ICTP School in Computational Condensed Matter Physics:
From Atomistic Simulations to Universal Model Hamiltonians
September 2015

Lecture 3
Systematic finite-size scaling methods for analyzing critical points (and ordered phases)

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Lecture outline

- 2D Heisenberg antiferromagnets, order and criticality

- 3D dimerized models and $TlCuCl_3$

- Crossing-point methods for critical points
    - formal analysis of scaling function
    - tests on 2D Ising model

- Pitfalls in order-parameter extrapolations

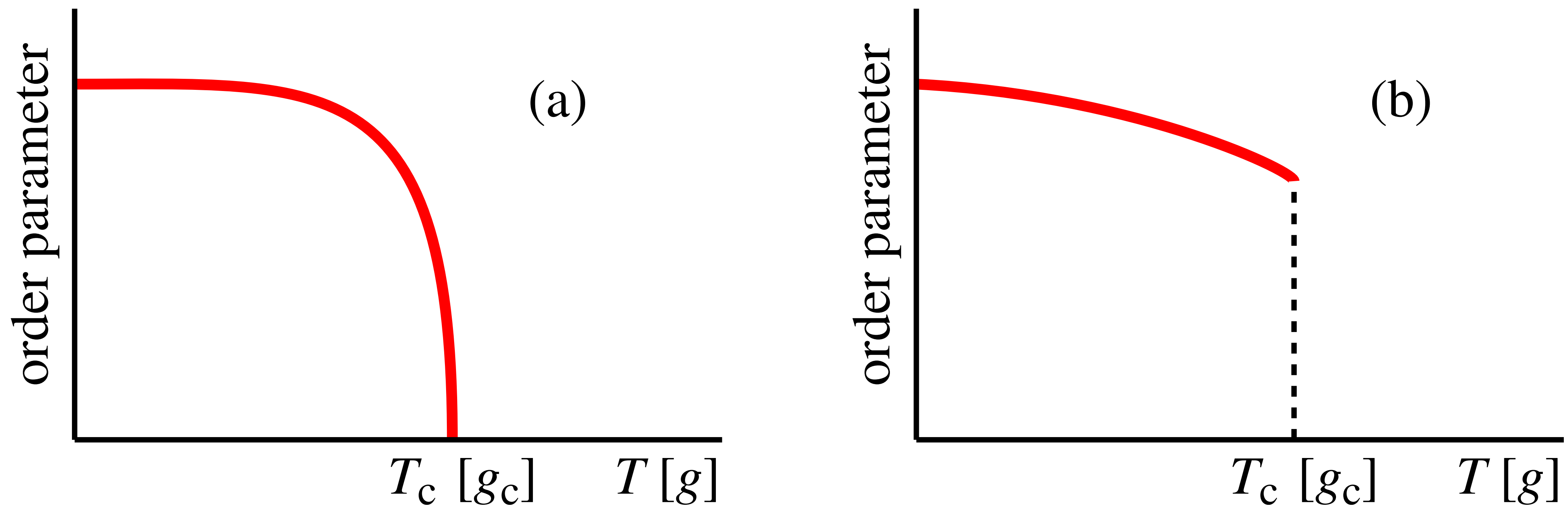
Classical and quantum phase transitions

Classical (thermal) phase transition

- Fluctuations regulated by temperature T>0

Quantum (ground state, T=0) phase transition

- Fluctuations regulated by parameter g in Hamiltonian



In both cases phase transitions can be

- <u>first-order (discontinuous):</u> finite correlation length ξ as $g \to g_c$ or $g \to g_c$
- <u>continuous:</u> correlation length diverges, **$\xi \sim |g-g_c|^{-\nu}$** or **$\xi \sim |T-T_c|^{-\nu}$**

There are many similarities between classical and quantum transitions
- and also important differences

We will discuss continuous phase transitions

Finite-size scaling and extrapolations

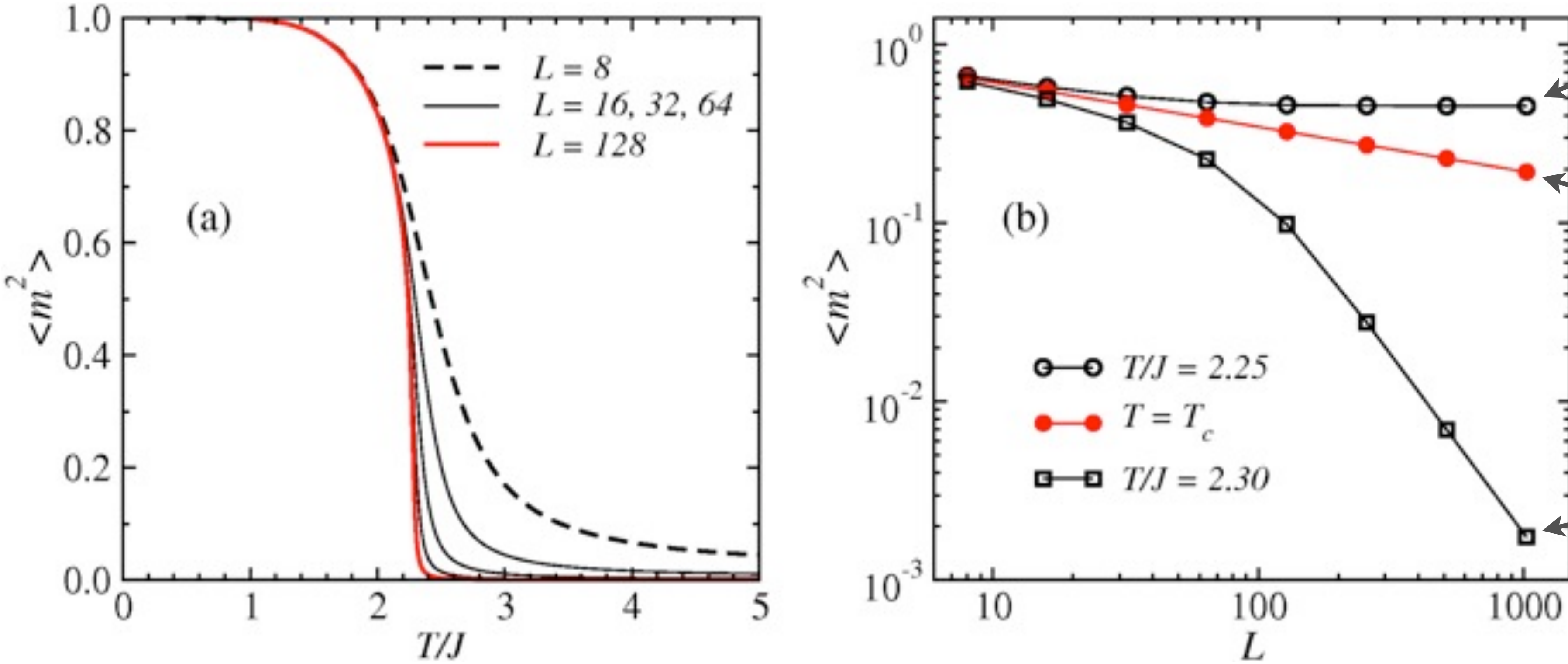
Monte Carlo simulations are done on finite lattices
- typically periodic boundary conditions

We have to analyze the size dependence of computed quantities and extract the behavior in the thermodynamic limit
- using input from theoretical expectations as much as possible

Example: 2D Ising model

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \qquad m = \frac{1}{N} \sum_{i=1}^{N} \sigma_i, \qquad \sigma_i \in \{-1, +1\}$$

Squared magnetization (order parameter) for L×L Ising lattices



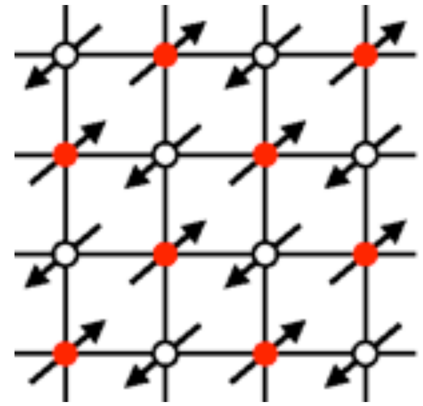
ordered (size independent)

critical scaling (non-trivial power-law)

disordered (trivial power-law $1/N = 1/L^{-2}$)

Long-range order in 2D S=1/2 Heisenberg antiferromagnet

$$\mathbf{H} = \mathbf{J} \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \mathbf{S_i} \cdot \mathbf{S_j}$$



Sublattice magnetization

$$\vec{m}_s = \frac{1}{N} \sum_{i=1}^{N} \phi_i \vec{S}_i, \qquad \phi_i = (-1)^{x_i+y_i} \quad \text{(2D square lattice)}$$

