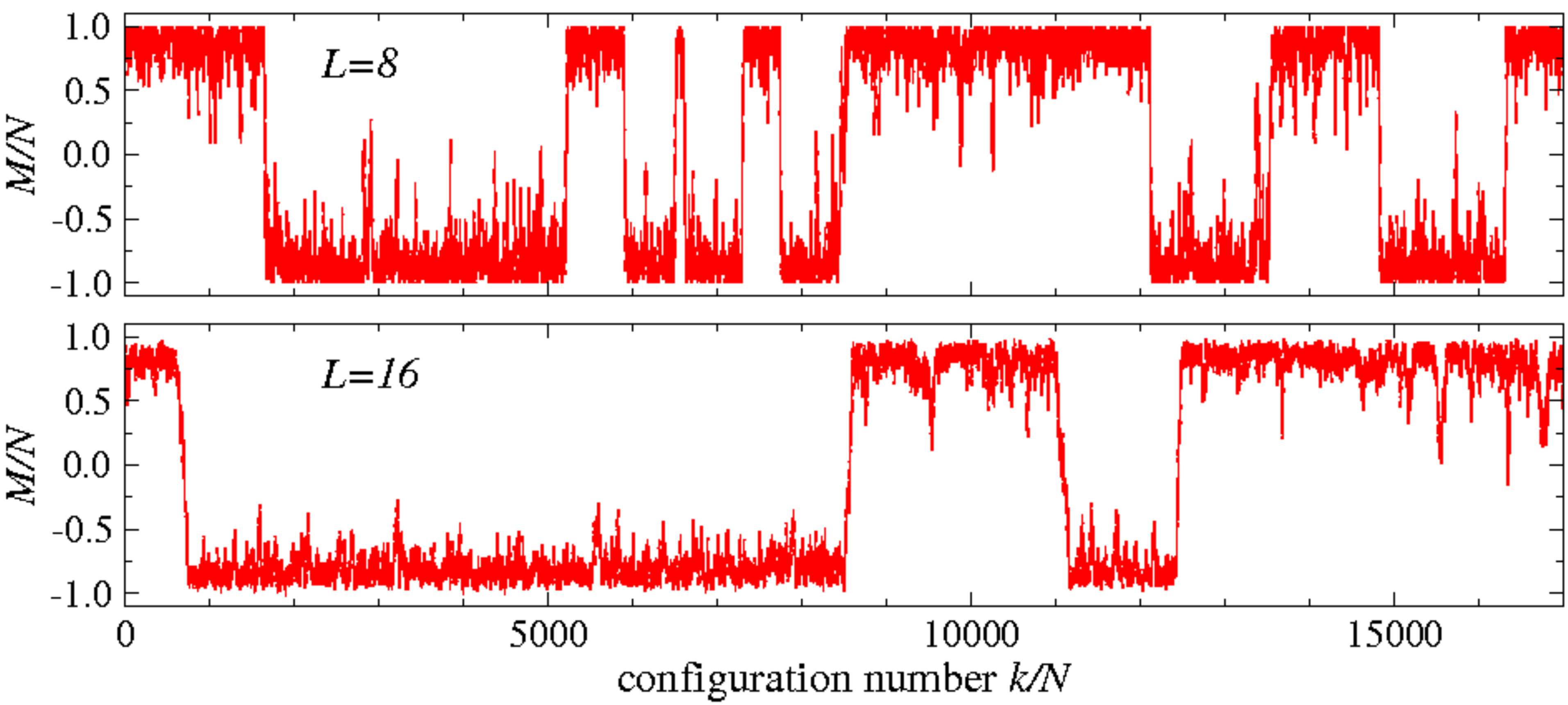
Illustration of simulation

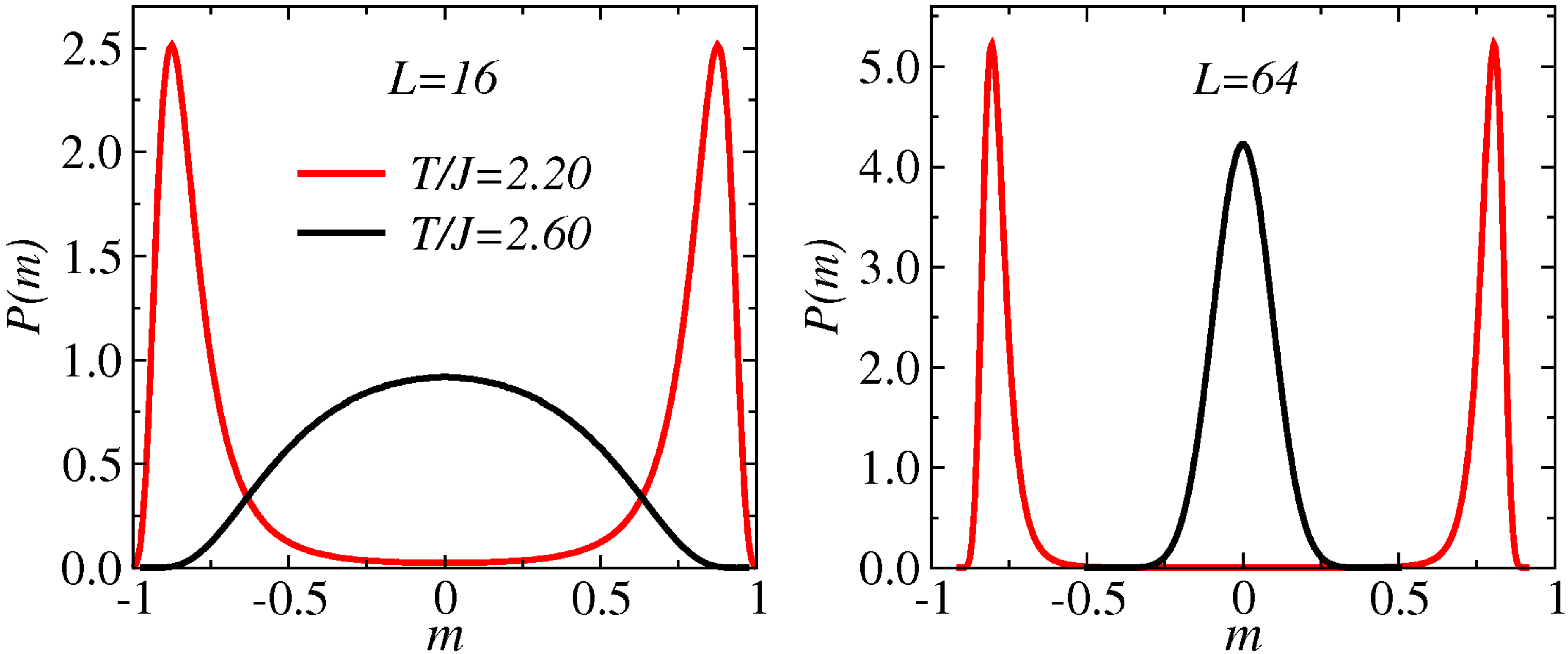
Evolution of the magnetization, 2D Ising model, T/J=2.2 (below Tc)

- <M>=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>Tc
- double peak around +<m> and-<m> for T<Tc



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

Measuring physical observables

Order parameter of ferromagnetic transition: Magnetization

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

Expectation vanishes for finite system; calculate $\langle |m| \rangle, \ \langle m^2 \rangle$

Susceptibility: Linear response of <m> to external field

$$E = E_0 - hM, \qquad E_0 = J \sum_{i,j} \sigma_i \sigma_j$$

$$\chi = \left. \frac{d\langle m \rangle}{dh} \right|_{h=0}$$

Deriving Monte Carlo estimator

$$\langle m \rangle = \frac{1}{Z} \sum_S m \mathrm{e}^{-(E_0 - hM)/T}, \quad Z = \sum_S \mathrm{e}^{-(E_0 - hM)/T}$$

$$\chi = -\frac{dZ/dh}{Z^2} \sum_S m \mathrm{e}^{-(E_0 - hM)/T} + \frac{1}{Z}\frac{1}{T} \sum_S m M \mathrm{e}^{-(E_0 - hM)/T}$$

$$\frac{dZ}{dh} = \frac{1}{T} \sum_S M \mathrm{e}^{-(E_0 - hM)/T}$$

$$\chi = \frac{1}{N}\frac{1}{T}\left(\langle M^2\rangle - \langle M\rangle^2\right) = \frac{1}{N}\frac{1}{T}\langle M^2\rangle, \quad (h=0)$$

