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Criticality in classical and quantum magnts

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Part I

- classical and quantum phase transitions, relation to path integrals
- finite-size scaling to study critical points

Part II

- criticality in dimerized S=1/2 Heisenberg models in 2D, 3D
- valence-bond solids and "deconfined" quantum criticality in 2D

Related review articles

- AW Sandvik, *Computational studies of quantum spin systems*, AIP Conference Proc. 1297, 135 (2010) [ArXiv:1101.3281]
- RKK. Kaul, RG Melko, and AW Sandvik, *Bridging lattice-scale physics and continuum field theory with quantum Monte Carlo simulations*, Annual Review of Condensed Matter Physics 4, 179 (2013) [arXiv:1204.5405]

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Part I

- classical and quantum phase transitions, relation to path integrals
- finite-size scaling to study critical points

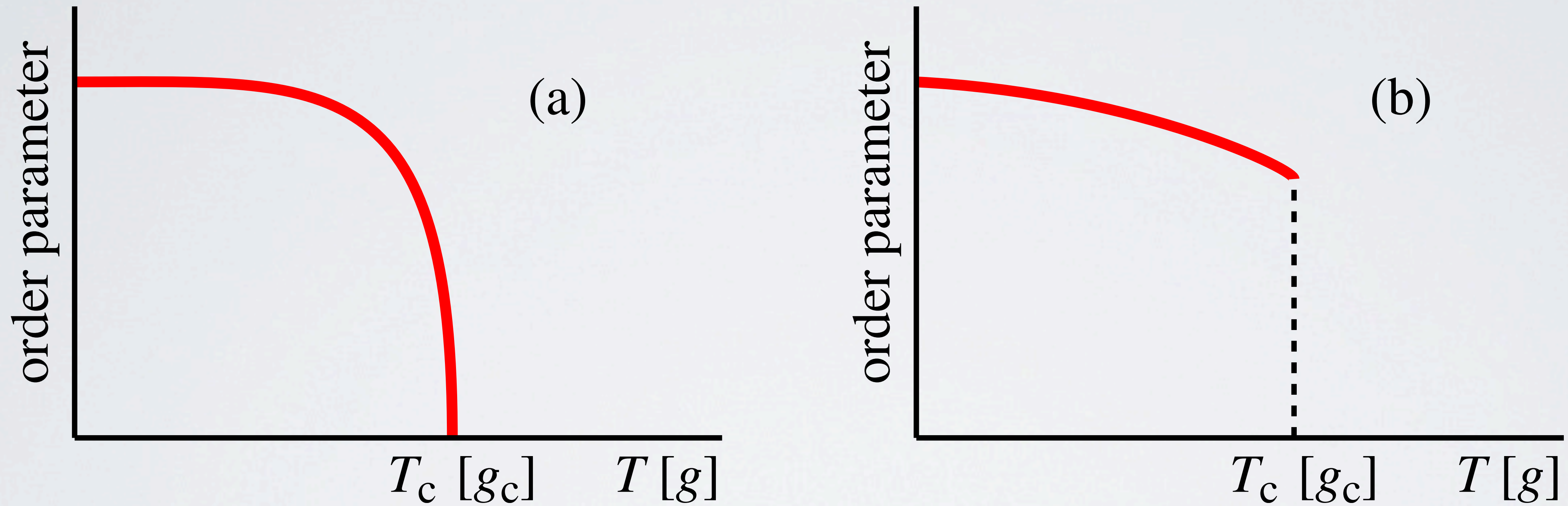
Classical and quantum phase transitions

Classical (thermal) phase transition

- Fluctuations regulated by temperature $T>0$

Quantum (ground state, T=0) phase transition

- Fluctuations regulated by parameter g in Hamiltonian



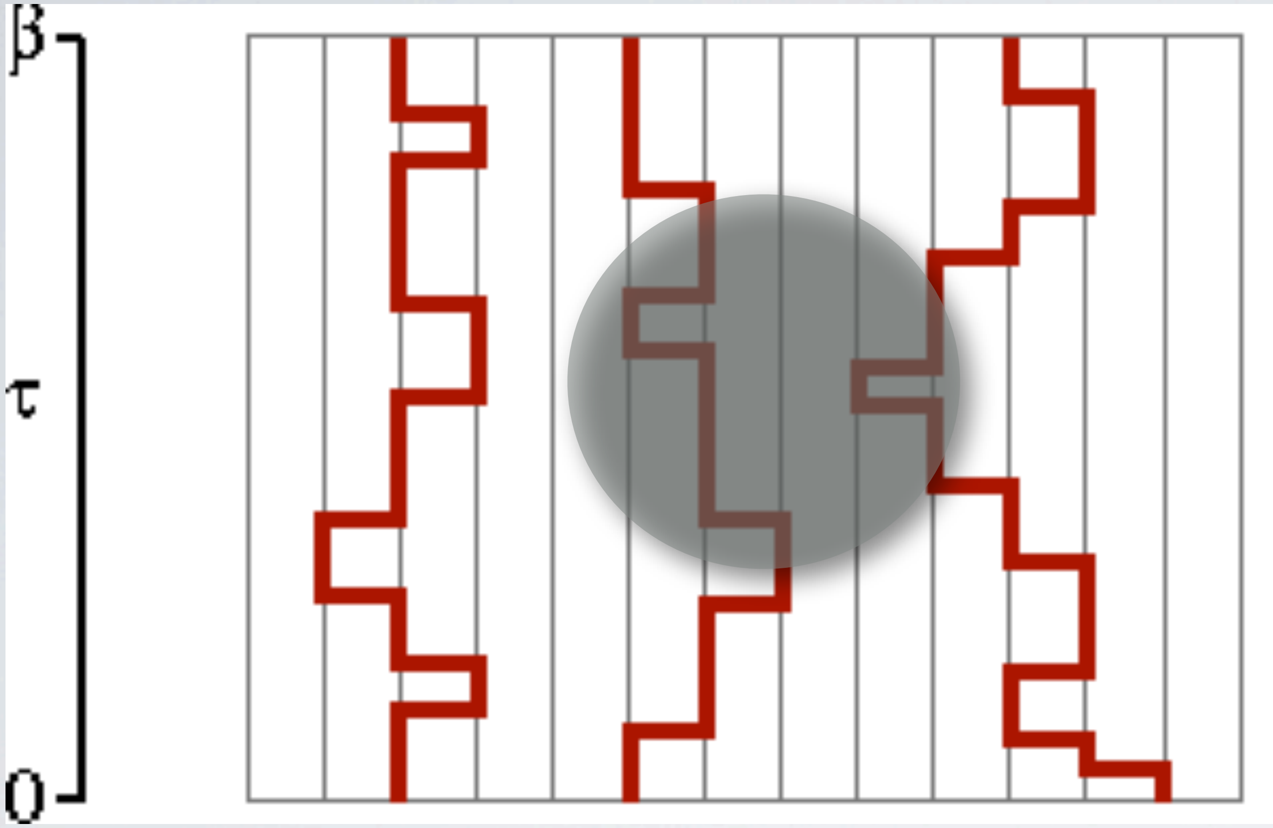
In both cases phase transitions can be

- first-order (discontinuous): finite correlation length ξ as $g \rightarrow g_c$ or $g \rightarrow g_c$
- continuous: 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

Path integrals and quantum field theories



The path integral maps the quantum system in D dimensions onto an equivalent system in D+1 dimensions

The space dimensions can be taken to infinity; $L \to \infty$

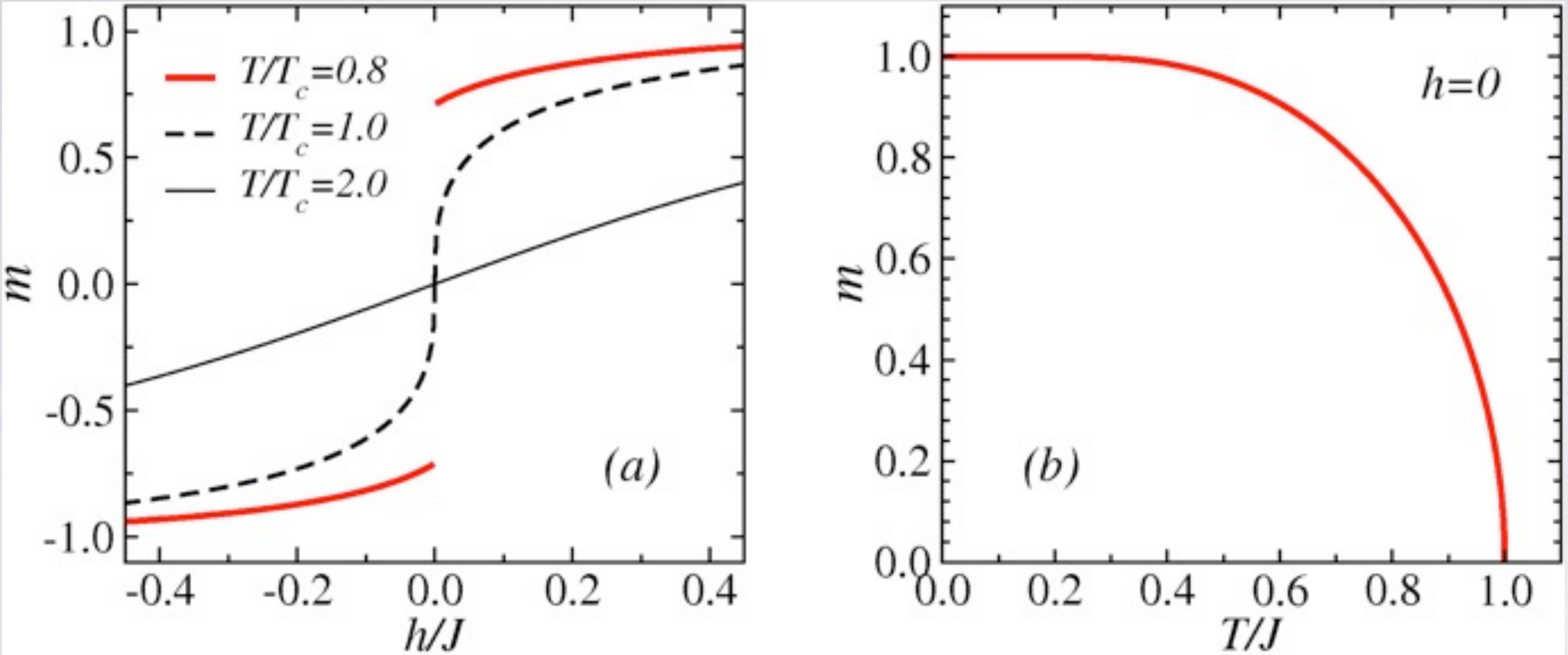
The time dimension is finite for $T > 0$
- $L_\tau = 1/T = \beta$
- $L_\tau \to \infty$ when $T \to 0$

Coarse graining → Continuum field theory in D+1 dimensions
- important approach for studying phase transitions

Finding the correct quantum field theory can be challenging
- Often difficult to derive rigorously from a lattice-scale model
- Quantum mechanics introduces complications; phases
- Symmetries and dimensionality not always enough! Topological defects...

Solving the field theory is in general difficult
- Important exchanges between field theory and lattice numerics
  - classical and quantum Monte Carlo (QMC) simulations

Phase transition, spontaneous symmetry breaking (Ising model)



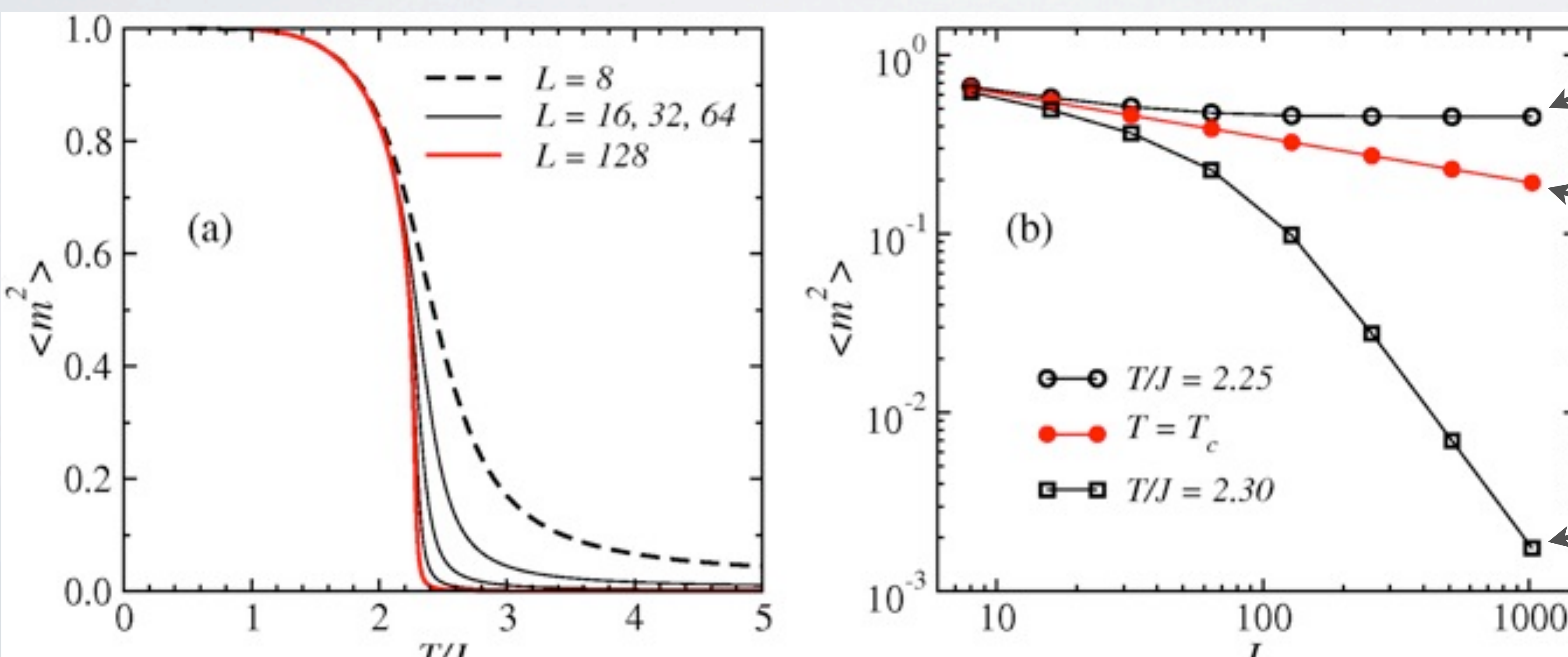
←Mean-field solution

Order parameter (magnetization)

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

MC: Compute time-average of $\langle m^2 \rangle$ to carry out **finite-size scaling**

Squared magnetization for L×L Ising lattices



ordered (size independent)

critical scaling (non-trivial power-law)

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

Finite-size scaling hypothesis

In general there are two relevant length scales
- system length **L**, physical correlation length **ξ(T)** (defined on infinite lattice)

In general physical quantities depend on both

$$\langle A \rangle = f(T, L) = g(\xi, L)$$

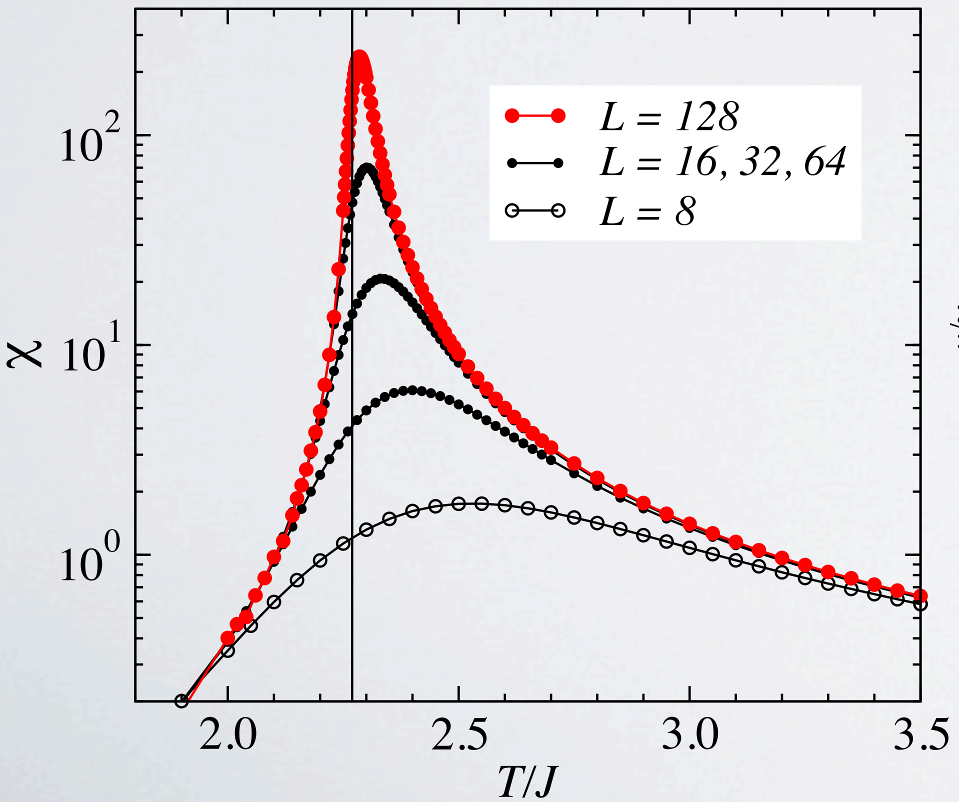
For ξ << L or ξ >> L one argument becomes irrelevant:

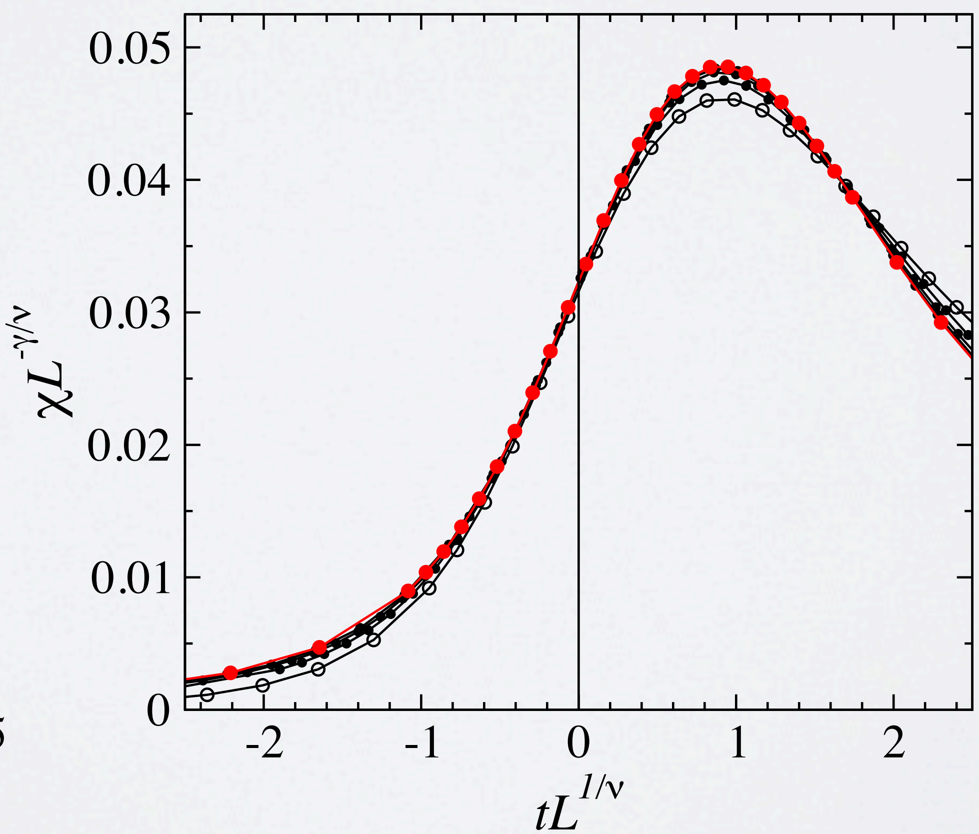
$$g \to g(L) \quad \text{or} \quad g \to g(\xi) = f(T)$$

Close to critical point: **$\xi(T) \sim |T-T_c|^{-\nu}$** (ν is a critical exponent) and when L ~ ξ(T):

$$g \to L^{\kappa} g(\xi/L) \sim L^{\kappa} g(|T-T_c|^{-\nu} L^{-1}) = L^{\kappa} g^{*}(|T-T_c| L^{1/\nu})$$

Use in "data collapse". Example: susceptibility $\chi = (\langle m^2 \rangle - \langle |m| \rangle^2)/T$





$$t = |T - T_c|$$

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

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

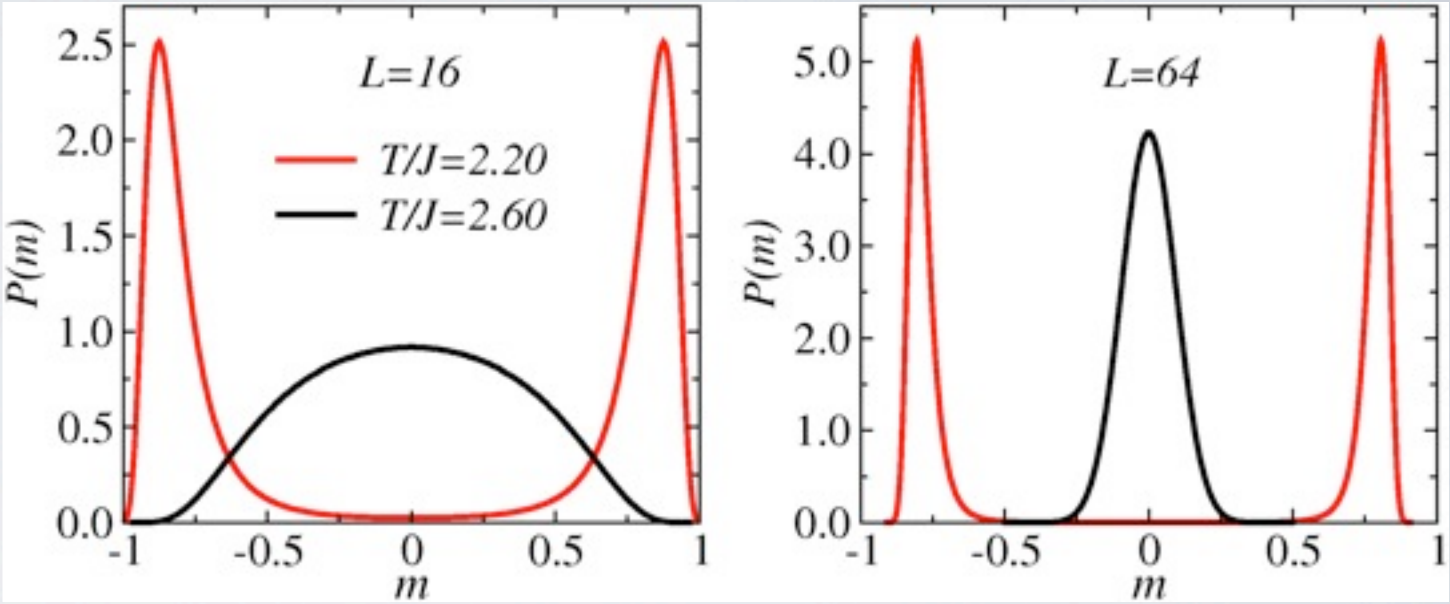
Binder ratios and cumulants

Consider the dimensionless ratio

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

We know R_2 exactly for $N \to \infty$

order parameter distribution

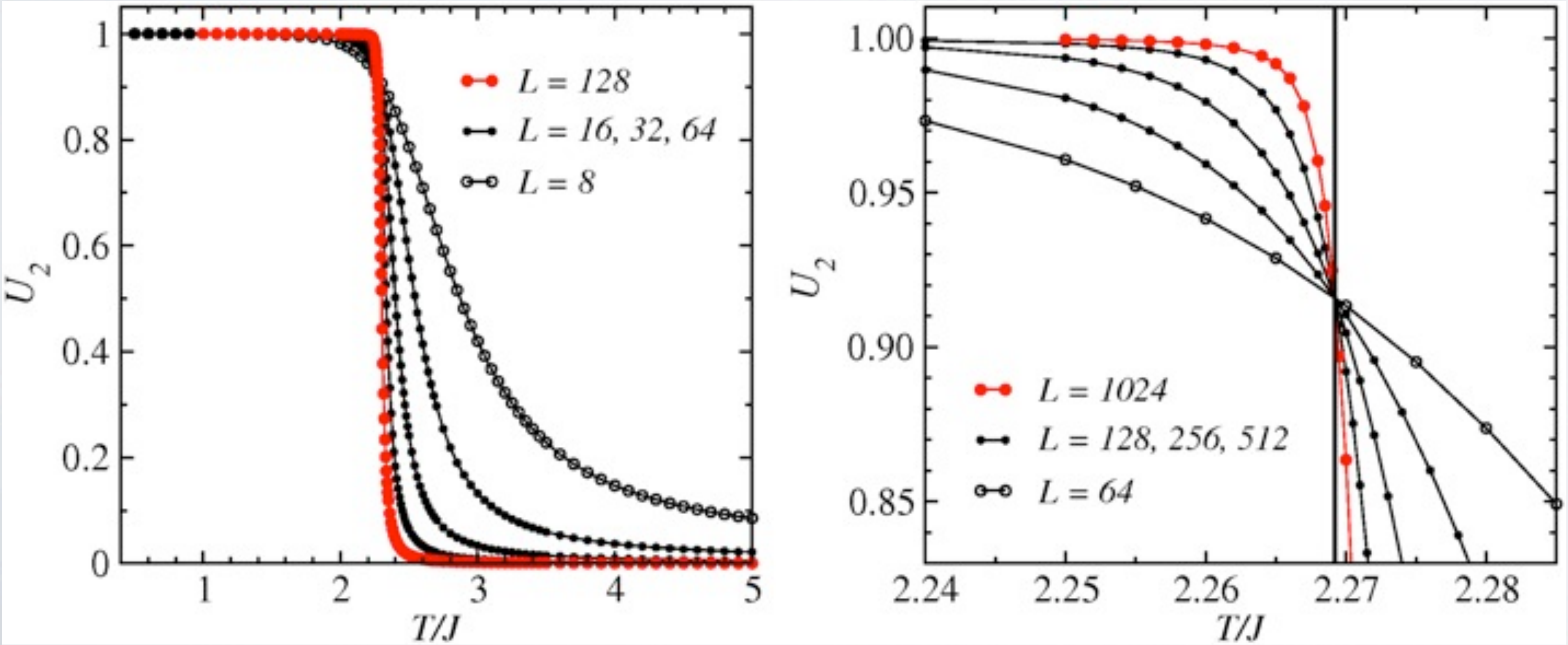


- **for $T<T_c$:** $P(m) \to \delta(m-m^*)+\delta(m+m^*)$
  m^*=|peak m-value|. **$R_2 \to 1$**
- **for $T>T_c$:** $P(m) \to \exp[-m^2/a(N)]$
  $a(N) \sim N^{-1}$ **$R_2 \to 3$** (Gaussian integrals)

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 asymptotically cross each other at T_c

Extrapolate crossing for sizes L and 2L to infinite size

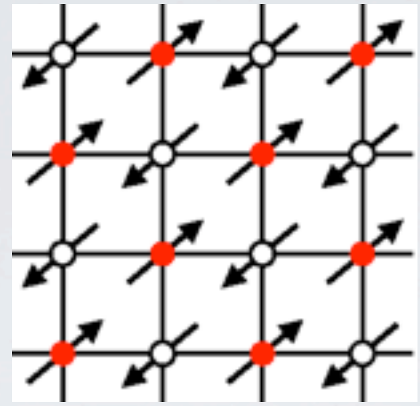
- converges faster than single-size T_c defs.

Part II

- criticality in dimerized S=1/2 Heisenberg models in 2D, 3D
- valence-bond solids and “deconfined” quantum criticality in 2D

Starting point: 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

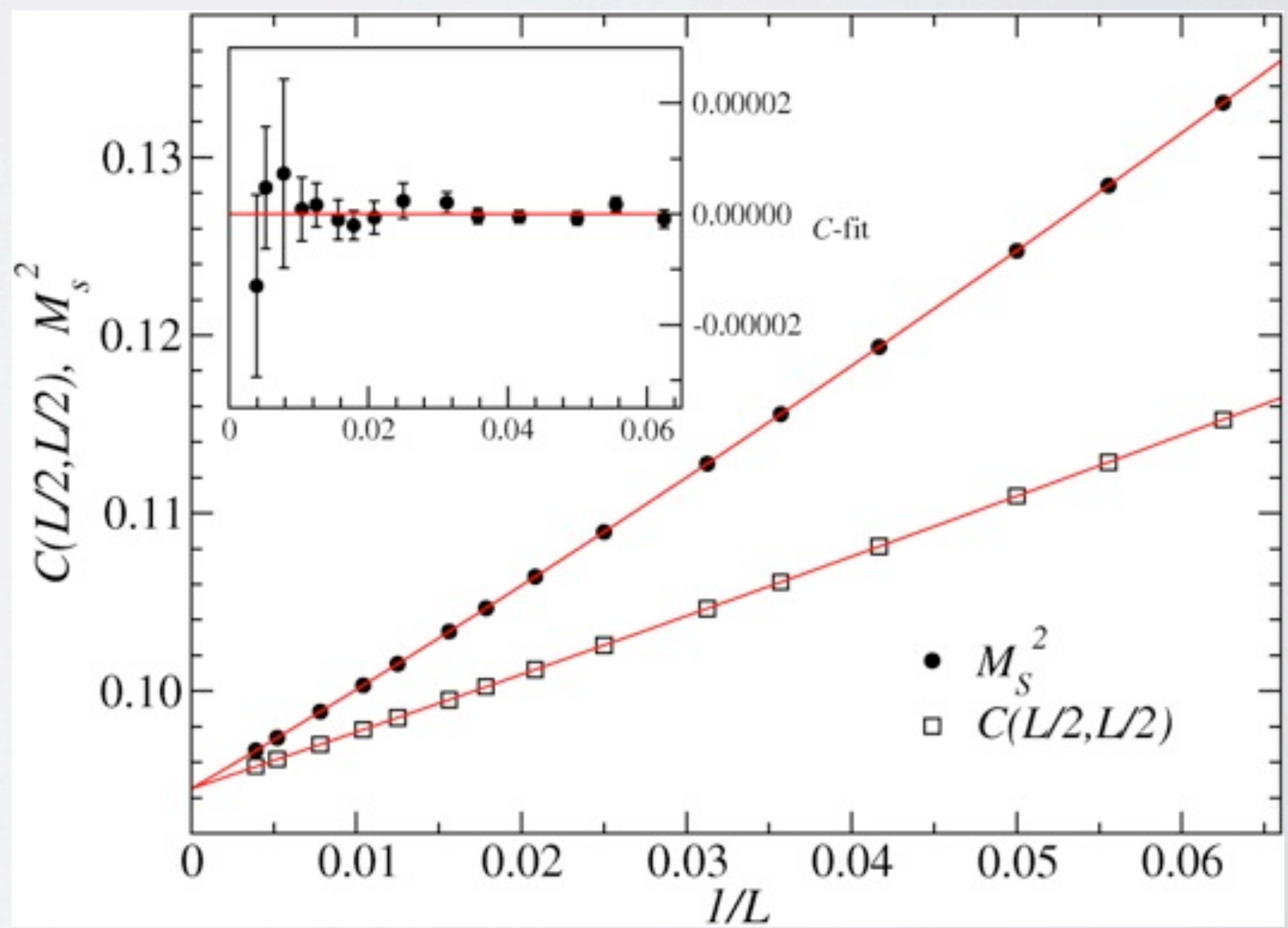
$$m_s = 0.30(2)$$

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

AWS & HG Evertz 2010

$$m_s = 0.30743(1)$$

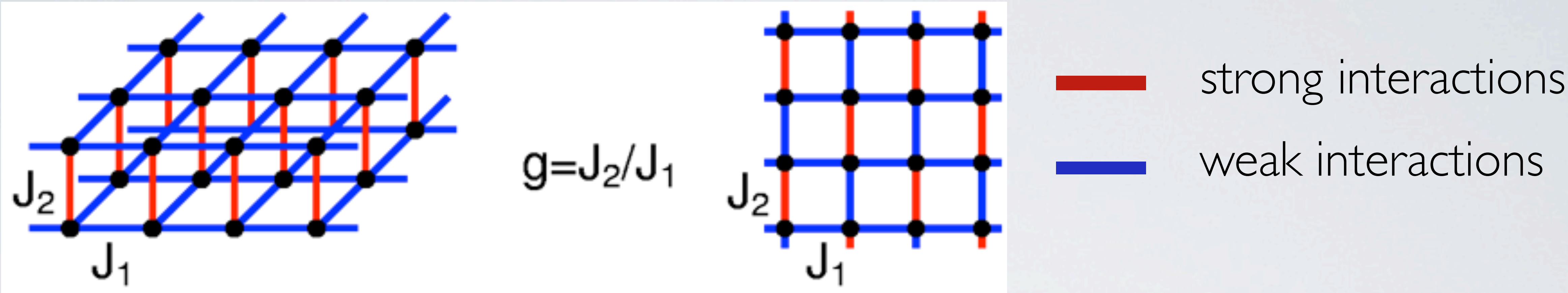
L×L lattices up to 256×256, T=0



T=0 Néel-paramagnetic quantum phase transition

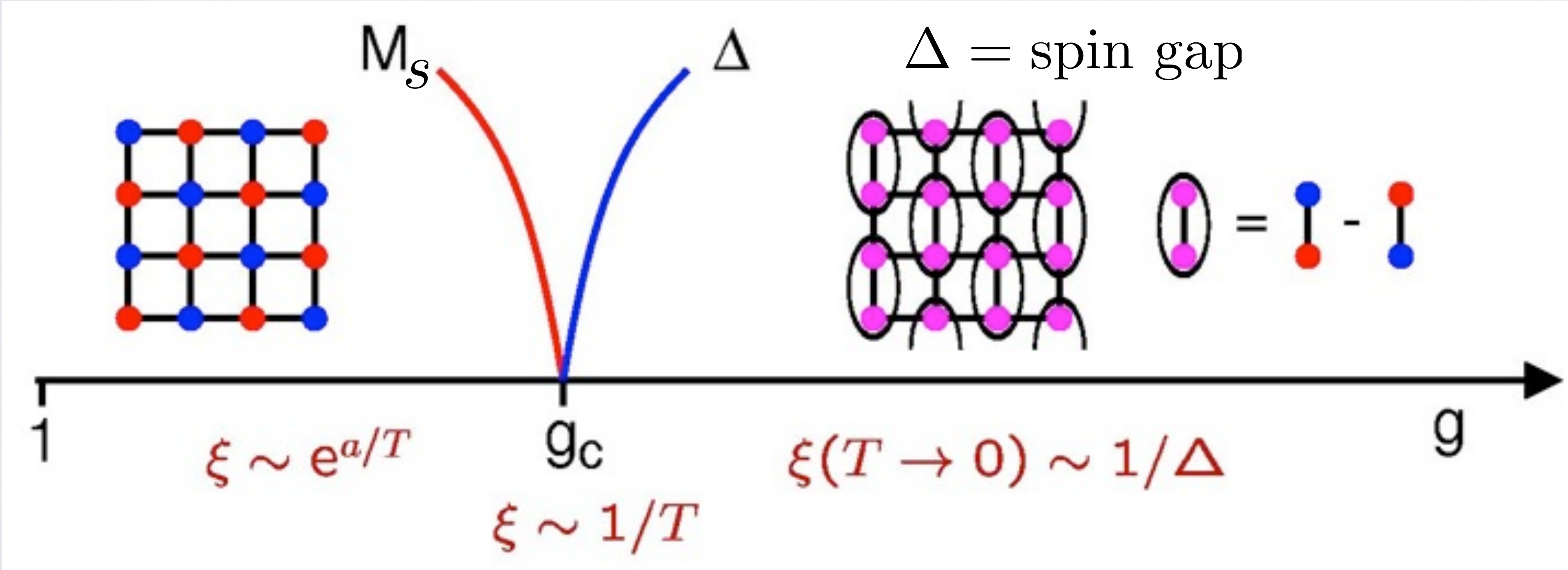
Example: Dimerized S=1/2 Heisenberg models