Long-range order: **$\langle m_s^2 \rangle > 0$ for $N \to \infty$**

Quantum Monte Carlo

- finite-size calculations
- no approximations
- extrapolation to infinite size

Reger & Young 1988

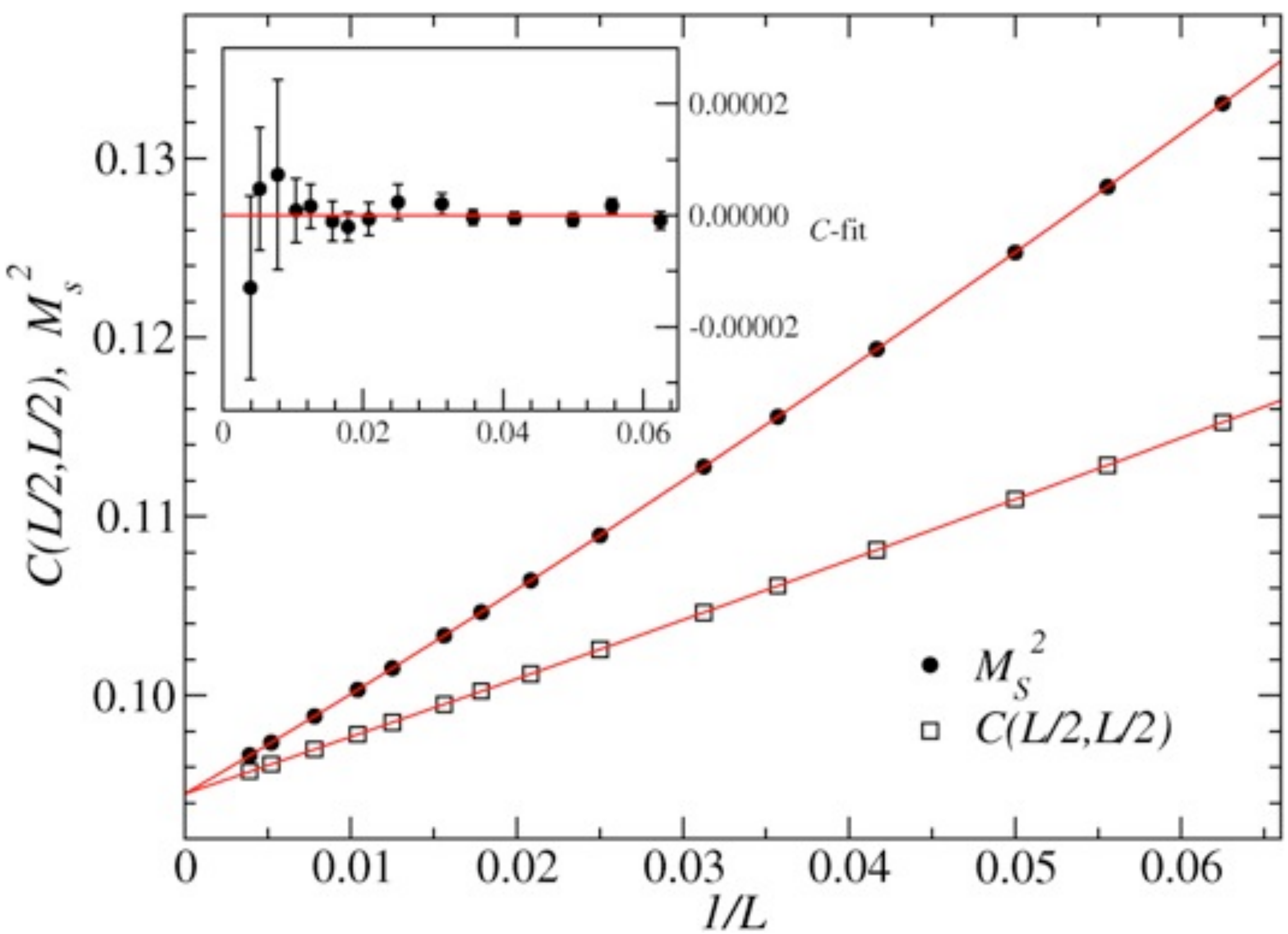
$$m_s = 0.30(2)$$

$$\approx 60\ \%\ \text{of classical value}$$

AWS & HG Evertz 2010

$$m_s = 0.30743(1)$$

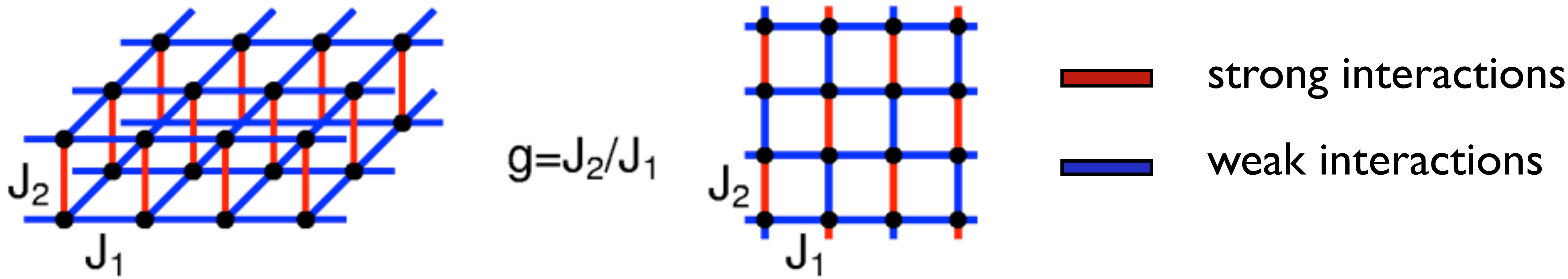
L×L lattices up to 256×256, T=0



T=0 Néel-paramagnetic quantum phase transition

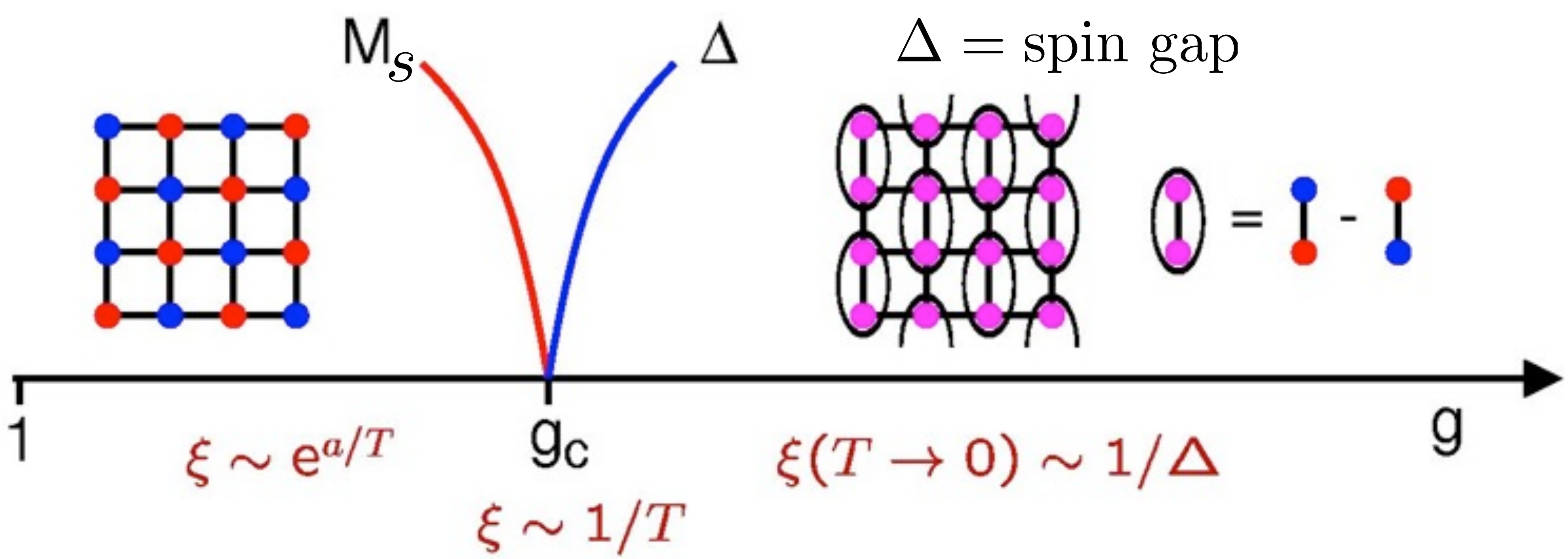
Example: Dimerized S=1/2 Heisenberg models

- every spin belongs to a dimer (strongly-coupled pair)
- many possibilities, e.g., bilayer, dimerized single layer



Singlet formation on strong bonds ➙ Néel - disordered transition

Ground state (T=0) phases

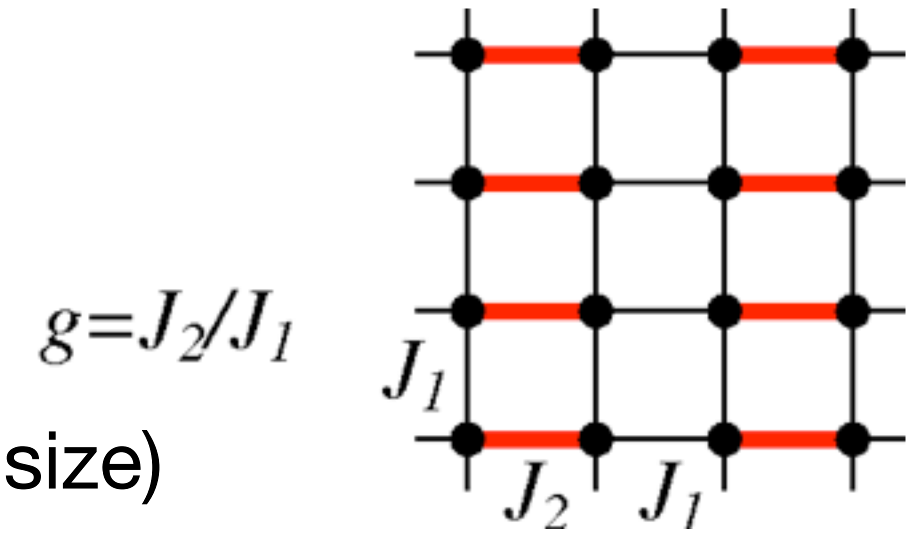


⇒ 3D classical Heisenberg (O3) universality class

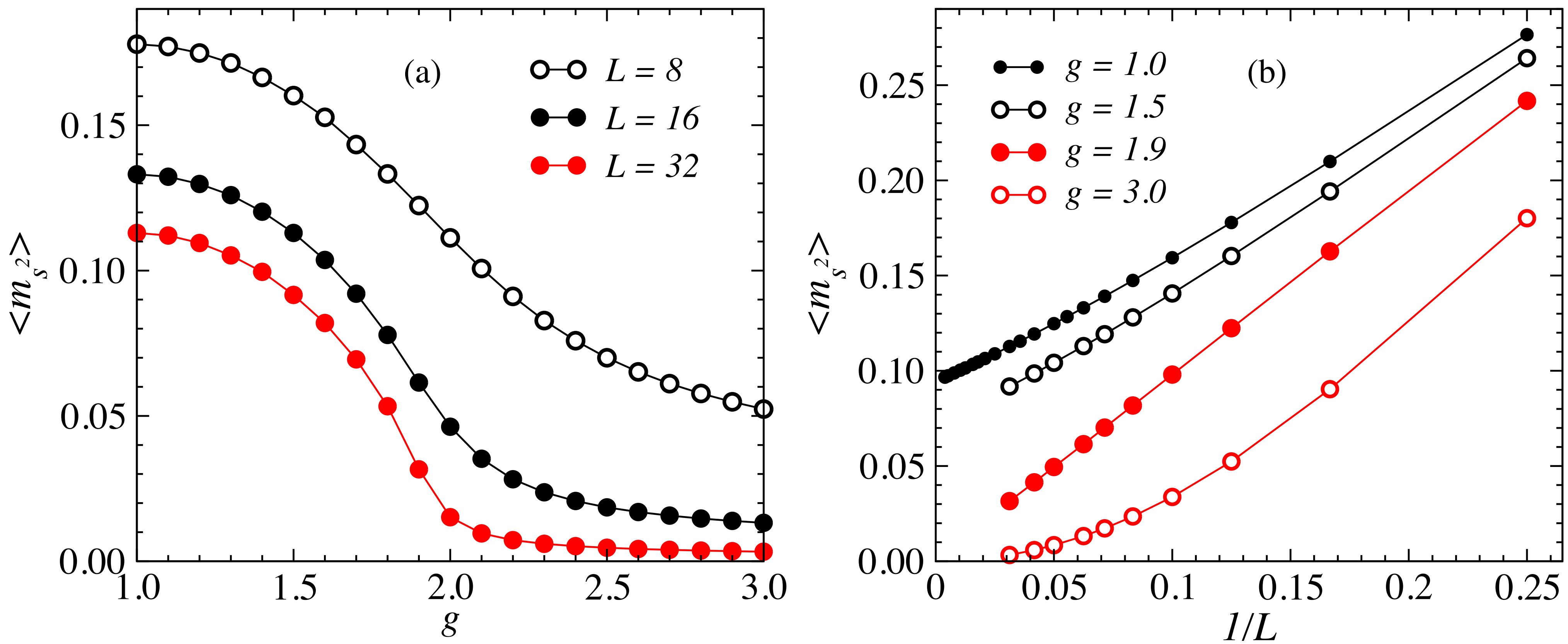
- QMC confirmed

SSE simulations of the loss of order

Single-layer columnar coupled dimers



T low enough to give the ground state
- T = a/L, a=2-4 (a may have to increase with size)



A linear behavior on 1/L is expected throughout the ordered phase
- becomes more difficult to see as the critical point is approached

Power-law form $\langle m_s^2 \rangle \sim 1/L^{1-\eta}$, $\eta \approx 0.03$, expected at g_c
- we will discuss extraction of critical points later

Experimental realization: $TlCuCl_3$ (a 3D coupled-dimer system)

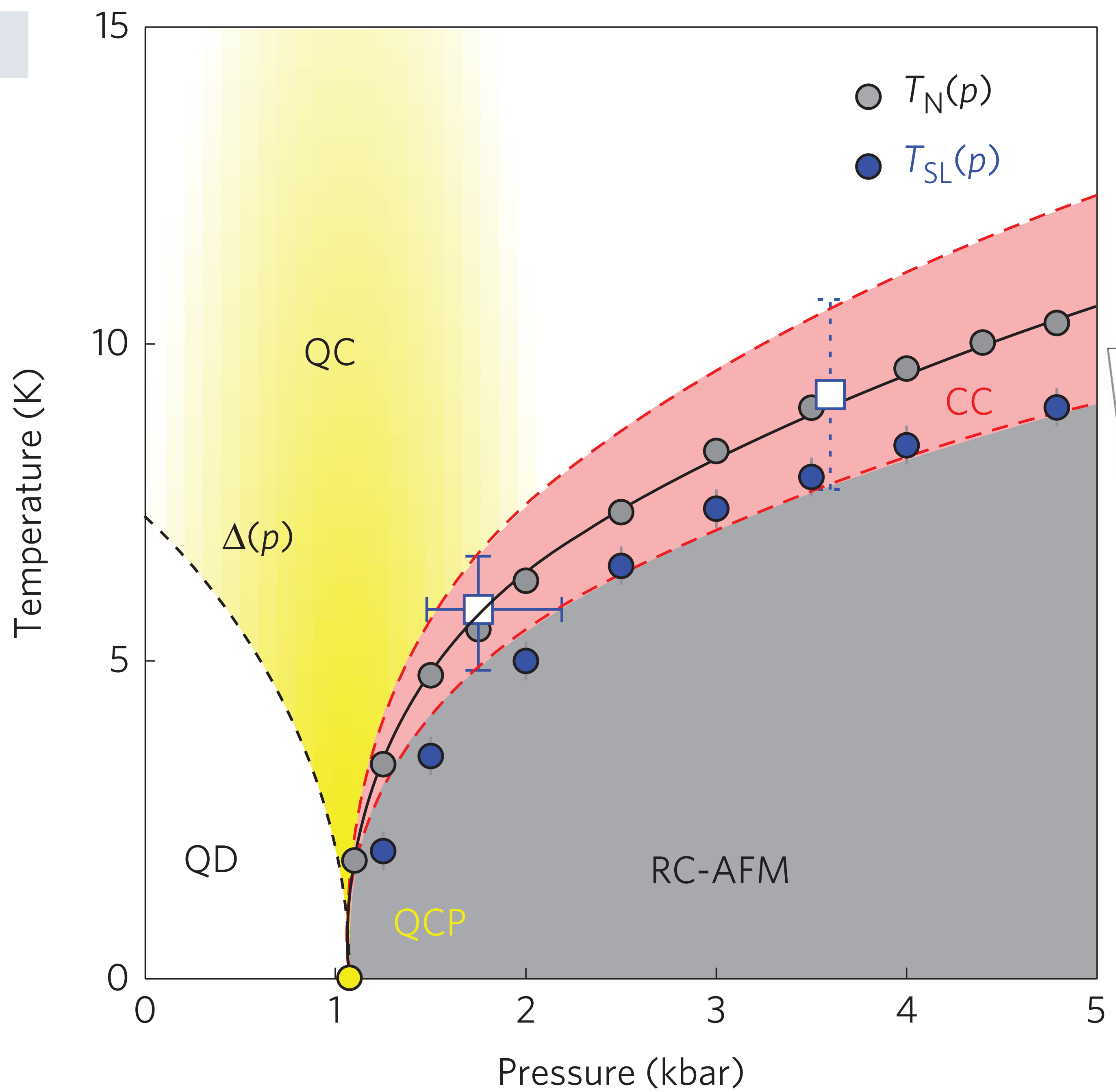
nature physics
ARTICLES
PUBLISHED ONLINE: 6 APRIL 2014 | DOI: 10.1038/NPHYS2902