Extrapolating to infinite size, this gives the correct result only in the disordered phase (gives infinite susceptibility for T<Tc)

We can also define the susceptibility estimator as

$$\chi = \frac{1}{N}\frac{1}{T}\left(\langle M^2\rangle - \langle |M|\rangle^2\right)$$

Gives correct infinite-size extrapolation for any T

Specific heat

$$C = \frac{1}{N}\frac{dE}{dT} = \frac{1}{N}\frac{d}{dT}\sum_C E(C)\mathrm{e}^{-E(C)/T} = \frac{1}{N}\frac{1}{T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right)$$

Correlation function

$$C(\vec{r}) = \langle \sigma_i \sigma_{j(\vec{r},i)}\rangle$$

Average over all spins i

$$C(\vec{r}) = \frac{1}{N}\sum_{i=1}^{N}\langle \sigma_i \sigma_{j(\vec{r},i)}\rangle$$

Statistical errors ("error bars")

Calculation based on M "bins". What is the statistical error?
Consider M independent calculations (each based on n configs)

Statistically independent averages $\bar{A}_i, \; i = 1, \ldots, M$

Full average

$$\bar{A} = \frac{1}{M}\sum_{i=1}^{M} A_i$$

Standard deviation

$$\sigma' = \sqrt{\frac{1}{M}\sum_{i=1}^{M}(\bar{A}_i^2 - \bar{A}^2)}$$

But, we want the standard deviation of the average

$$\sigma = \sqrt{\frac{1}{M(M-1)}\sum_{i=1}^{M}(\bar{A}_i^2 - \bar{A}^2)}$$

The bins have to be long enough (n large enough)
to be essentially statistically independent
(can be quantified by "autocorrelations" - later)

Adding an external magnetic field

$$E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i$$

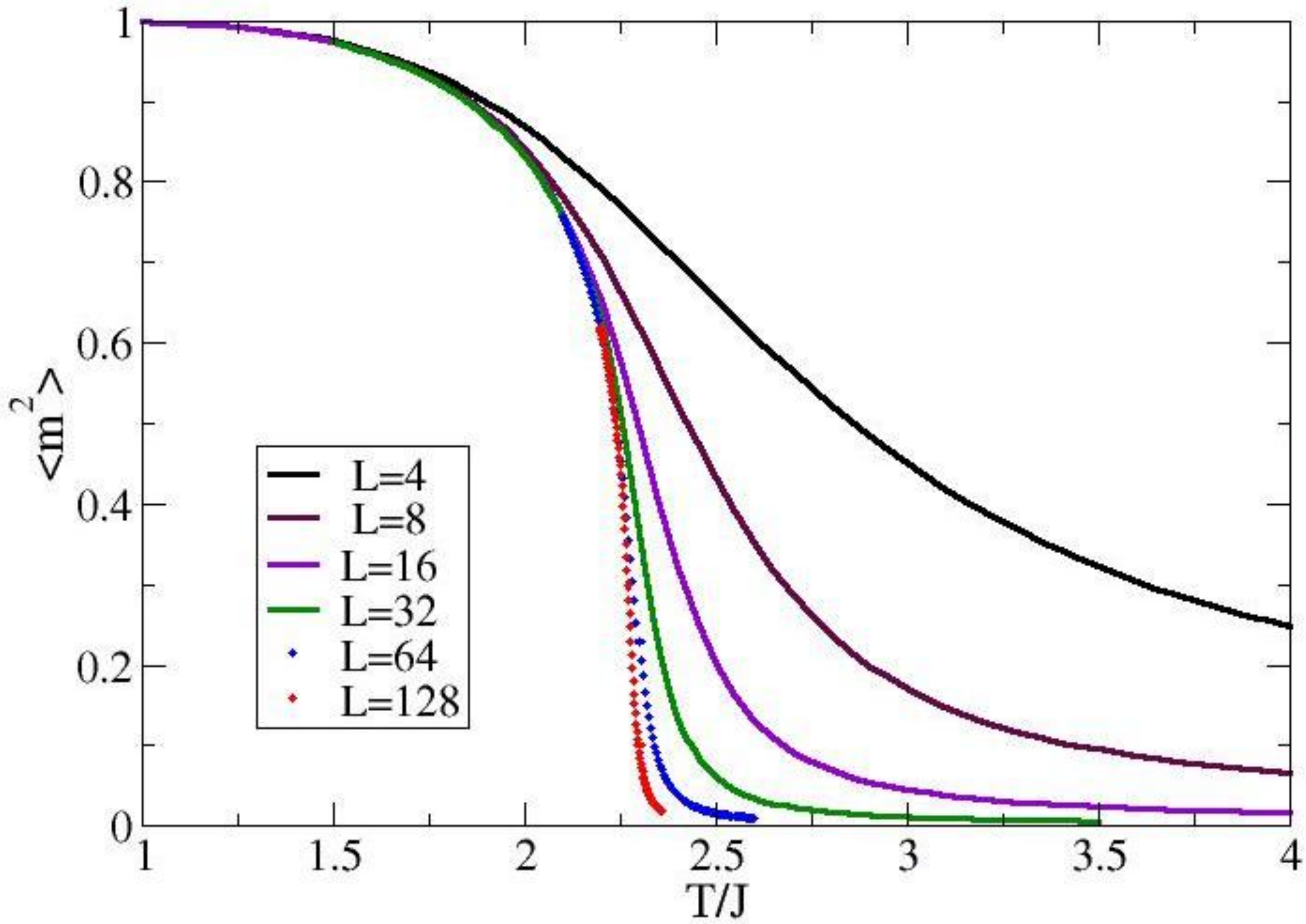
For h>0, the average magnetization <M> > 0

