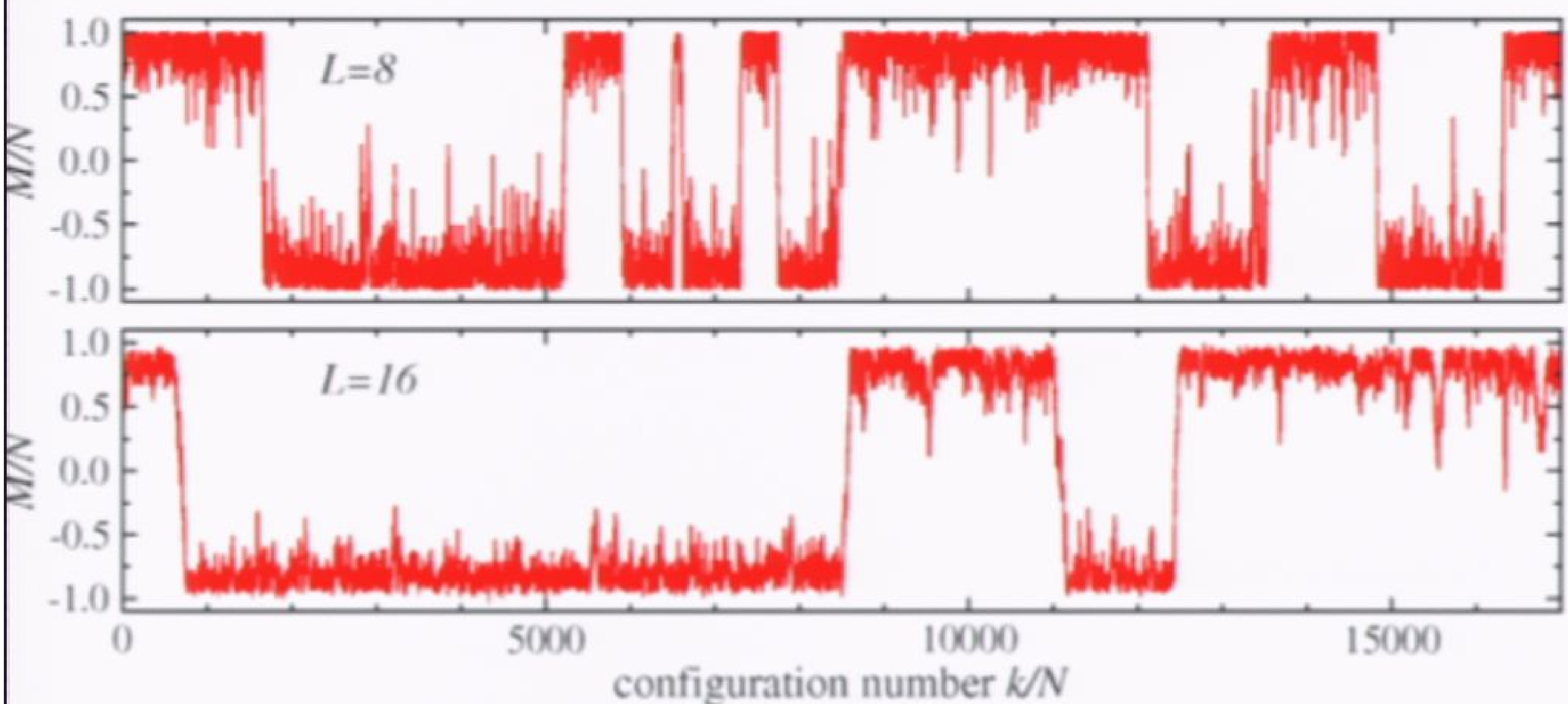

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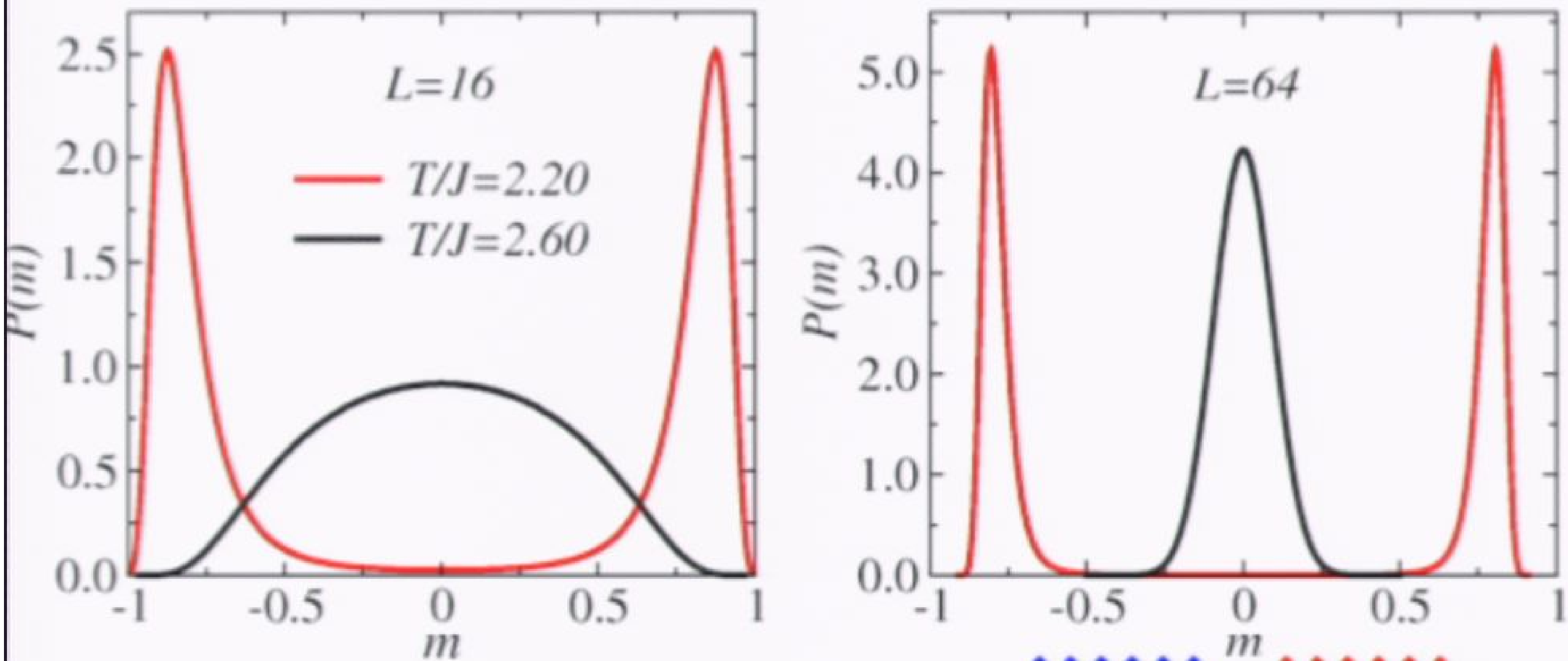

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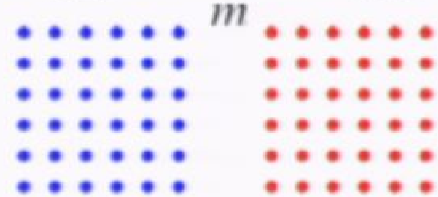

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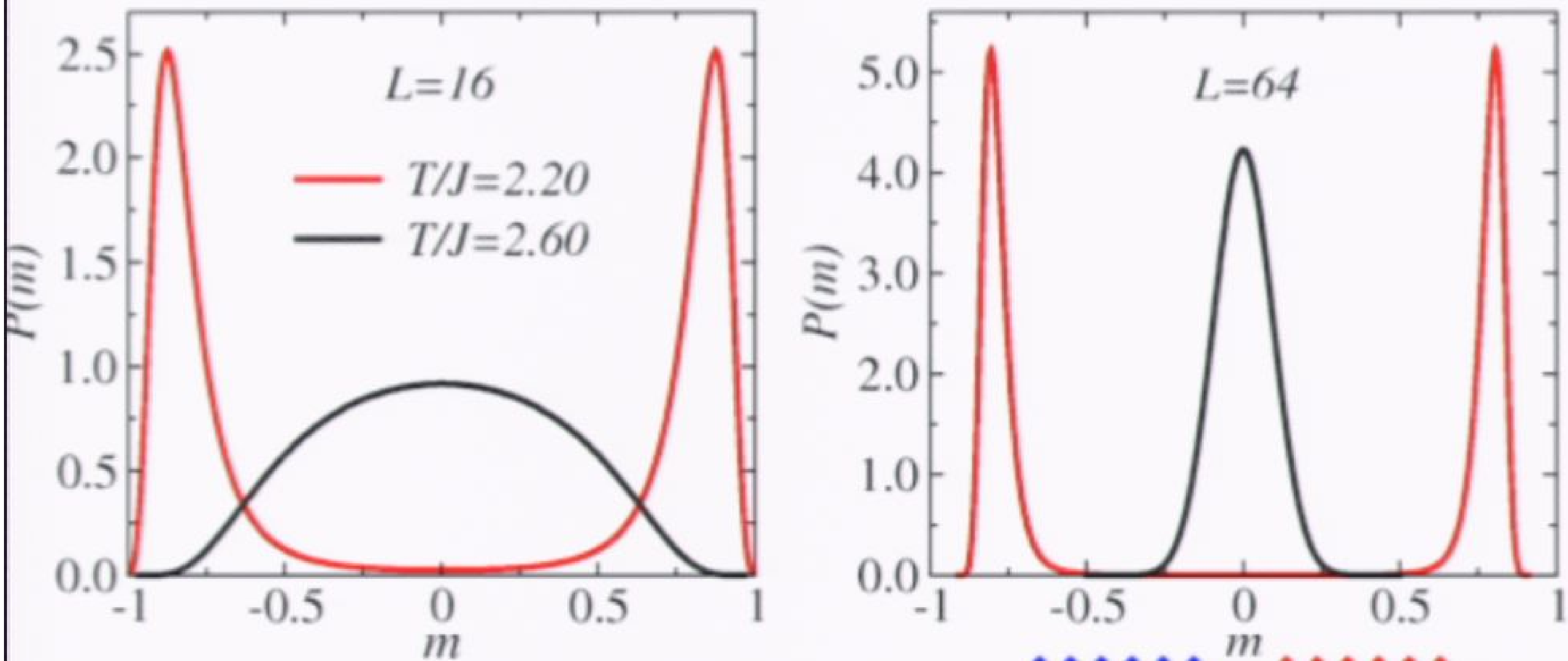