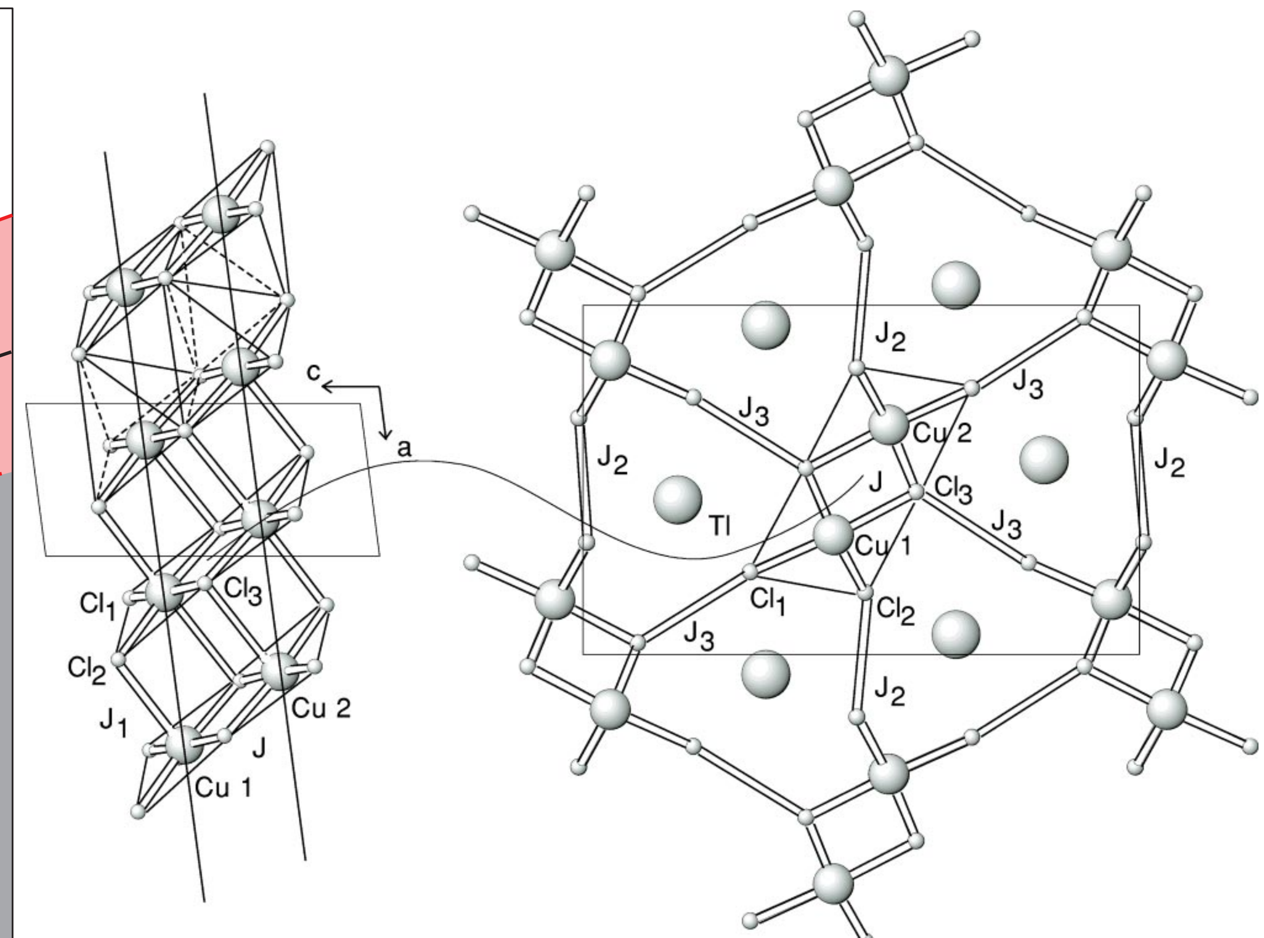
$TlCuCl_3$

Quantum and classical criticality in a dimerized quantum antiferromagnet

P. Merchant[1], B. Normand[2], K. W. Krämer[3], M. Boehm[4], D. F. McMorrow[1] and Ch. Rüegg[1,5,6★]

3D Network of dimers
- couplings can be changed by pressure

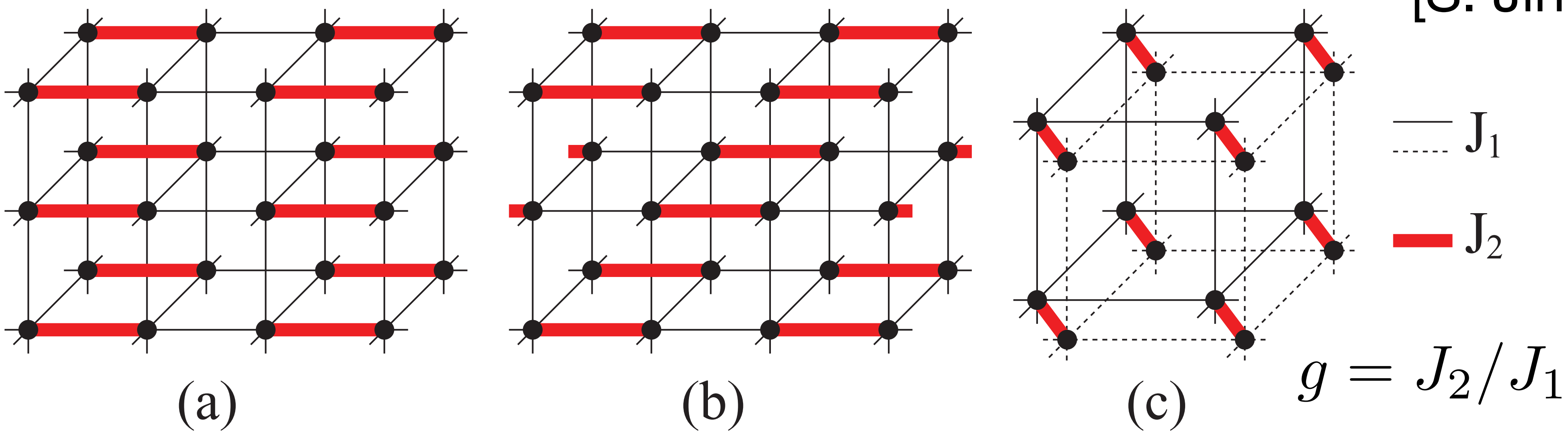




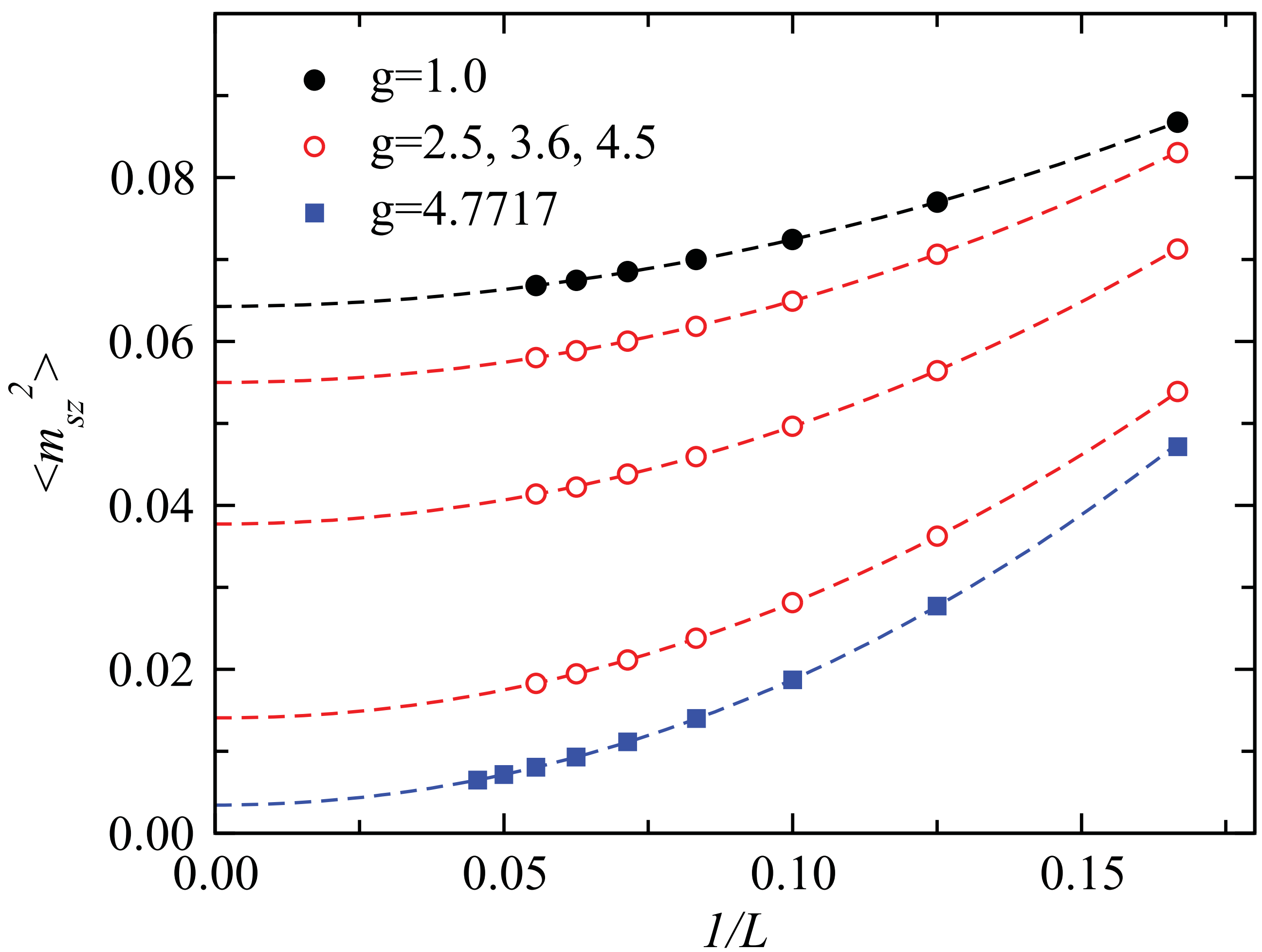
From: M Matsumoto, B Normand, TM Rice, M Sigrist, PRB (2004)

Universality of the Neel temperature in 3D dimerized systems?

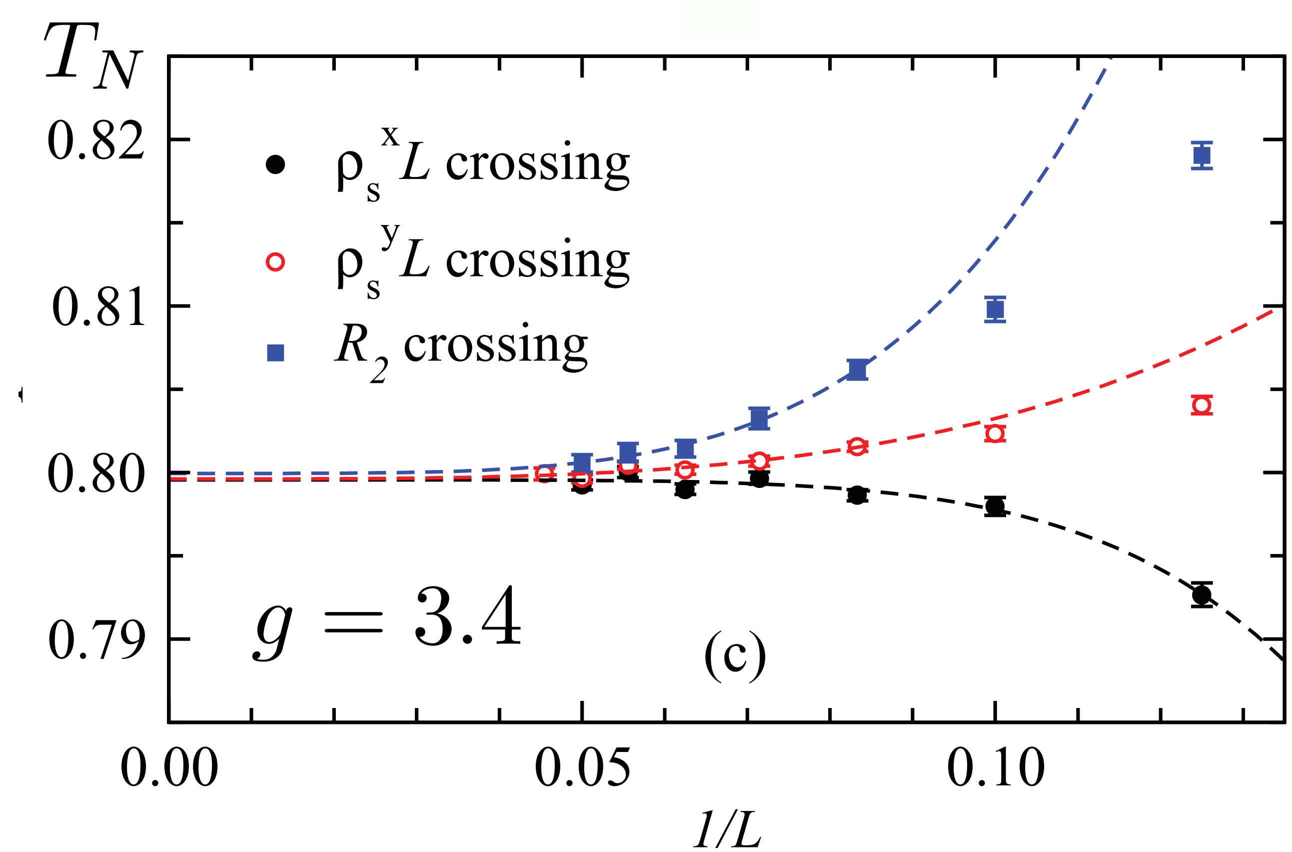
[S. Jin, AWS, PRB2012]



