Computational Studies of Quantum Criticality

Examples of quantum Monte Carlo studies of critical quantum magnets

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Related review articles

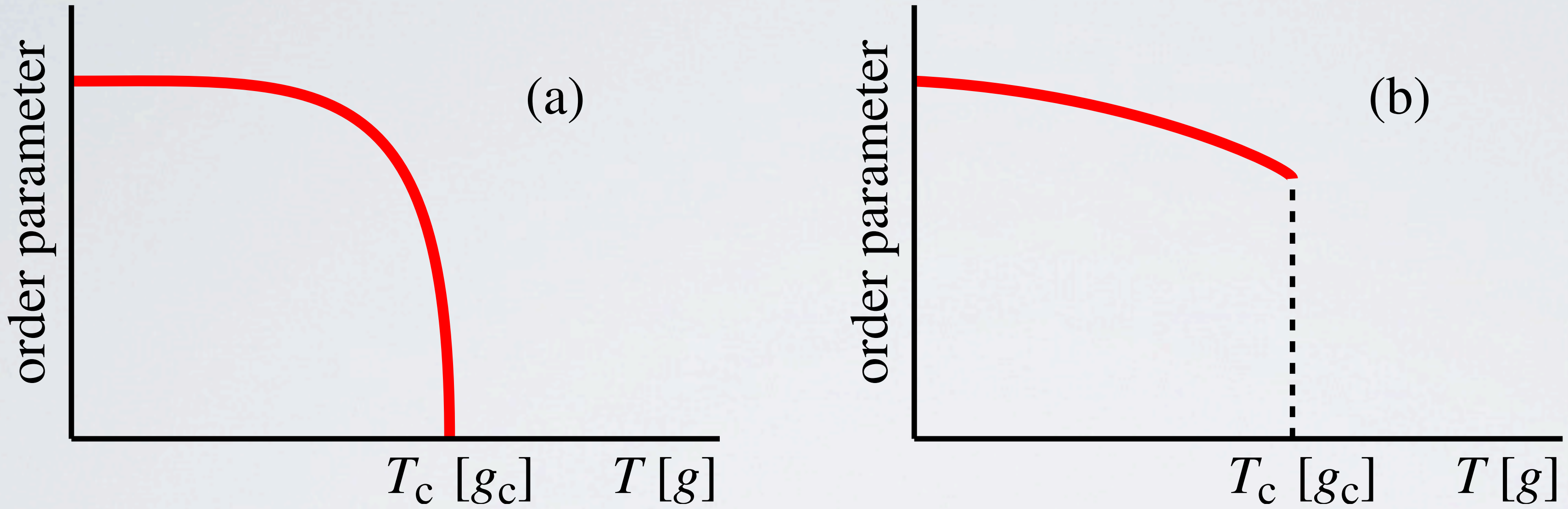
- AW Sandvik, *Computational studies of quantum spin systems*, AIP Conference Proc. 1297, 135 (2010) [ArXiv:1101.3281]
- RKK. Kaul, RG Melko, and AW Sandvik, *Bridging lattice-scale physics and continuum field theory with quantum Monte Carlo simulations*, Annual Review of Condensed Matter Physics 4,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

Thermal (classical) phase transition

- Fluctuations regulated by temperature T>0

Quantum (ground state, T=0) phase transition

- Fluctuations regulated by parameter g in Hamiltonian



Lecture outline

Part I

- classical spin models
- Monte Carlo simulations
- finite-size scaling to study critical points

Part II

- quantum spin models
- quantum Monte Carlo methods (S=1/2 quantum spins)
- criticality in dimerized systems on 2 and 3 dimensions

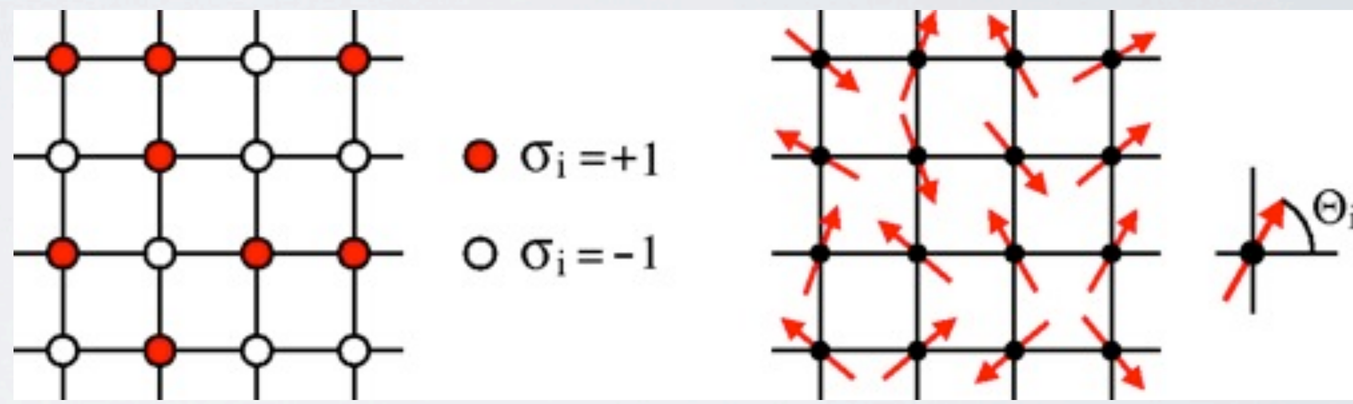
[- valence-bond solids and “deconfined” quantum criticality in 2D]

Classical spin models

Lattice models with “spin” degrees of freedom at the vertices

Classified by type of spin:

- **Ising model:** discrete spins, normally two-state $\sigma_i = -1, +1$
- **XY model:** planar vector spins (fixed length)
- **Heisenberg model:** 3-dimensional vector spins.



Statistical mechanics

- spin configurations C
- energy E(C)
- some quantity Q(C)
- temperature T (k_B=1)

$$\langle Q \rangle = \frac{1}{Z} \sum_{C} Q(C) \mathrm{e}^{-E(C)/T}$$

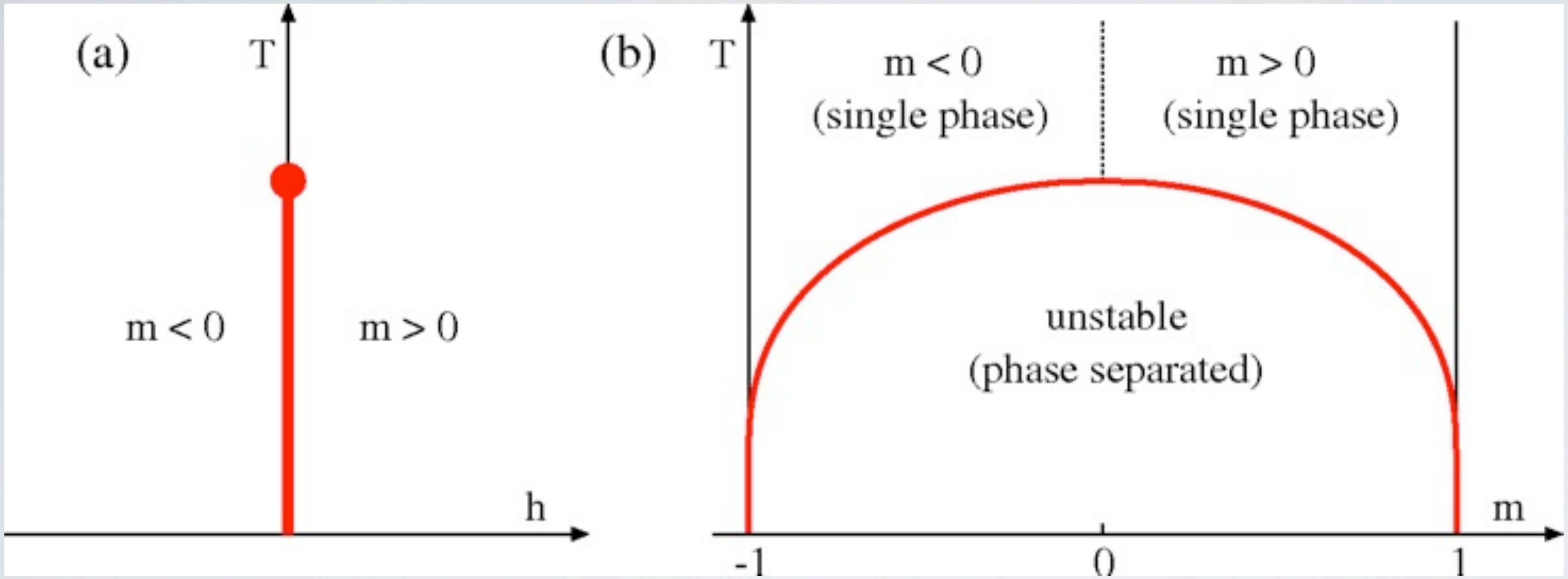
$$Z = \sum_{C} \mathrm{e}^{-E(C)/T}$$

$$E = \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \qquad \text{(Ising)}$$

$$E = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} \cos(\Theta_i - \Theta_j) \qquad \text{(XY)}$$

$$E = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \qquad \text{(Heisenberg)}$$

Phase transition in the Ising model



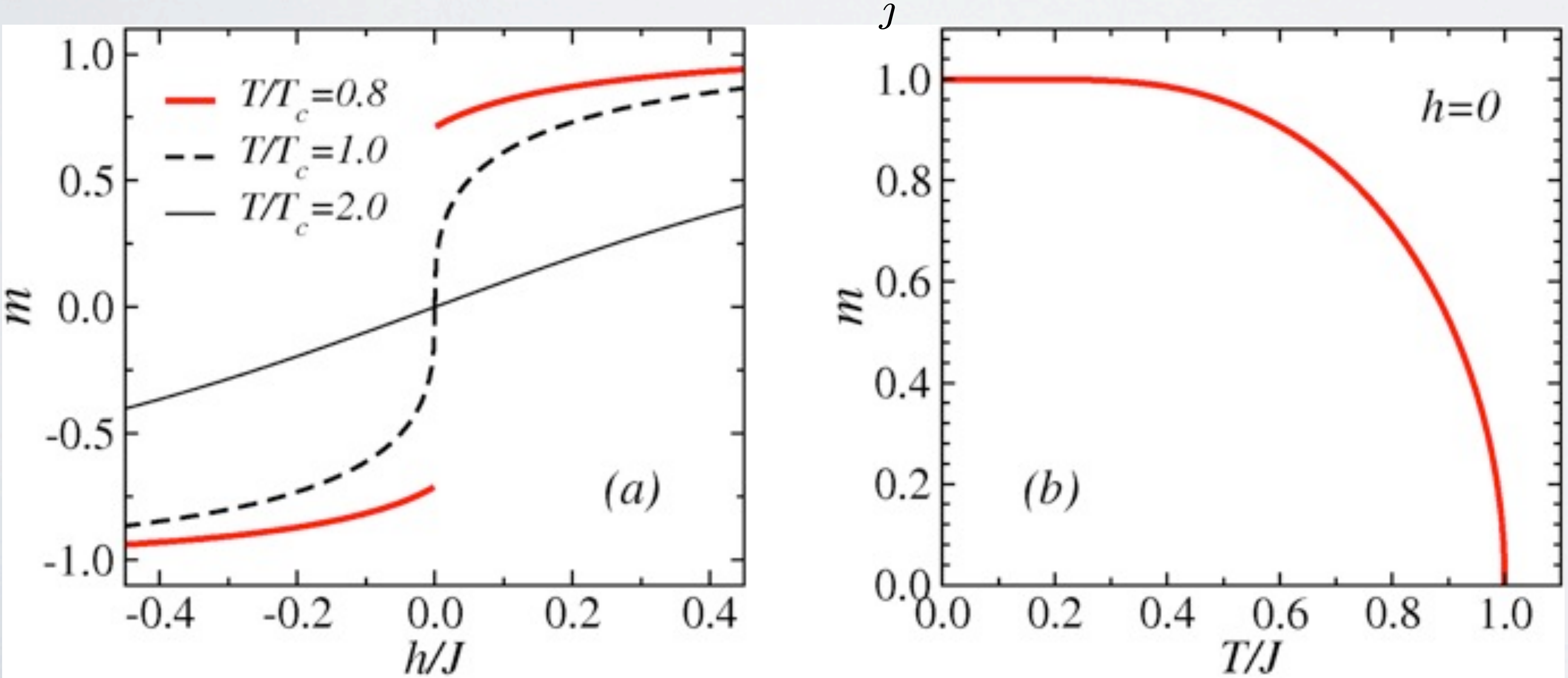
For 2D square lattice with nearest-neighbor couplings