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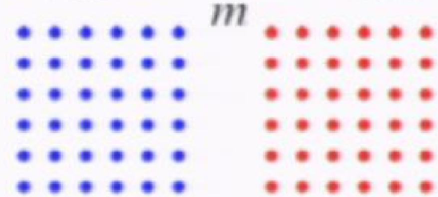

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Why this peak structure? balance between

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

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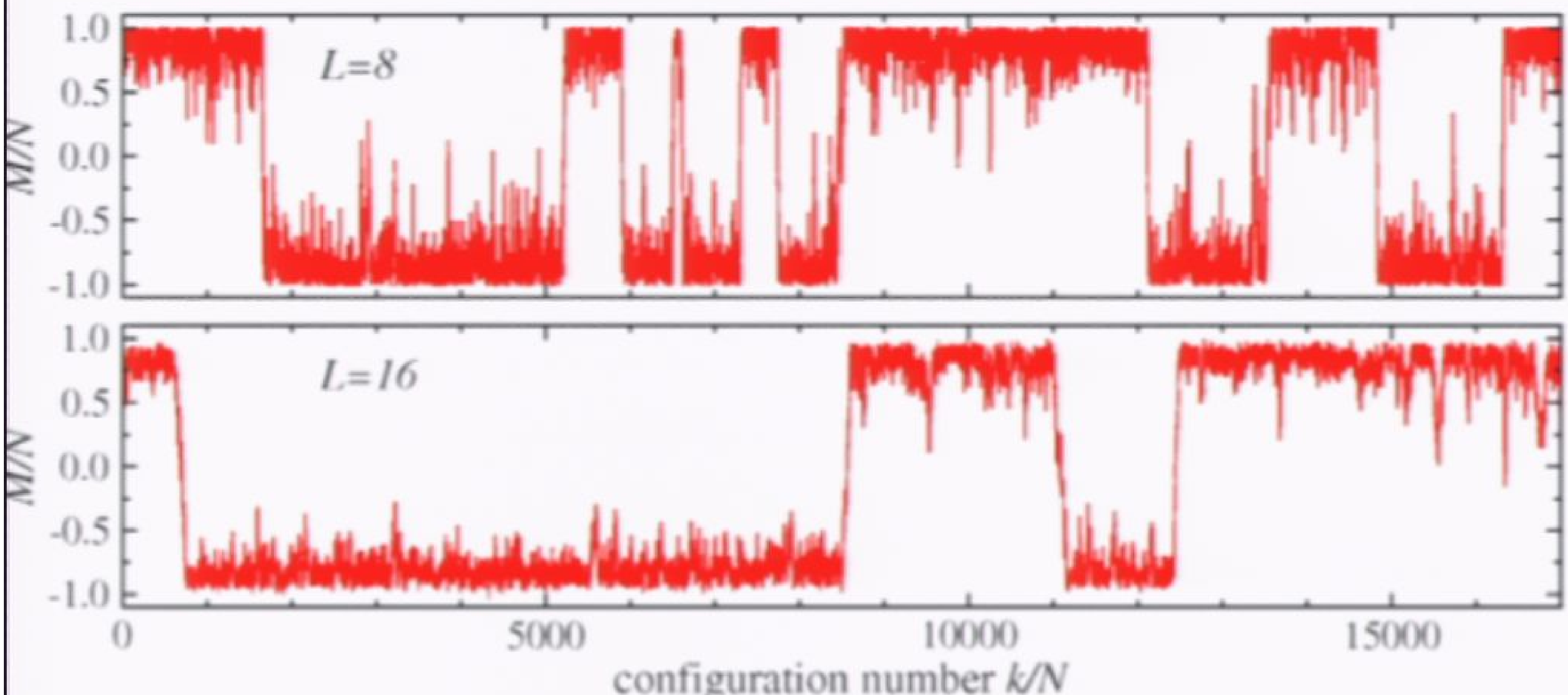

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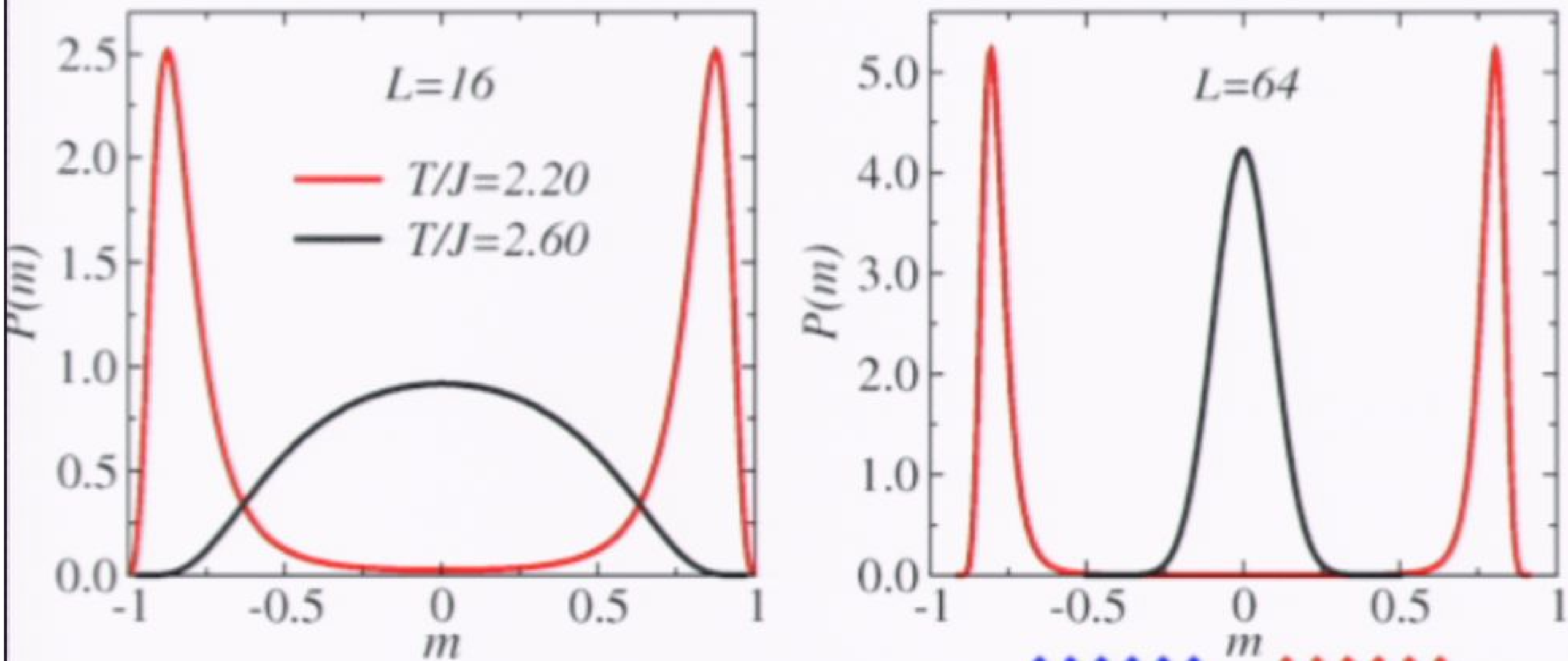

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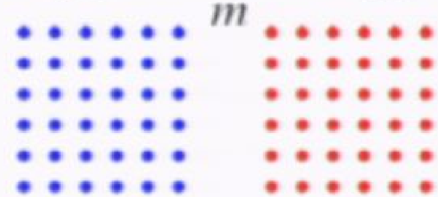

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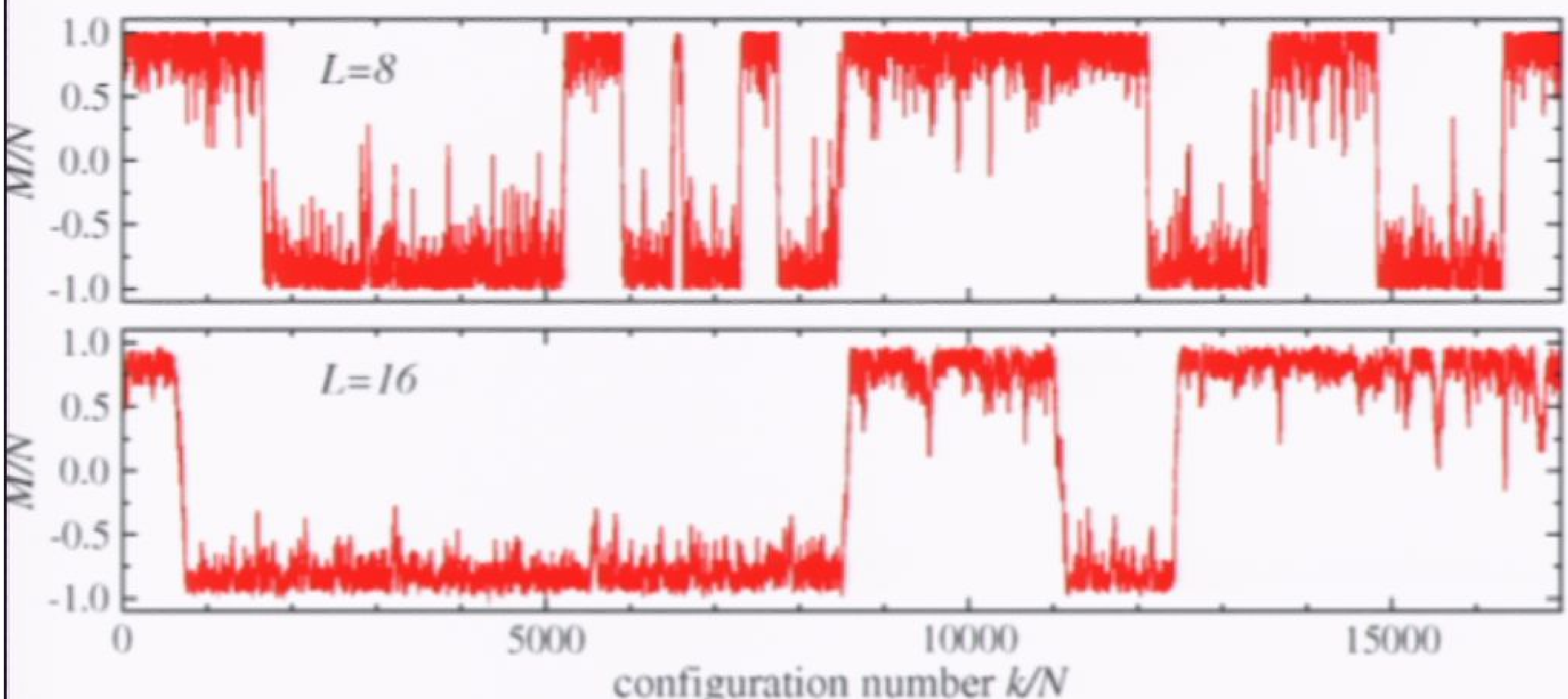