Determine the Neel ordering temperature **T_N** and the T=0 ordered moment **m_s** for 3 different dimerization patterns

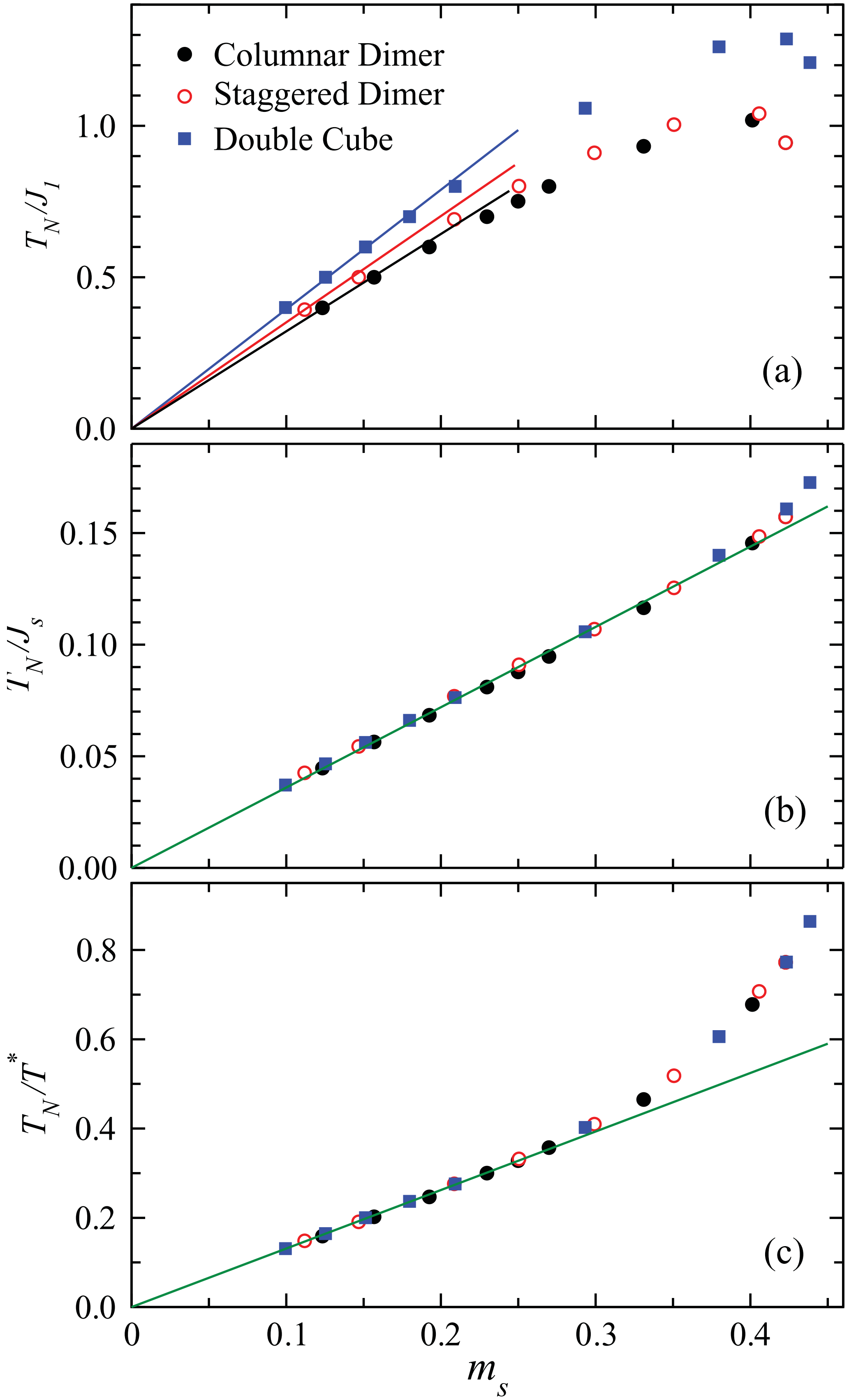


Example: Columnar dimers



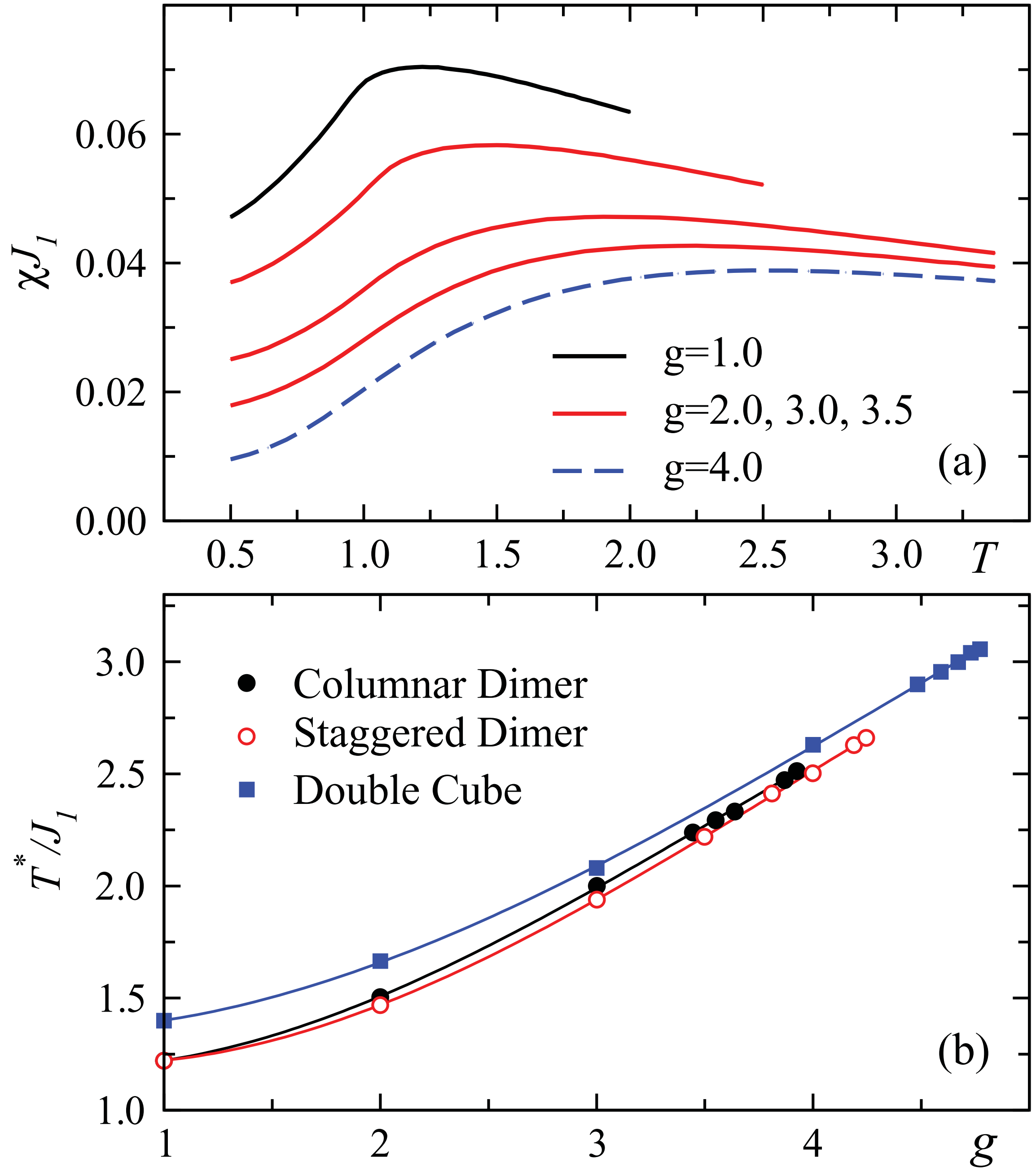
Couplings vs pressure not known experimentally

- plot T_N vs m_s to avoid this issue and study universality
- but how to normalize T_N?



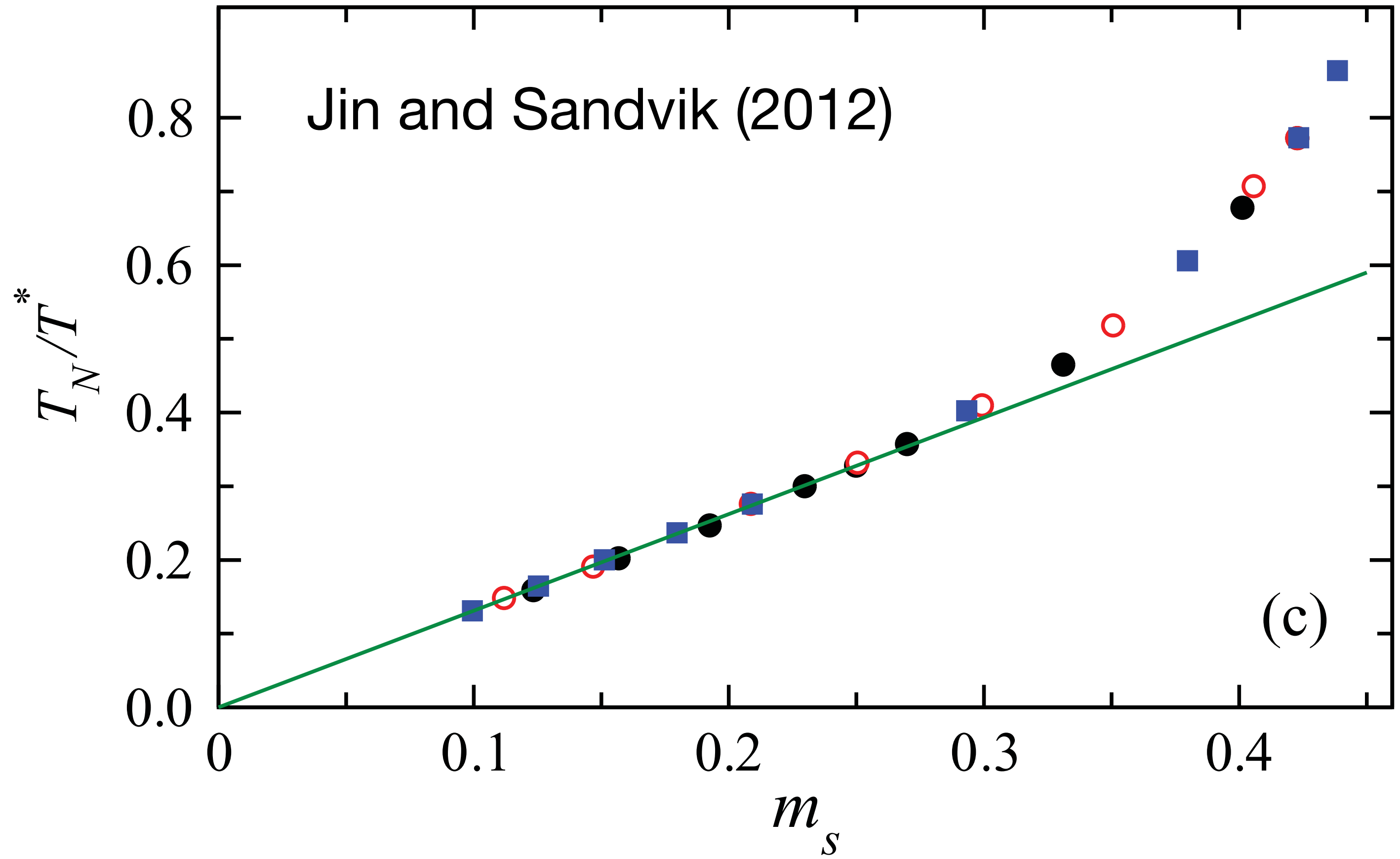
Three normalizations

(a) weaker copling J_1
(b) sum J_s of couplings per spin
(c) peak T^* of magnetic susceptibility