Simple change in the acceptance probability

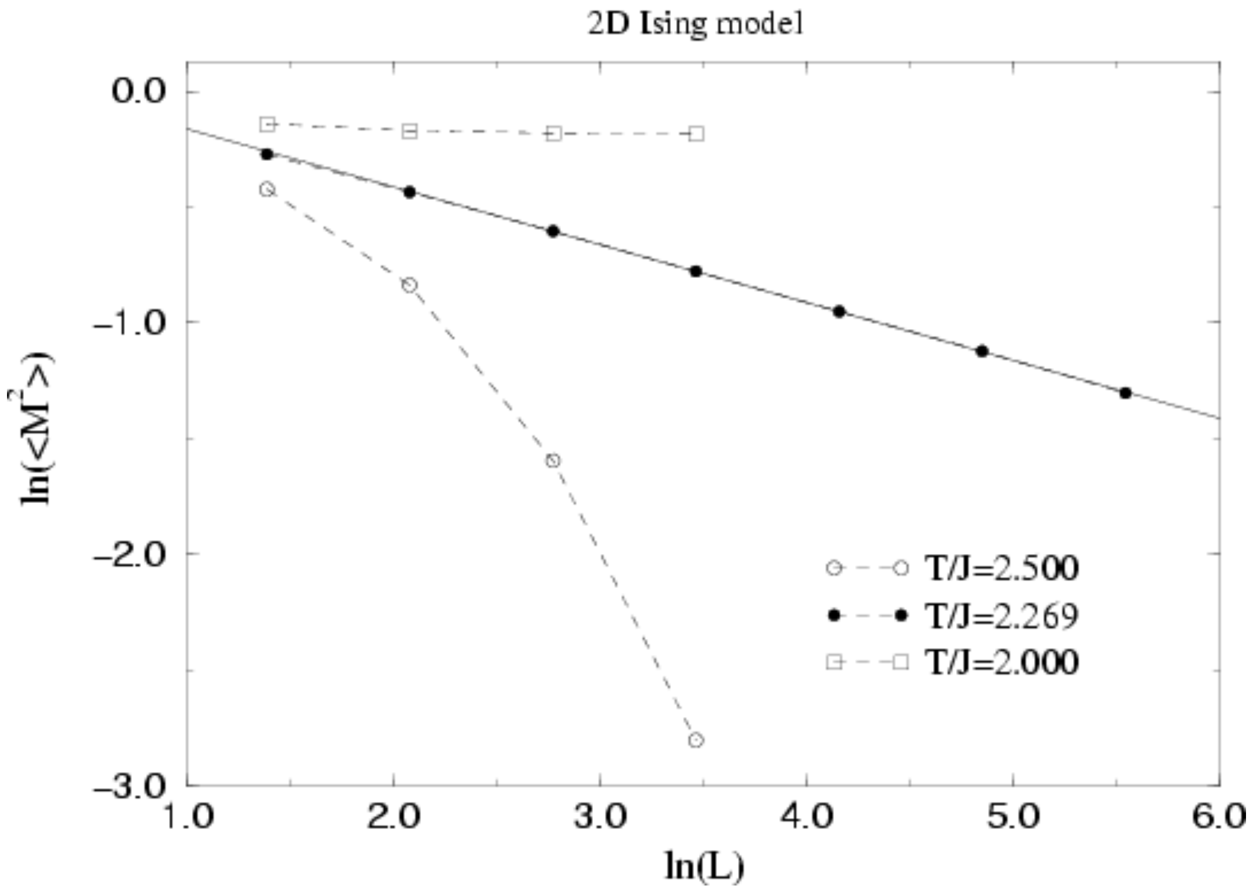
$$P(S \to \tilde{S}_j) = \min \left[\frac{W(\tilde{S}_j)}{W(S)}, 1 \right]$$