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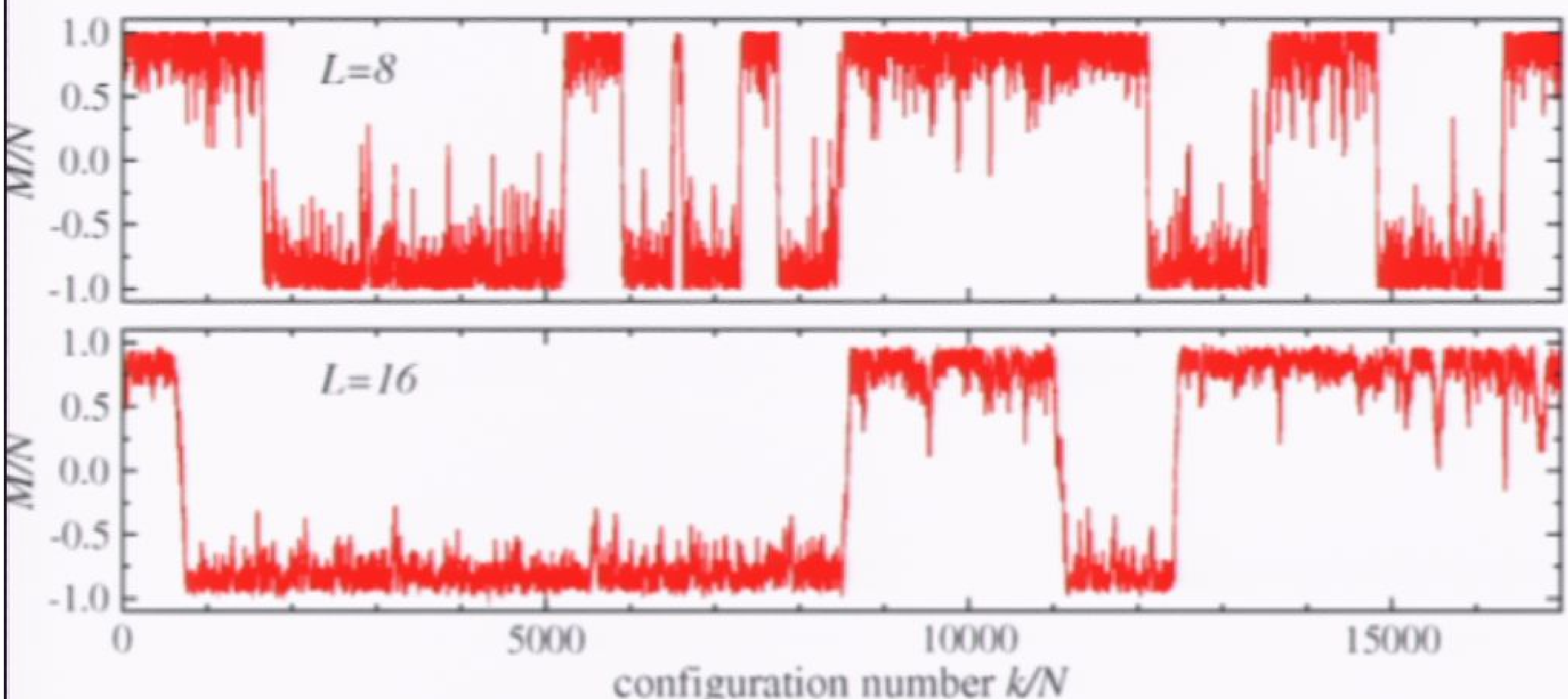

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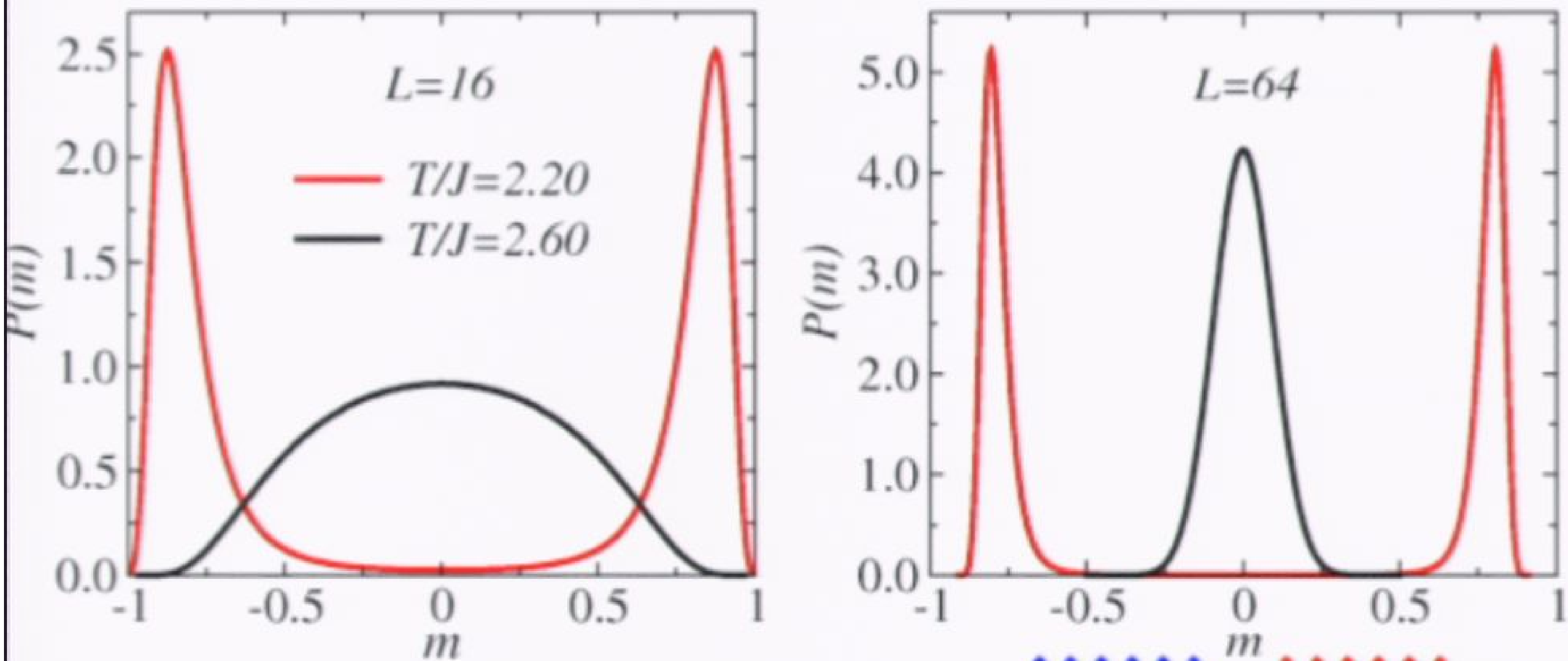

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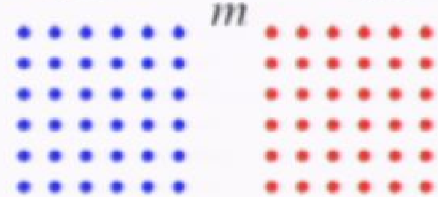