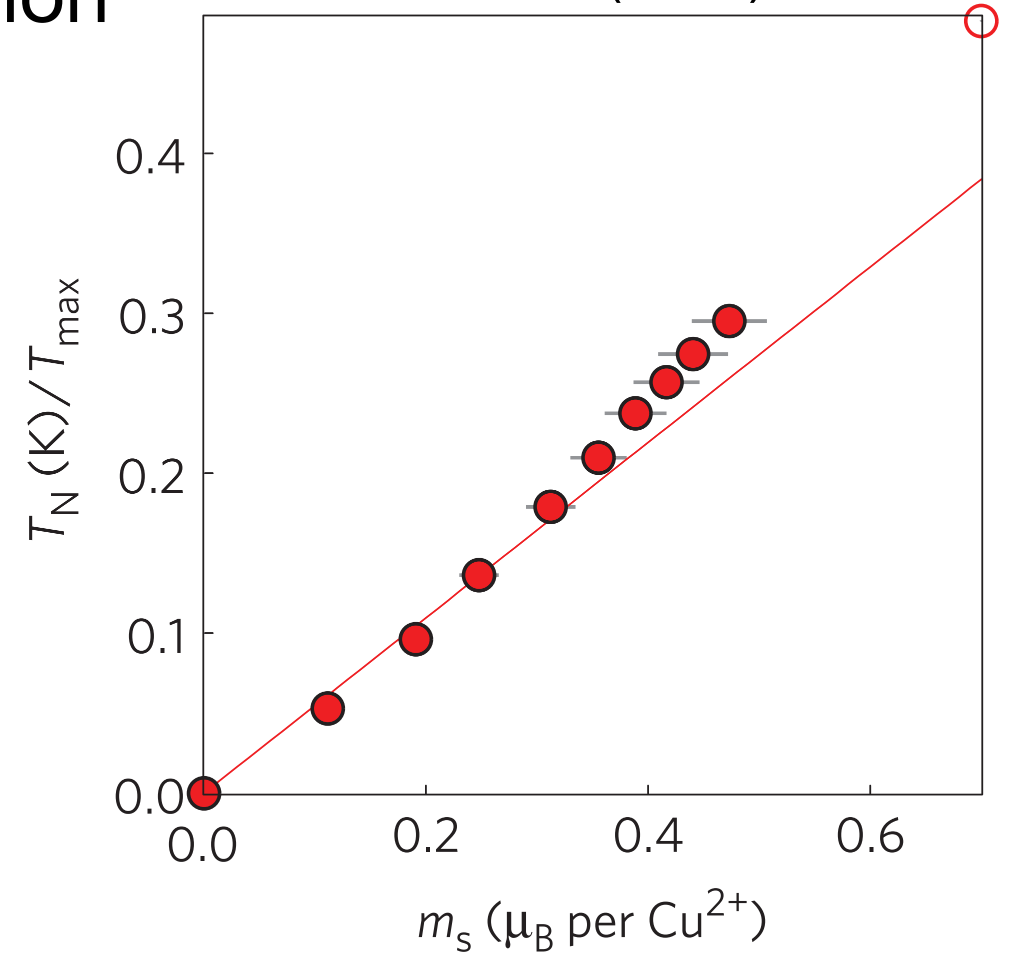


T* normalization is in principle accessible experimentally

- some experimental susc. results available
- neutron data analyzed with this normalization



Merchant et al (2014)



Universality is not a feature of quantum-criticality

- extends far from the quantum critical point
- linear behavior is expected from semiclassical theory (decoupling of quantum and thermal fluctuations)
- deviations show coupling of quantum and thermal fluctuations

Same features observed in models and experiment

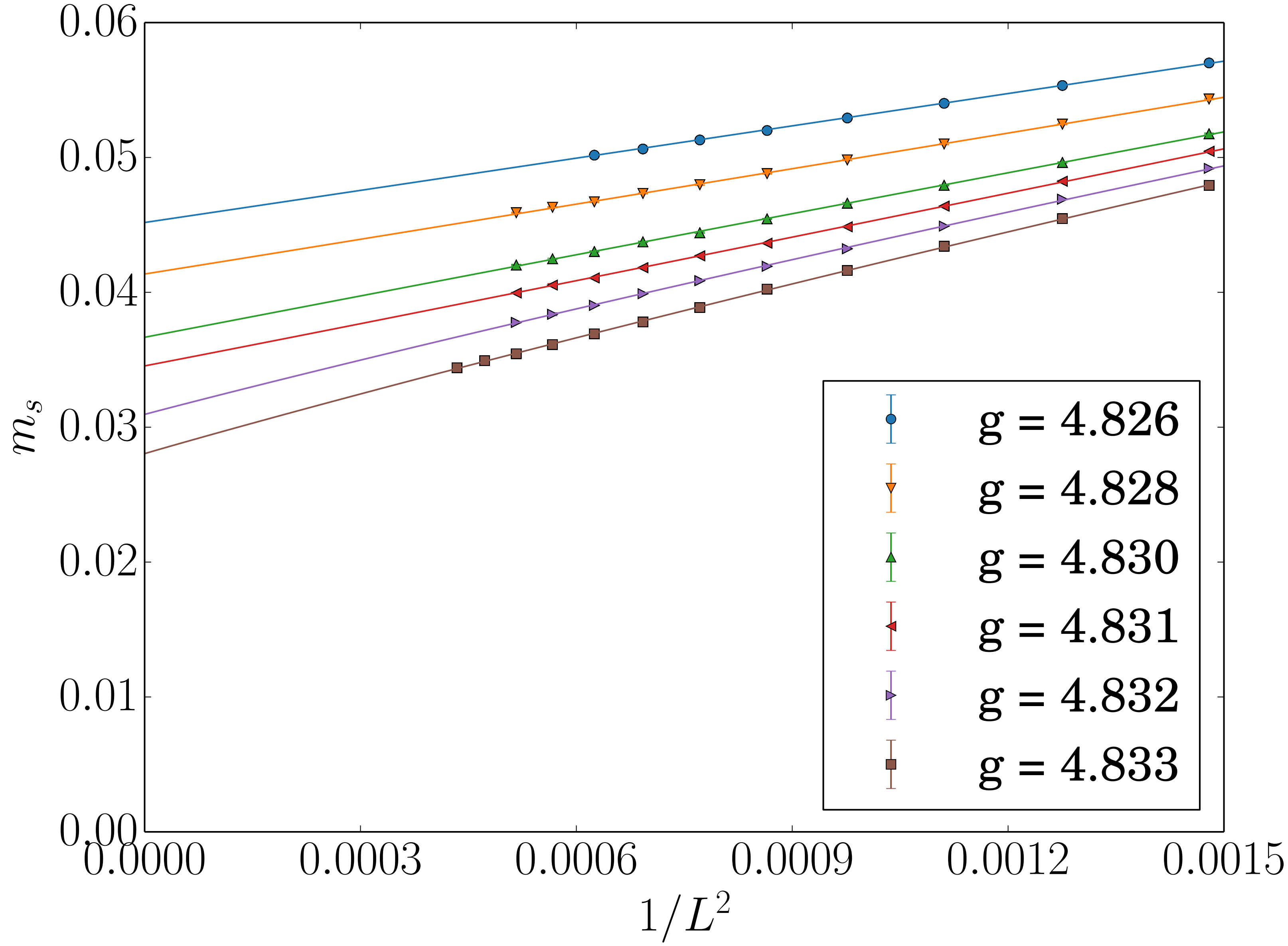
- experimental slope about 25% lower if g-factor 2 assumed (what exactly is the g-factor?)

Logarithmic corrections [YQ Qin, B. Normand, AWS, ZY Meng, arXiv:1506:0607]

The quantum-critical (T=0) point corresponds to d=3+1=4
- the upper critical dimension of the O(N) transition

Mean-field behavior with log corrections expected
- can the logs be detected (numerically and experimentally)?

SSE Simulations close to the critical point (double cube)
- T → 0 (T=1/2L) results for $N=L^3$ spins with L up to 40 (128000 spins)



$g_c \approx 4.837$
determined first
(curve-crossing method)

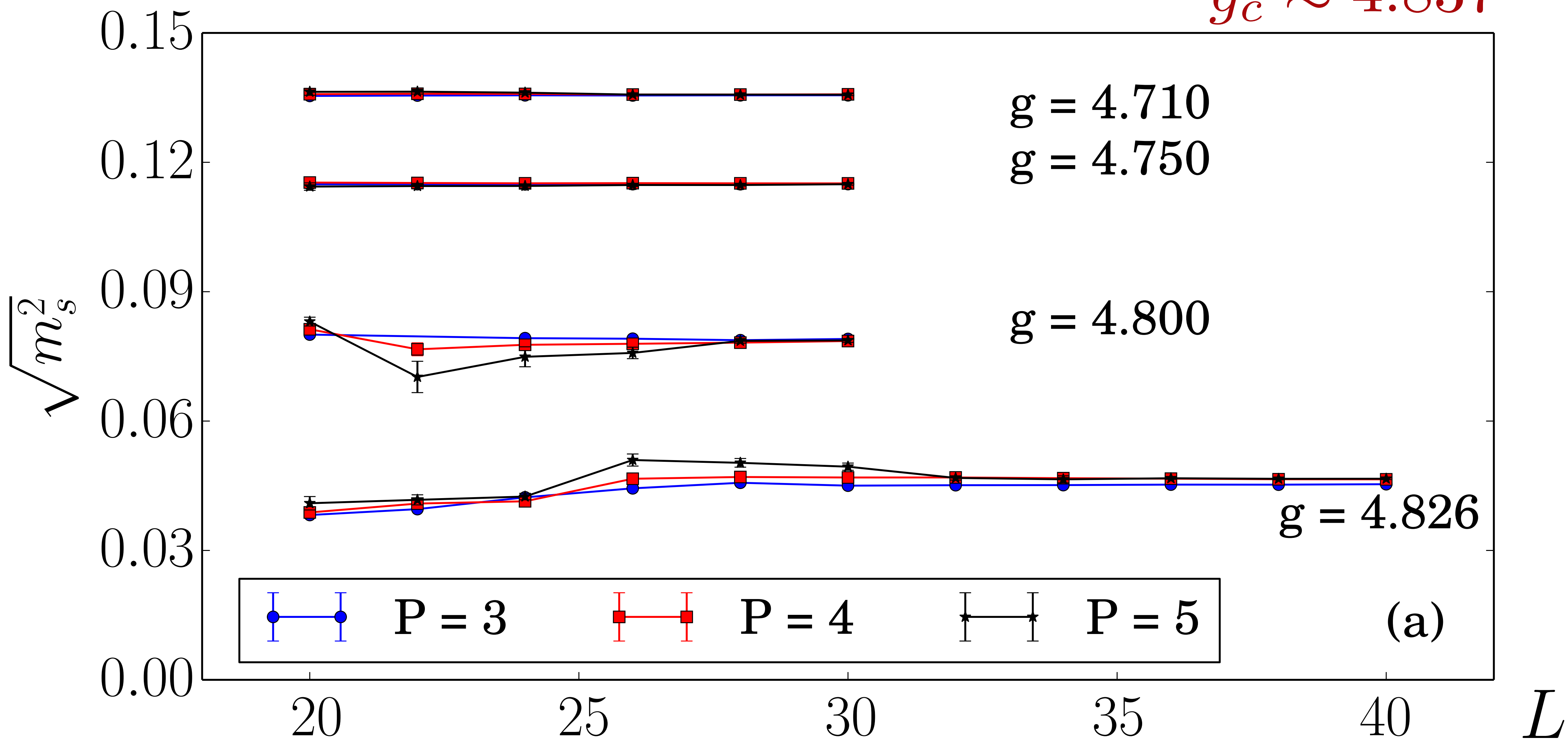
Extrapolations of m_s close to g_c point are challenging:
- use polynomials without linear term (expected)
- check dependence on order of polynomial and L-range used

When is a fit good? Using the criterion:

$$\frac{\chi^2}{\text{dof}} - 1 = \frac{\chi^2}{n_L - n_p} - 1 \leq 3\sqrt{\frac{2}{n_L - n_p}}$$