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

Squared magnetization for different system sizes (no external field): development of phase transition



Finite-size scaling



$T > T_c$: $\langle M^2 \rangle \rightarrow 0$ (exponentially)

$T = T_c$: $\langle M^2 \rangle \rightarrow 0$ (power law)

$T < T_c$: $\langle M^2 \rangle \rightarrow$ constant > 0

Extracting an exponent: $A = aL^\alpha \longrightarrow \ln(A) = \ln(a) + \alpha \ln(L)$

- Power-law: straight line when plotted on log-log scale

Critical behavior and scaling

Correlation length ξ defined in terms of correlation function

$$C(\vec{r}_j - \vec{r}_j) = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle^2 \sim \mathrm{e}^{-|\vec{r}_j - \vec{r}_j|/\xi}$$

The correlation length diverges at the critical point

$$\xi \sim t^{-\nu}, \qquad t = \frac{|T - T_c|}{T_c} \quad \text{(reduced temperature)}$$

ν is an example of a critical exponent

Universality

Critical exponents do not depend on microscopic details of the interactions; only on the dimensionality of the system and the order parameter:

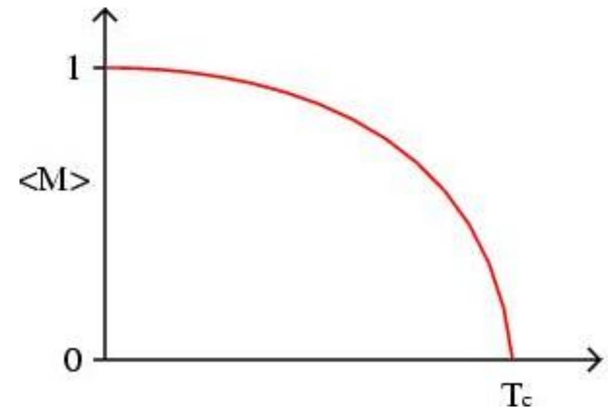
- Ising, gas/liquid (scalar Z2-symmetric order parameter)
- XY spins, phase of superconductor (2D, O(2) order parameter)
- Heisenberg spins (3D, O(3) order parameter)

Phase transitions fall into universality classes characterized by different sets of critical exponents

Other critical exponents

Order parameter for T < Tc (e.g., magnetization)

$$\langle m \rangle \sim (T_c - T)^\beta$$



In practice, calculate $\langle |m| \rangle, \quad \langle m^2 \rangle$

Susceptibility corresponding to order

$$\chi = \frac{1}{N}\frac{1}{T}\left(\langle M^2 \rangle - \langle |M| \rangle^2\right)$$