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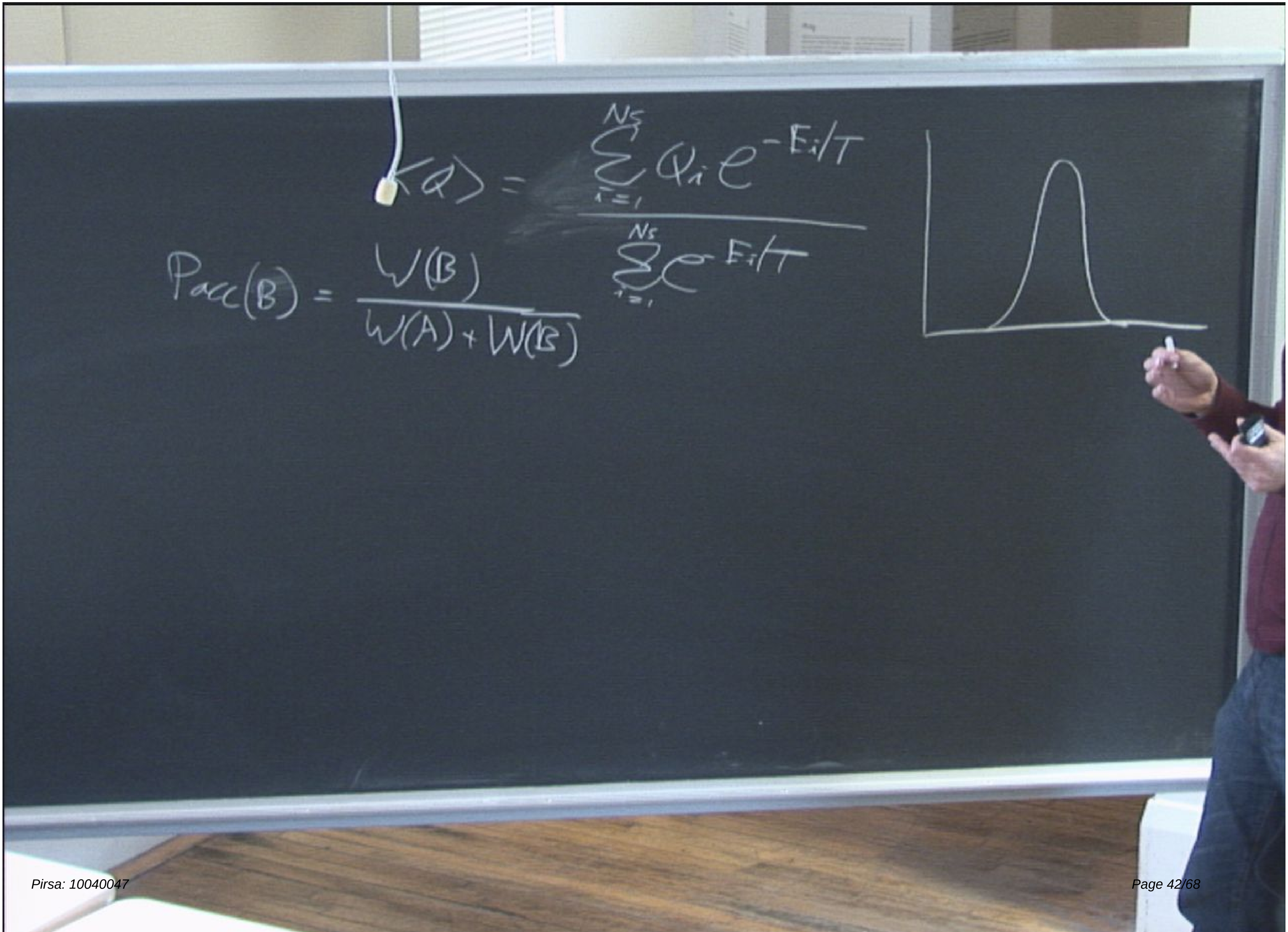
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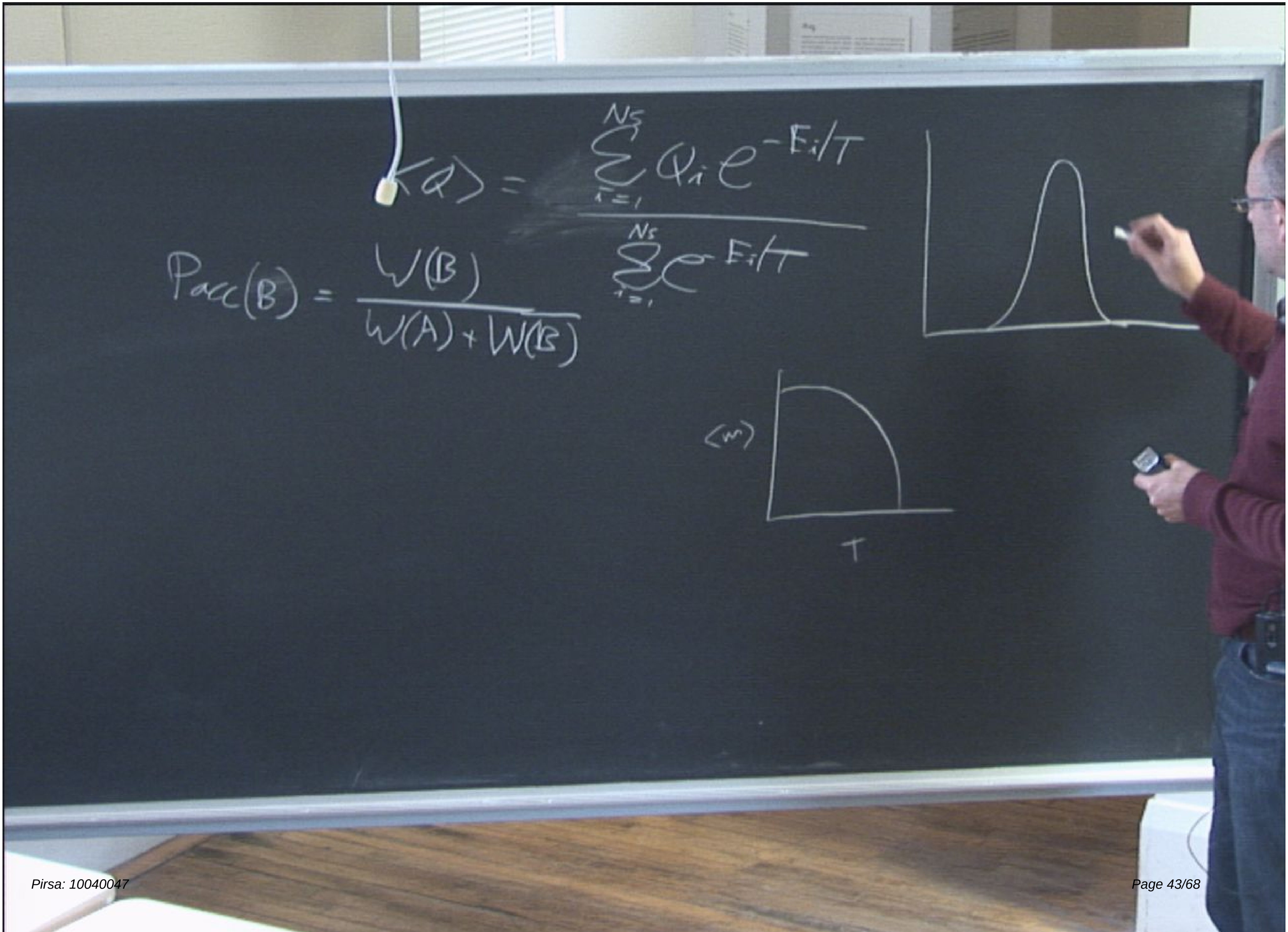
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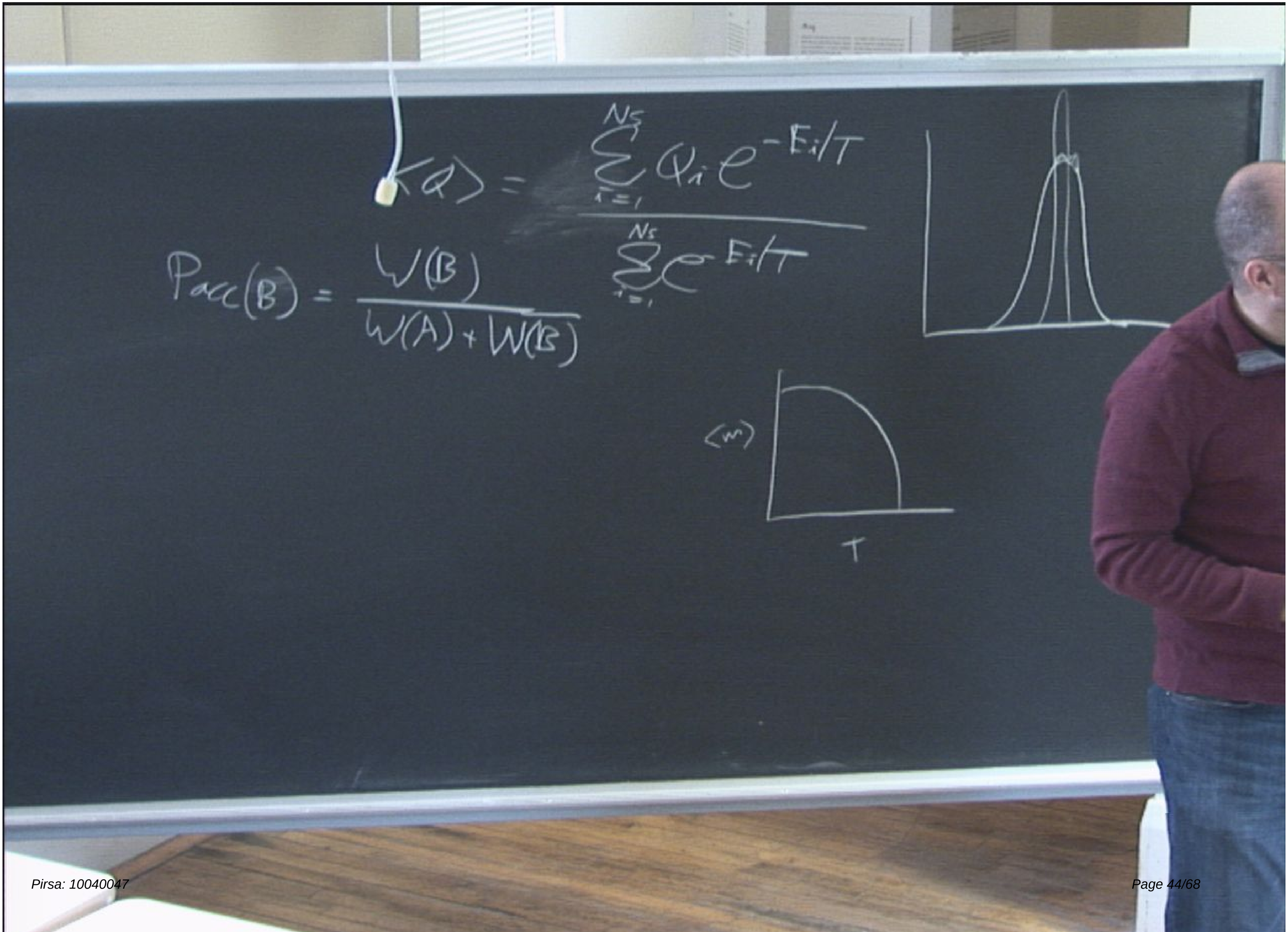
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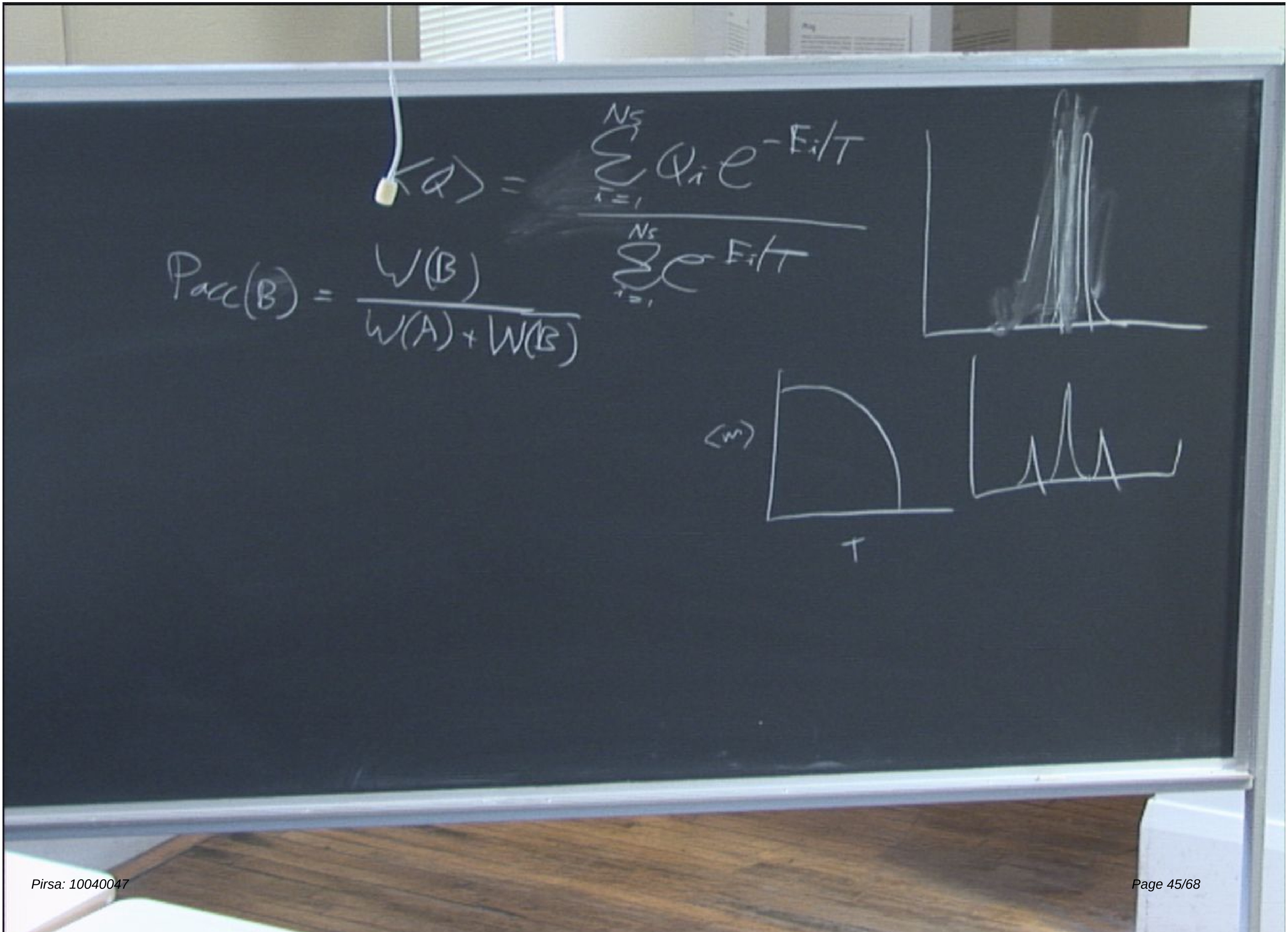
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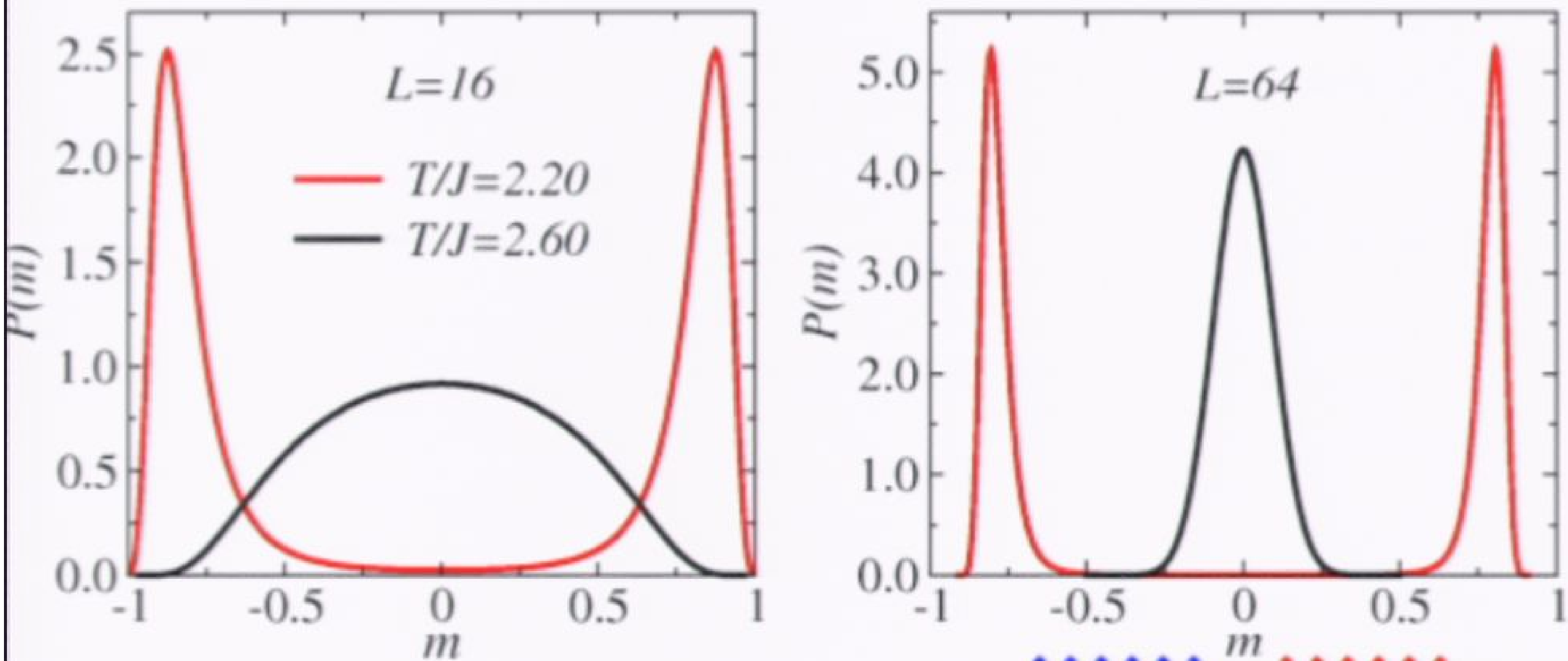