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

$$\approx 2.269$$

- first-order transition versus h (at h=0) for $T<T_c$
- continuous transition at h=0

Mean-field solution: $J = J_i = \sum_j J_{ij} \qquad m = \tanh[(Jm+h)/T], \qquad (m = \langle \sigma_i \rangle)$



- Here J is the sum of local couplings

$$J = \sum_j J_{ij}$$

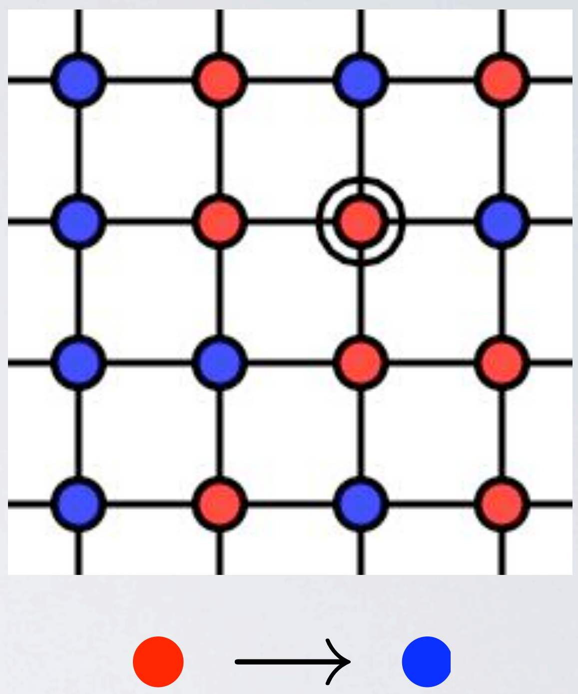
Monte Carlo simulation of the Ising model

The Metropolis algorithm

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

Generate a series of configurations (Markov chain); $C_1 \rightarrow C_2 \rightarrow C_3 \rightarrow C_4 \rightarrow \ldots$

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



- changes satisfy the **detailed-balance principle**

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

$$P_{\rm change}(A \to B) = P_{\rm select}(B|A) P_{\rm accept}(B|A)$$

$$P_{\rm select} = 1/N, \quad P_{\rm accept} = \min[W(B)/W(A), 1]$$

$$\frac{W(B)}{W(A)} = e^{-\Delta_E/T} = e^{[E(A)-E(B)]/T}$$

is easy to calculate (only depends on spins interacting with lipped spin)

Starting from any configuration, such a repeated stochastic process leads to configurations distributed according to W

- the process has to be **ergodic**
  - any configuration reachable in principle
- it takes some time to reach equilibrium (typical configurations of the Boltzmann distribution)

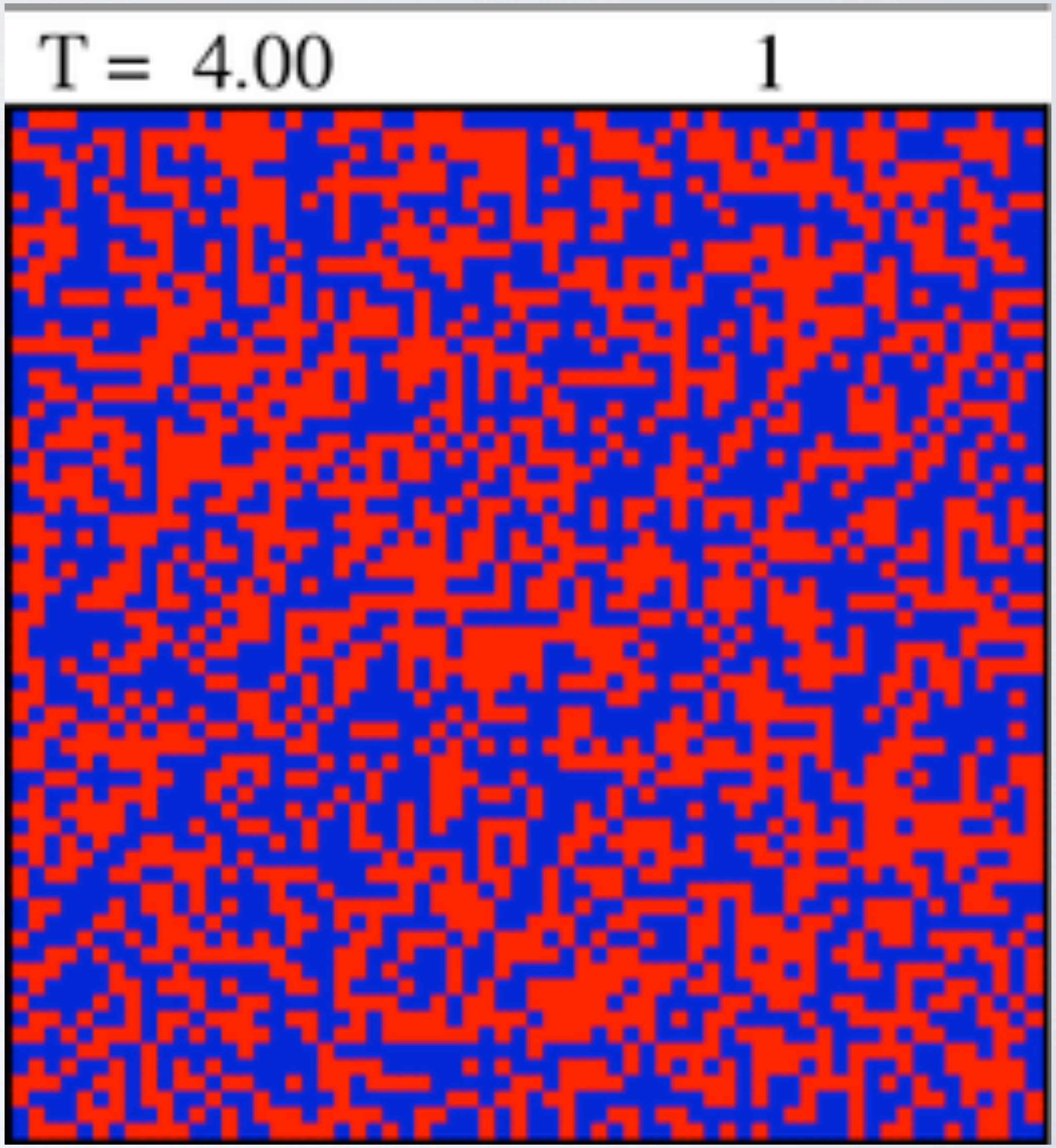
Metropolis algorithm for the Ising model. For each update perform:

- select a spin i at random; consider flipping it $\sigma_i \to -\sigma_i$
- compute the ratio $R=W(\sigma_1,\ldots-\sigma_i,\ldots,\sigma_N)/W(\sigma_1,\ldots\sigma_i,\ldots,\sigma_N)$
  - for this we need only the neighbor spins of i
- generate **random number $0<r\leq 1$; accept flip if $r<R$** (stay with old config else)
- repeat (many times...)

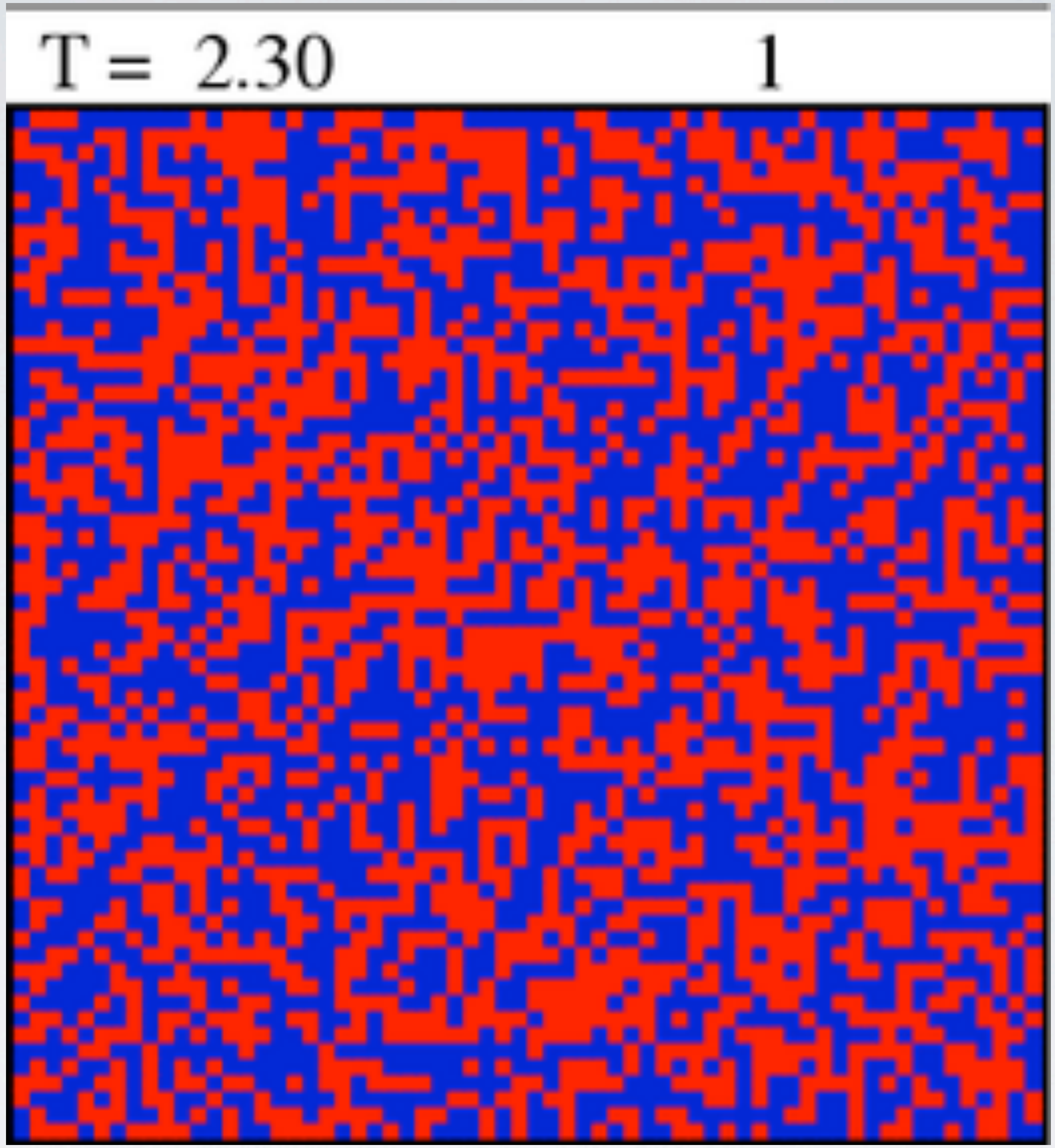
Simulation time unit
(Monte Carlo step or sweep)
- N spin flip attempts