Diverges at the critical point

$$\chi \sim t^{-\gamma}$$

Specific heat $\quad C = \frac{1}{N}\frac{1}{T^2}\left(\langle E^2 \rangle - \langle E \rangle^2\right)$

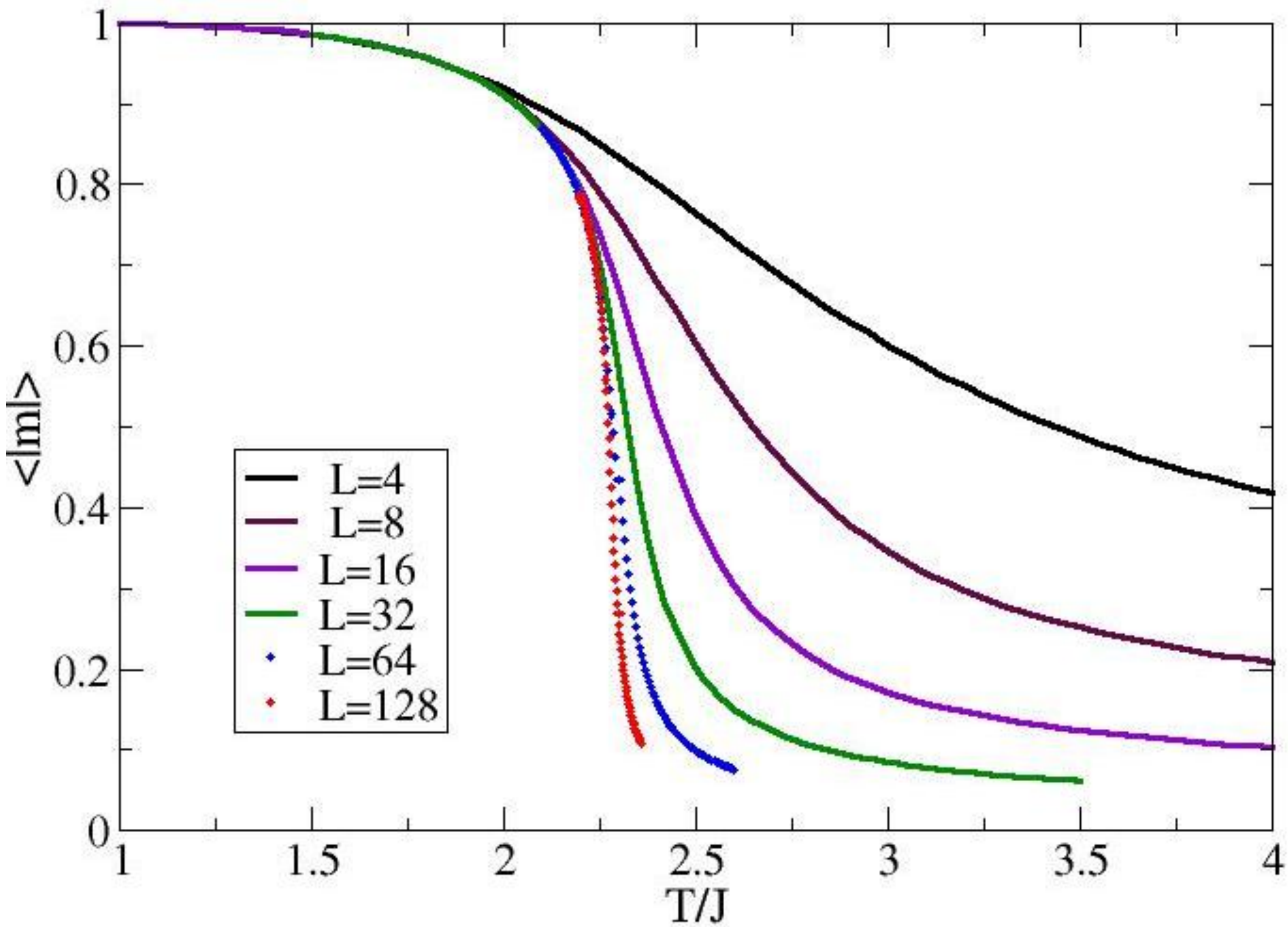
Singular at Tc

$$C \sim t^{-\alpha}$$