- 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

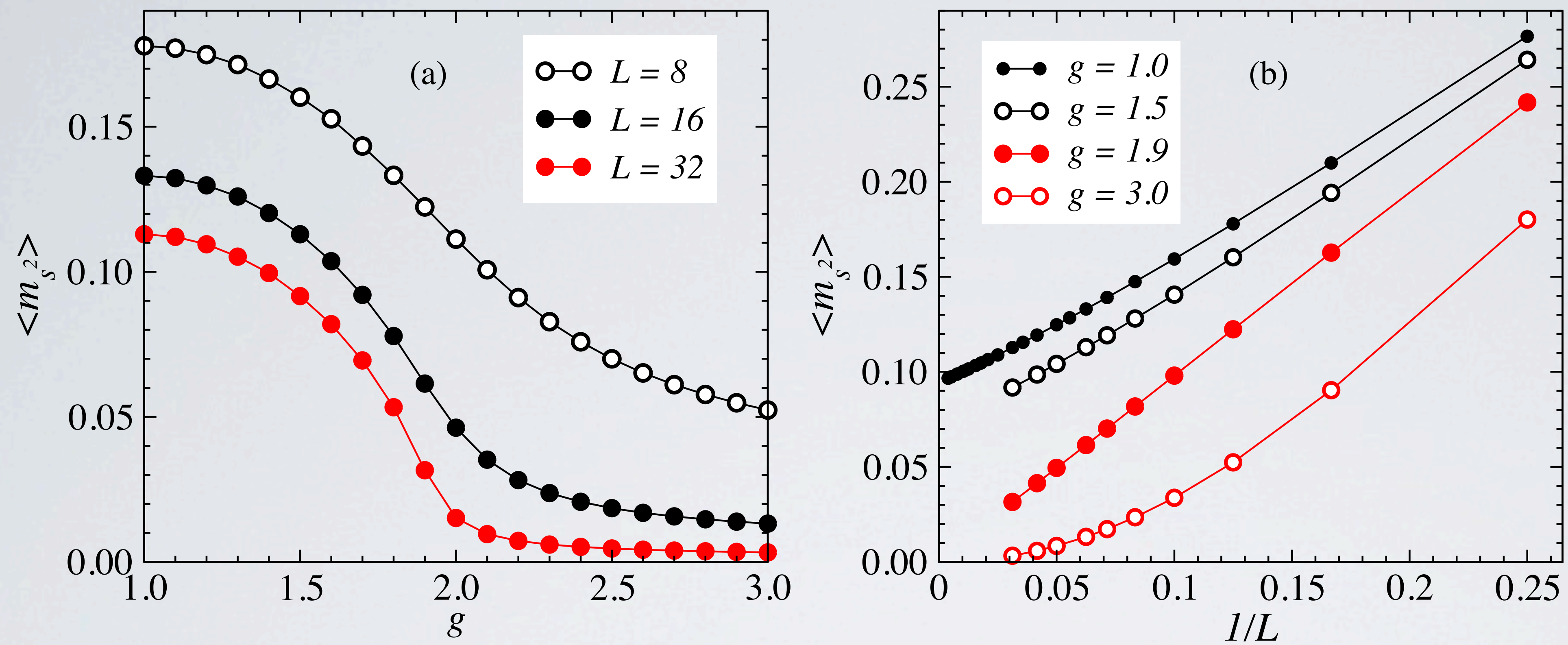
Ground state (T=0) phases



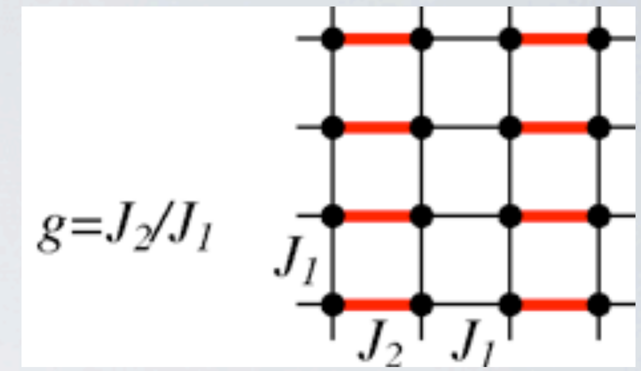
⇒ 3D classical Heisenberg (O3) universality class; QMC confirmed

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

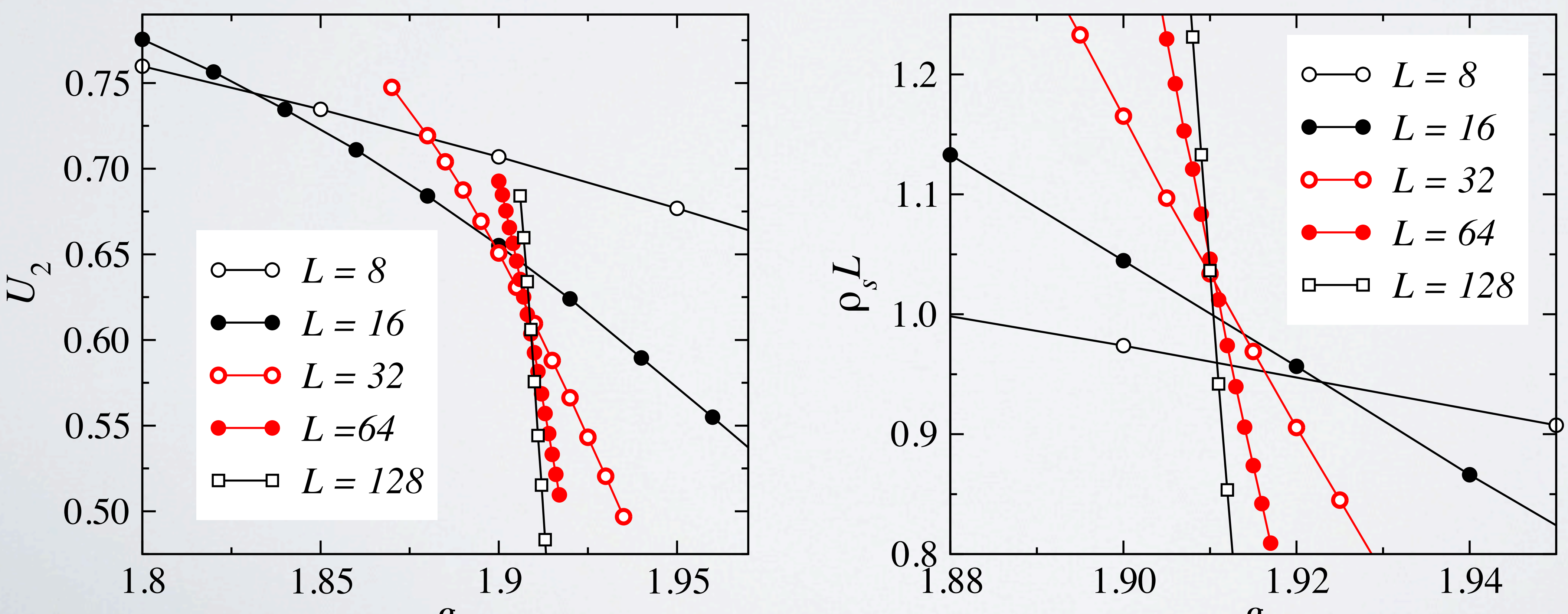
SSE calculations to locate the critical point



Columnar dimer system



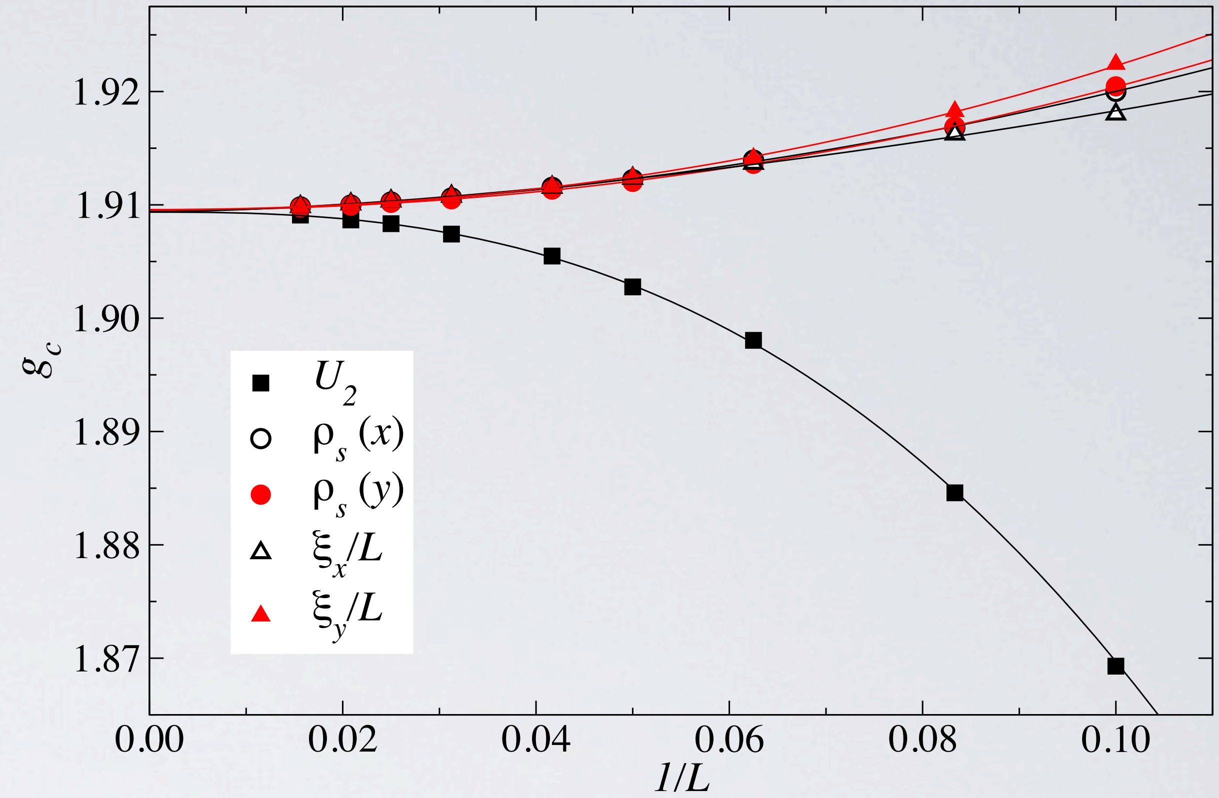
Curve crossing analysis: dimensionless quantities



Crossing points drift as the system size is increased
- extrapolations necessary
- can use (L,2L) crossing points

$$g_c(L) = g_c(\infty) + aL^{-b}$$

Different quantities give consistent results: **g_c=1.90948(4)**



Knowing g_c, we can analyze the ordering process

Correlations and susceptibility in Fourier space: $S^z_q = \frac{1}{\sqrt{N}} \sum_r \mathrm{e}^{-iqr} S^z_r$

$$S(q) = \langle S^z_{-q} S^z_q \rangle$$ (static structure factor)

$$\chi(q) = \int_0^\beta d\tau \langle S^z_{-q}(\tau) S^z_q(0) \rangle$$ (susceptibility of quantum system)

The ordering wave vector is q=Q=(π,π).

$$\frac{S(Q)}{N} = \langle m_s^2 \rangle \qquad \xi = \frac{L}{2\pi}\sqrt{\frac{S(Q)}{S(Q-2\pi/L)} - 1}$$ (correlation length)

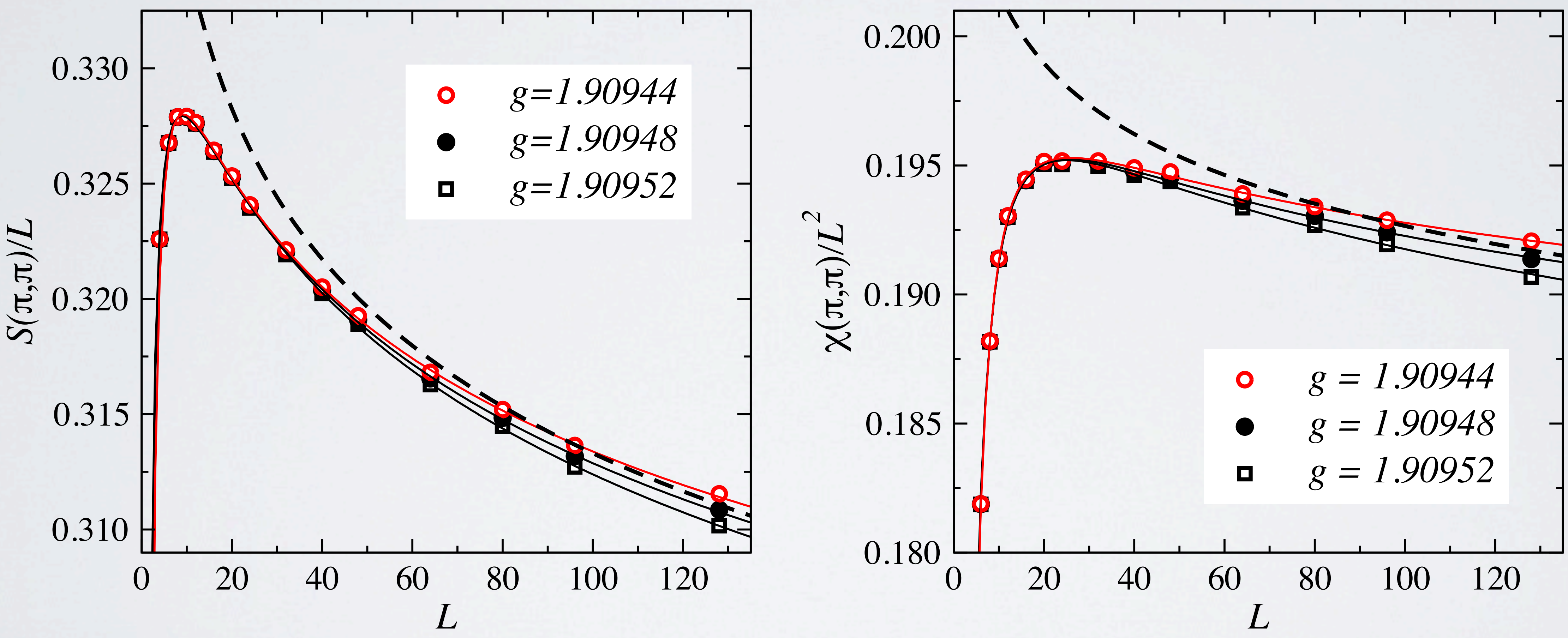
Critical exponents from finite-size scaling

It is often necessary to include scaling corrections. At g_c:

$$S(\pi,\pi) = aL^{1-\eta} + bL^{\omega}$$

$$\chi(\pi,\pi) = aL^{2-\eta} + bL^{\omega}$$

Do fits at the critical point and close to it (for error estimate)



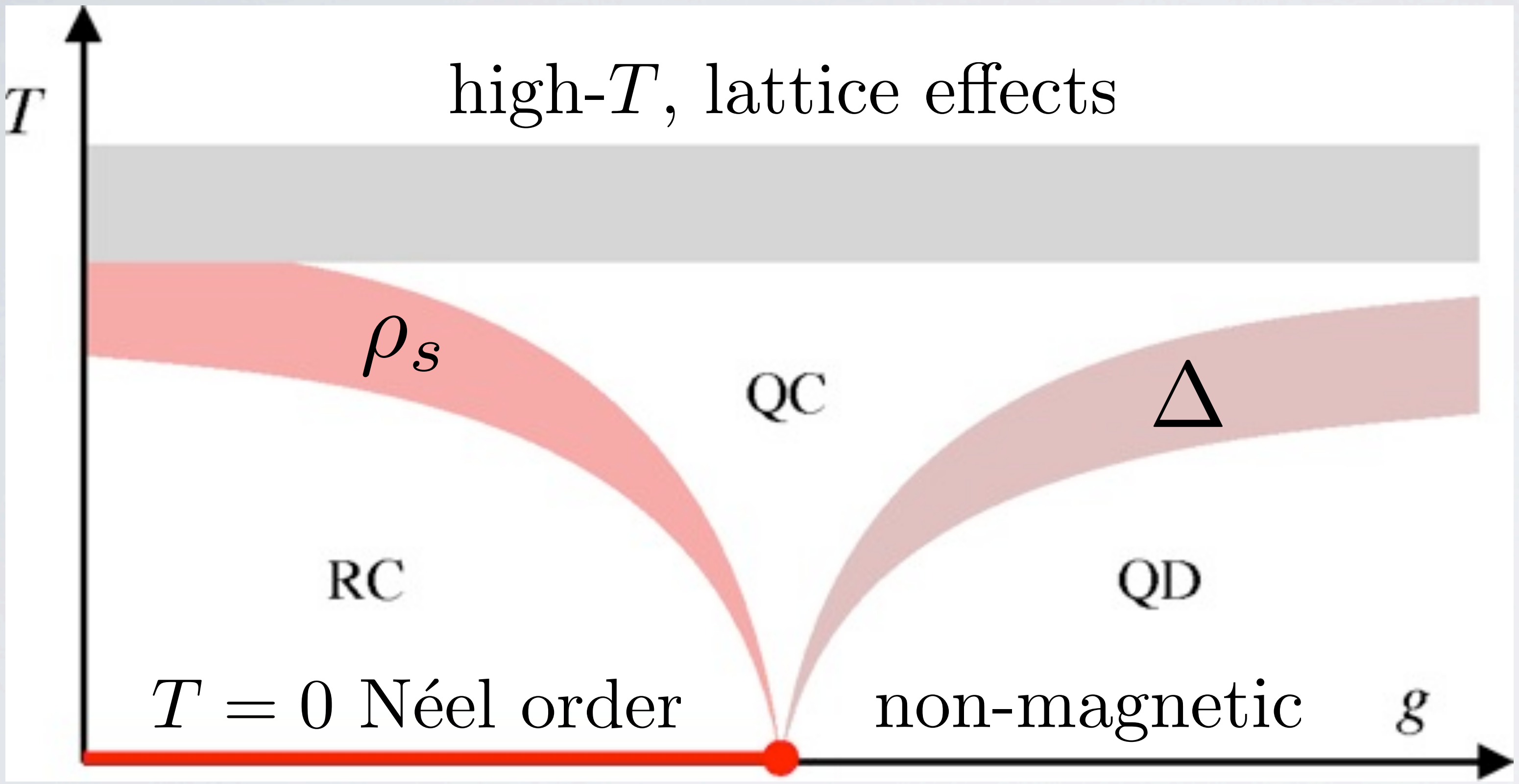
(dashed curves: correction terms removed)

Result: η=0.029(3) from S and 0.020(4) from X

- consistent with 3D O(3) (Heisenberg) universality class

What's so special about quantum-criticality?