"**Measure**" physical observables (averaged over time) on the generated configurations
- begin **after equilibration** (when configurations are typical representatives of the Boltzmann distribution)

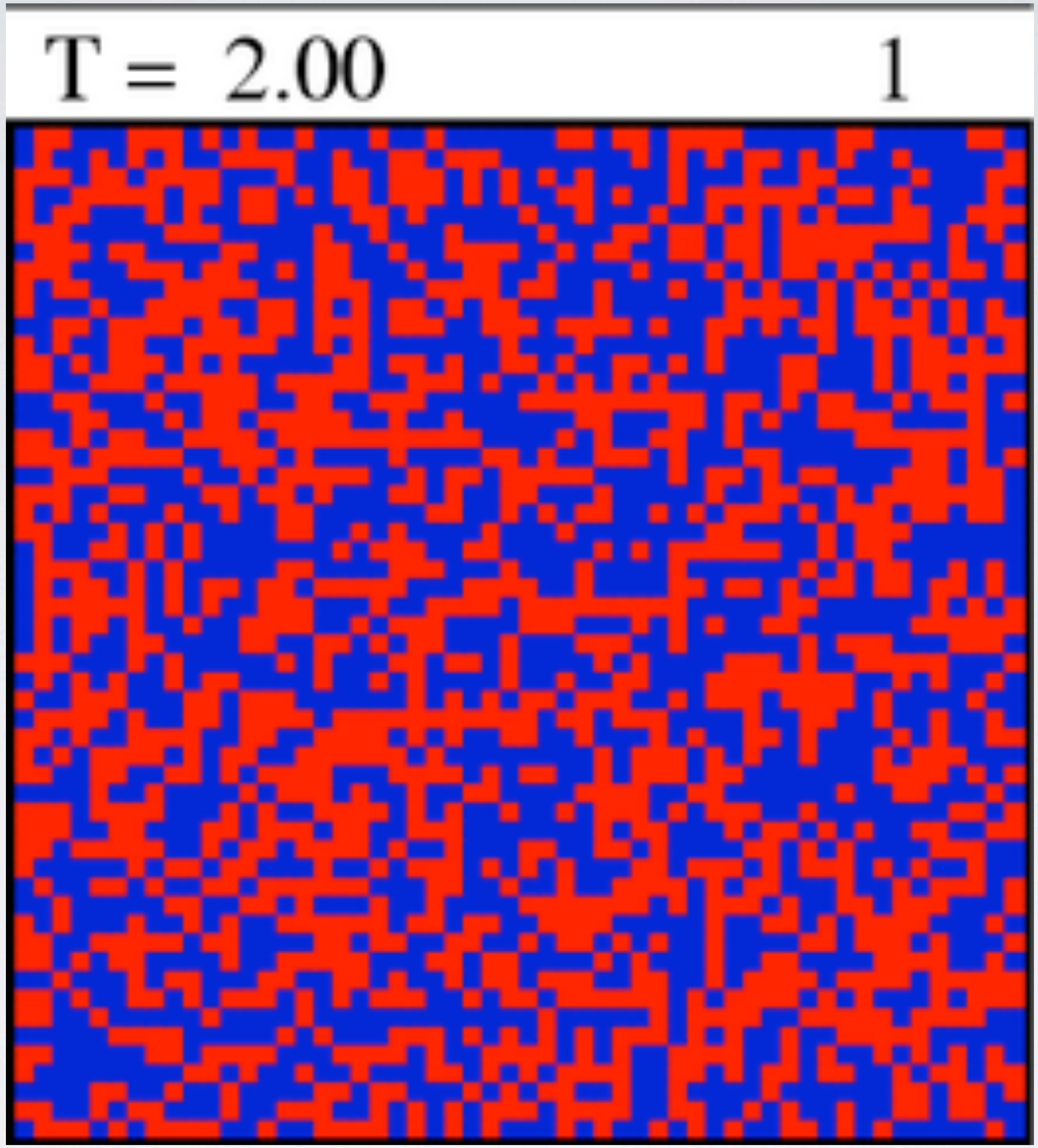
Example
- 128×128 lattice (N=16384) at T/J=4 (> $T_c/J \approx 2.27$)



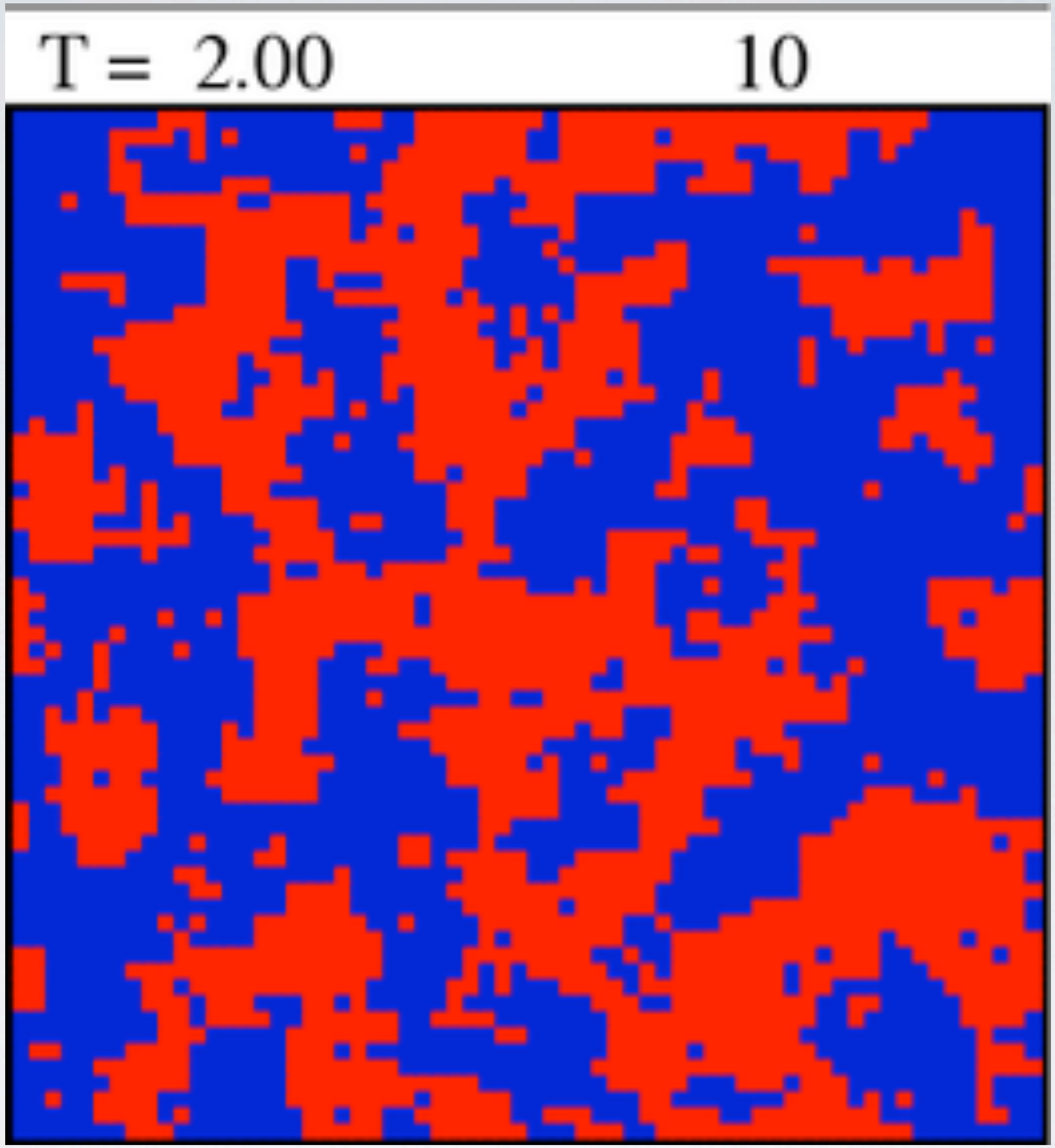
Going closer to Tc



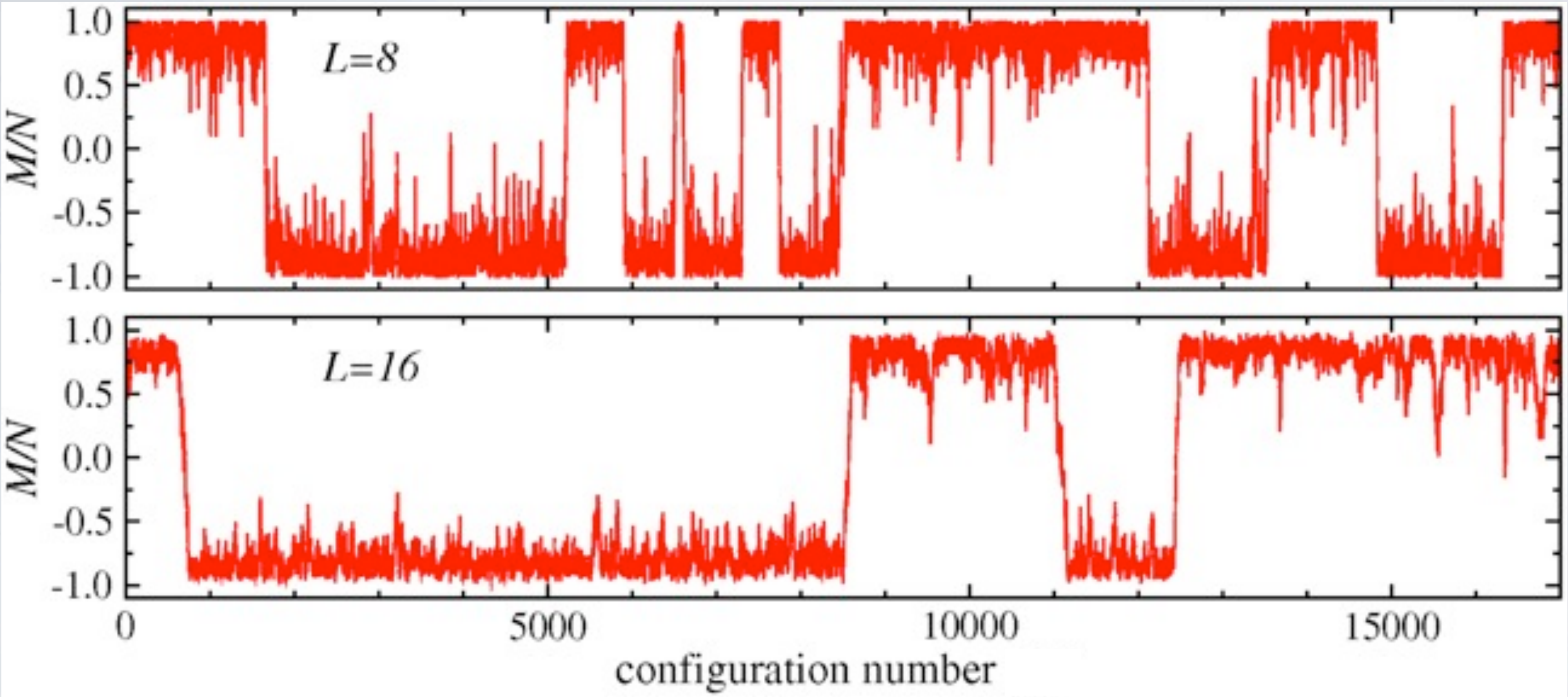
Going below Tc....