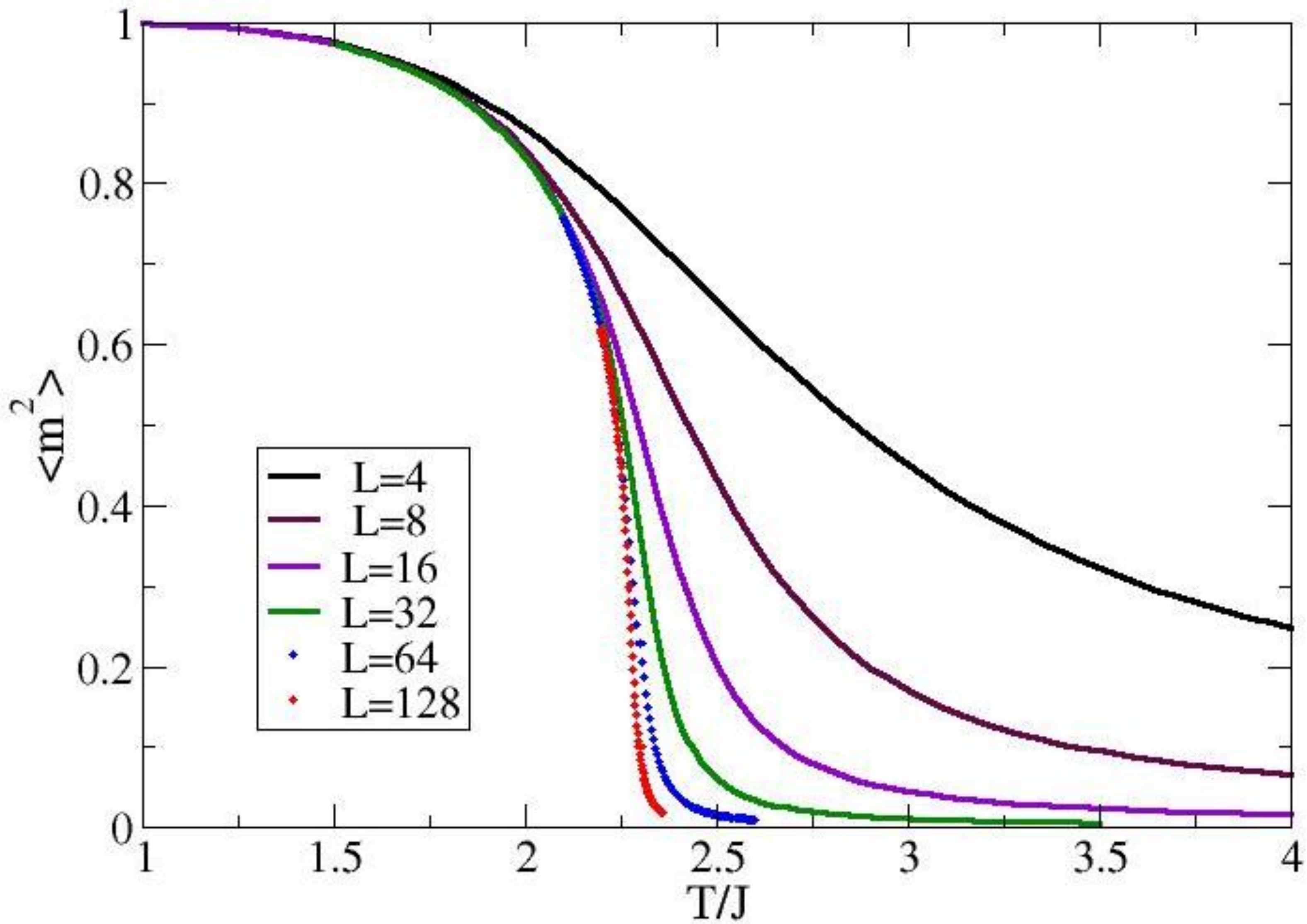
The exponent α can be positive or negative (no divergence
If negative; 0 can correspond to log divergence)

Magnetization of 2D Ising ferromagnet

$\langle |m| \rangle \sim (T_c - T)^{\beta}, \quad (T < T_c)$ for infinite system