- large T>0 quantum-critical "fan" where T is the only relevant energy scale
- physical quantities show power laws governed by the T=0 critical point



2D Neel-paramegnet **"cross-over diagram"** [Chakravarty, Halperin, Nelson, PRB 1988]

QC: Universal quantum critical scaling regime

Changing T is changing the imaginary-time size L_τ:

- Finite-size scaling at g_c leads to power laws

$\xi \sim T^{-1}$ (correlation length)

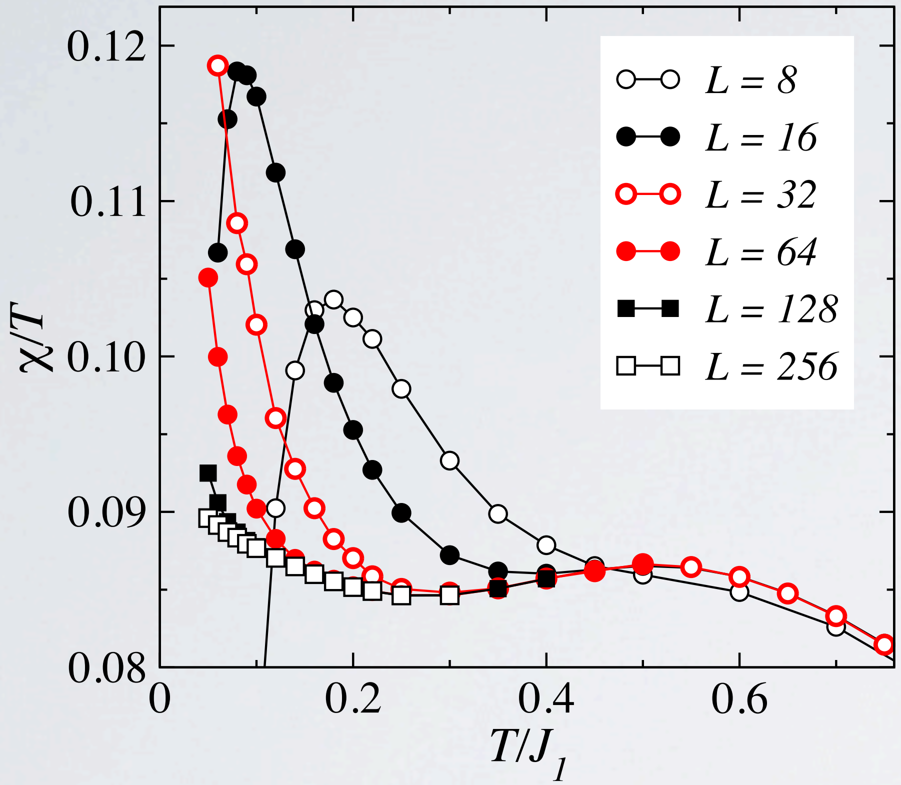
$C \sim T^2$ (specific heat)

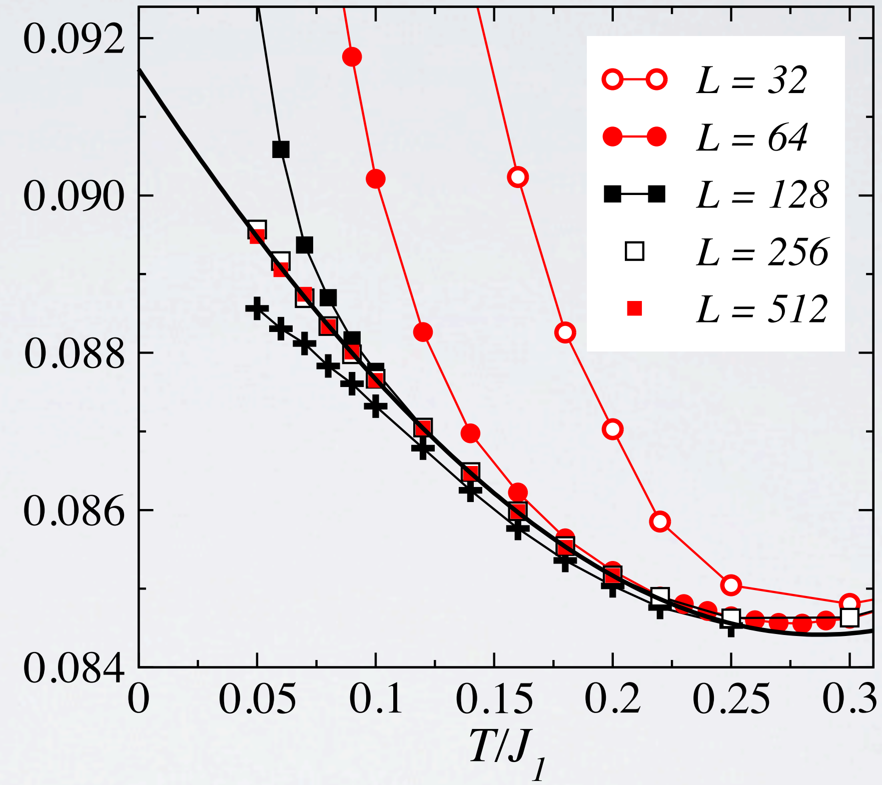
$\chi(0) \sim T$ (uniform magnetic susceptibility)

Test of predictions. Example, susceptibility

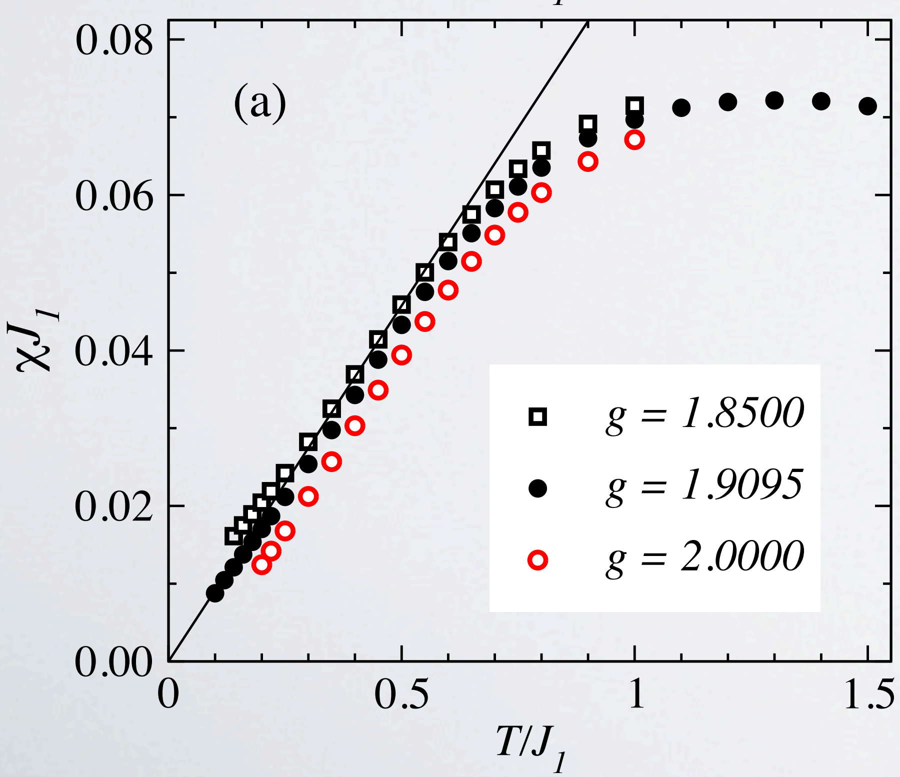
$$\chi(0) \sim T \Rightarrow \chi(0)/T \rightarrow \text{constant when } T \rightarrow 0$$

This prediction is for the thermodynamic limit
- has to use system size large enough for L→∞ convergence





convergence slower for decreasing T (increasing ξ)



Away from the critical point (in the quantum-critical fan) the behavior is still linear:

$$\chi(0) = a + bT$$

Making connections with quantum field theory

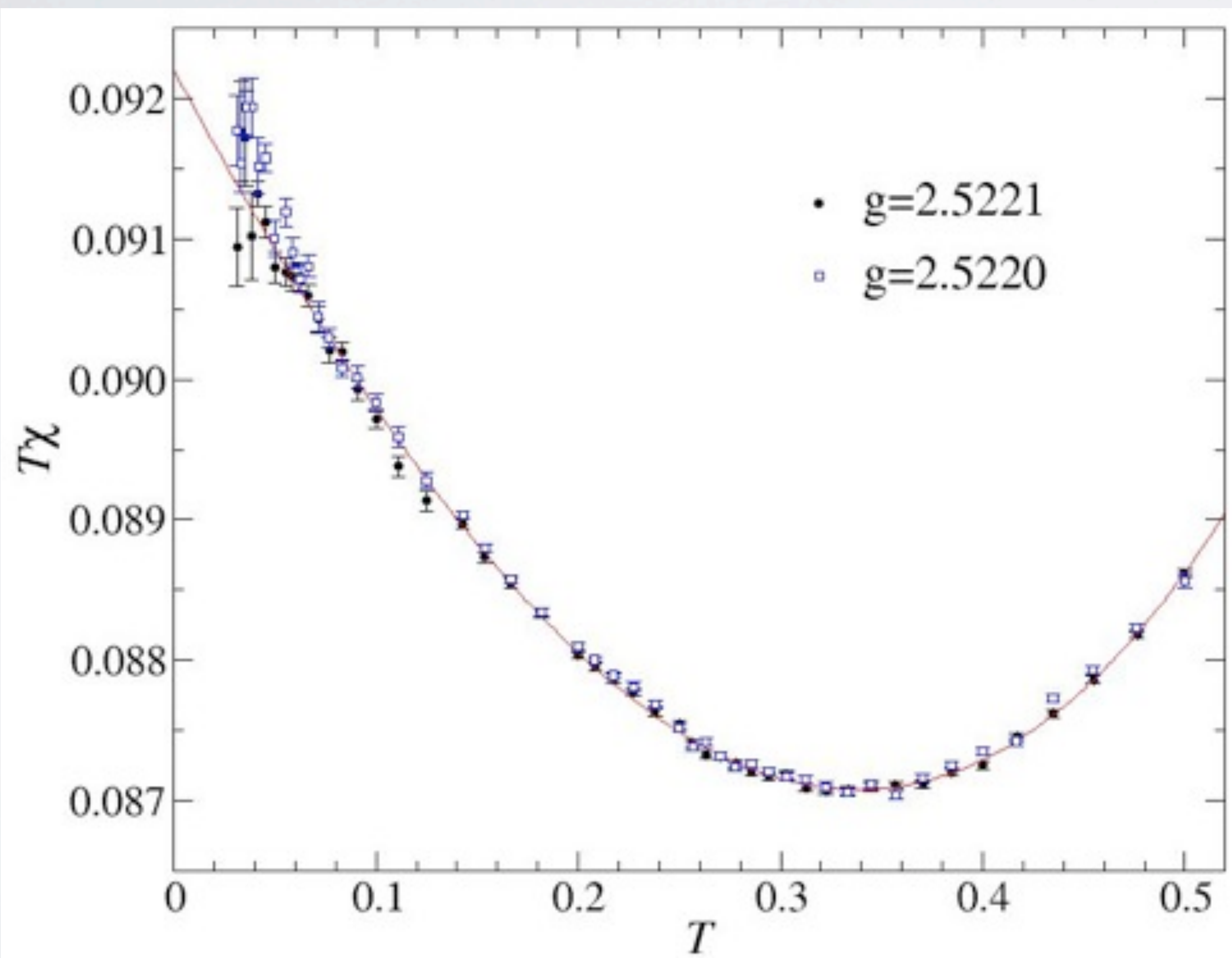
Low-energy properties described by the (2+1)-dimensional nonlinear σ-model
- Chakravarty, Halperin, Nelson (1989), Chubukov, Sachdev, Ye (1994)

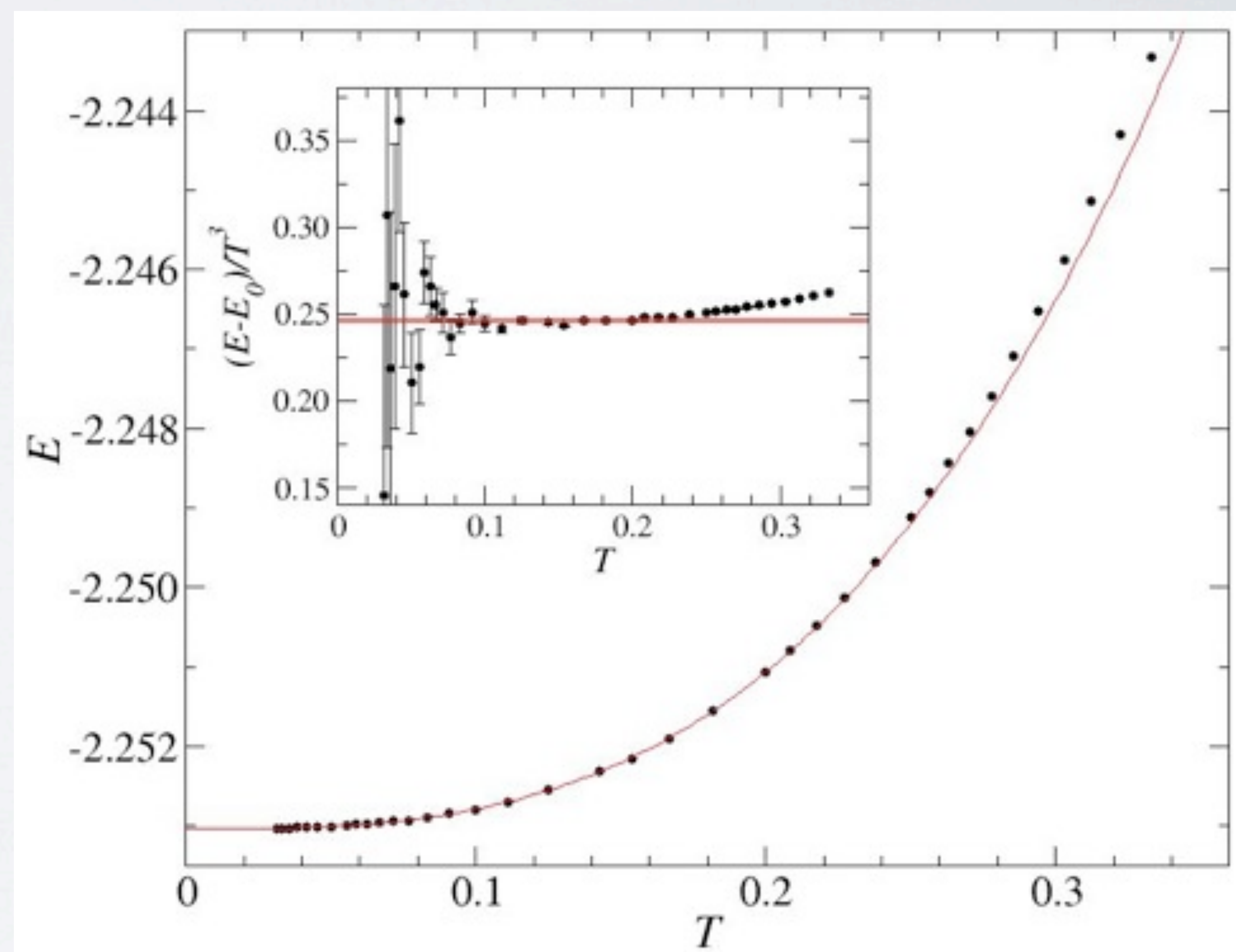
Expand O(3) order-parameter symmetry to O(N), large-N calculations

T>0 properties at quantum-critical coupling (N=3):

$$\chi(T) = \frac{1.0760}{\pi c^2} T \qquad\qquad E(T) = E_0 + \frac{12 \cdot 1.20206}{5\pi c^2} T^3$$

QMC results for **bilayer model**: g_c = 2.5220(1), $c(g_c)$=1.9001(2)
- L×L lattices with L up to 512 (no size-effects for $T/J_1 \gtrsim 0.03$)





T and T^3 prefactors agree with theory to within 3%

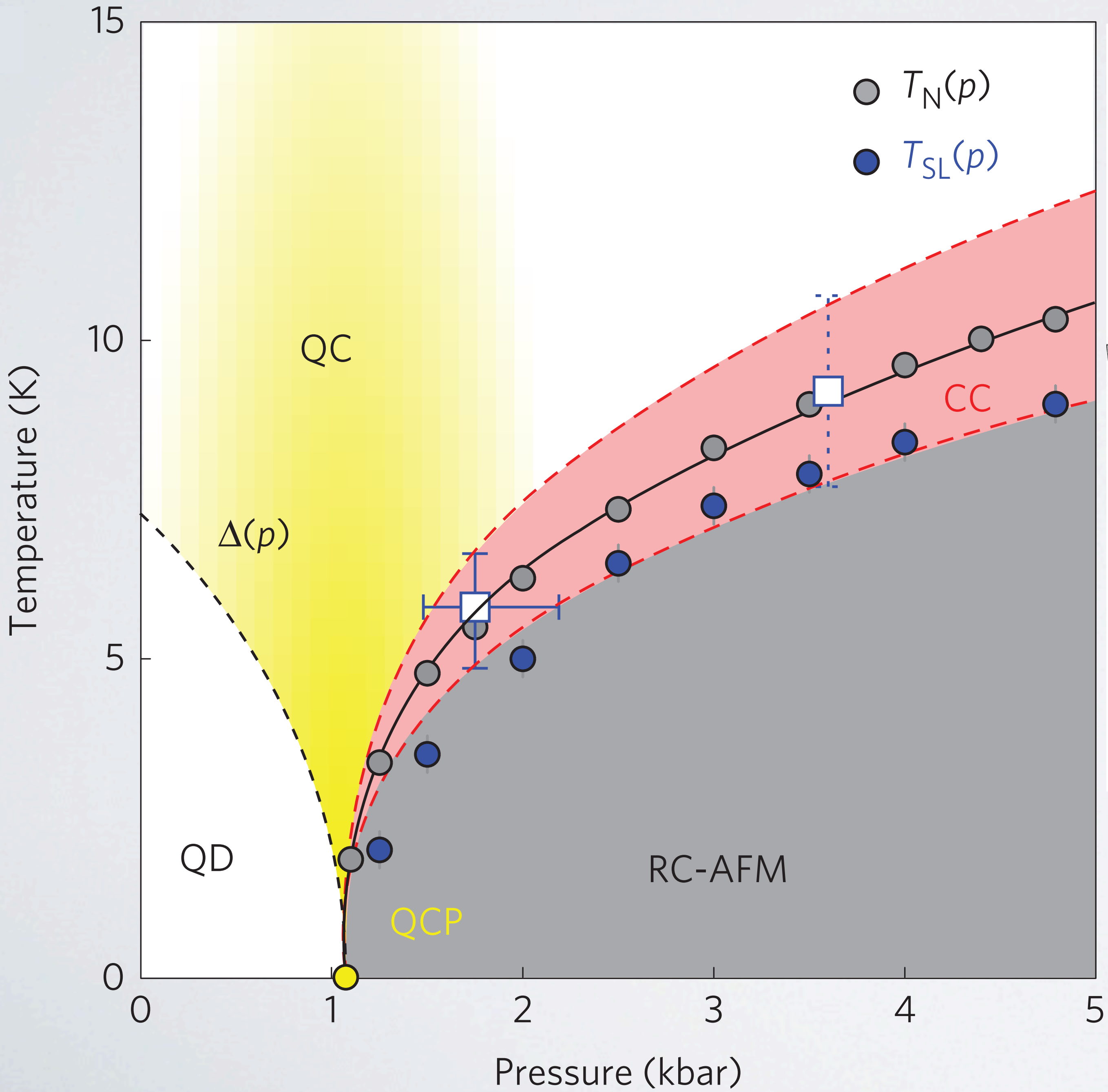
nature physics
ARTICLES
PUBLISHED ONLINE: 6 APRIL 2014 | DOI: 10.1038/NPHYS2902