Use data for up to size L, exclude small sizes until criterion satisfied

$g_c \approx 4.837$



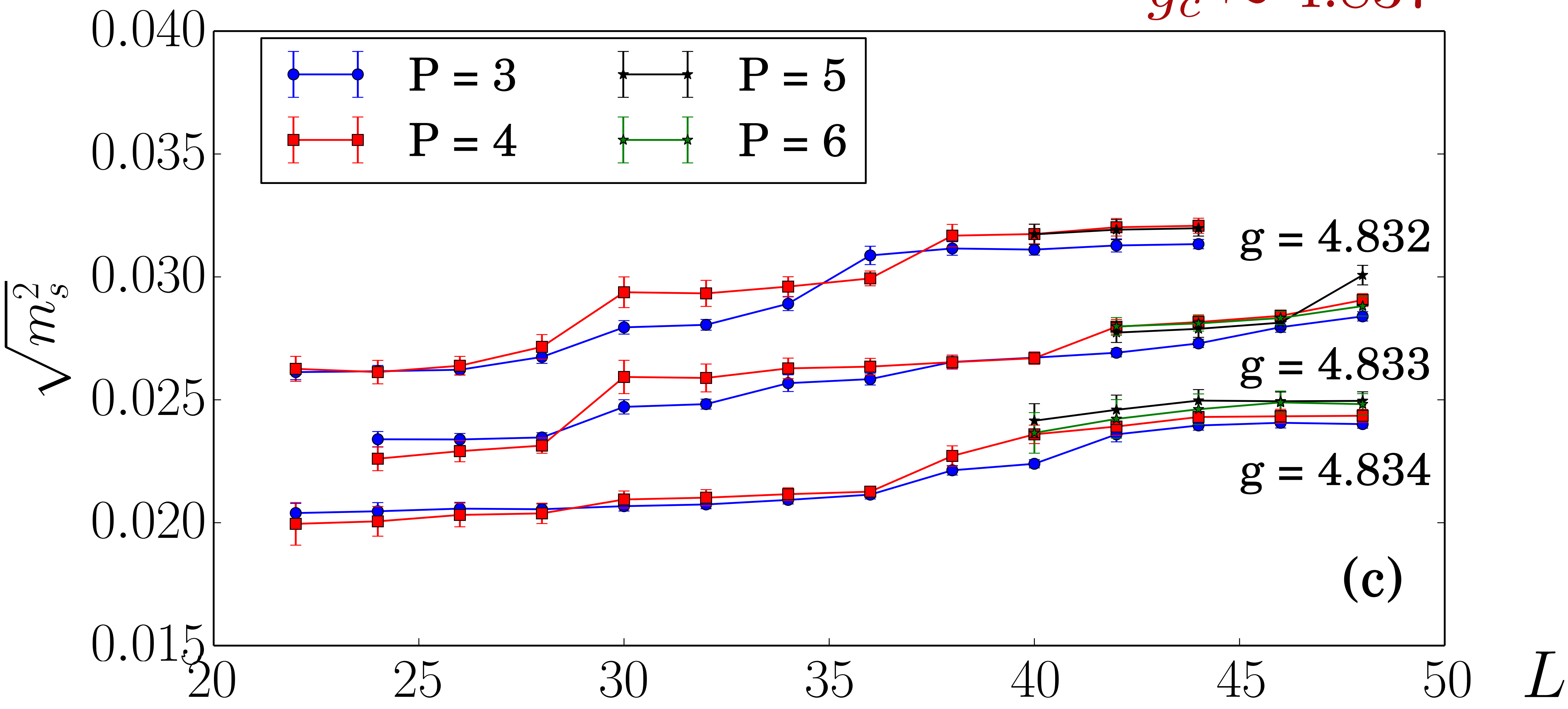
The procedure is very stable sufficiently far away from g_c

When is a fit good? Using the criterion:

$$\frac{\chi^2}{\mathrm{dof}} - 1 = \frac{\chi^2}{n_L - n_p} - 1 \leq 3\sqrt{\frac{2}{n_L - n_p}}$$

Use data for up to size L, exclude small sizes until criterion satisfied

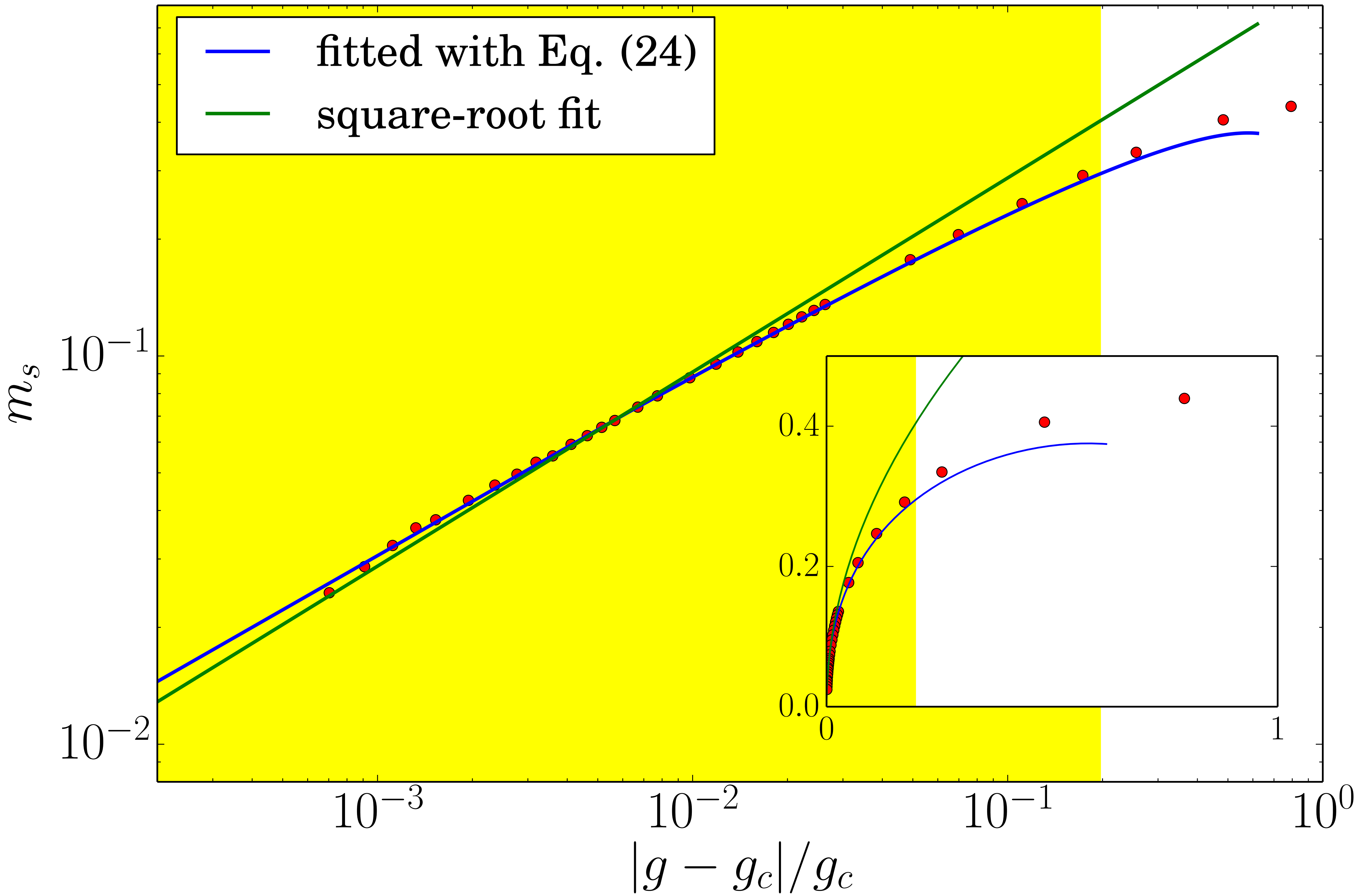
$g_c \approx 4.837$



The procedure becomes increasingly sensitive to the range of points as L increases, and some effects of order P as well (we use P=4).

The log corrections to the mean-field behavior can be seen
- expected form (RG calculations: Zinn-Justin, Kenna,...)

$$m_s(g) = a|g-g_c|^{\beta}\,|\ln(|g-g_c|/c)|^{\hat{\beta}} \qquad \beta = 1/2, \quad \hat{\beta} = 3/11$$



Critical points: Finite-size scaling

The correlation length diverges at the critical point

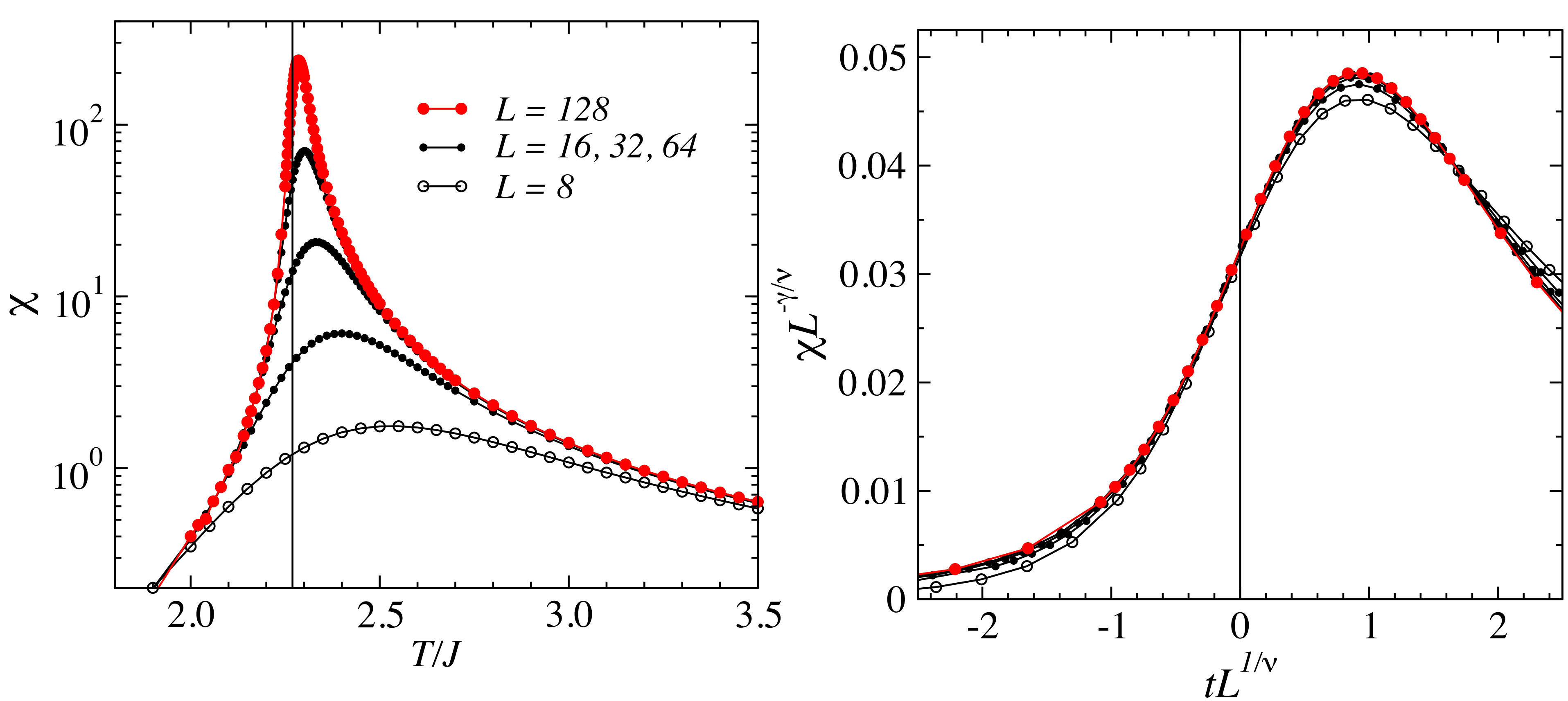
$$\delta = T - T_c \quad \text{or} \quad \delta = g - g_c, \qquad \xi(\delta) \propto \delta^{-\nu}$$

A singular quantity A exhibits finite-size scaling according to

$$A(\delta) \propto \delta^{\kappa} \to A(\delta, L) \propto L^{-\kappa/\nu} f(\delta L^{1/\nu})$$

Commonly used in “data collapse” of simulation data

Example: susceptibility of the 2D Ising model: $\chi = (\langle m^2 \rangle - \langle |m| \rangle^2)/T$



$$t = |T - T_c|$$

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

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

When Tc and/or exponents not known, use them as parameters
- to obtain “best” data collapse

Not very reliable, need more systematic approach

Crossing-point analysis [S. Hui, W. Guo, AWS, unpublished manuscript]

Aim: Completely systematic and unbiased method to extract the location of a critical point and the critical exponents

Starting point: Scaling function known from RG

$$A(\delta, L) = L^{-\kappa/\nu} f(\delta L^{1/\nu}, \lambda_1 L^{-\omega_1}, \lambda_2 L^{-\omega_2}, \cdots)$$

κ = critical exponent corresponding to A: $A \sim \delta^{\kappa}$
ν = correlation-length exponent; $\xi \sim \delta^{-\nu}$
δ = distance to the critical point (relevant field)
λ_i = irrelevant fields, $\omega_{i+1} \geq \omega_i > 0$

We only keep the leading irrelevant variable, $\omega_1=\omega$ (and leave out λ)

$$A(q, L) = L^{-\kappa/\nu} f(\delta L^{1/\nu}, L^{-\omega})$$

The scaling function f can be Taylor expanded:

$$A(\delta, L) = L^{-\kappa/\nu}(a + b\delta L^{1/\nu} + cL^{-\omega} + \ldots)$$

Crossing-point analysis: Consider two system sizes
$L_1 = L$, $L_2 = rL$, r=constant (e.g., r=2)

Study points $\delta^*(L)$ such that $A(\delta^*,L_1)=A(\delta^*,L_2)$

Large-L crossing point from Taylor expansion:

$$\delta^* = \frac{a}{b}\frac{1-r^{-\kappa/\nu}}{r^{(1-\kappa)/\nu}-1}L^{-1/\nu} + \frac{c}{b}\frac{1-r^{-\kappa/\nu-\omega}}{r^{(1-\kappa)/\nu}-1}L^{-1/\nu-\omega}$$

κ=0 (dimensionless quantity A) is a special case
- faster convergence to critical point:

$$g(L) - g_c \equiv \delta^* \propto dL^{-1/\nu-\omega}$$

If the exponent κ/ν is known, $L^{\kappa/\nu}A$ can be used and is dimensionless
- some quantities are explicitly dimensionless (Binder ratio,...)