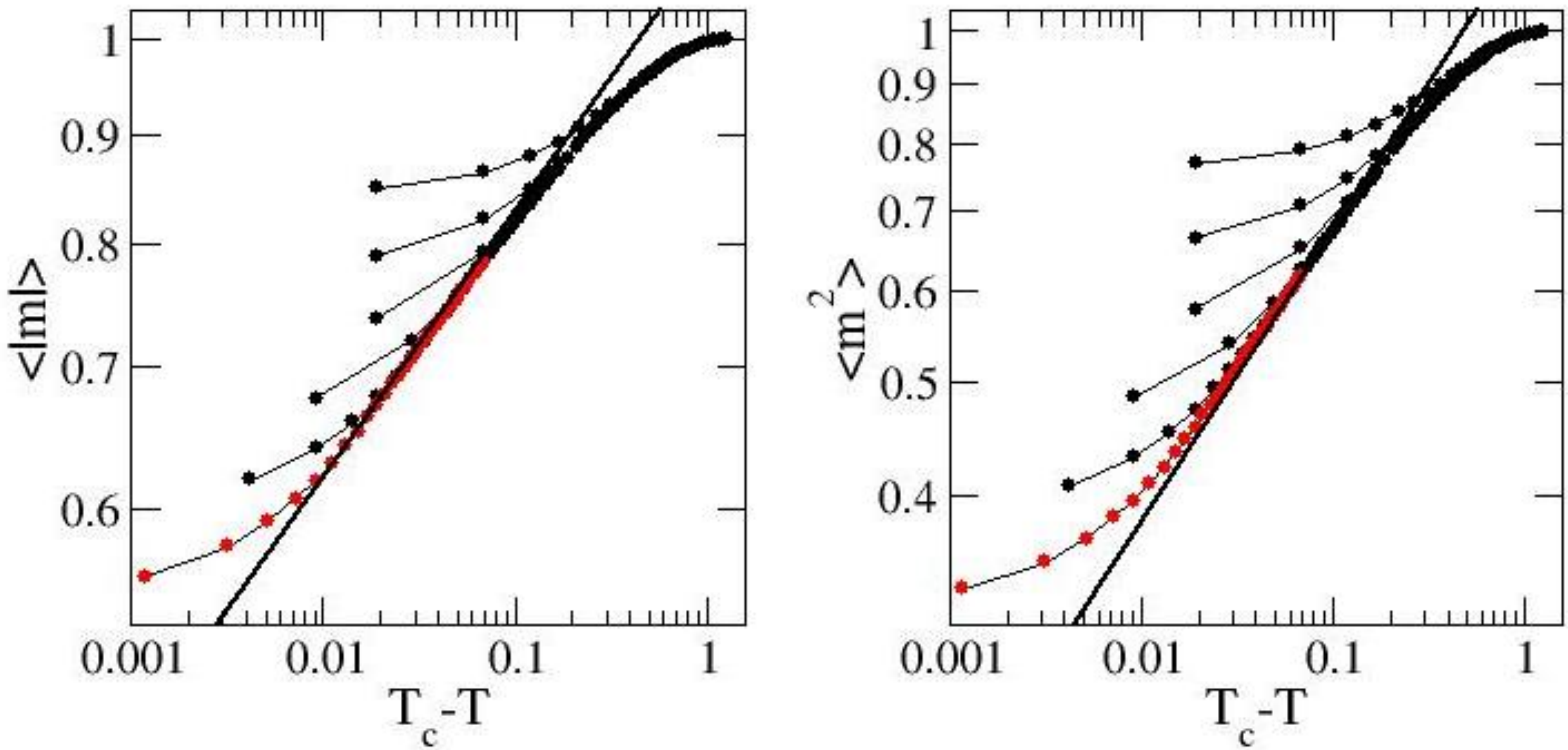
Magnetization squared $\langle m^2 \rangle \sim (T_c - T)^{2\beta}, \quad (T < T_c)$



The exponent β can be extracted for large L

Comparison with known 2D Ising model exponent

$$\beta = 1/8$$



If Tc is not known, use it as an adjustable parameter and look for power-law behavior