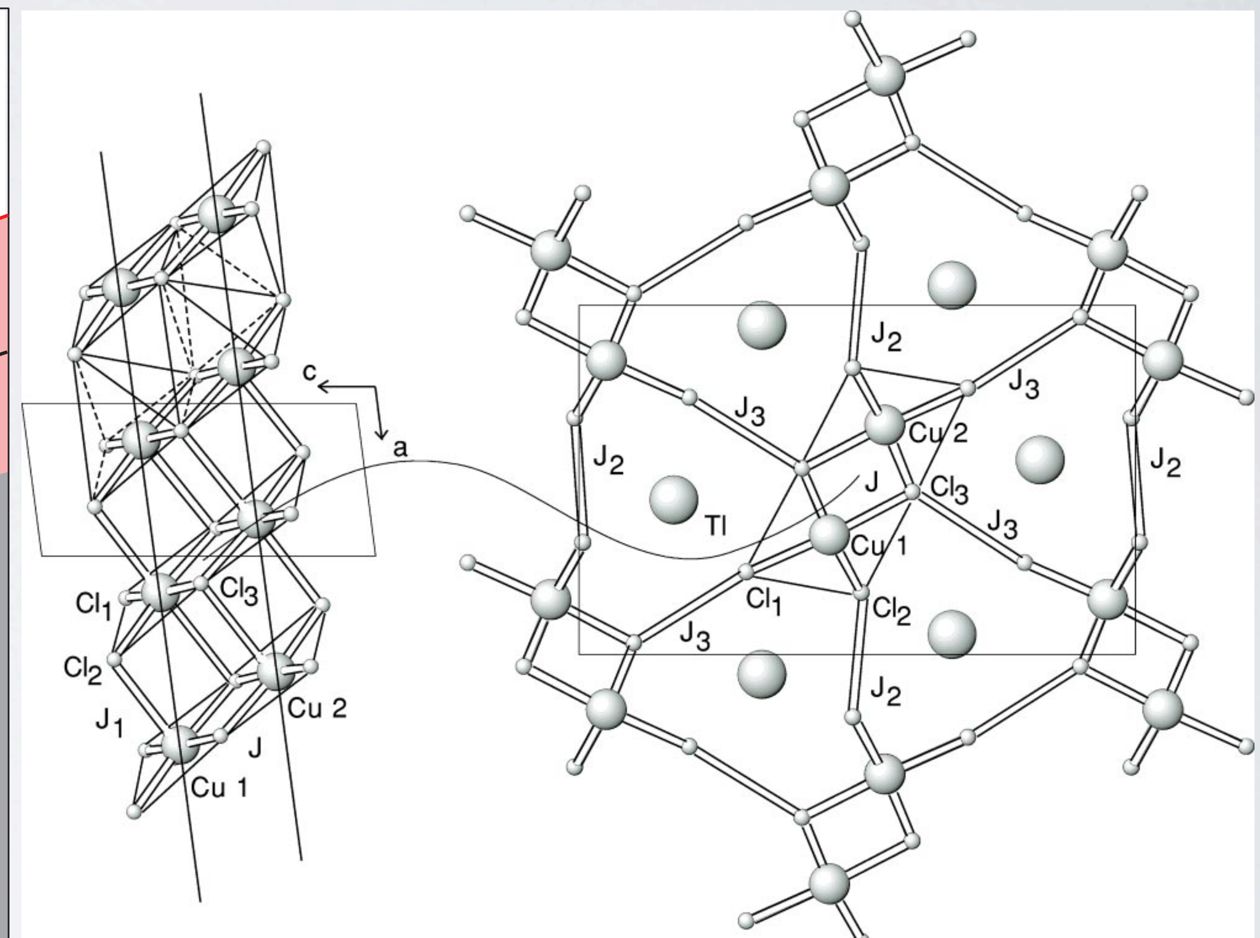
$TlCuCl_3$

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



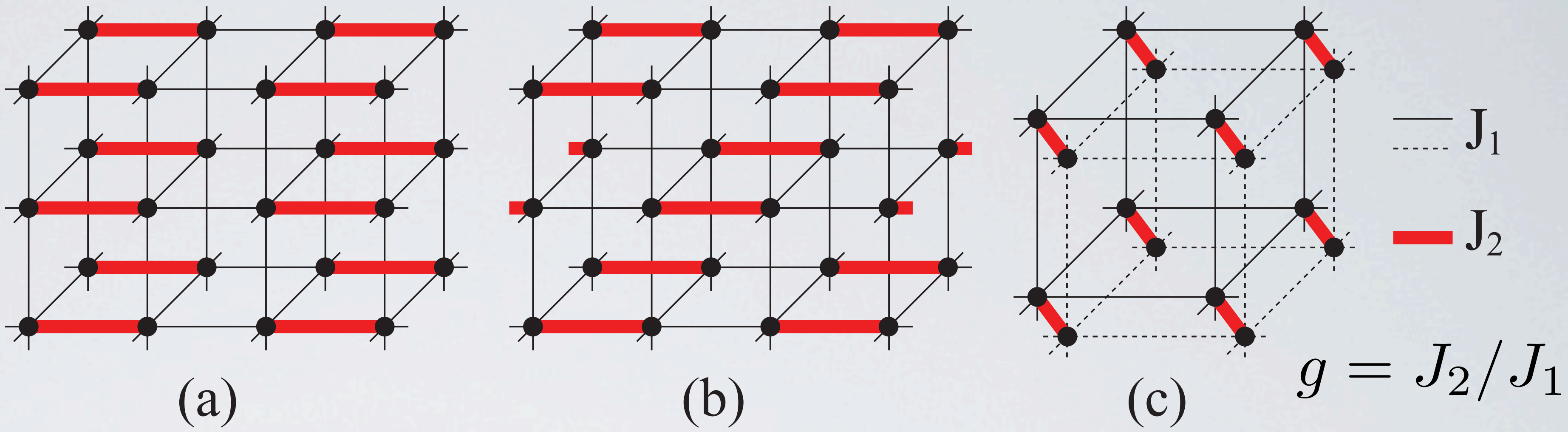


From: M Matsumoto, B Normand, TM Rice, M Sigrist, PRB (2004)

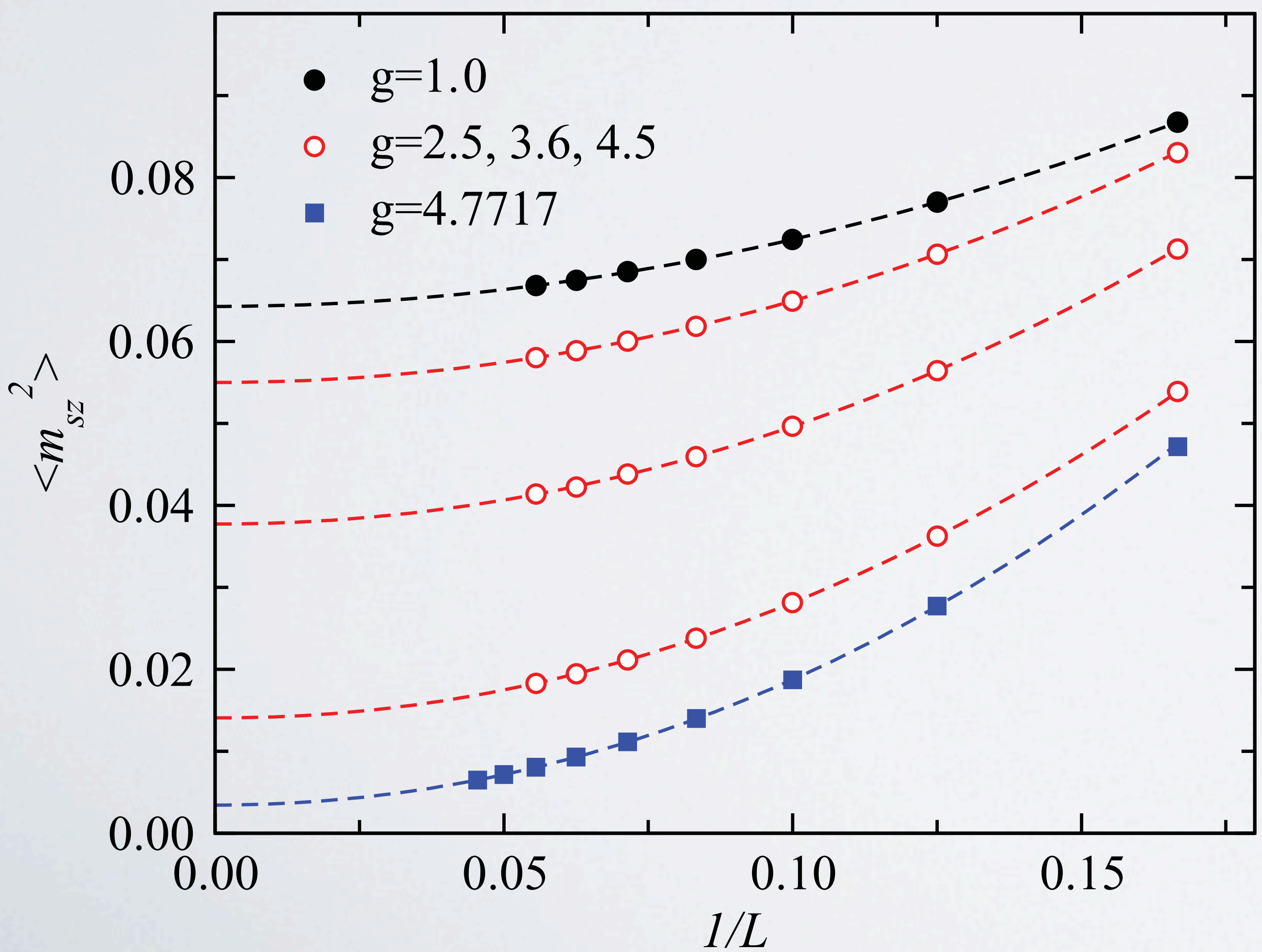
Universality of the Neel temperature in 3D dimerized systems?

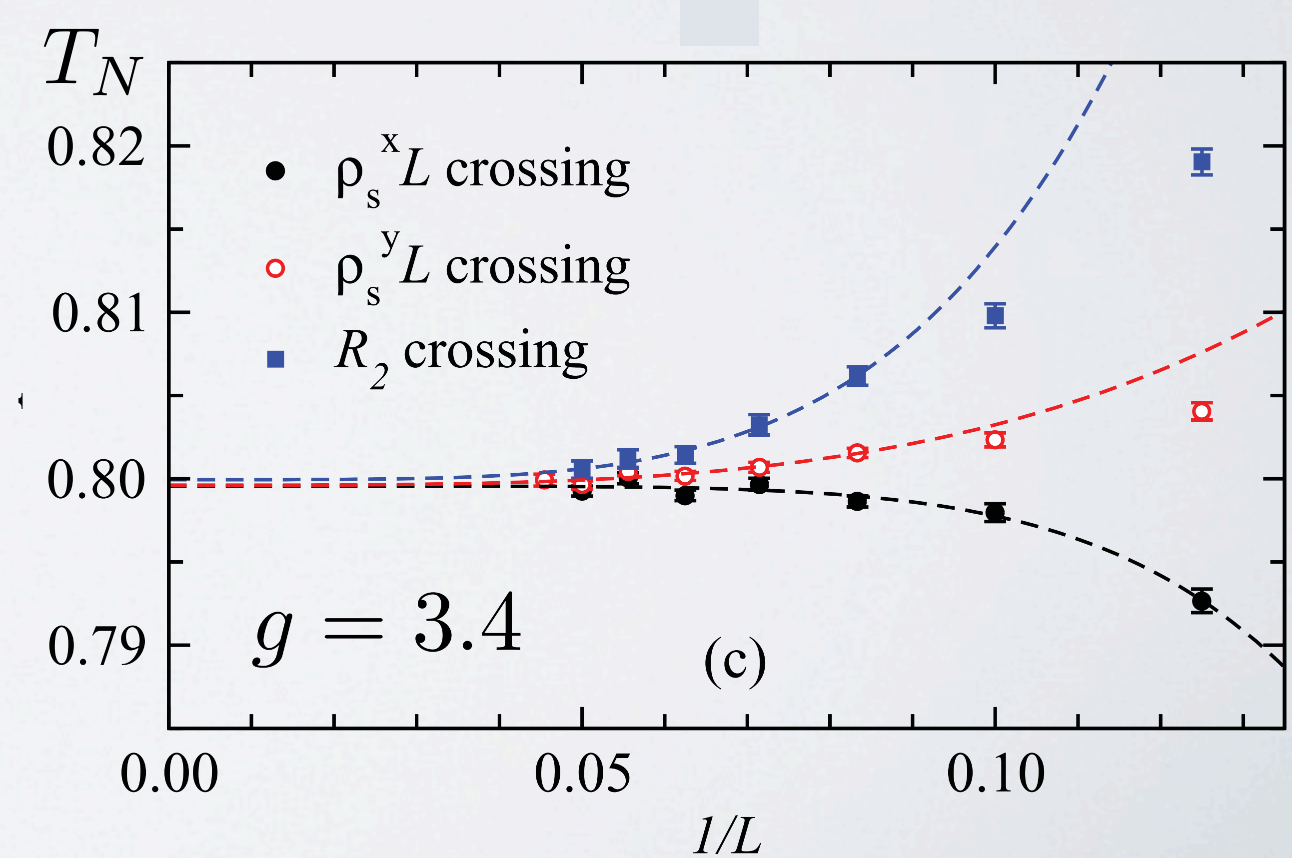
[S. Jin, AWS, PRB2012]