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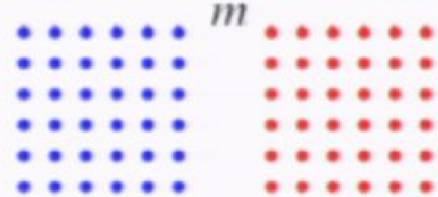

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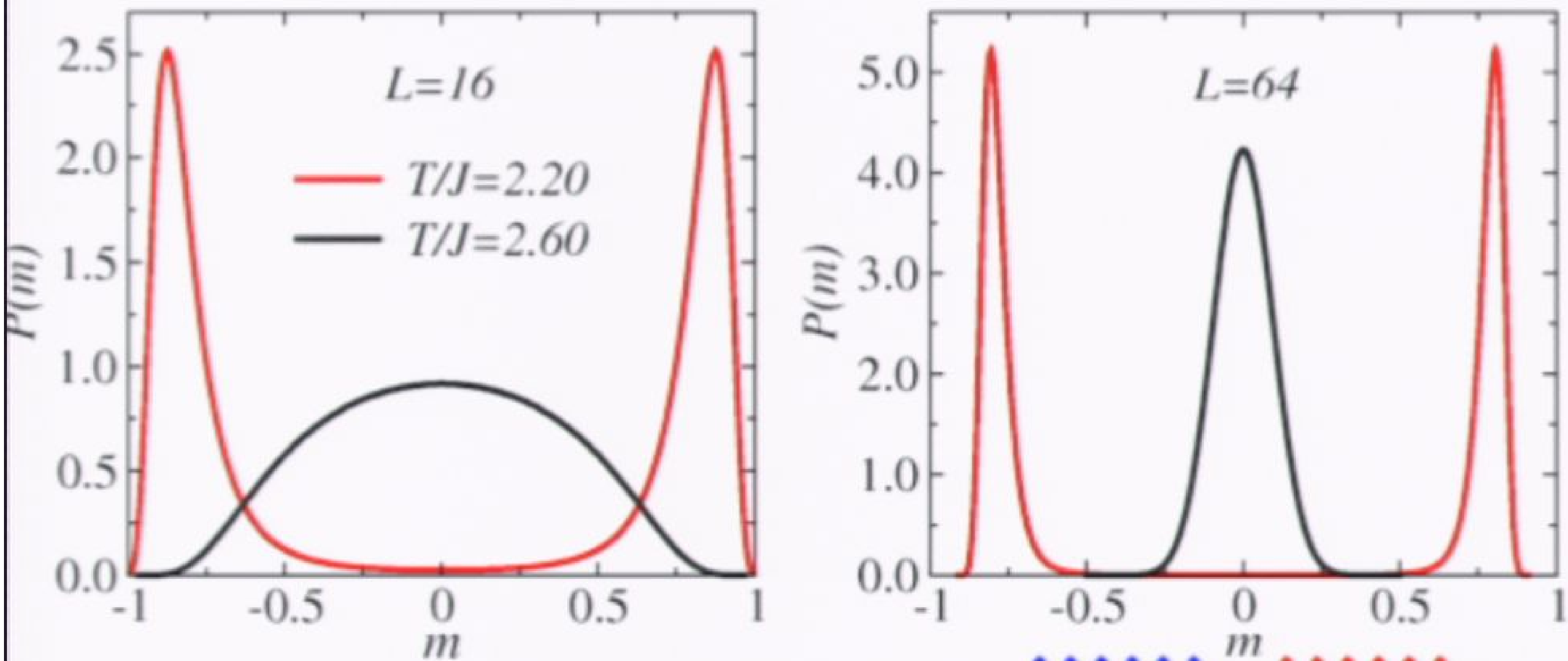