Staying at same T, speeding up time by factor 10



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



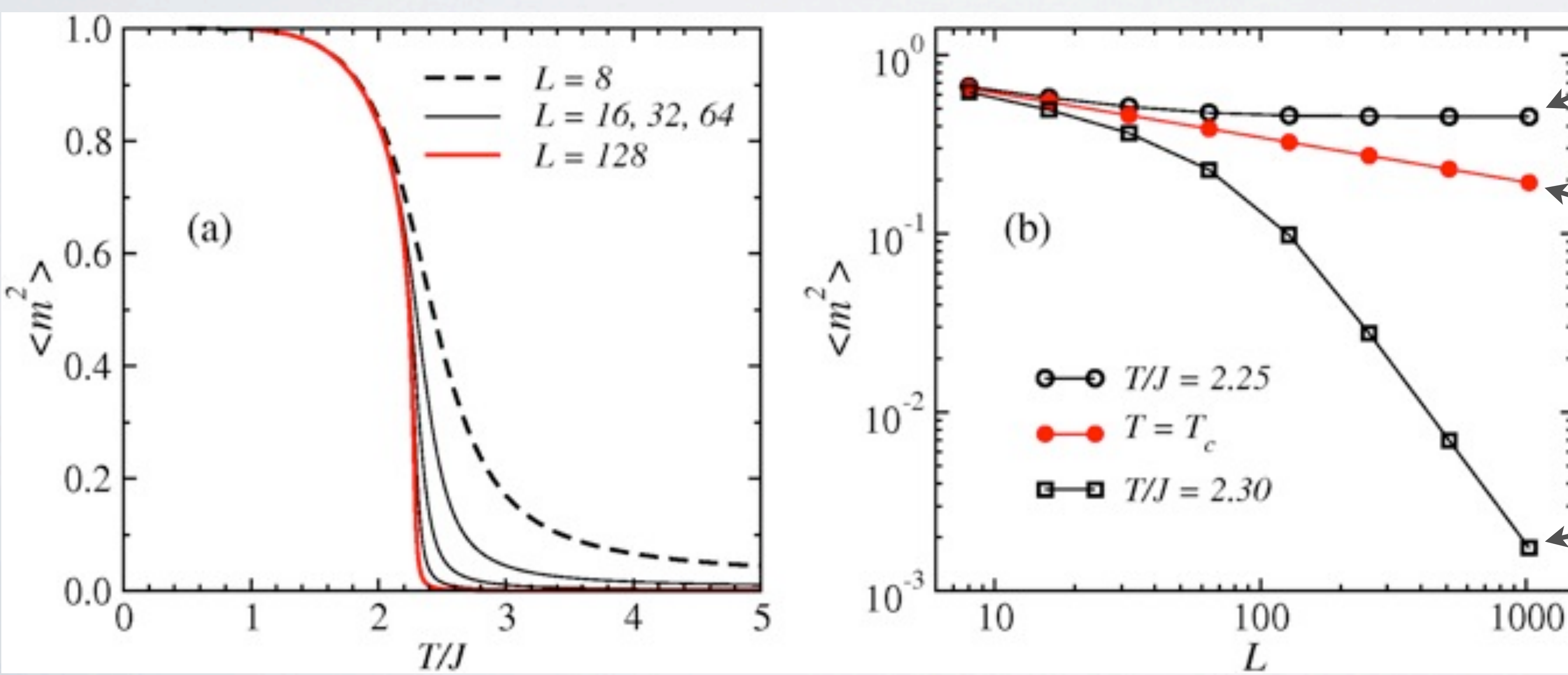
Order parameter (magnetization)

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

Time-scale of m reversals diverges when L →∞
- symmetry breaking

Compute time-average of $<m^2>$ 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

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

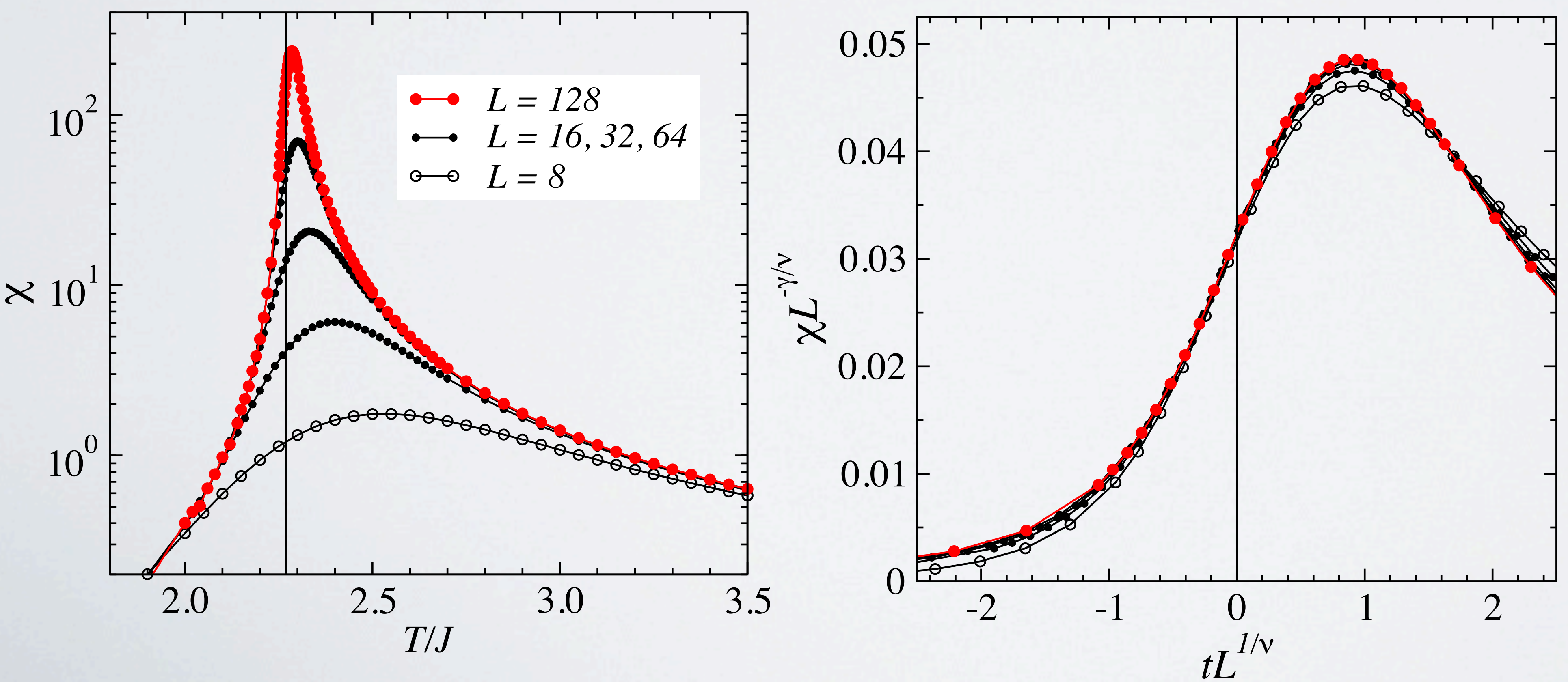
For ξ << L or ξ >> L one argument becomes irrelevant:

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

Close to critical point: **$\xi(T) \sim |T-T_c|^{-\nu}$** ($\nu$ 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 $\chi = (\langle m^2 \rangle - \langle |m| \rangle^2)/T$



$$t = |T - T_c|$$

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

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

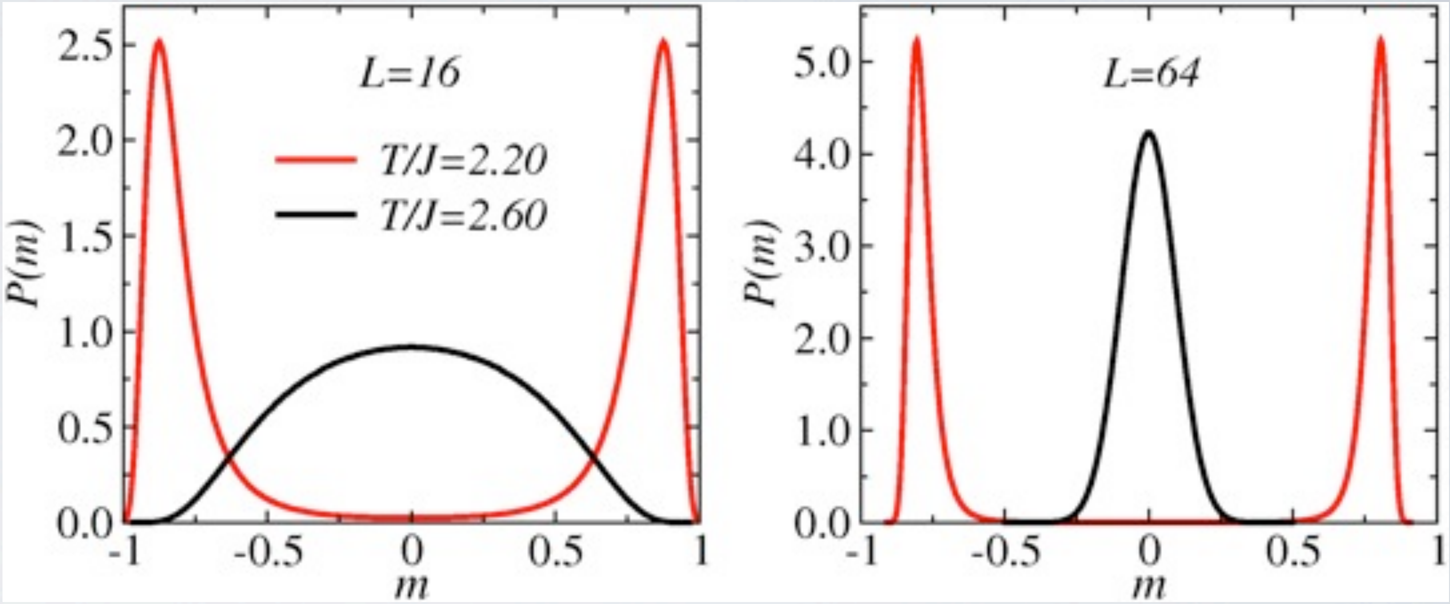
Binder ratios and cumulants

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



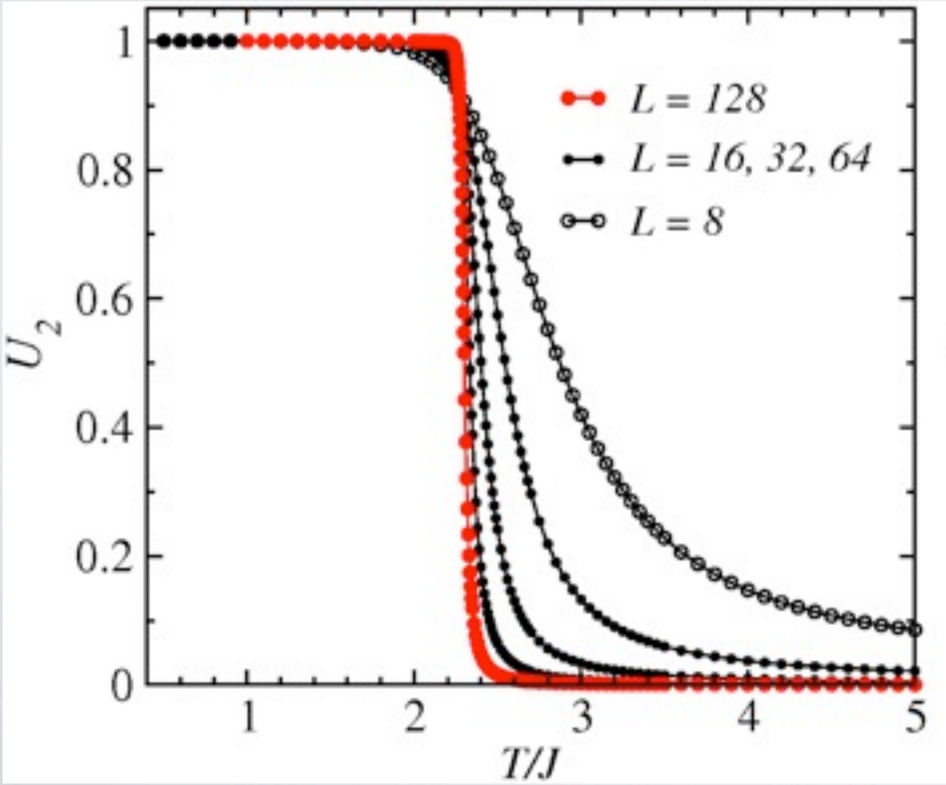
- **for $T<T_c$:** $P(m) \to \delta(m-m^*)+\delta(m+m^*)$
  m^*=|peak m-value|. **$R_2 \to 1$**