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



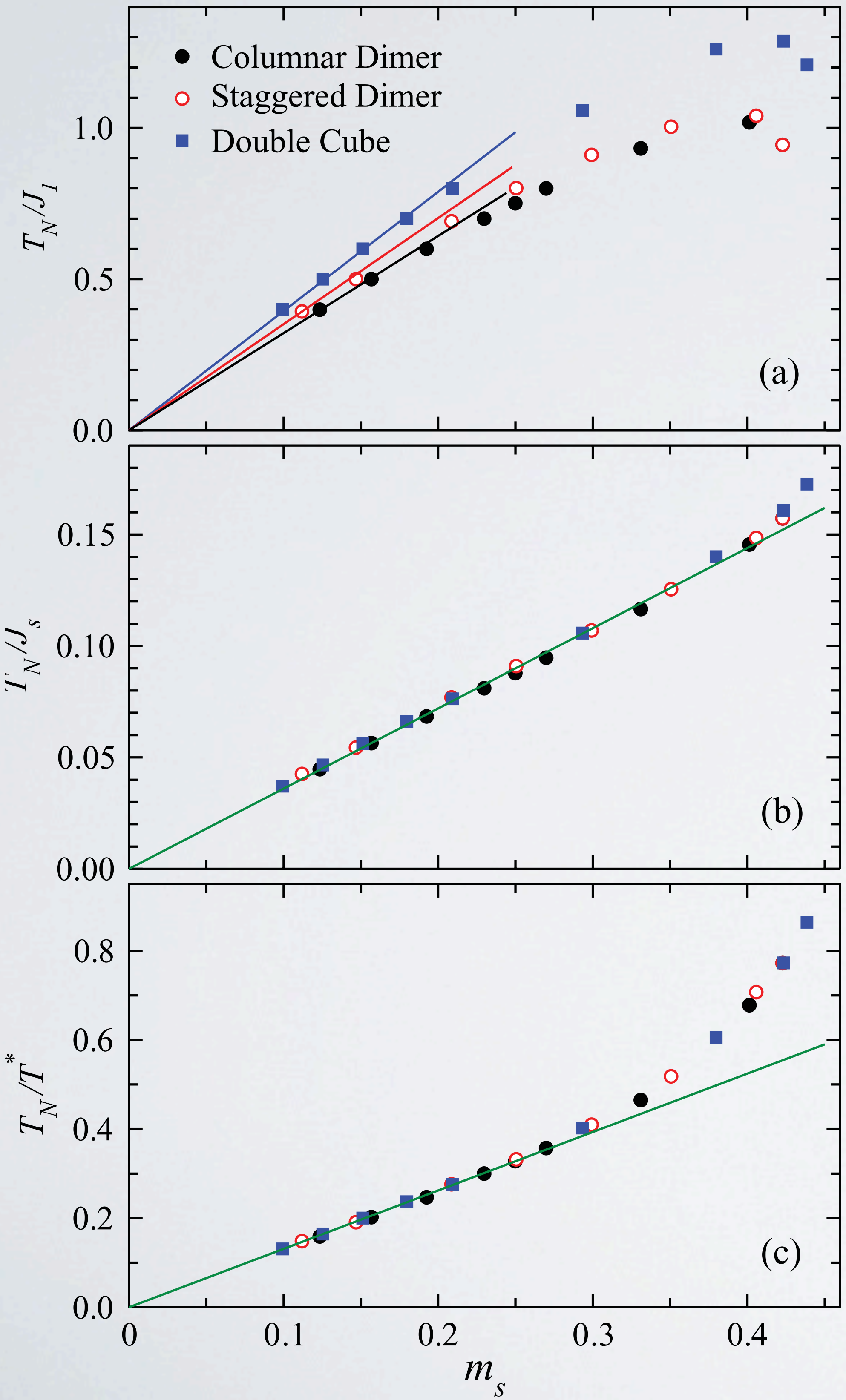
Example: Columnar dimers





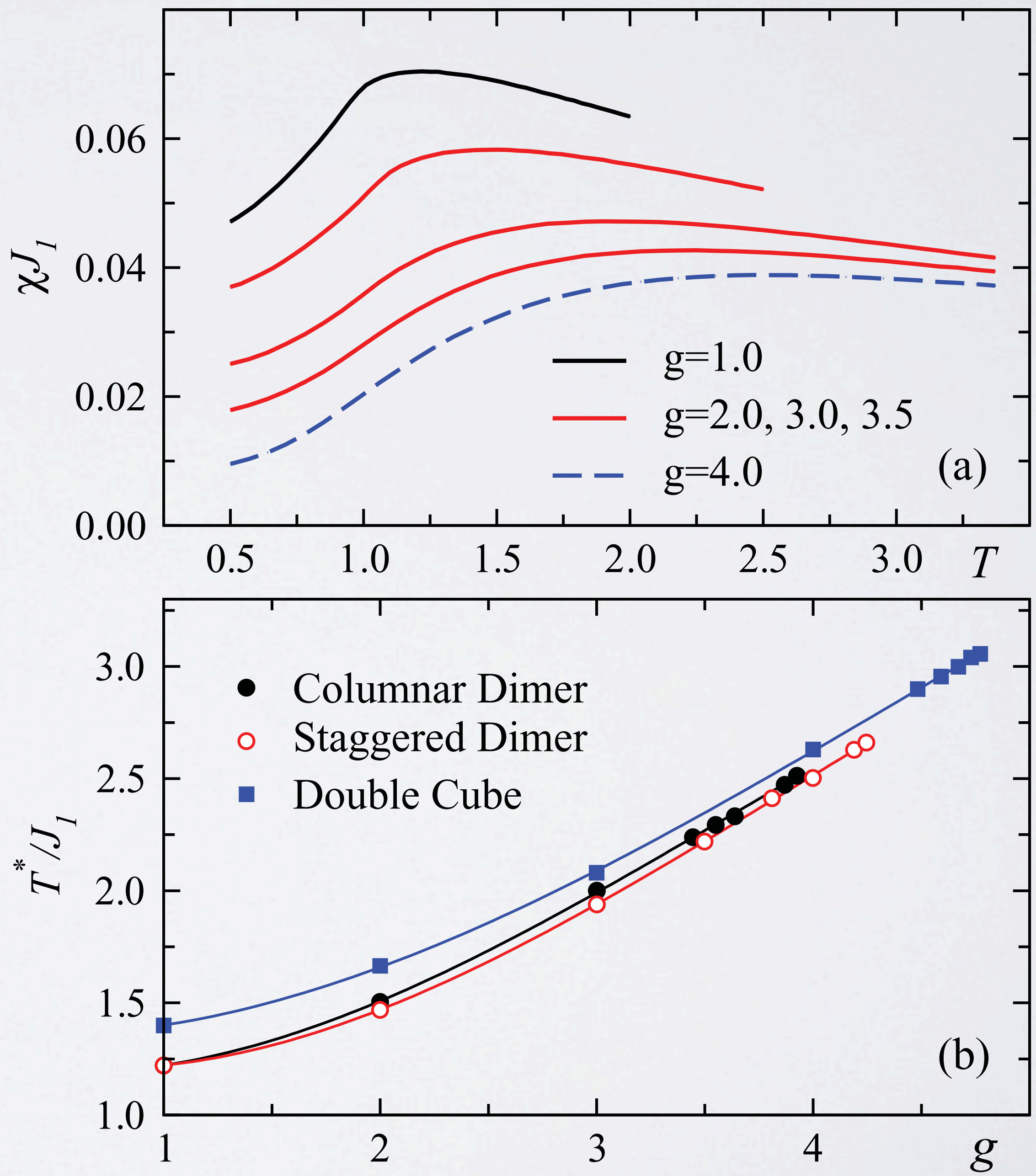
Couplings vs pressure not known experimentally

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



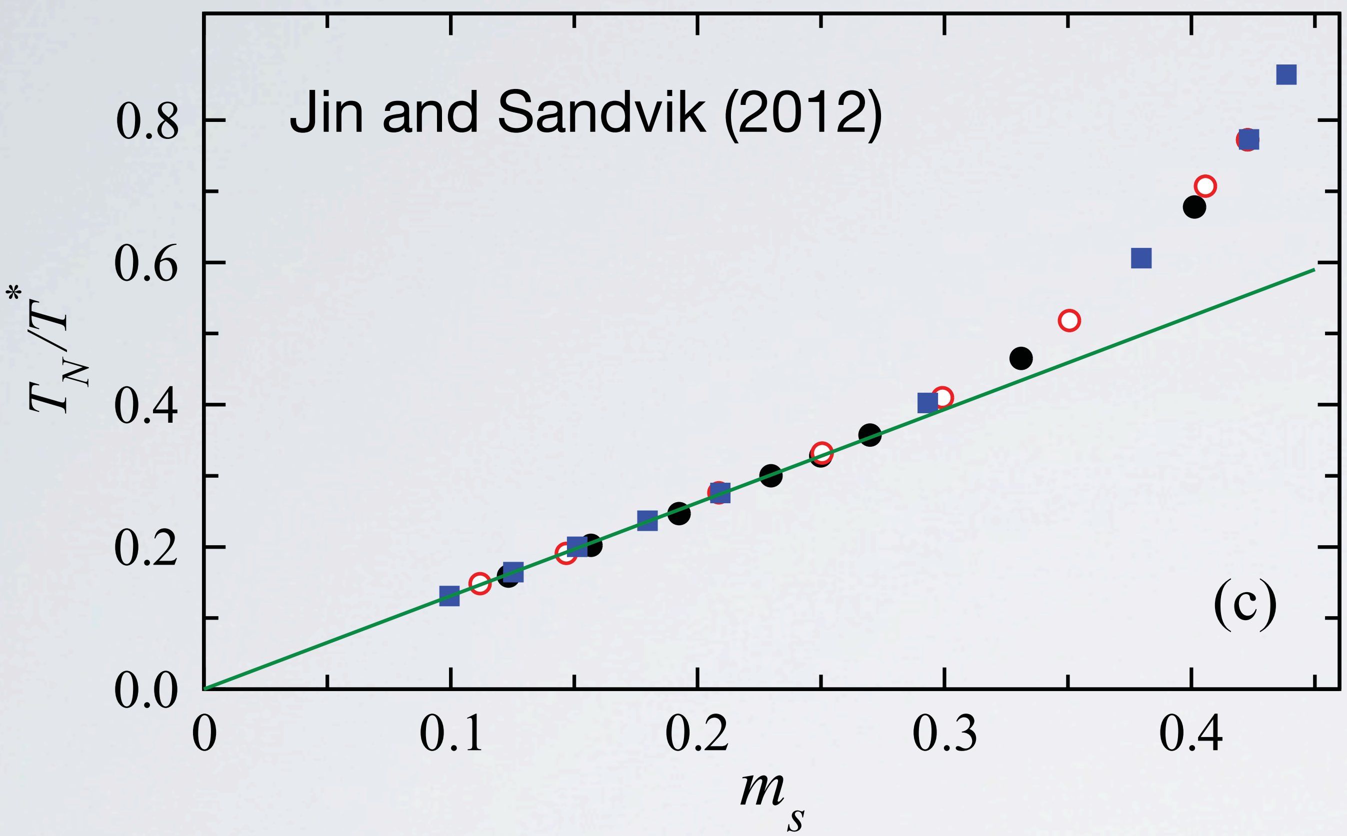
Three normalizations

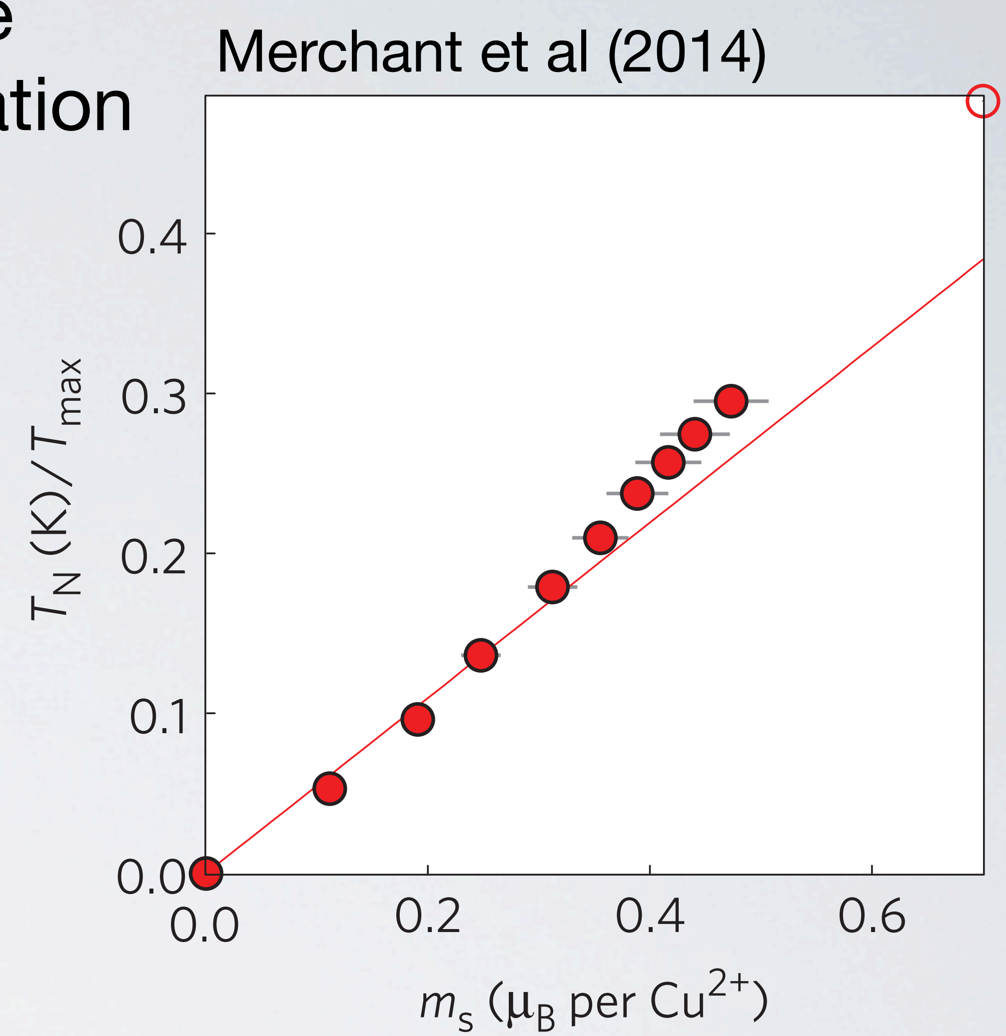
- weaker copling J_1
- sum J_s of couplings per spin
- peak T^* of magnetic susceptibility



T* normalization is in principle accessible experimentally

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





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 (high T_N, high density of excited spin waves)

Same features observed in models and experiment

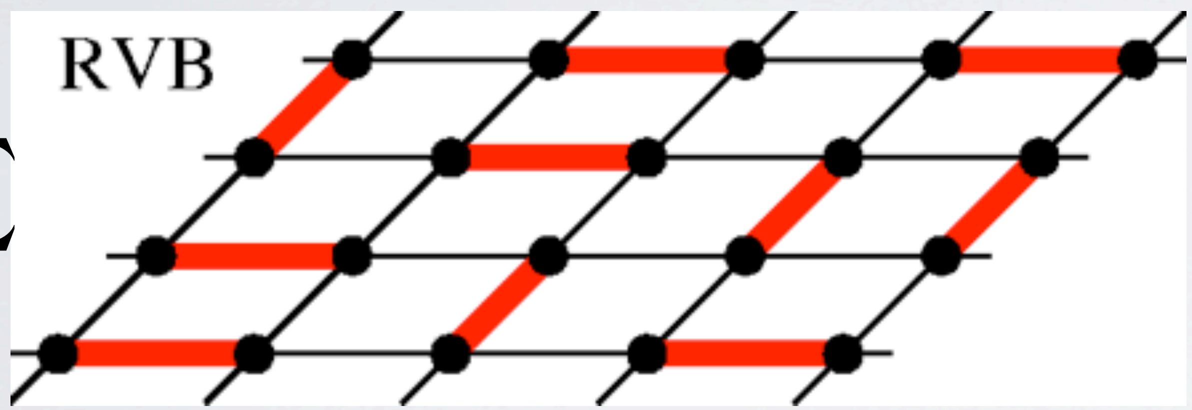
- experimental slope about 25% lower of g-factor 2 assumed (what exactly is the g-factor?)

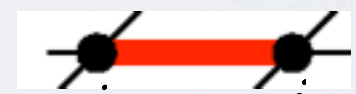
More complex non-magnetic states; systems with 1 spin per unit cell

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

- **non-trivial non-magnetic ground states are possible, e.g.,**
  - ➡ resonating valence-bond (RVB) spin liquid
  - ➡ valence-bond solid (VBS)

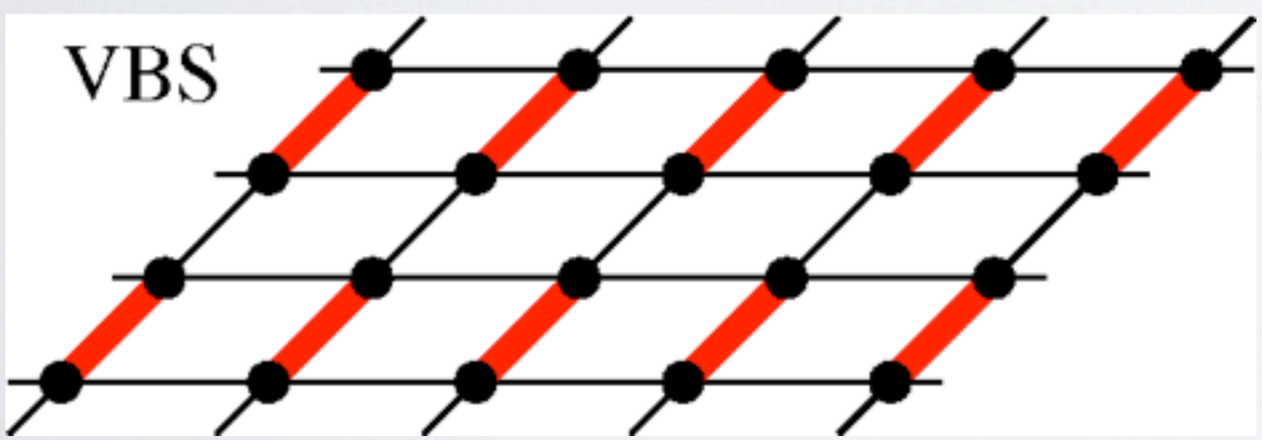
Non-magnetic states often have natural descriptions with **valence bonds**

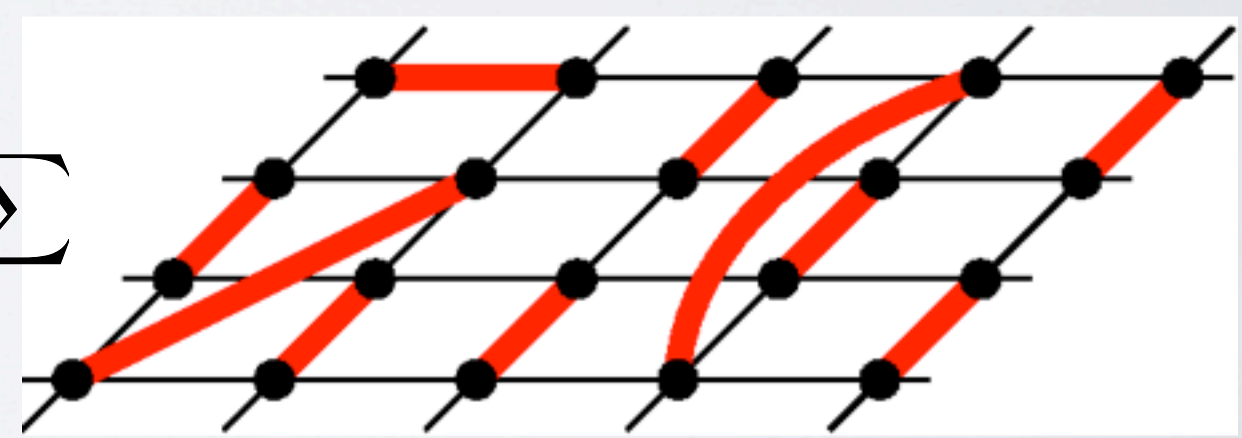
$\sum$ 



$$= (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j)/\sqrt{2}$$

The basis including bonds of all lengths is **overcomplete** in the singlet sector



$\sum$ 

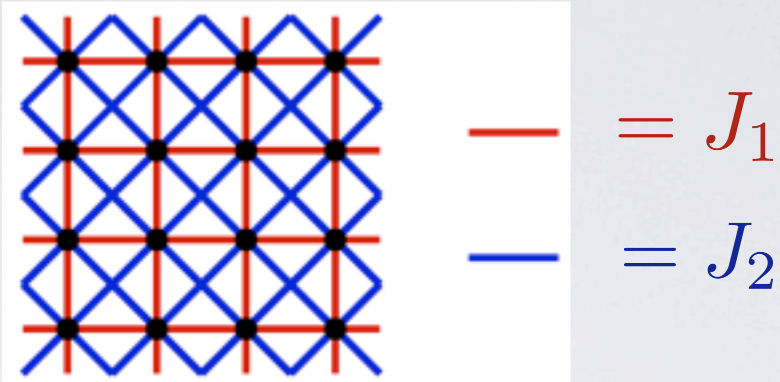
• non-magnetic states dominated by short bonds

Frustrated spin interactions

Quantum phase transitions as some coupling (ratio) is varied

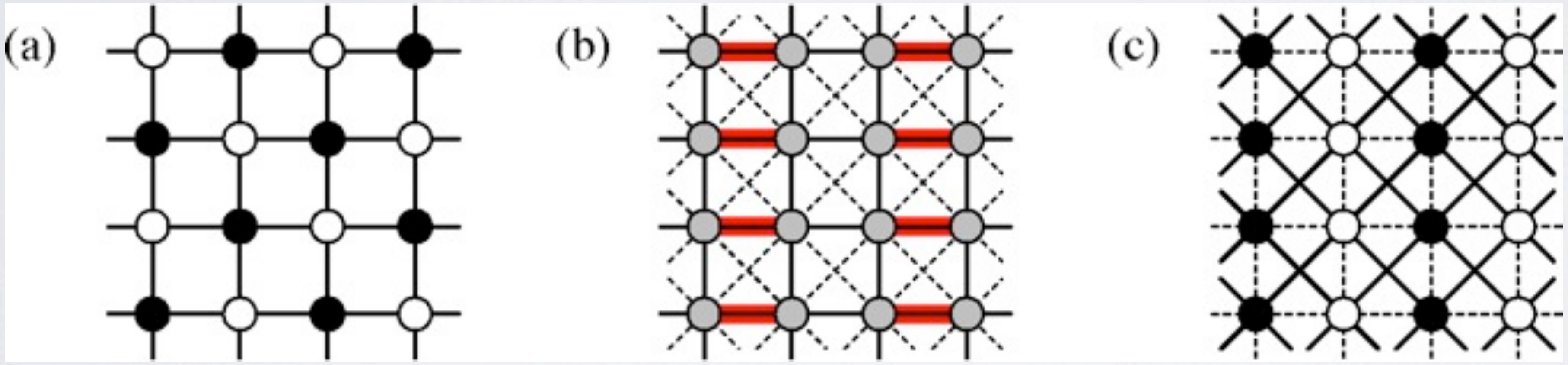
- J_1-J_2 Heisenberg model is the prototypical example

$$H = \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$



$$g = J_2/J_1$$

- Ground states for small and large g are well understood
  - Standard **Néel order up to g≈0.45; collinear magnetic order for g>0.6**