$$A^*(L) = A(\delta^*, L) = L^{-\kappa/\nu}(\tilde{a} + \tilde{b}L^{-\omega} + \ldots)$$

With a set of points g*(L), one can use the known power-law form to extrapolate to g_c, and ã, with 1/ν and ω as fitting parameters
- works well for g_c, exponents often "effective", slowly changing with L

One can derive a better expression for extrapolating ν directly from the crossing points
- using dimensionless quantity Q hereafter (κ=0)

Taylor expansion of the scaling function:

$$Q(\delta, L) = a_0 + a_1 \delta L^{1/\nu} + a_2 \delta^2 L^{2/\nu} + b_1 L^{-\omega} + c_1 \delta L^{1/\nu - \omega} + \ldots$$

Define the **slope** (derivative)

$$s(\delta) = \frac{dQ(\delta, L)}{d\delta} = \frac{dQ(\delta, L)}{dg} = a_1 L^{1/\nu} + c_1 L^{1/\nu - \omega} + a_2 \delta L^{2/\nu} + \ldots .$$

The **log-slope** at the critical point

$$\ln[s(0)] = a + \frac{1}{\nu} \ln(L) + bL^{-\omega} + \ldots$$

This is a well-known way to extract the exponent v
- find the critical point first
- plot log-slope versus ln(L), try to extract its slope 1/v for large L
- scaling corrections make it non-trivial

New proposal: Use the two slopes at the crossing point

$$s(\delta^*, L_n) = a_1 L_n^{1/\nu} + c_1 L_n^{1/\nu - \omega} + a_2 d L_n^{1/\nu - \omega} + \ldots \quad (n = 1, 2)$$

$$\ln[s(\delta^*, rL)] - \ln[s(\delta^*, L)] = \frac{1}{\nu} \ln(r) + aL^{-\omega} + \ldots$$

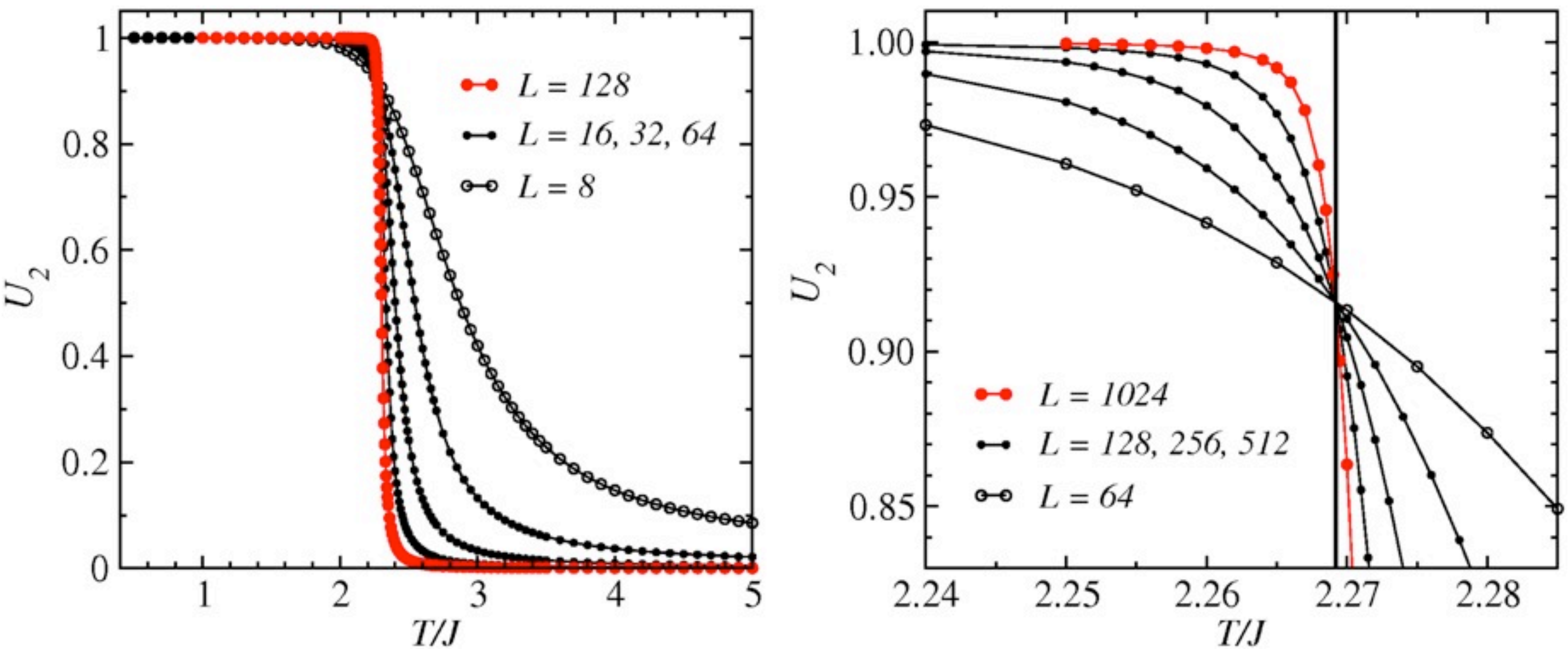
Much easier to fit and extrapolate for 1/v and don't need g_c first !

$$\frac{1}{\nu^*(L)} = \frac{\ln[s(\delta^*, rL)] - \ln[s(\delta^*, L)]}{\ln(r)}$$

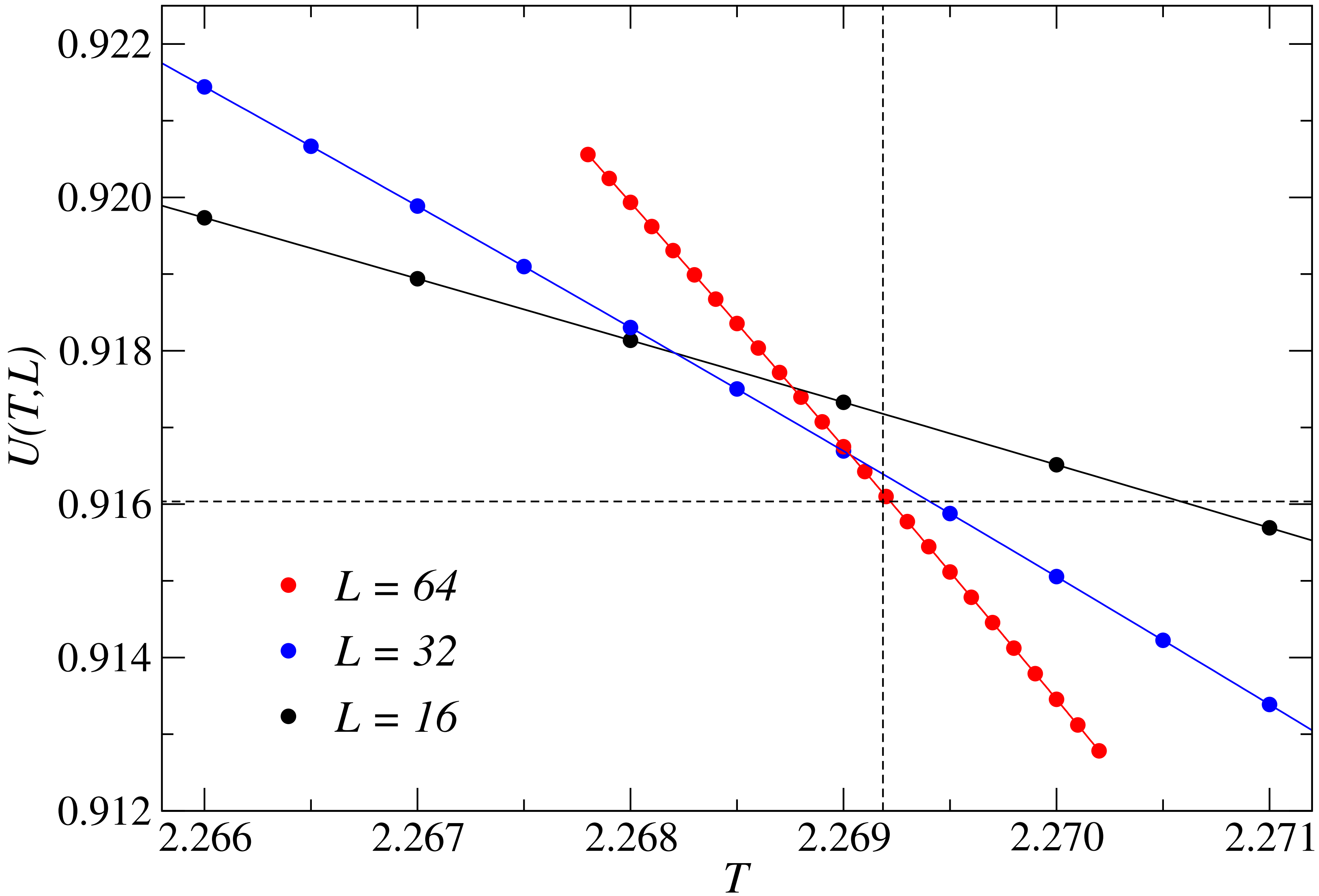
$$\frac{1}{\nu^*(L)} = \frac{1}{\nu} + bL^{-\omega} + \ldots$$

Good quantity Q to use: Binder cumulant: $U = \frac{1}{2}\left(3 - \frac{\langle m^4\rangle}{\langle m^2\rangle^2}\right)$

2D Ising model; MC results



We need a very fine grid of points close to T_c (+interpolate)



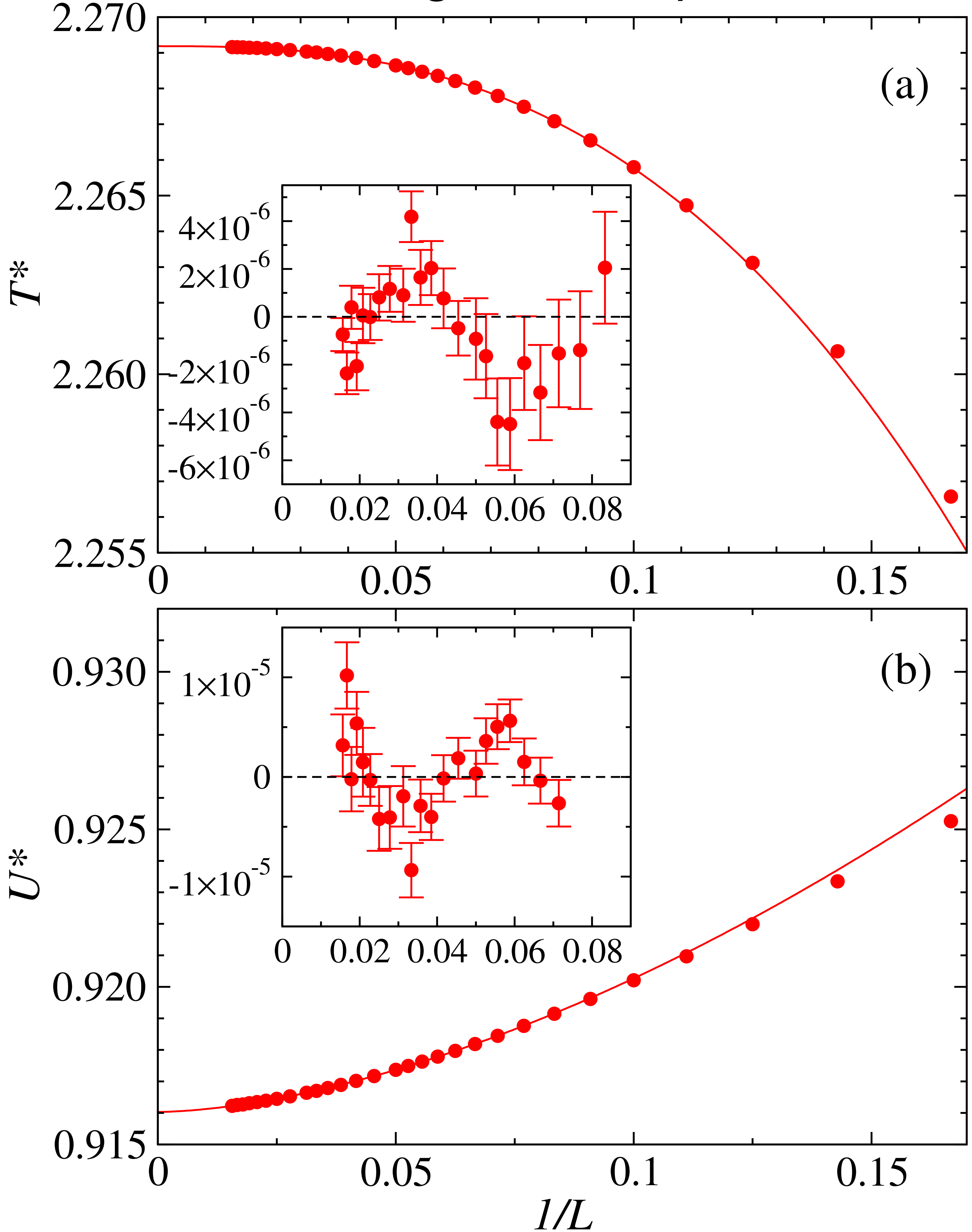
- use ~20-30 points
- use polynomials for interpolation
- bootstrap sampling to compute stat. errors of quantities at the crossing points