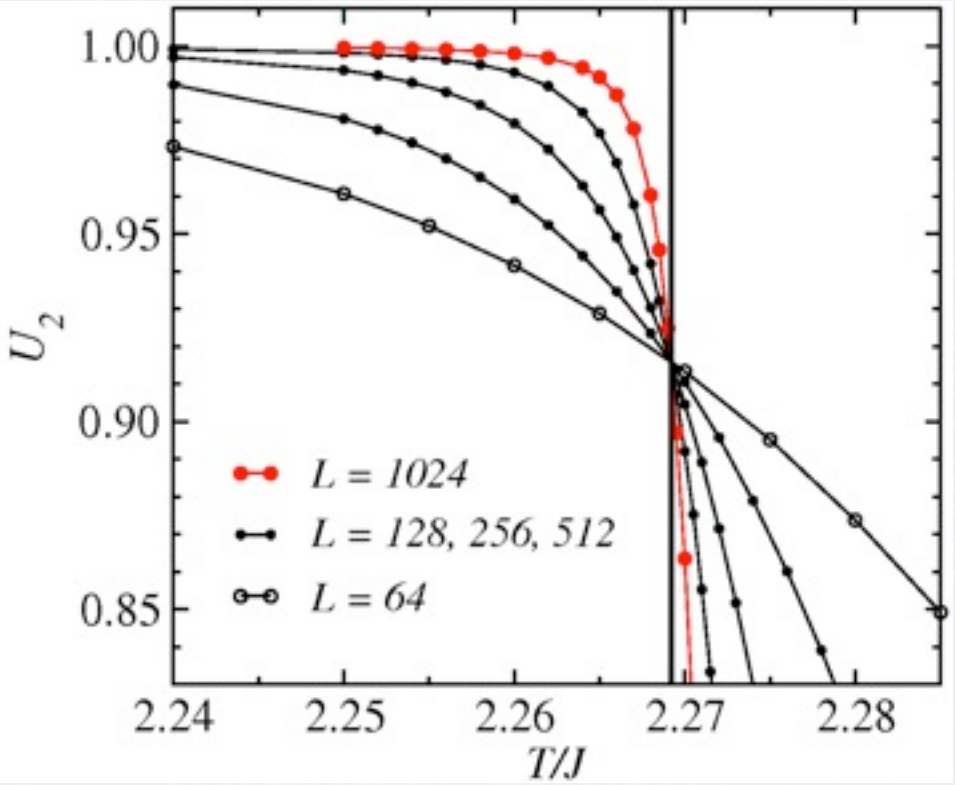
- **for $T>T_c$:** $P(m) \to \exp[-m^2/a(N)]$
  $a(N) \sim N^{-1}$ **$R_2 \to 3$** (Gaussian integrals)

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.

Quantum spin models

- the spins have three (x,y,z) components, satisfy commutation relations
- interactions may contain 1 (Ising), 2 (XY), or 3 (Heisenberg) components

$$H = \sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z = \frac{1}{4} \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \qquad \textbf{(Ising)}$$

$$H = \sum_{\langle ij \rangle} J_{ij} [S_i^x S_j^x + S_i^y S_j^y] = \frac{1}{2} \sum_{\langle ij \rangle} J_{ij} [S_i^+ S_j^- + S_i^- S_j^+] \qquad \textbf{(XY)}$$

$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} [S_i^z S_j^z + \tfrac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)] \qquad \textbf{(Heisenberg)}$$

+ many modifications and extensions... and local spin S=1/2,1,3/2,....

Quantum statistical mechanics

$$\langle Q \rangle = \frac{1}{Z} \mathrm{Tr} \left\{ Q \mathrm{e}^{-H/T} \right\} \qquad Z = \mathrm{Tr} \left\{ \mathrm{e}^{-H/T} \right\} = \sum_{n=0}^{M-1} \mathrm{e}^{-E_n/T}$$

Large size M of the Hilbert space; $M=2^N$ for S=1/2

- difficult problem to find the eigenstates and energies
- we may be especially interested in the ground state (T→0)
  (for classical systems the ground state is often trivial)

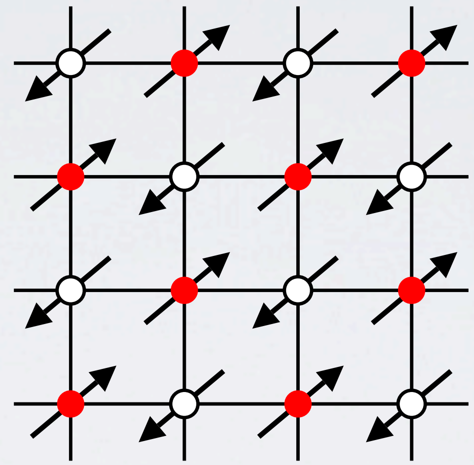
Quantum antiferromagnets

Nearest-neighbor <i,j> interactions (Heisenberg) on some lattice

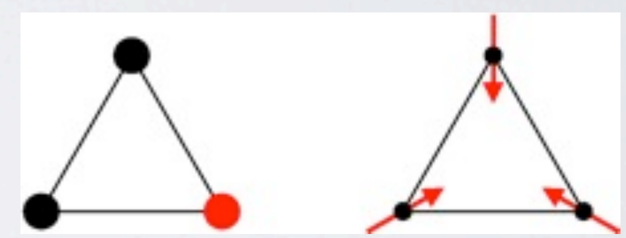
$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, \qquad J > 0$$

Lattices can be classified as

Bipartite
- nearest-neighbors i,j always on different sublattices
- compatible with Neel order
- but other states possible



Non-bipartite
- no bipartition is possible
- frustrated antiferromagnetic interactions
- different kinds of order or no long-range order (spin liquid)



Fully ordered Neel state (ground state of H for classical spins) **is not an eigenstate** of H even on a bipartite lattice
- if there is order at T=0 it is reduced by quantum fluctuations

Mermin-Wagner theorem (on breaking a continuous symmetry) implies:
- No Neel order in 1D Heisenberg model
- Neel order possible only at T=0 in 2D system
- Order possible also at T>0 in 3D

Quantum Monte Carlo

Rewrite the quantum-mechanical expectation value into a classical form

$$\langle A\rangle = \frac{\mathrm{Tr}\{Ae^{-\beta H}\}}{\mathrm{Tr}\{e^{-\beta H}\}} \to \frac{\sum_c A_c W_c}{\sum W_c}$$

Monte Carlo sampling in the space **{c} with weights W_c** (if positive-definite...) ("sign problem" if not the case)

Different ways of doing it

- World-line methods for spins and bosons
- Stochastic series expansion for spins and bosons
- Fermion determinant methods

For ground state calculations we can also do projection from a "trial state"

$$|\Psi_m\rangle \sim H^m|\Psi_0\rangle \qquad |\Psi_m\rangle \to |0\rangle \quad \text{when} \quad m \to \infty$$

$$|\Psi_\beta\rangle \sim \mathrm{e}^{-\beta H}|\Psi_0\rangle \qquad |\Psi_\beta\rangle \to |0\rangle \quad \text{when} \quad \beta \to \infty$$

Particularly simple and efficient schemes exist for S=1/2 models

$$H = -J\sum_{b=1}^{N_b}\left(\frac{1}{4} - \mathbf{S}_{i(b)}\cdot\mathbf{S}_{j(b)}\right)$$

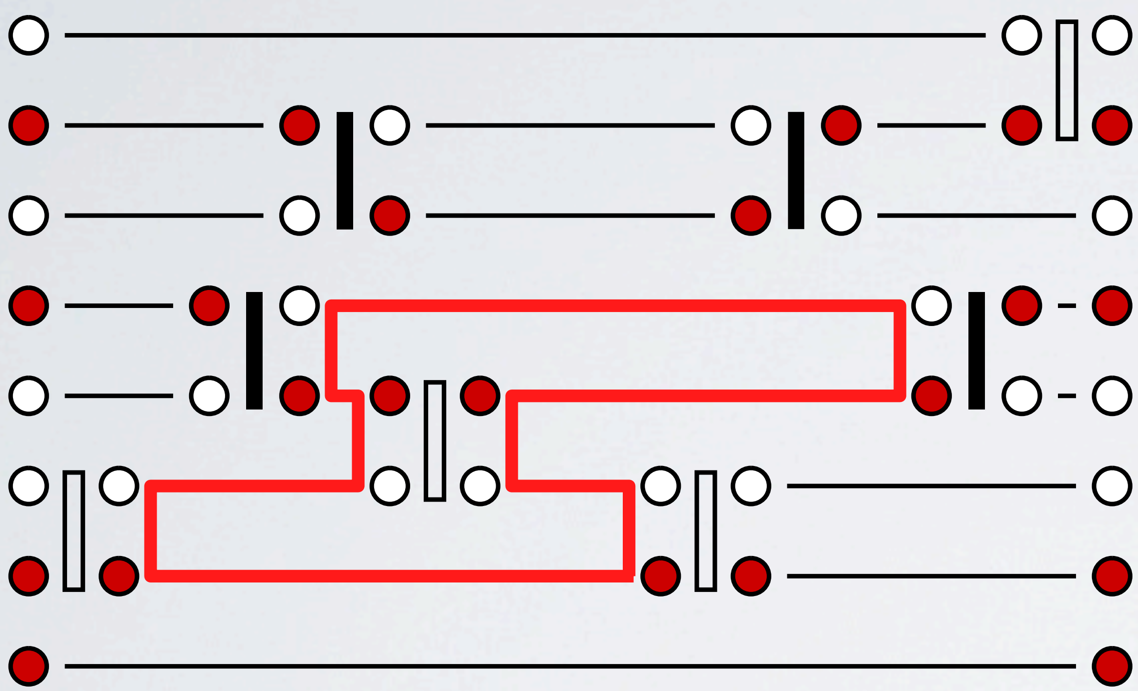
(+ certain multi-spin terms)

No sign problem on **bipartite lattices**

Finite-temperature QMC

(Stochastic series expansion, SSE)

$$\mathrm{tr}\{\mathrm{e}^{-\beta H}\} = \sum_n \frac{\beta^n}{n!} \langle\alpha|(-H)^n|\alpha\rangle$$

