"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

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

$$\chi = \left. \frac{d\langle m \rangle}{dh} \right|_{h=0}$$ (we can also consider h>0 here)

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

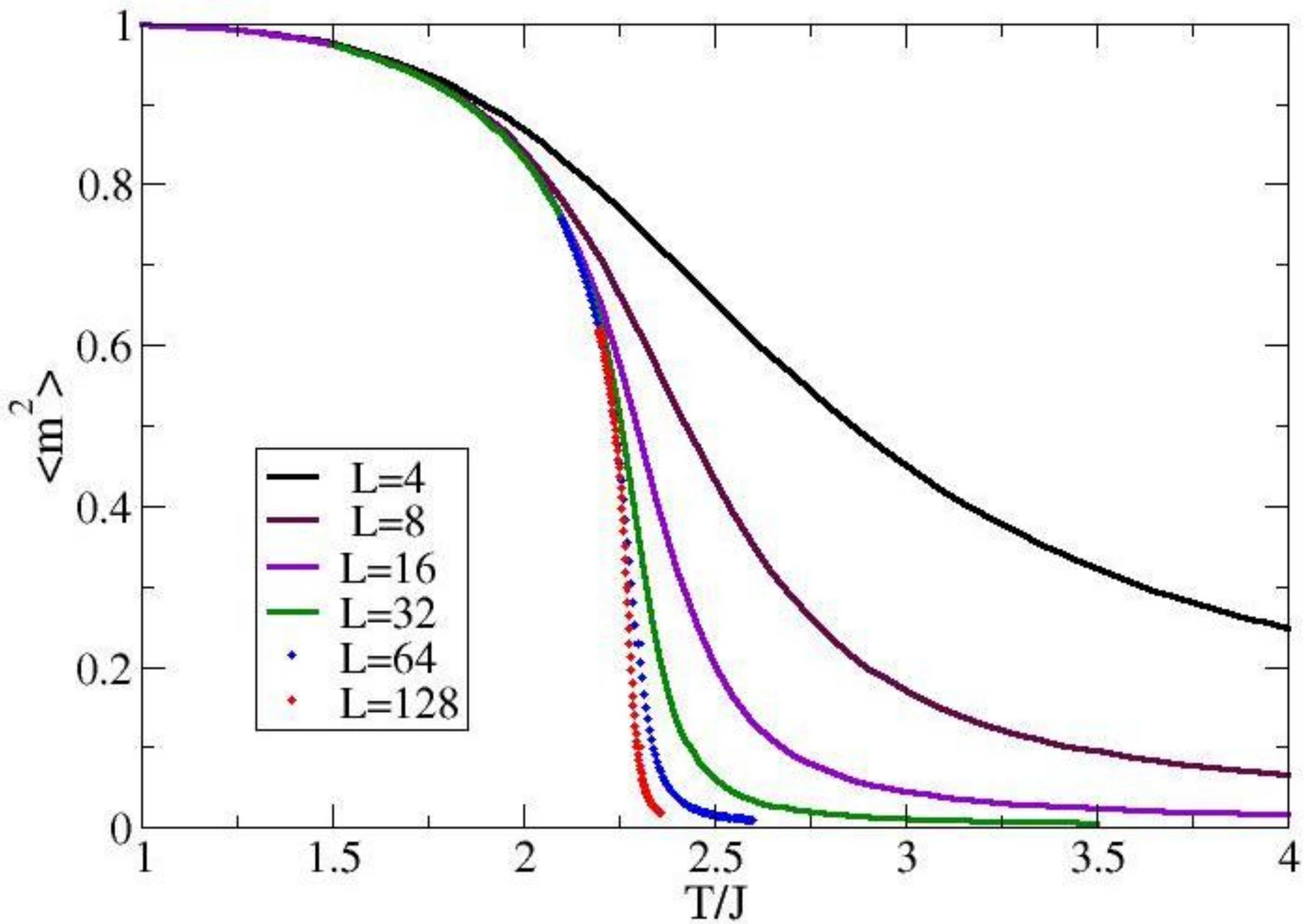
$$\sigma' = \sqrt{\frac{1}{M} \sum_{i=1}^{M} (\bar{A}_i^2 - \bar{A}^2)}$$