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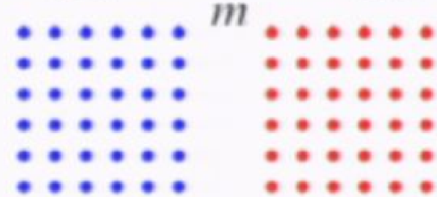

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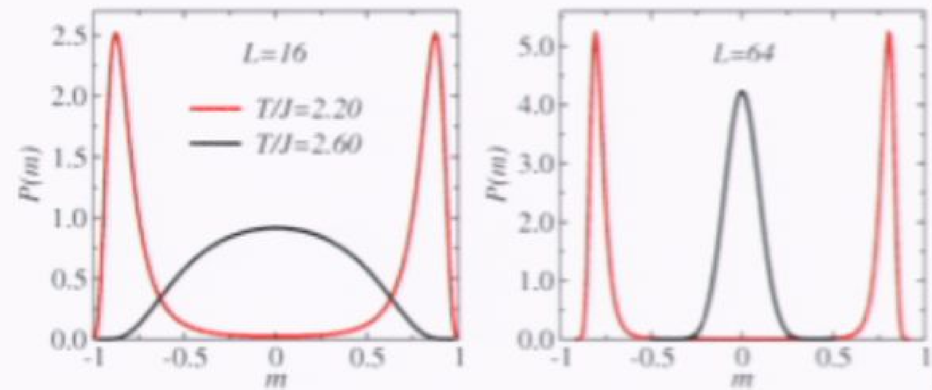
Why this peak structure? balance between

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

Binder ratios and cumulants



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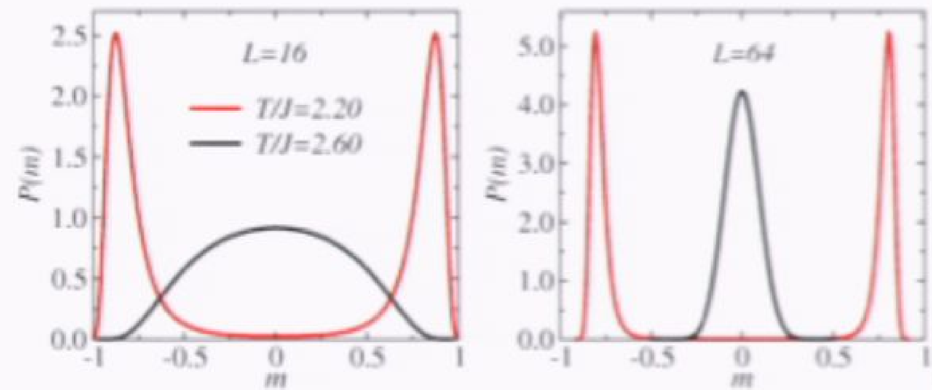

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$$R_2 = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}$$

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

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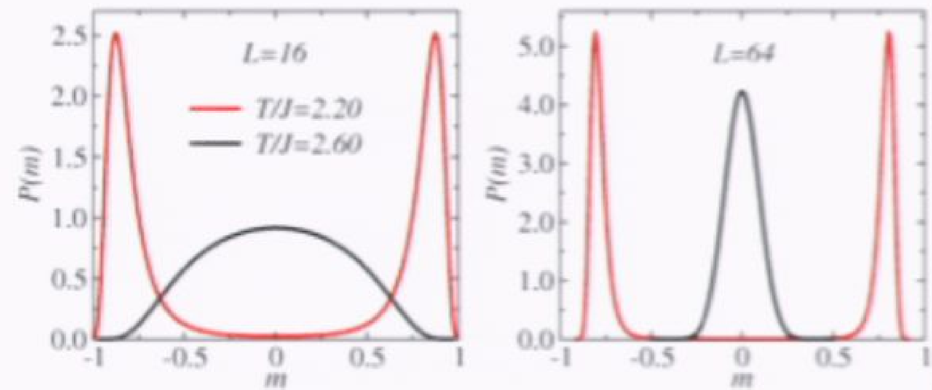

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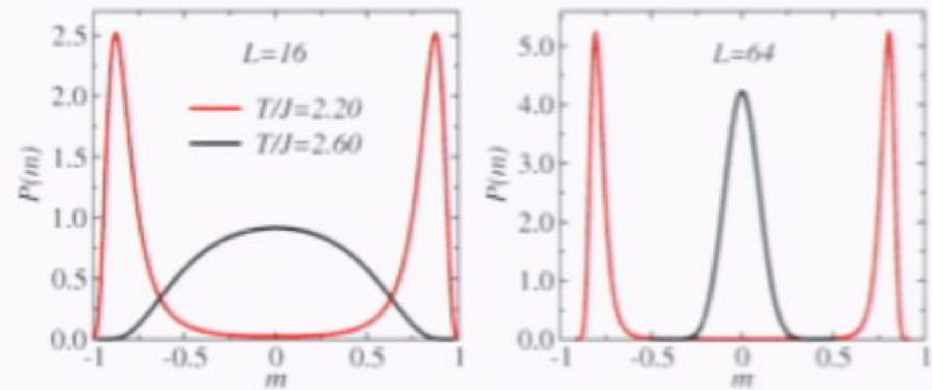

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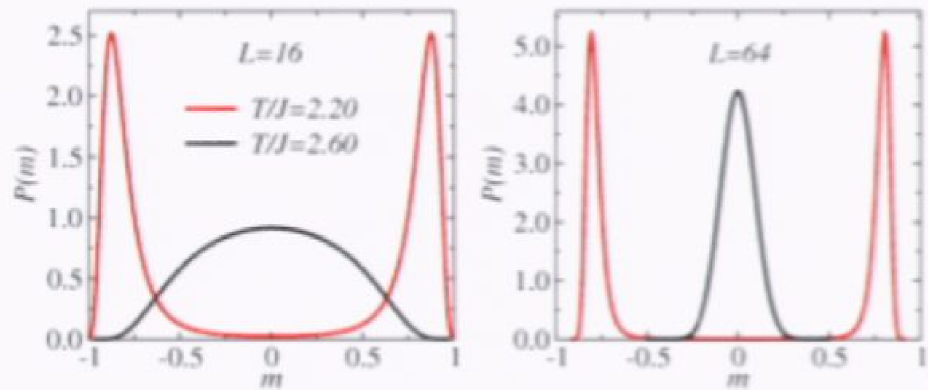

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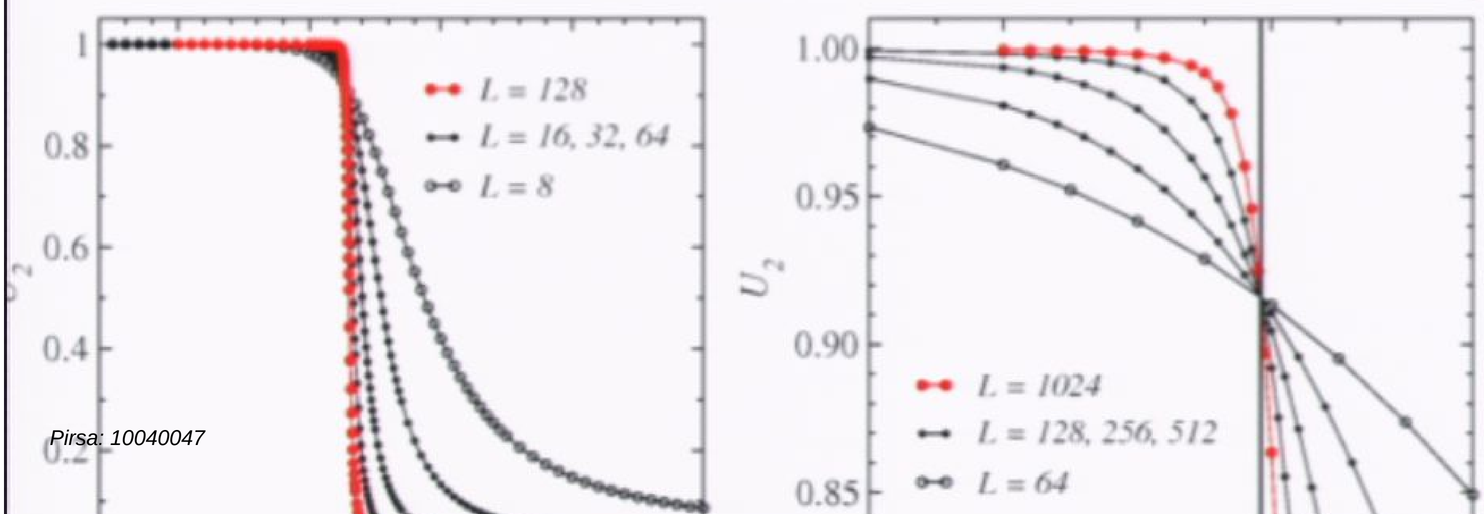
2D Ising model; MC results



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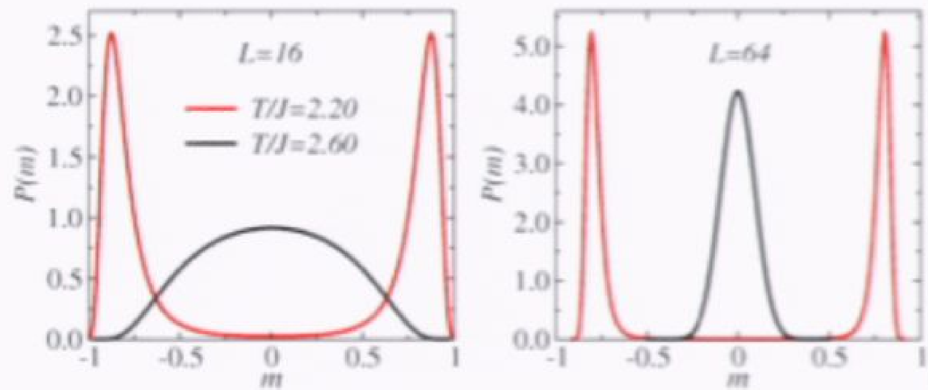