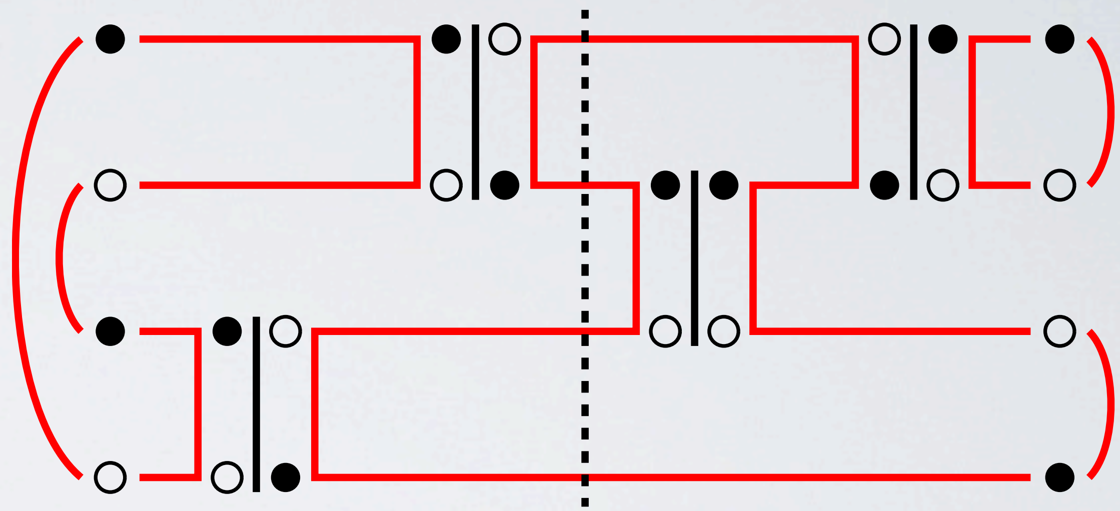


periodic “time” boundary conditions

Sampling of operator sequences and boundary states using efficient loop updates

Ground state projection

$$\sum_{\alpha\beta} f_\beta f_\alpha \langle\beta|(-H)^m|\alpha\rangle$$



open boundaries capped by valence bonds (2-spin singlets) [AWS, HG Evertz, PRB 2010]

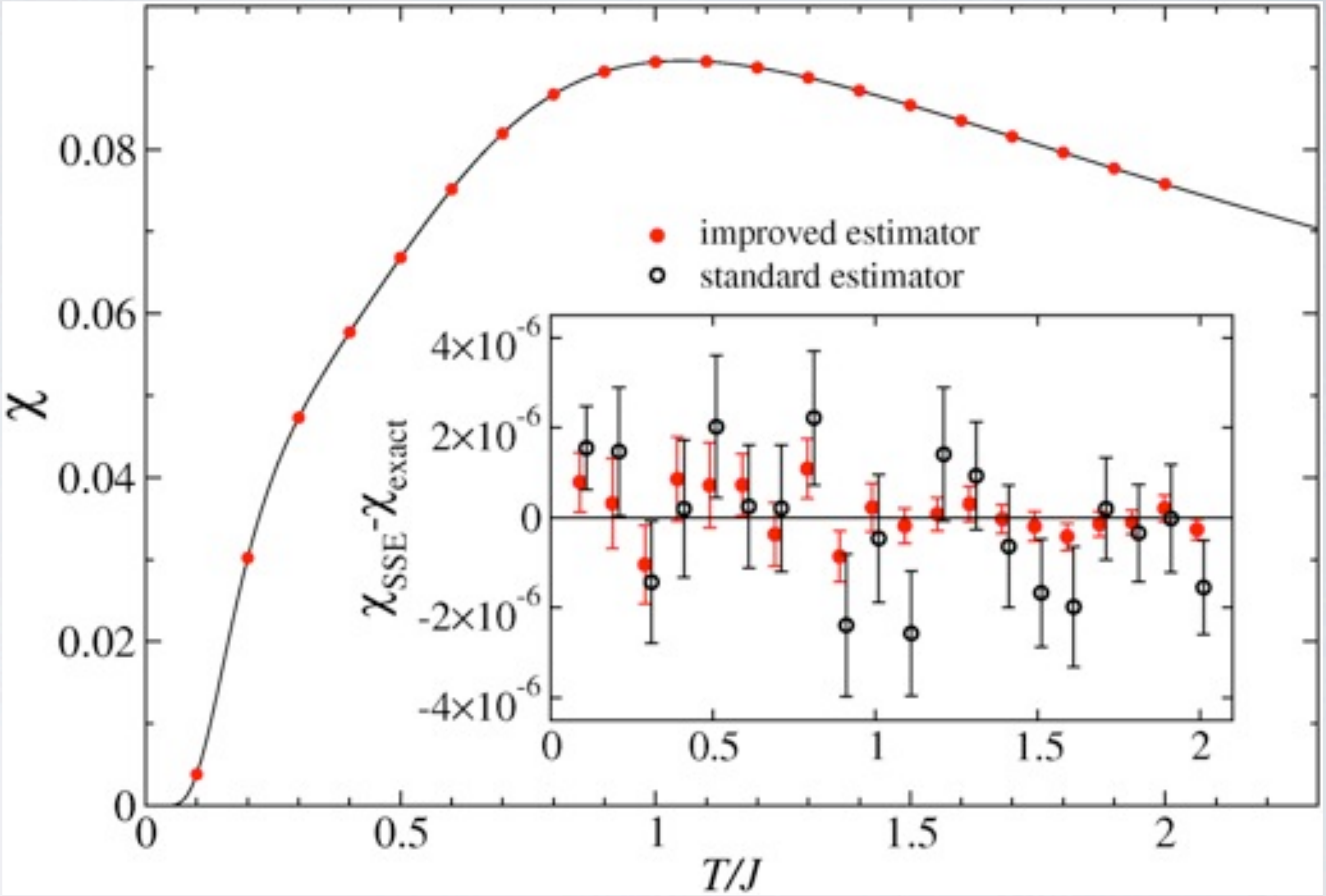
Trial state can conserve relevant ground state quantum numbers (S=0, k=0,...)

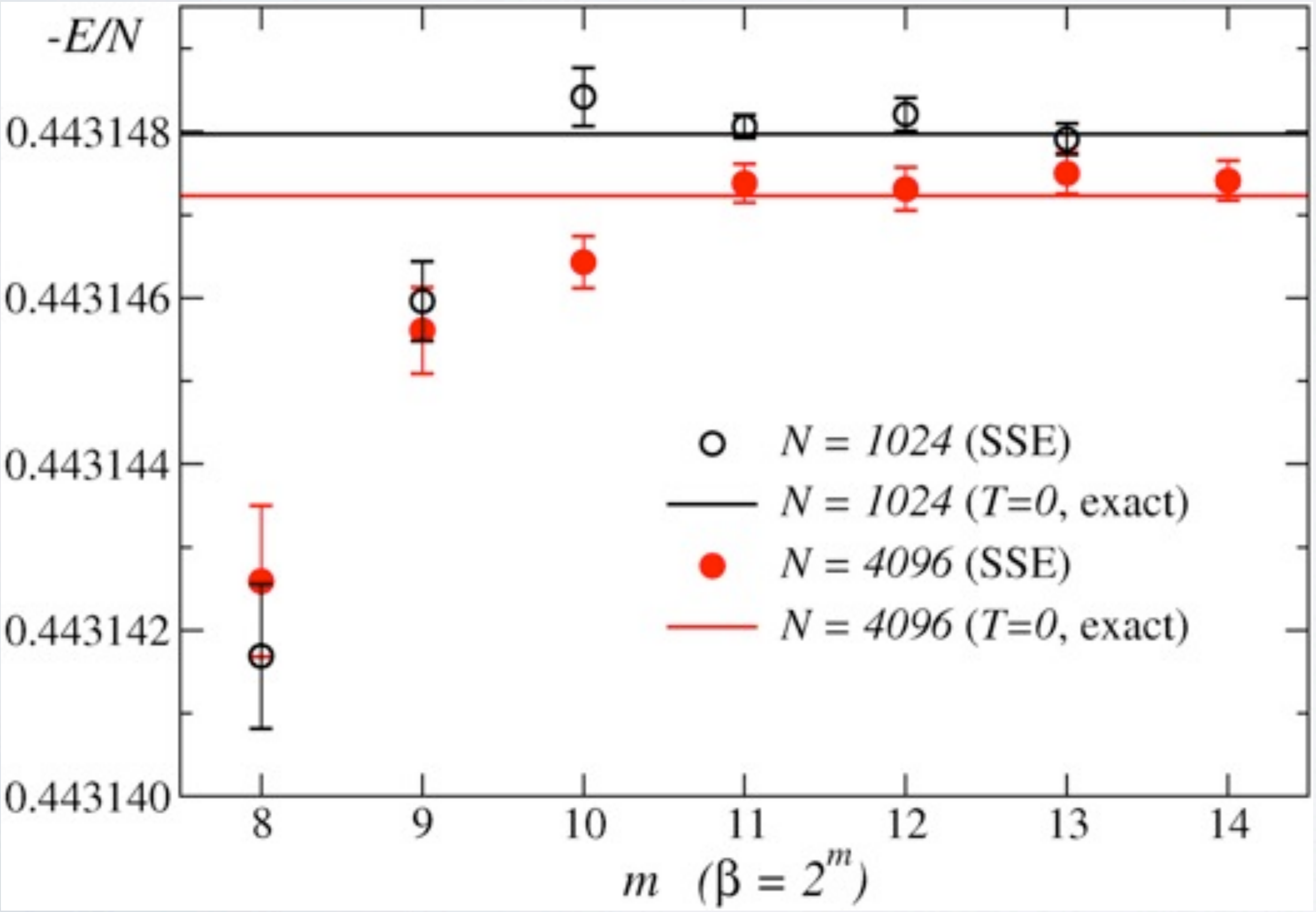
Does it work?
Compare with exact results

- 4×4 exact diagonalization
- Bethe Ansatz; long chains

Susceptibility of the 4×4 lattice ⇒

- SSE results from 10^{10} sweeps
- improved estimator gives smaller error bars at high T (where the number of loops is larger)





⇐ Energy for long 1D chains

- SSE results for 10^6 sweeps
- Bethe Ansatz ground state E/N
- SSE can achieve the ground state limit (T→0)

Spin correlation function of the Heisenberg chain (T=0)