But, we want the standard deviation of the average

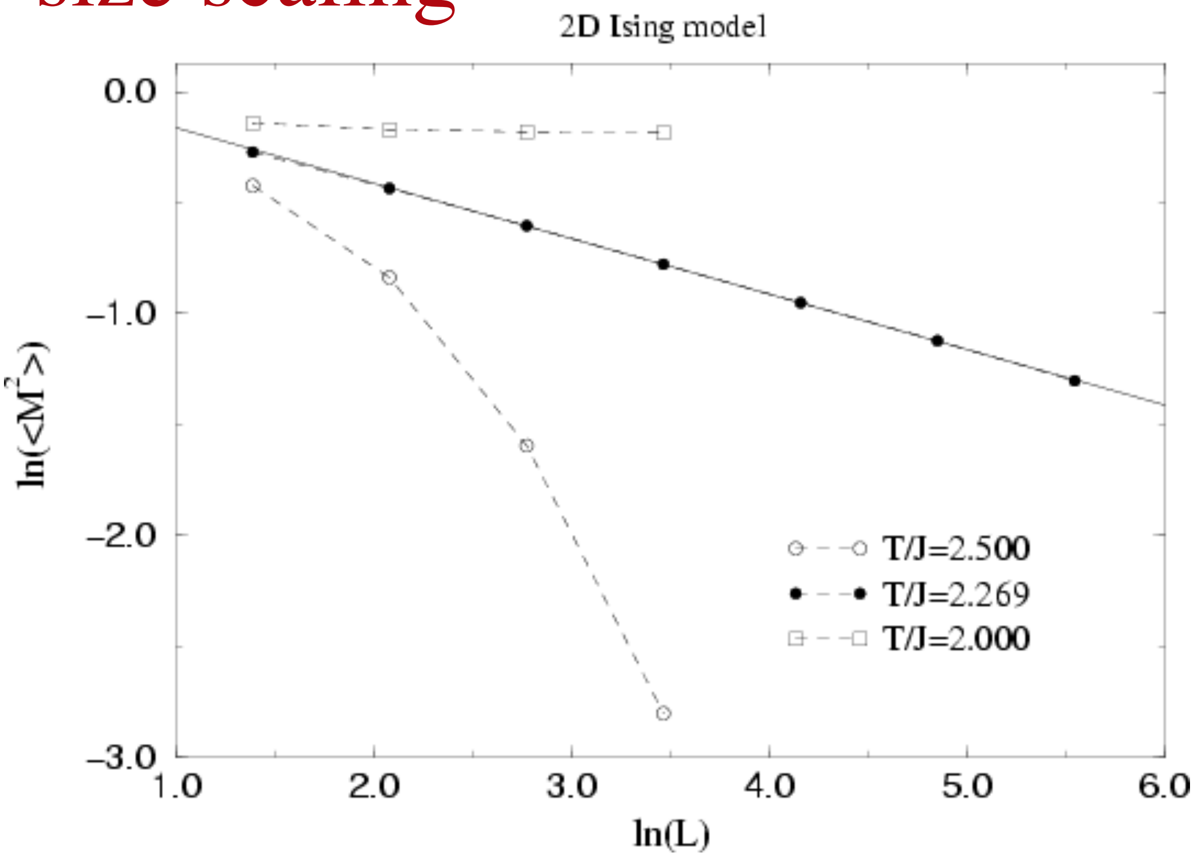
$$\sigma = \sqrt{\frac{1}{M(M-1)} \sum_{i=1}^{M} (\bar{A}_i^2 - \bar{A}^2)}$$

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

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



Finite-size scaling



$T > T_c$: $\langle M^2 \rangle \rightarrow 0$ (as $1/L^2$, trivial from short-range correlations)

$T = T_c$: $\langle M^2 \rangle \rightarrow 0$ (non-trivial 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
- The $1/L^2$ form for T/J=2.5 not yet seen because of cross-over behavior; close to the critical point, larger L required

Critical behavior and scaling

Correlation length ξ defined in terms of correlation function

$$C(\vec{r}_{ij}) = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle^2 \sim \mathrm{e}^{-r_{ij}/\xi}, \quad \vec{r}_{ij} \equiv |\vec{r}_i - \vec{r}_j|$$

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