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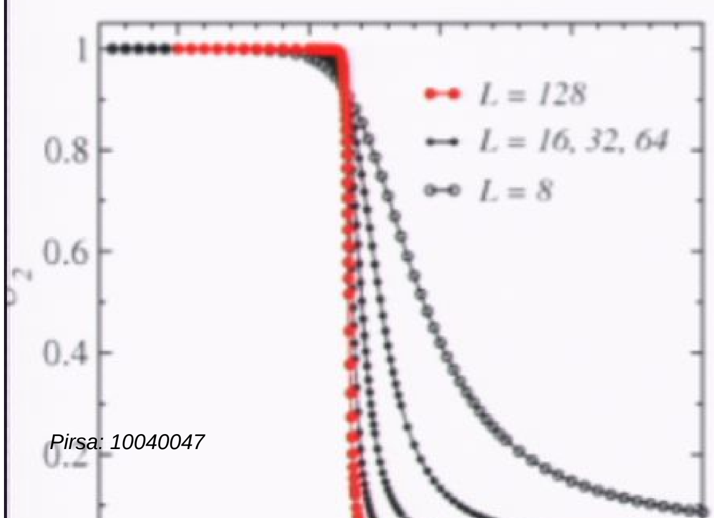

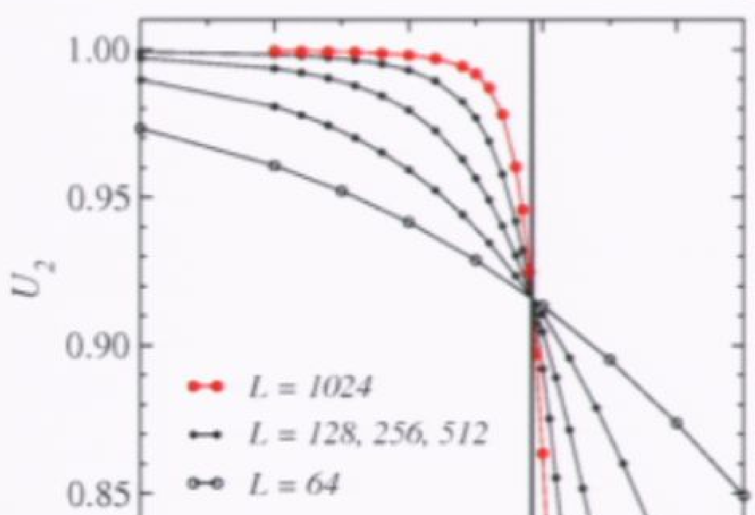

Curves for different L normally cross each other close to T_c

Extrapolate crossing for sizes L and 2L to infinite size

- converges faster than

Computing expectation values and their statistical errors

Definition: Monte Carlo sweep = N spin-flip attempts

- a natural unit of simulation "time"
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If M is sufficiently large (>> autocorrelation time) the average and error are

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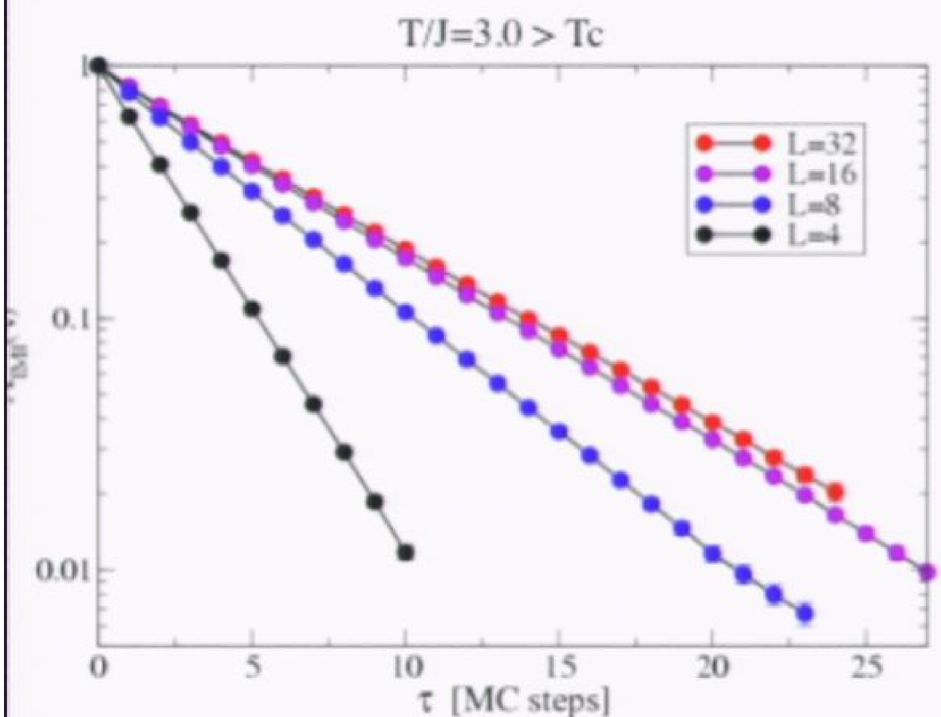

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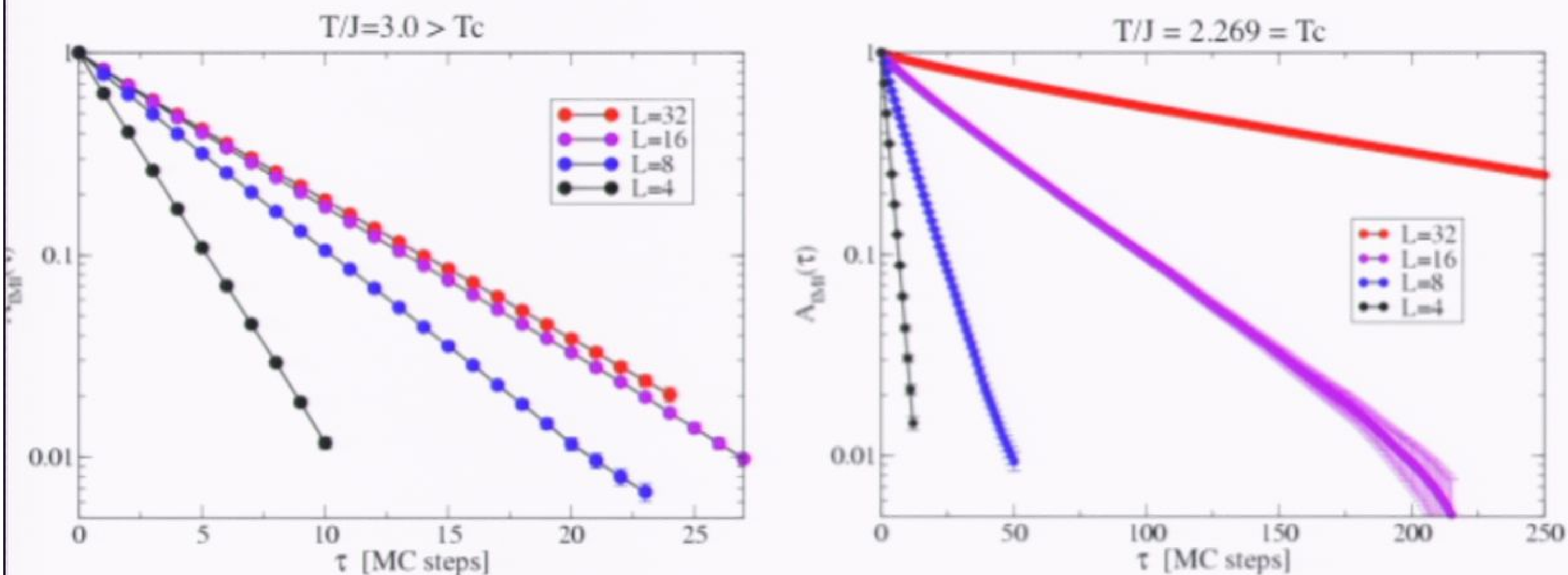

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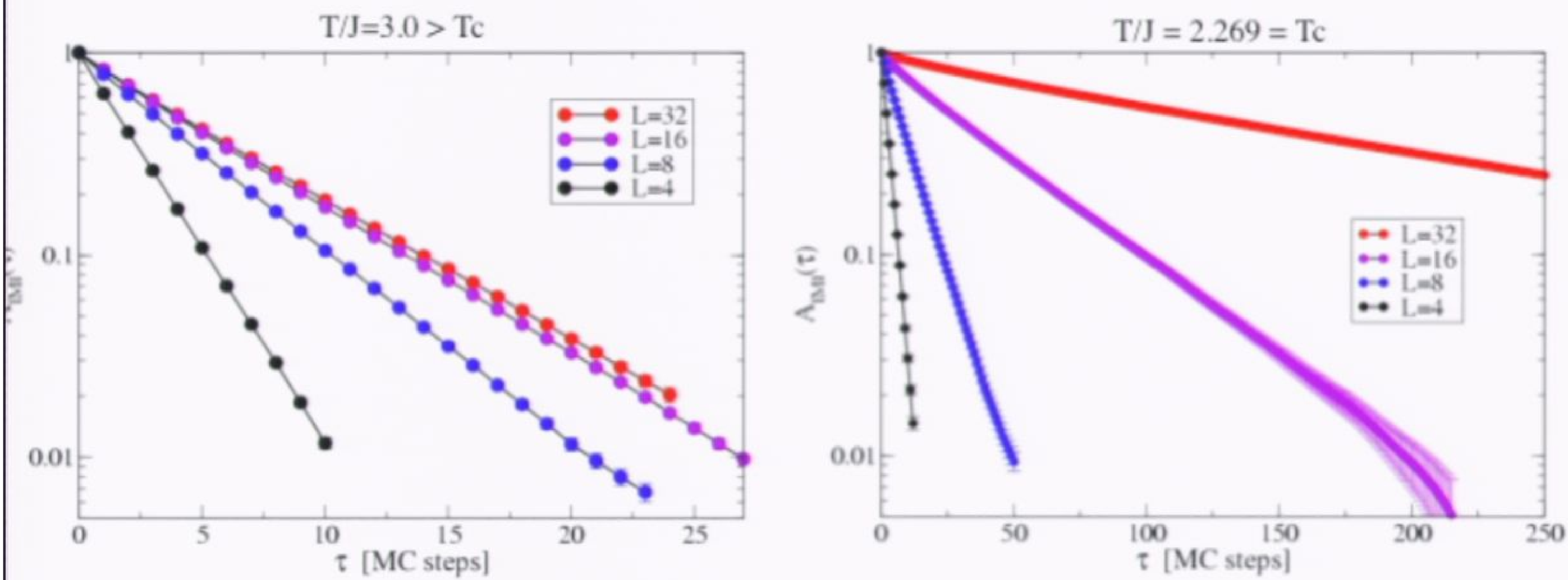