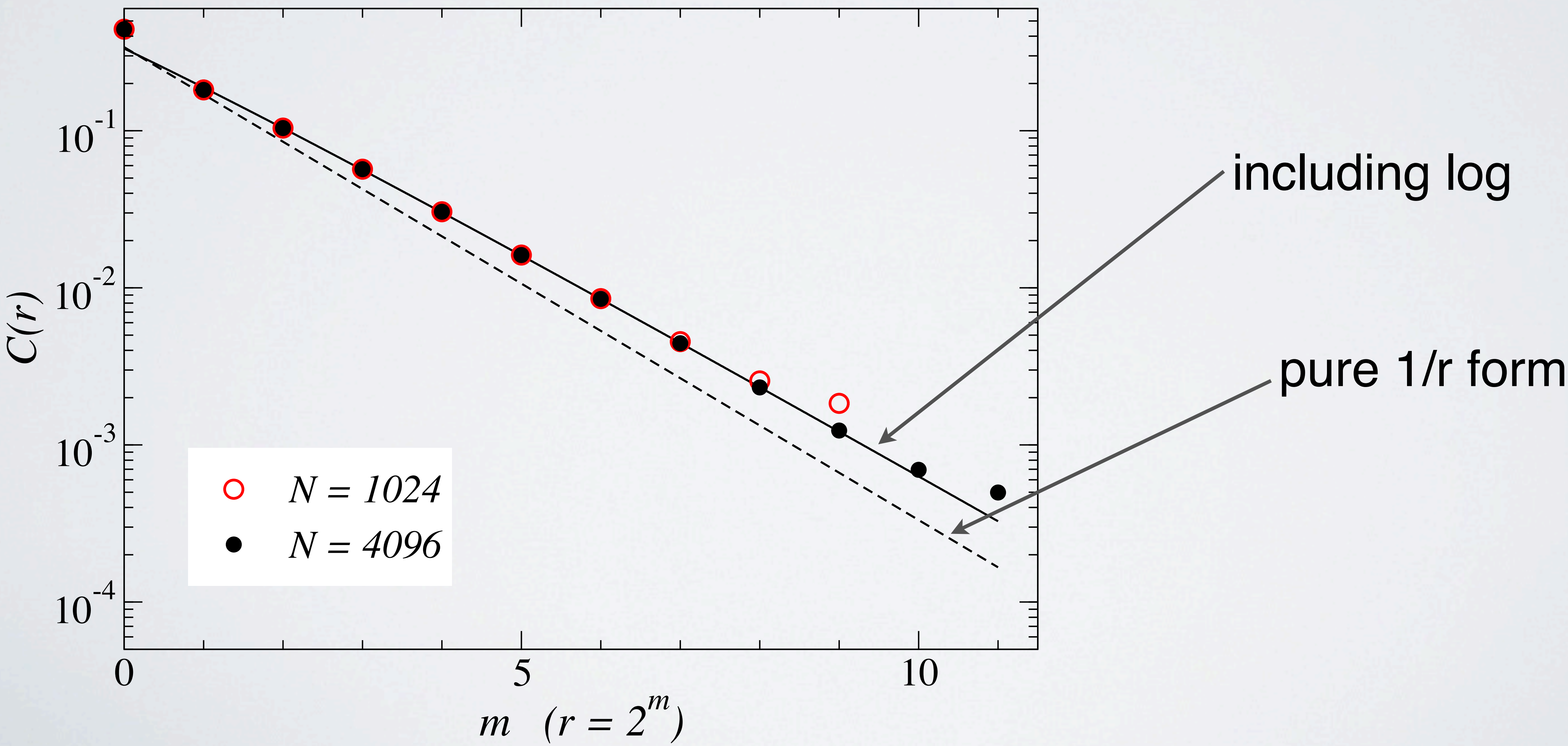
$$C(r) = \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle$$

If there is long-range Neel order $C(r) \to (-1)^r \langle m^2 \rangle$

- but not possible in 1D
- exact results and low-energy field theory predict critical state

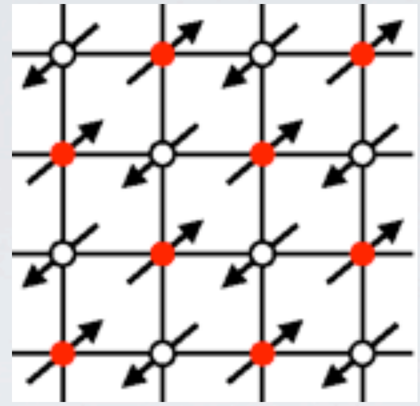
$$C(r) \to \frac{\ln^{1/2}(r/r_0)}{r}(-1)^r$$

SSE T→0 results agree with this form



2D S=1/2 antiferromagnetic Heisenberg model

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



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

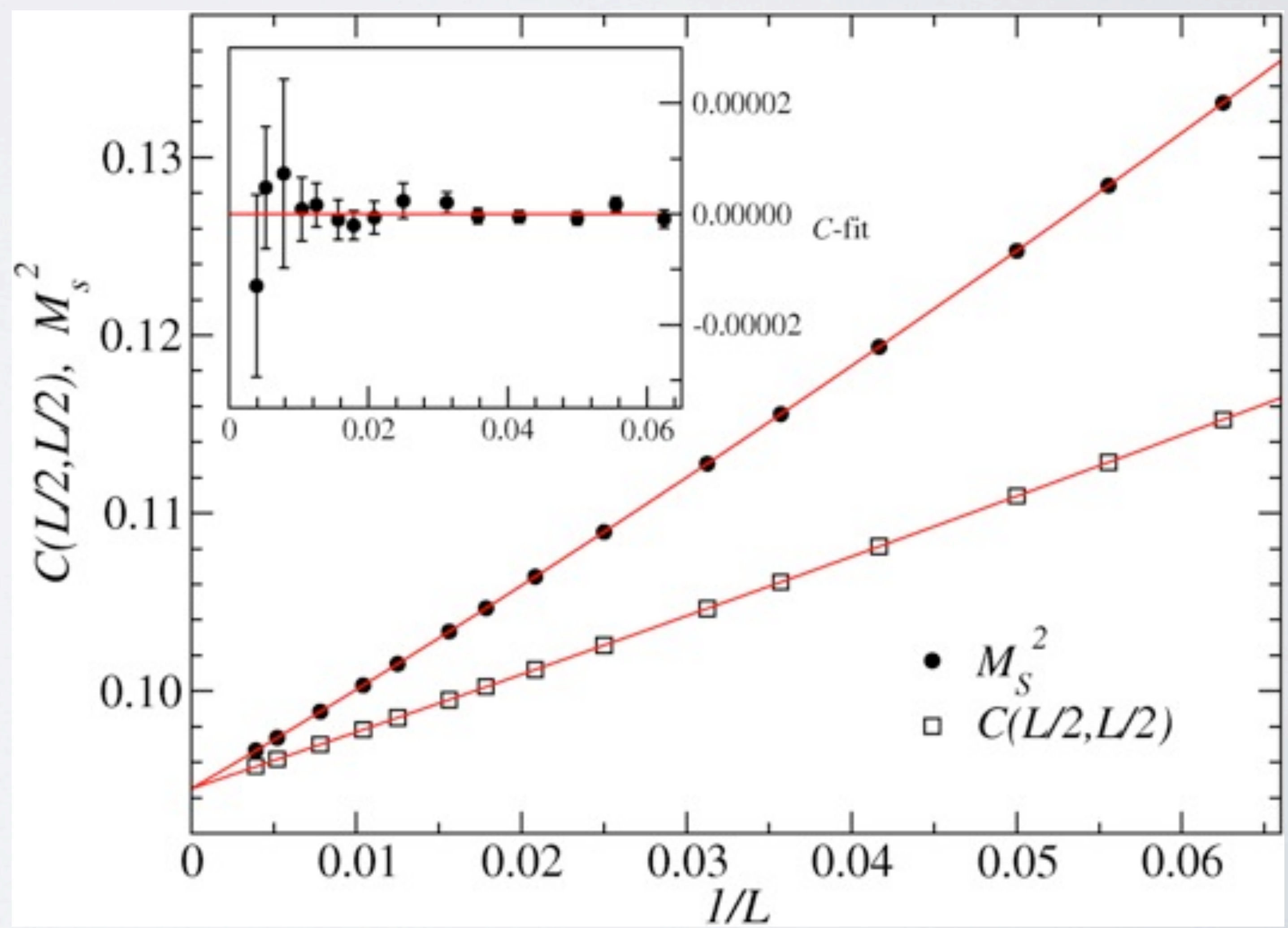
$$m_s = 0.30(2)$$

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

AWS & HG Evertz 2010

$$m_s = 0.30743(1)$$

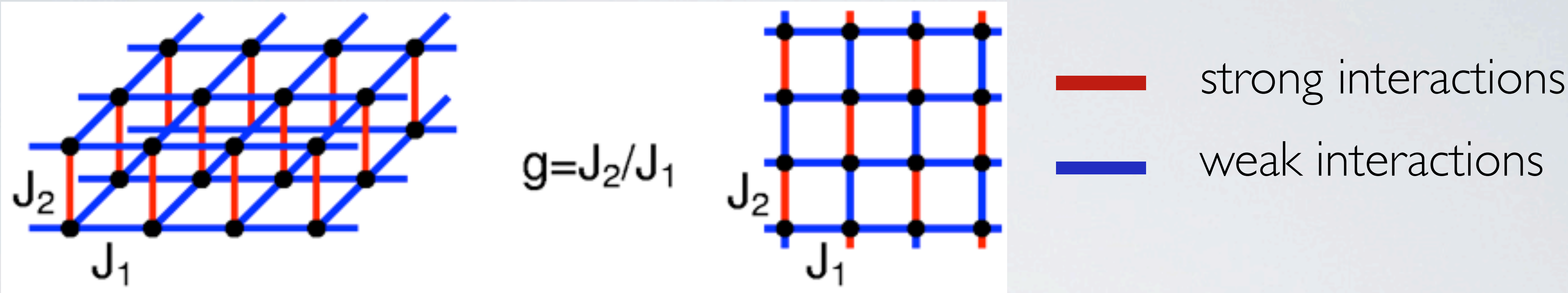
L×L lattices up to 256×256, T=0



T=0 Néel-paramagnetic quantum phase transition

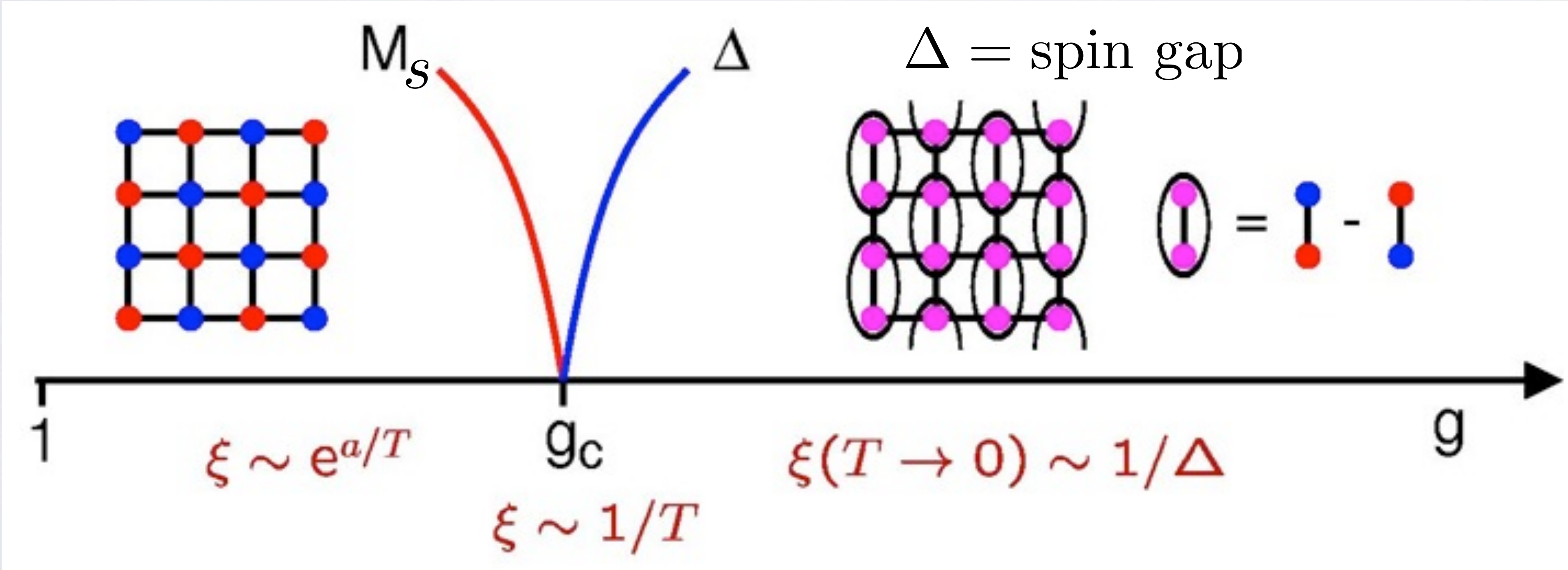
Example: Dimerized S=1/2 Heisenberg models