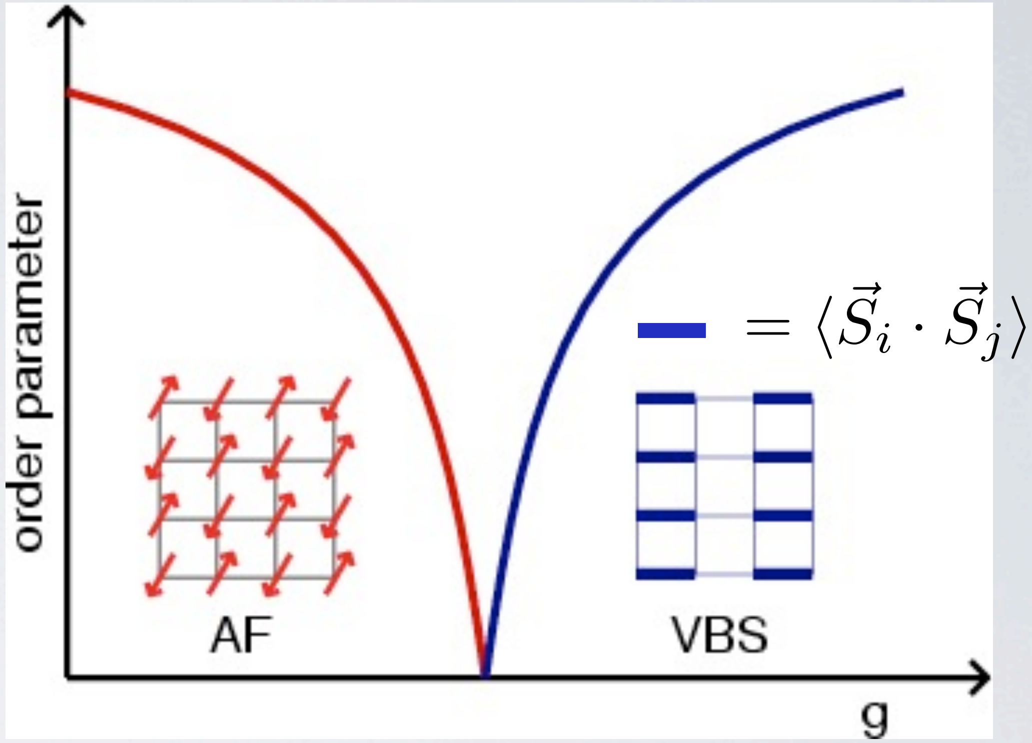
$0 \leq g < 0.45$ $\quad$ $0.45 \leq g < 0.6$ $\quad$ $g > 0.6$

- A non-magnetic state exists between the magnetic phases
  - May be a VBS (what kind? Columnar or "plaquette?)
  - Some calculations (interpretations) suggest spin liquid
- 2D frustrated models are challenging
  - QMC sign problems (non-positive-definite weights in path integral)

VBS states and "deconfined" quantum criticality

Read, Sachdev (1989),....,Senthil, Vishwanath, Balents, Sachdev, Fisher (2004)

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



Neel-VBS transition in 2D

- generically continuous
- violating the "Landau rule" stating 1st-order transition

Description with spinor field (2-component complex vector)

$\boldsymbol{\Phi} = z^*_\alpha \boldsymbol{\sigma}_{\alpha\beta} z_\beta$ gauge redundancy: $z \longrightarrow e^{i\gamma(r,\tau)} z$

$$\mathcal{S}_z = \int d^2 r d\tau \left[|(\partial_\mu - iA_\mu) z_\alpha|^2 + s|z_\alpha|^2 + u(|z_\alpha|^2)^2 + \frac{1}{2e_0^2}(\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda)^2 \right]$$

A is a U(1) symmetric gauge field

- CP^1 action (non-compact)
- large-N calculations for CP^{N-1} theory

- proposed as critical theory separating Neel and VBS states
- describes VBS state when additional terms are added

Competing scenario: first-order transition (Prokof'ev et al.)

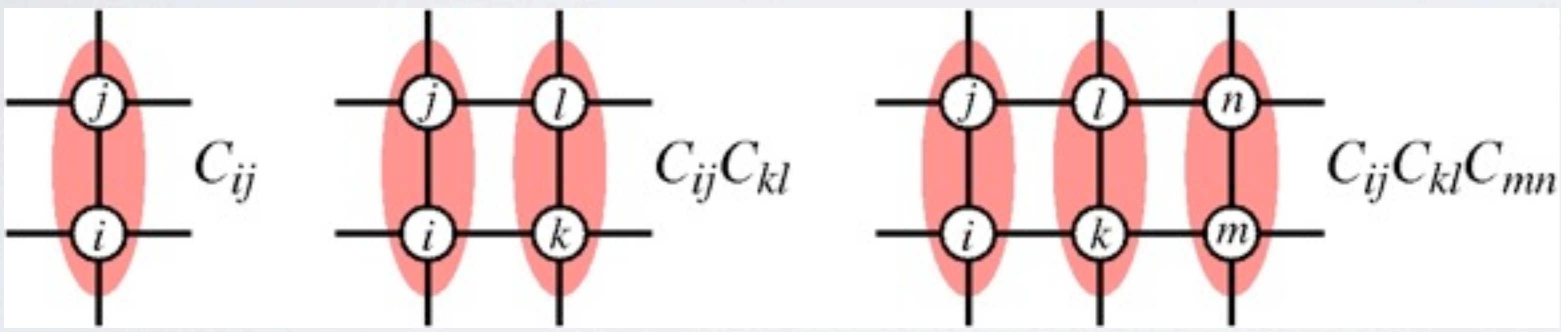
VBS states from multi-spin interactions (Sandvik, 2007)

The Heisenberg interaction is equivalent to a singlet-projector

$$C_{ij} = \frac{1}{4} - \vec{S}_i \cdot \vec{S}_j$$

$$C_{ij}|\phi^s_{ij}\rangle = |\phi^s_{ij}\rangle, \qquad C_{ij}|\phi^{tm}_{ij}\rangle = 0 \quad (m=-1,0,1)$$

- we can construct models with products of singlet projectors
- no frustration in the conventional sense (QMC can be used)
- correlated singlet projection reduces the antiferromagnetic order



+ all translations and rotations

The "J-Q" model with two projectors is

$$H = -J\sum_{\langle ij\rangle} C_{ij} - Q \sum_{\langle ijkl\rangle} C_{ij}C_{kl}$$

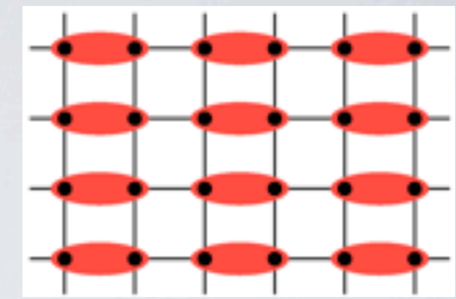
- Has Néel-VBS transition, appears to be continuous
- Not a realistic microscopic model for materials
- Intended to study VBS and Néel-VBS transition (universal physics)

T=0 Néel-VBS transition in the J-Q model

Ground-stae projector QMC calculations

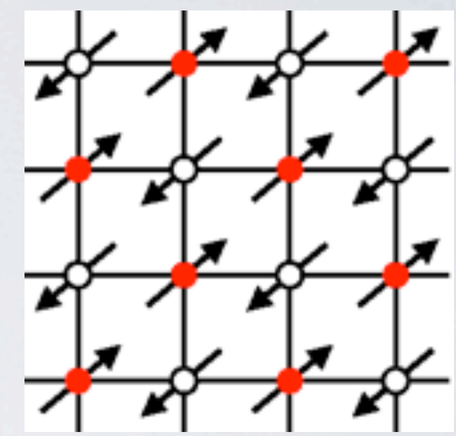
(Sandvik, 2007; Lou, Sandvik, Kawashima, 2009)

VBS vector order parameter (D_x,D_y) (x and y lattice orientations)



$$D_x = \frac{1}{N}\sum_{i=1}^{N}(-1)^{x_i}\mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}}, \quad D_y = \frac{1}{N}\sum_{i=1}^{N}(-1)^{y_i}\mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}}$$

Néel order parameter (staggered magnetization)



$$\vec{M} = \frac{1}{N}\sum_{i}(-1)^{x_i+y_i}\vec{S}_i$$

No symmetry-breaking in simulations; study the squares

$$M^2 = \langle \vec{M} \cdot \vec{M} \rangle, \qquad D^2 = \langle D_x^2 + D_y^2 \rangle$$

Finite-size scaling: a critical squared order parameter (A) scales as

$$A(L,q) = L^{-(1+\eta)} f[(q-q_c)L^{1/\nu}]$$

coupling ratio

$$q = \frac{Q}{J+Q}$$

Data "collapse" for different system sizes L of $AL^{1+\eta}$ graphed vs $(q-q_c)L^{1/\nu}$

J-Q$_2$ model; q$_c$=0.961(1)

$$\eta_s = 0.35(2)$$

$$\eta_d = 0.20(2)$$

$$\nu = 0.67(1)$$

J-Q$_3$ model; q$_c$=0.600(3)

$$\eta_s = 0.33(2)$$

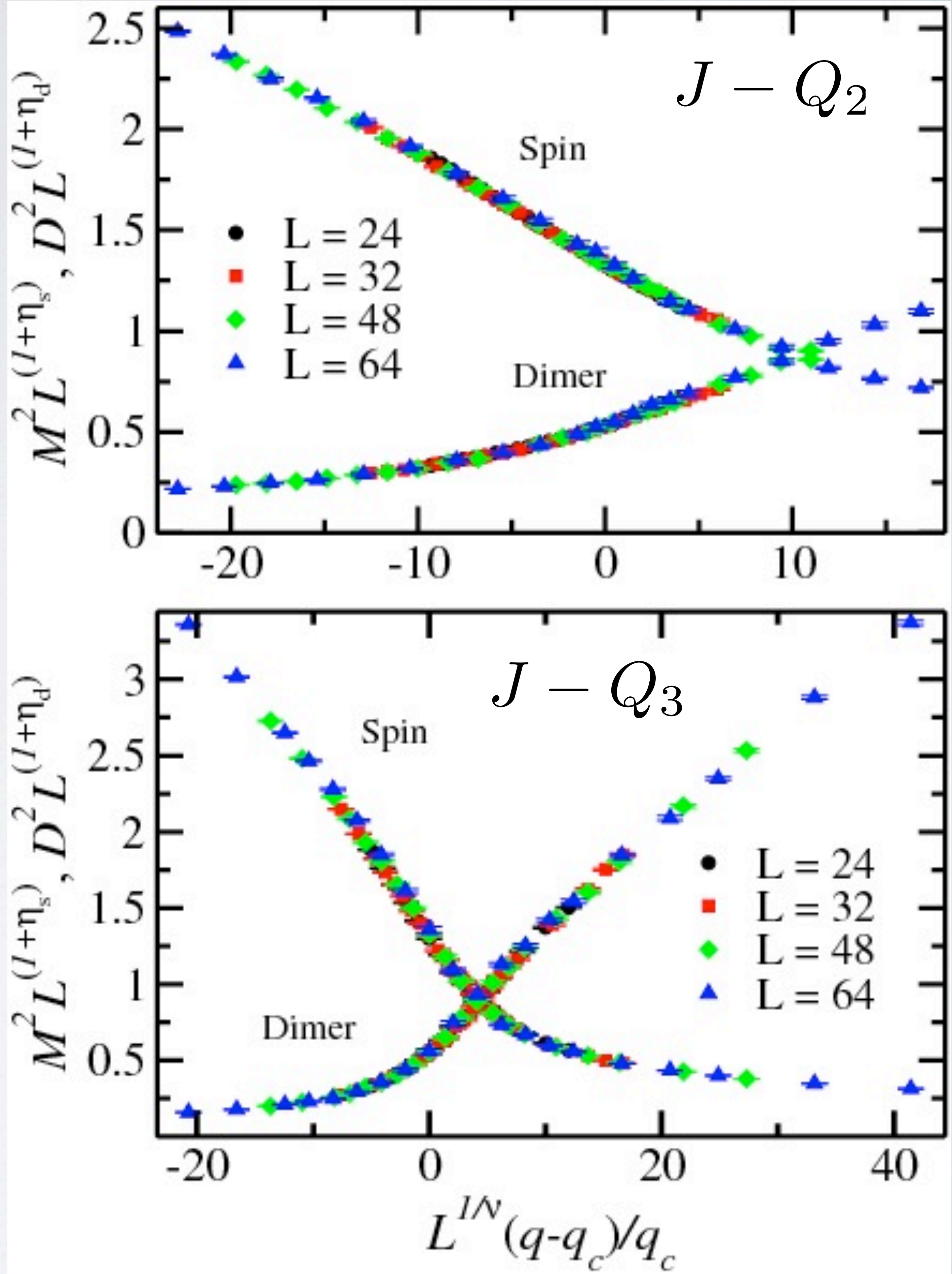
$$\eta_d = 0.20(2)$$

$$\nu = 0.69(2)$$

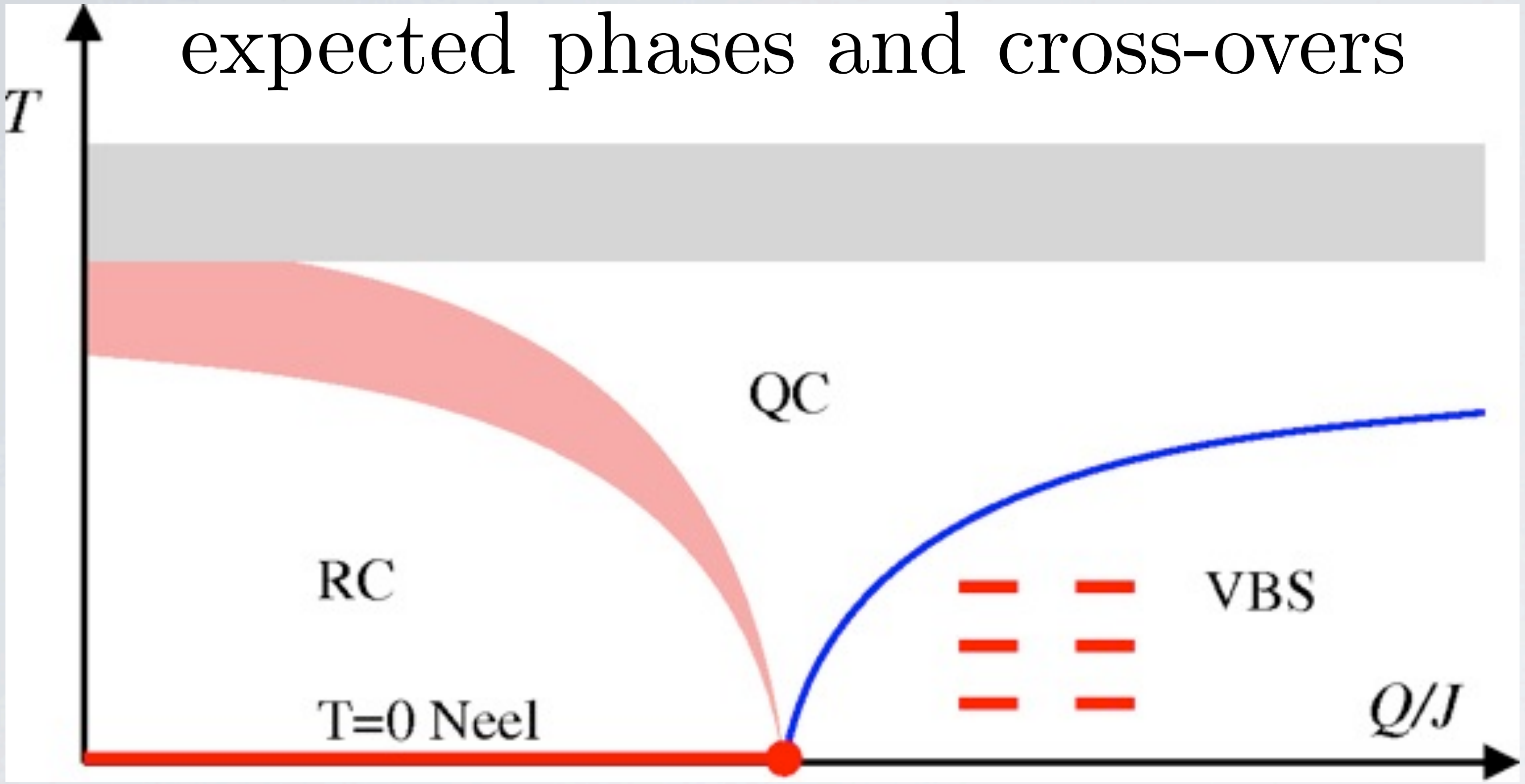
Exponents universal
(within error bars)

Comparable results for honeycomb J-Q model
Alet & Damle, PRB 2013

Dimer expansion calculations; strong fluctuations, hard to reproduce QMC results
D. Yao et al., PRB 2009



T>0 Paramagnet - VBS transition



What is the nature of the T>0 critical(?) curve (universality class)?
S. Jin, A. Sandvik, PRB 2013

The VBS pattern can be arranged in 4 different ways (translate, rotate)

- **Z_4 symmetric order param**

Scenarios for 2D Z_4 symmetry-breaking (conformal field theory, CFT):

4-state Potts — $\nu \to 2/3$ — $\eta = 1/4$ — $\nu \to 1$ — Ising

Ashkin-Teller and J_1-J_2 Ising models

XY (KT trans.) — $\nu \to \infty$ — $\eta = 1/4$ — $\nu \to 1$ — Ising

XY-model with cos(4θ) term

But a previous study found ν≈0.5 for J-Q_2 model at J=0:
- Tsukamoto, Harada, Kawashima, J. Phys. Conf. Ser. **150**, 042218 (2009)