This problem can be largely overcome by using **cluster algorithms**

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

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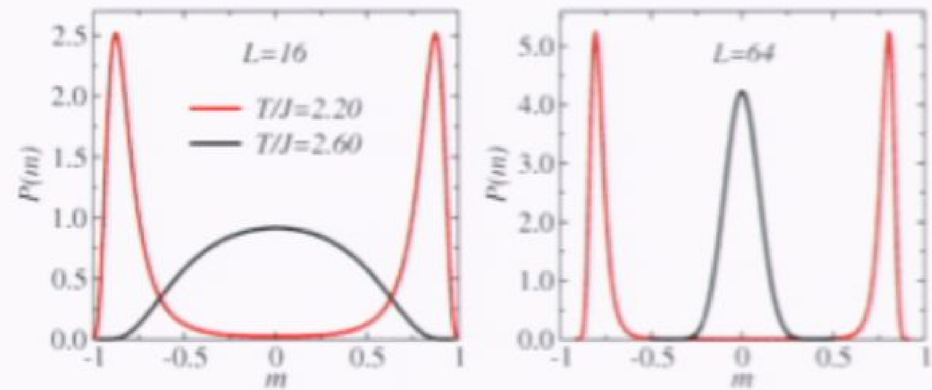
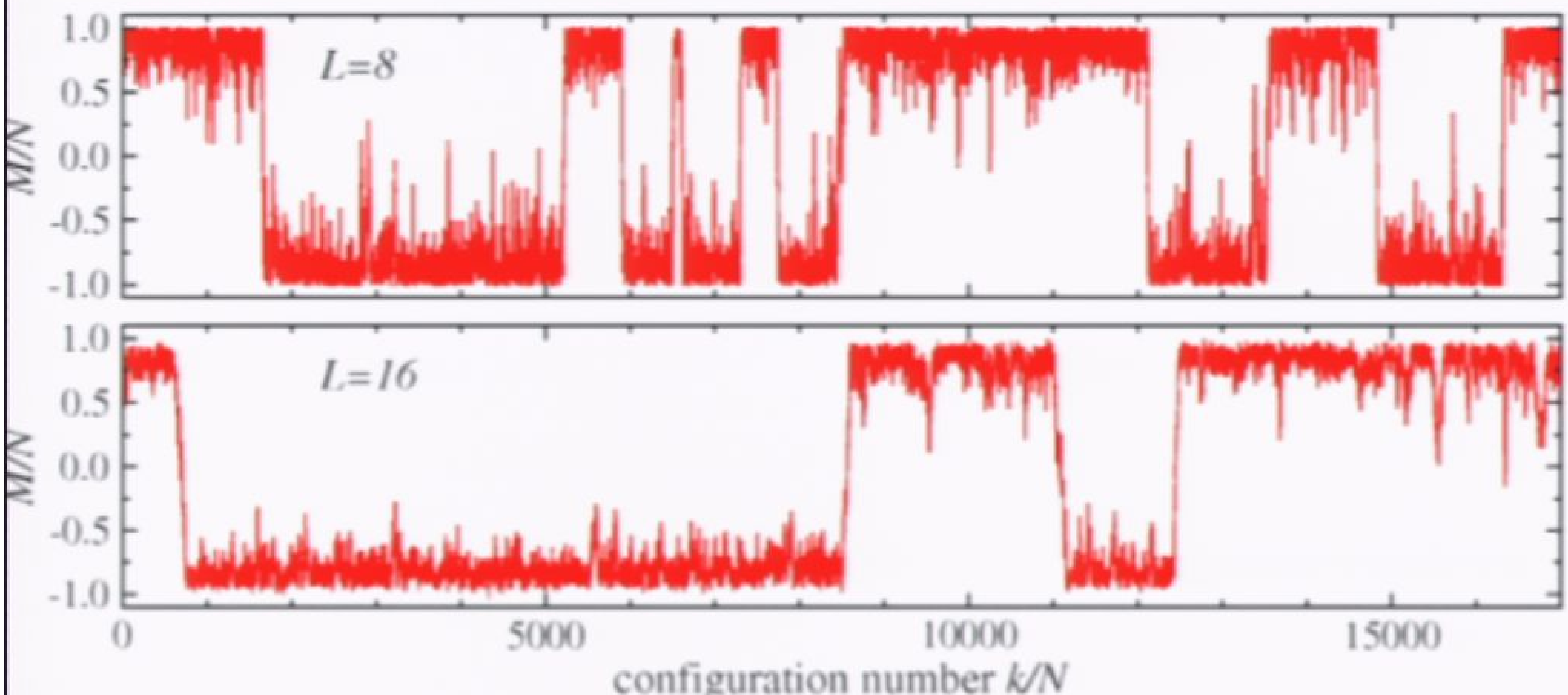


Symmetry breaking (magnetic phase transition) for h=0

A magnetized state, $\langle m \rangle \neq 0$, breaks a symmetry (E invariant under all $\boldsymbol{\sigma_i} \rightarrow \boldsymbol{-\sigma_i}$)

- strictly, mathematically we must have $\langle m \rangle = 0$
- symmetry breaking (phase transition) can take place when $N \rightarrow \infty$
- how can we understand the symmetry breaking for N large but finite?

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



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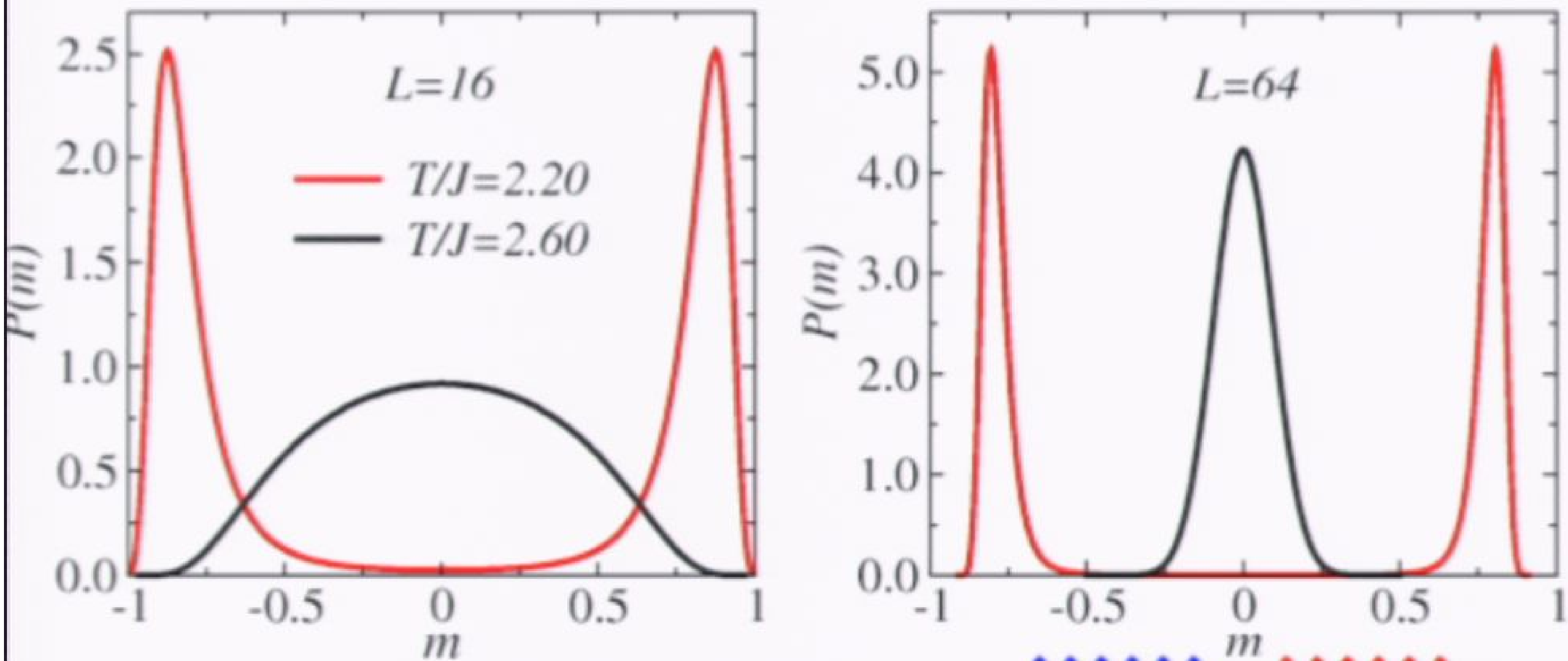

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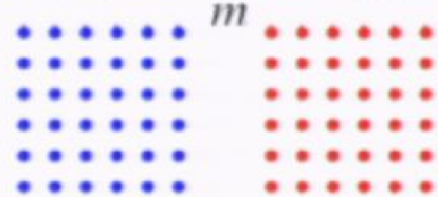

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