Note that crossing points are correlated
- same system size can appear in two different (L_1,L_2) pairs
- should use covariance matrix in goodness of fit

$$\chi^2 = \sum_{i=1}^{M} \sum_{i=1}^{M} (\langle U_i \rangle - U_i^{\text{fit}}) [C^{-1}]^2_{ij} (\langle U_j \rangle - U_j^{\text{fit}})$$

$$C_{ij} = \Big\langle (U_i - \langle U_i \rangle)(U_j - \langle U_j \rangle) \Big\rangle$$

2D Ising data, L up to 128



Fit to leading form with correction $\sim L^{-\omega}$

Higher-order corrections visible for small sizes and good data

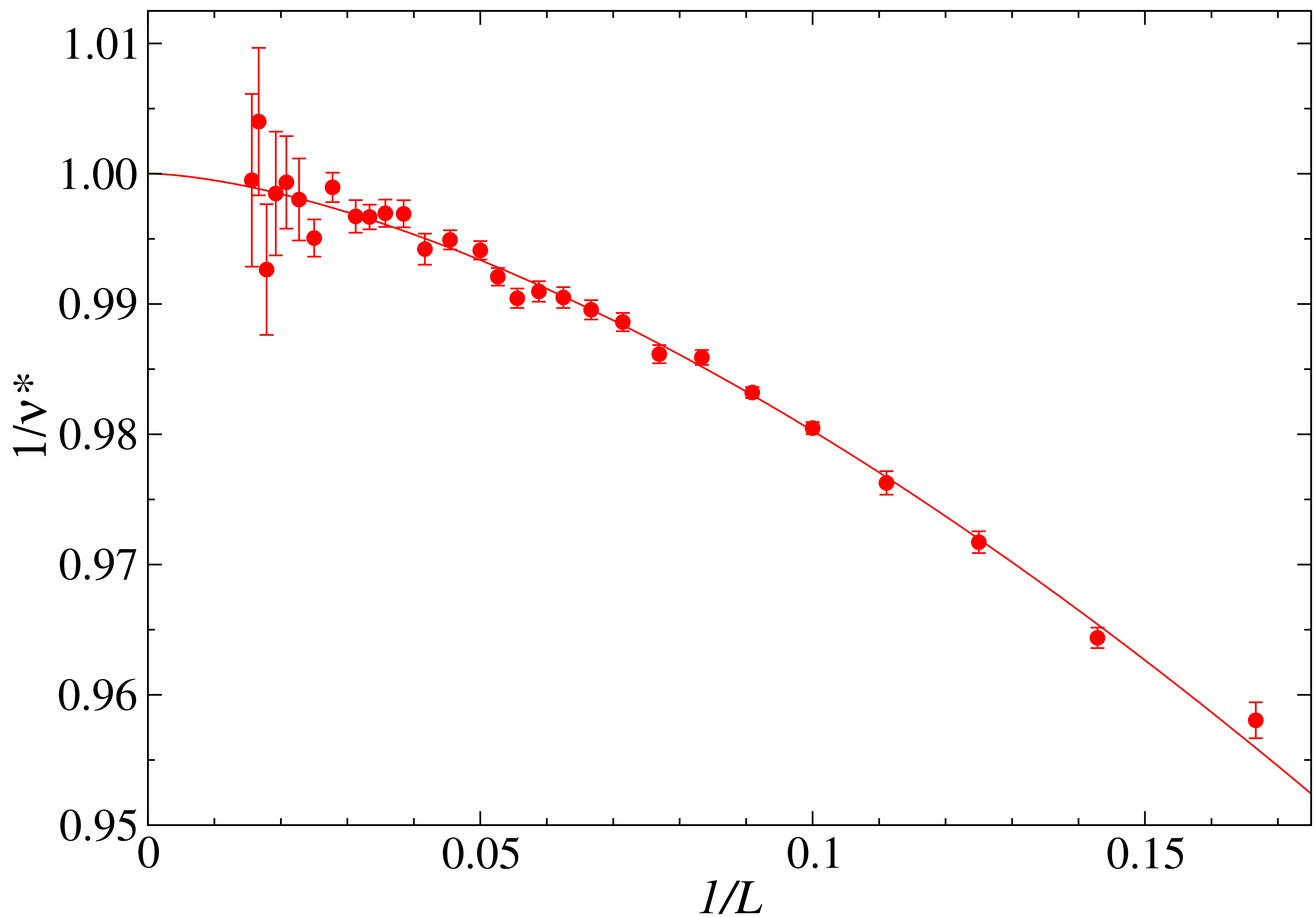
Exclude small sizes until good fit:

$$\frac{\langle \chi^2 \rangle}{N_{\rm dof}} - 1 < 2\sqrt{\frac{2}{N_{\rm dof}}}$$

Fit with L_{min}=12 gave
T_c=2.2691855(5)
- correct value is
T_c=2.2691853...

Some effects of higher-order correction seen in data (wiggles)
- did not affect T_c

Correlation-length exponent:
- data are much noisier (expected, slope...)

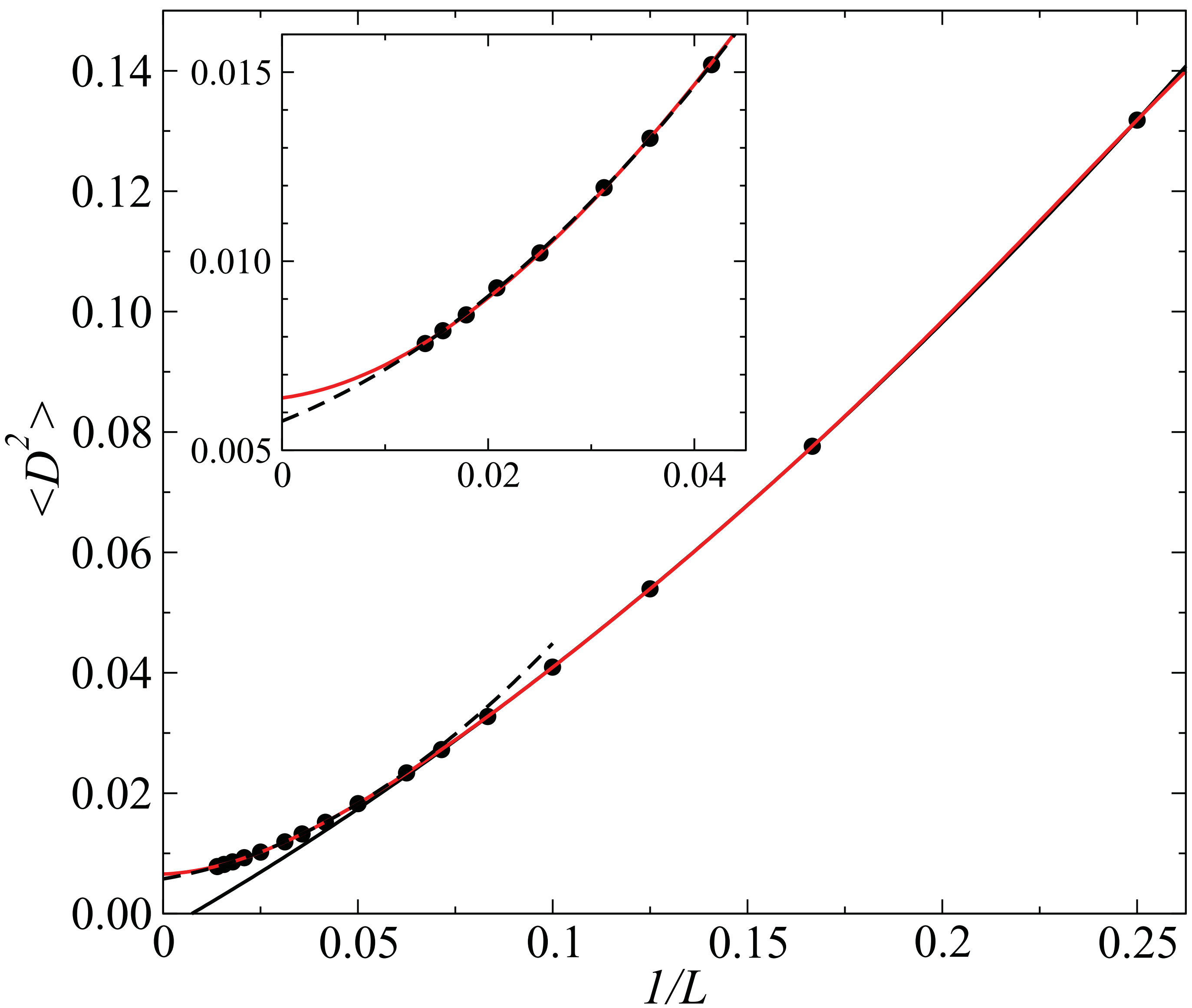


Extrapolations stable and give exponent 1/ν=1.0001(7)

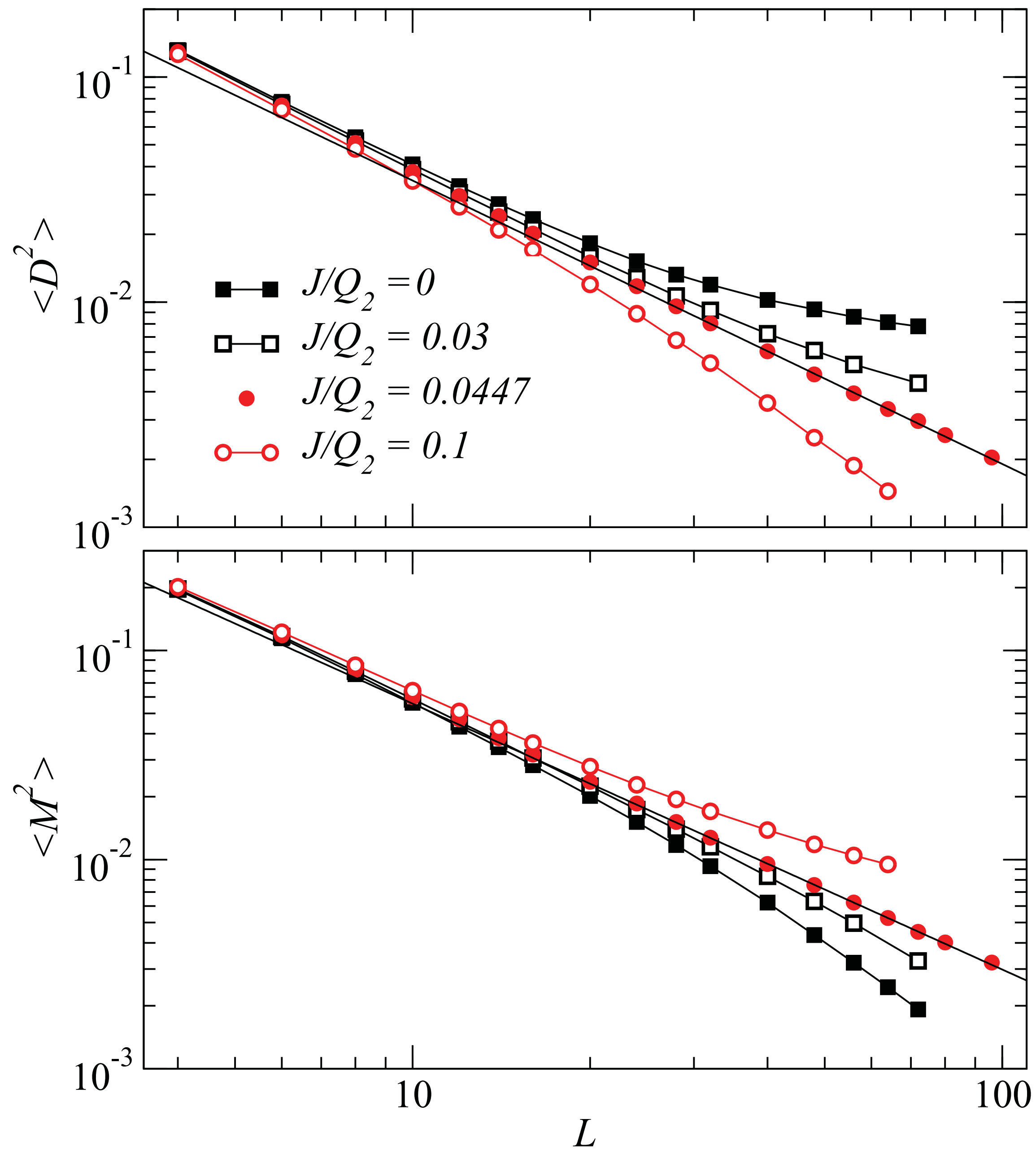
Other exponents can also be extracted
- by analyzing other quantities at the crossing points

Warning: finite-size extrapolations of order parameters are not reliable close to critical points!

Cross-over behaviors make extrapolations impossible when the order parameter (or a gap) is less than some L_{max} dependent value



Example: VBS order parameter of the J-Q model at J=0



Locate phase transitions first

- scaling behavior in L

- use Binder-cumulant crossings etc