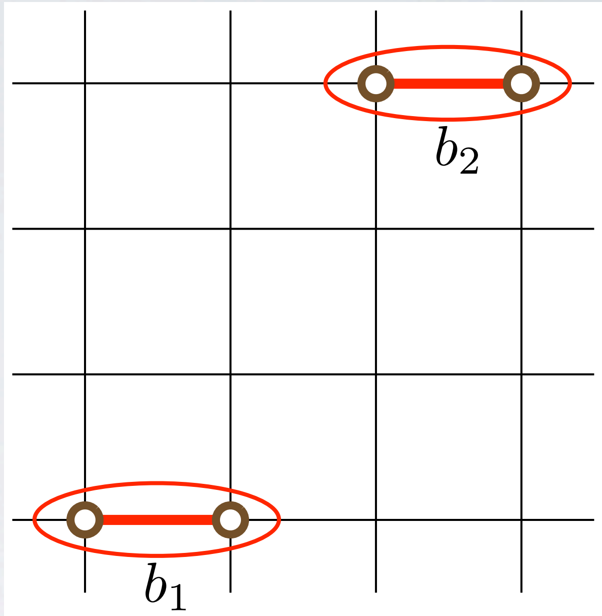
QMC study of J-Q$_3$ model at T>0

- T_c higher; further away from T=0 quantum-criticality

QMC calculations of the VBS correlation length

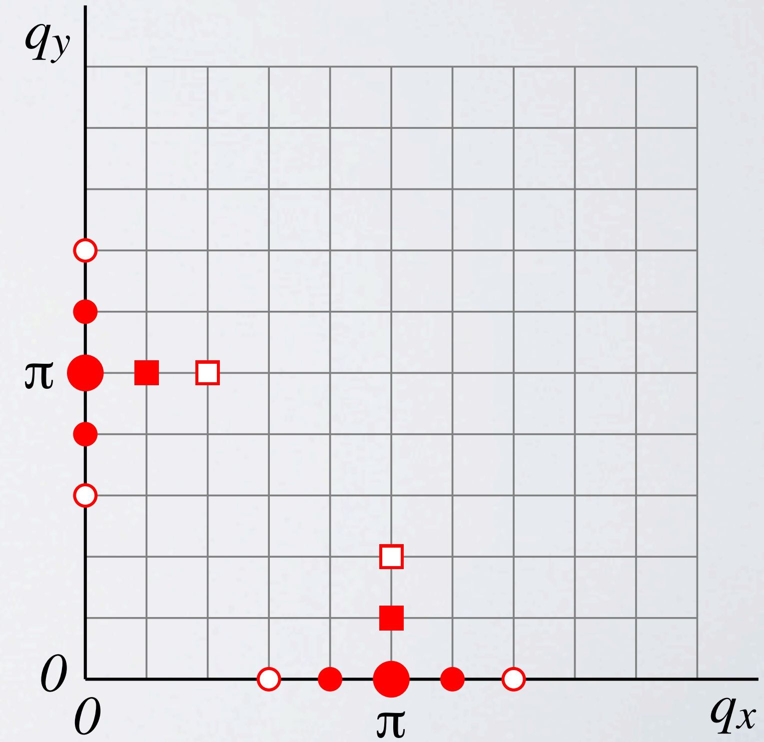
Using VBS real-space susceptibilities

$$\chi_{b_1,b_2} = \int_0^\beta d\tau \langle C_{b_2}(\tau) C_{b_1}(0) \rangle$$



Fourier transform to $\chi_{\rm VBS}(q_x, q_y)$

Two correlation lengths of the order parameter
- parallel and perpendicular to ordered bonds



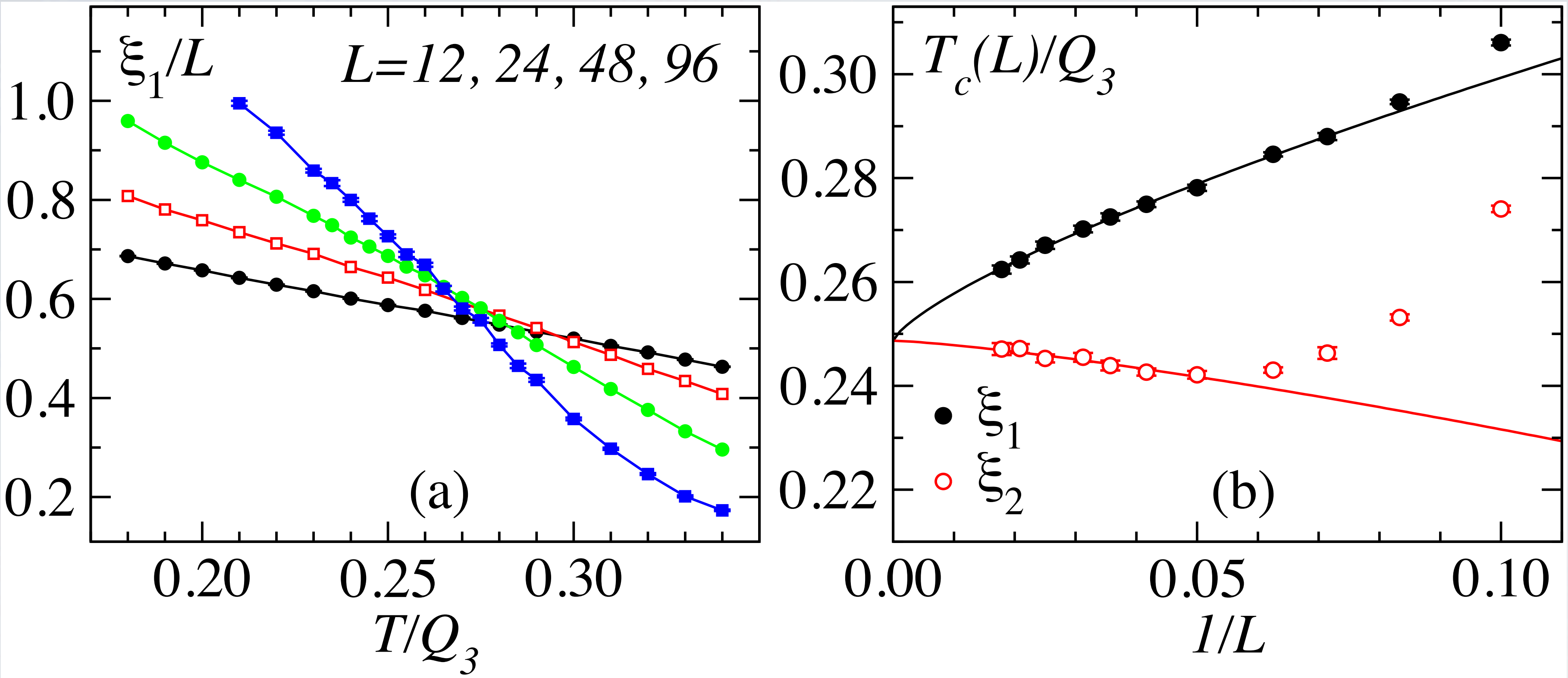
Second moment (q-space) definitions:

$$\xi_1^x = \frac{L}{2\pi}\sqrt{\frac{\chi^x_{\rm VBS}(\mathbf{q}_0)}{\chi^x_{\rm VBS}(\mathbf{q}_1)} - 1}, \quad \xi_2^x = \frac{L}{2\pi}\sqrt{\frac{\chi^x_{\rm VBS}(\mathbf{q}_0)}{\chi^x_{\rm VBS}(\mathbf{q}_2)} - 1},$$

$\mathbf{q}_0 = (\pi, 0)$, $\mathbf{q}_1 = (\pi + \frac{2\pi}{L}, 0)$ and $\mathbf{q}_2 = (\pi, \frac{2\pi}{L})$

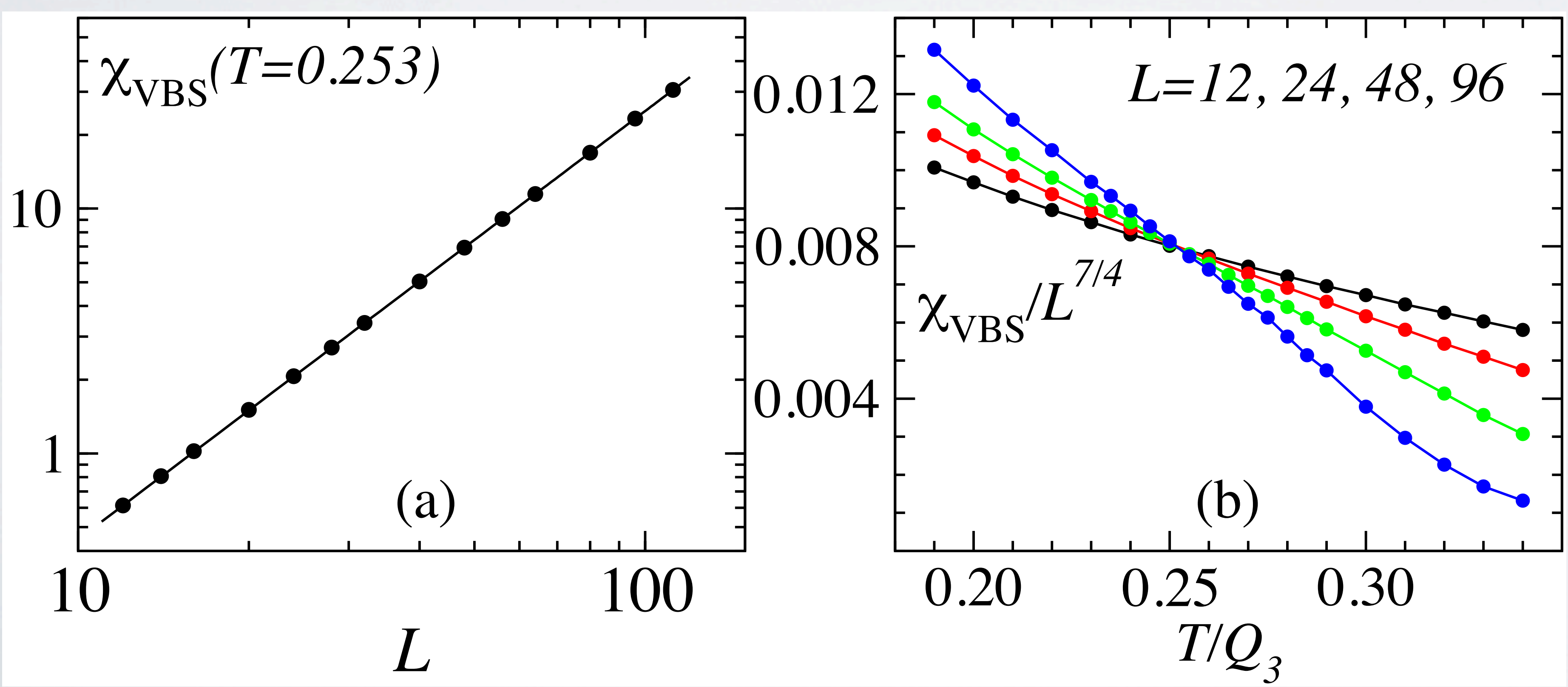
$$\chi^x_{\rm VBS} = \chi^x_{\rm VBS}(\mathbf{q}_0).$$

Finite-size scaling: ξ/L size independent at T_c



$Q_3/J = 5$

Alternative way: find T=T_c where $X_{VBS} \sim L^a$, $a=2-\eta$

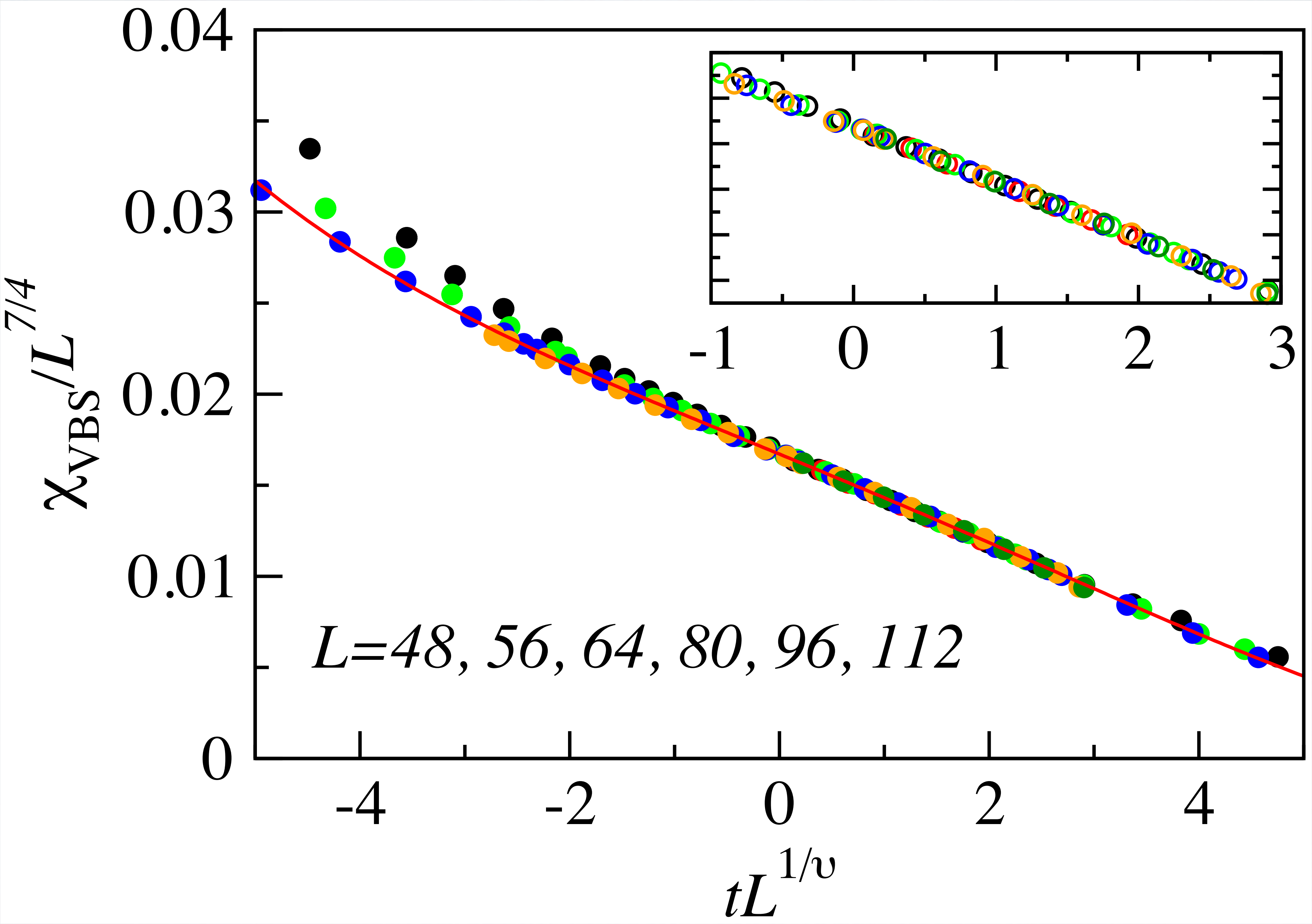


$Q_3/J = 5$

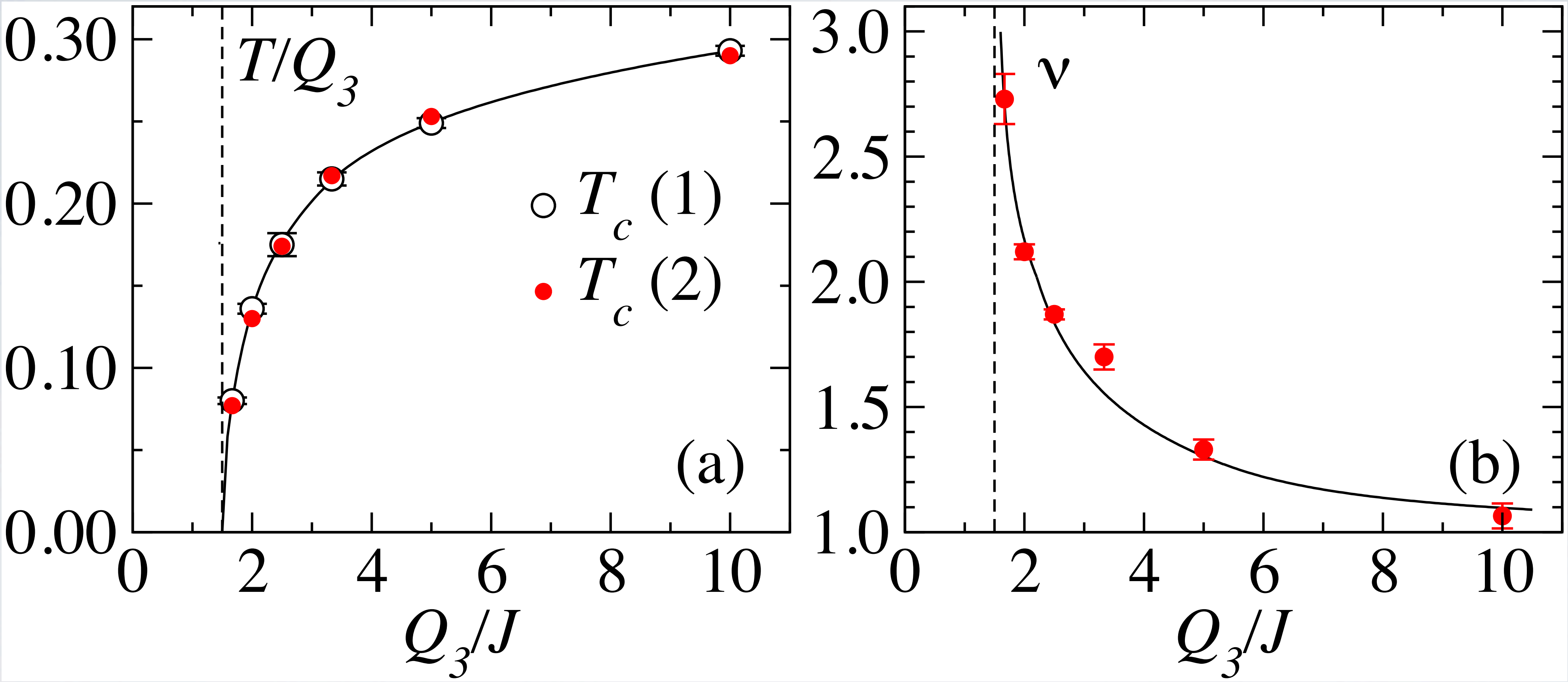
Gives same T_c and η=0.250(1)

Data collapse to extract correlation-length exponent ν

- plot size-normalized X_{VBS} vs $tL^{1/\nu}$, $t=(T-T_c)/T_c$
- exponent ν adjusted for best scaling collapse



Collecting the key results:



η very close to 1/4 (<1% deviation) for all cases studied

Procedures become difficult for low T_c

- larger scaling corrections → larger system sizes
- QMC simulations more time-consuming for low T

Results show Ising - XY (KT) critical curve realized (c=1 CFT)

Note: Limits T→0 and L →∞ do not commute

- L →∞ first gives 2-dim KT transition
- T → 0 first gives (2+1)-dim DQC universality class