- 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

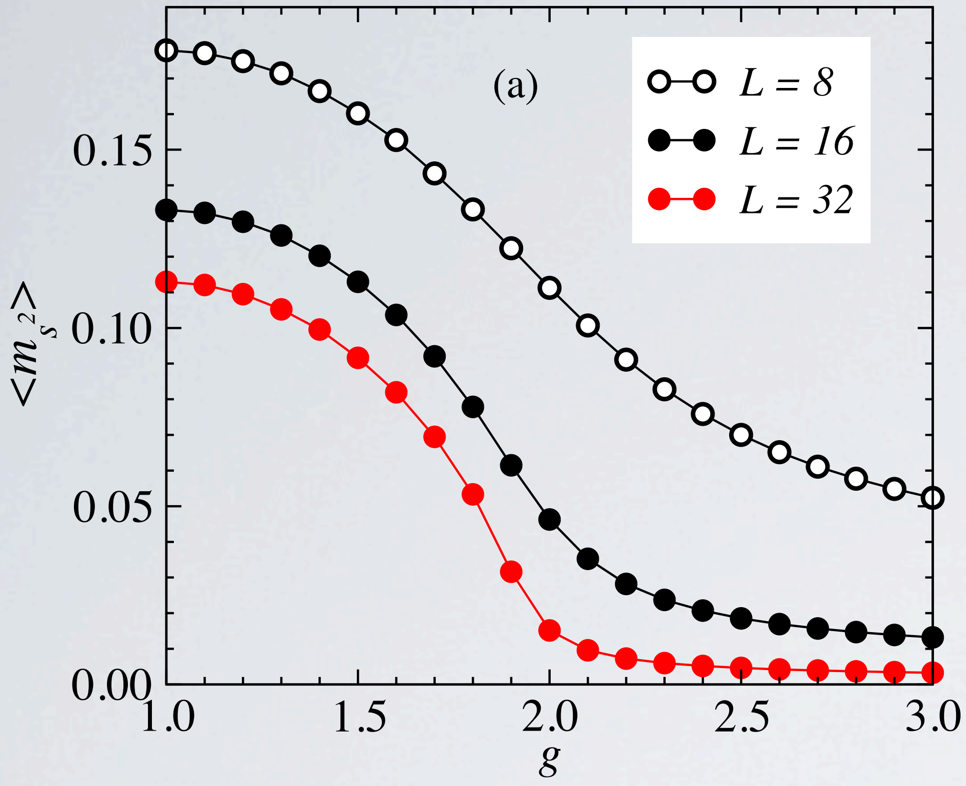
Ground state (T=0) phases

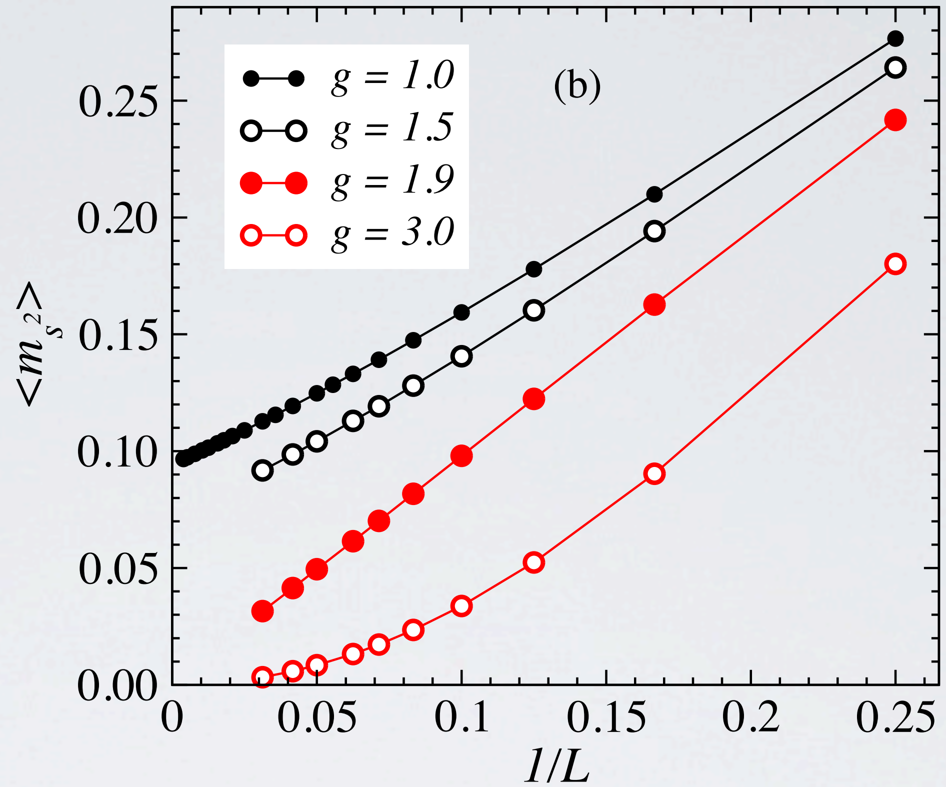


⇒ 3D classical Heisenberg (O3) universality class; QMC confirmed

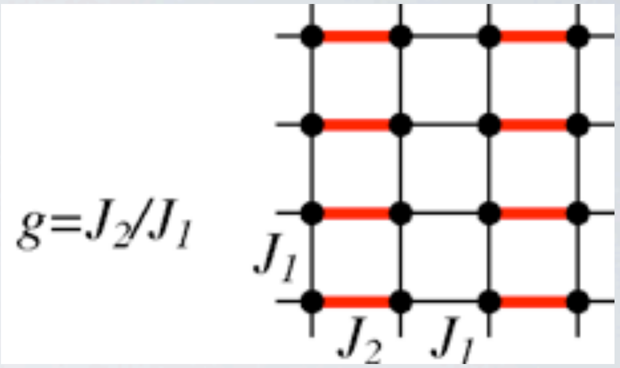
Experimental realization (3D coupled-dimer system): $TlCuCl_3$

SSE calculations to locate the critical point

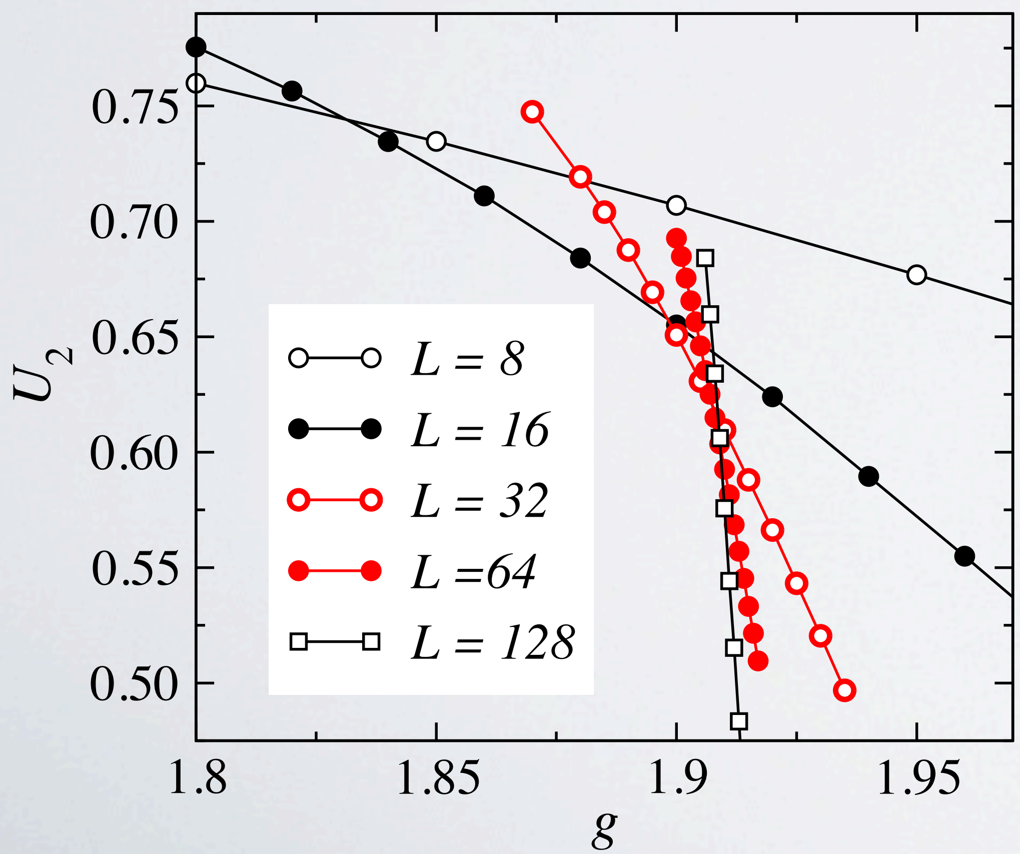


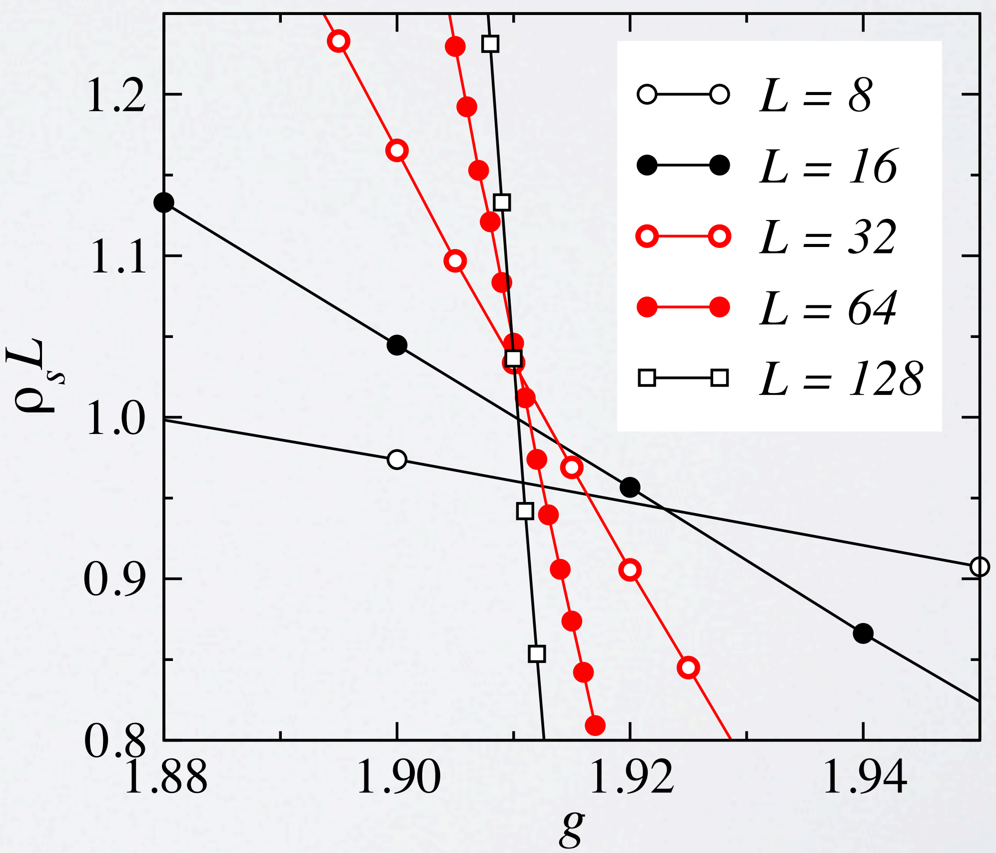


Columnar dimer system



Curve crossing analysis: dimensionless quantities

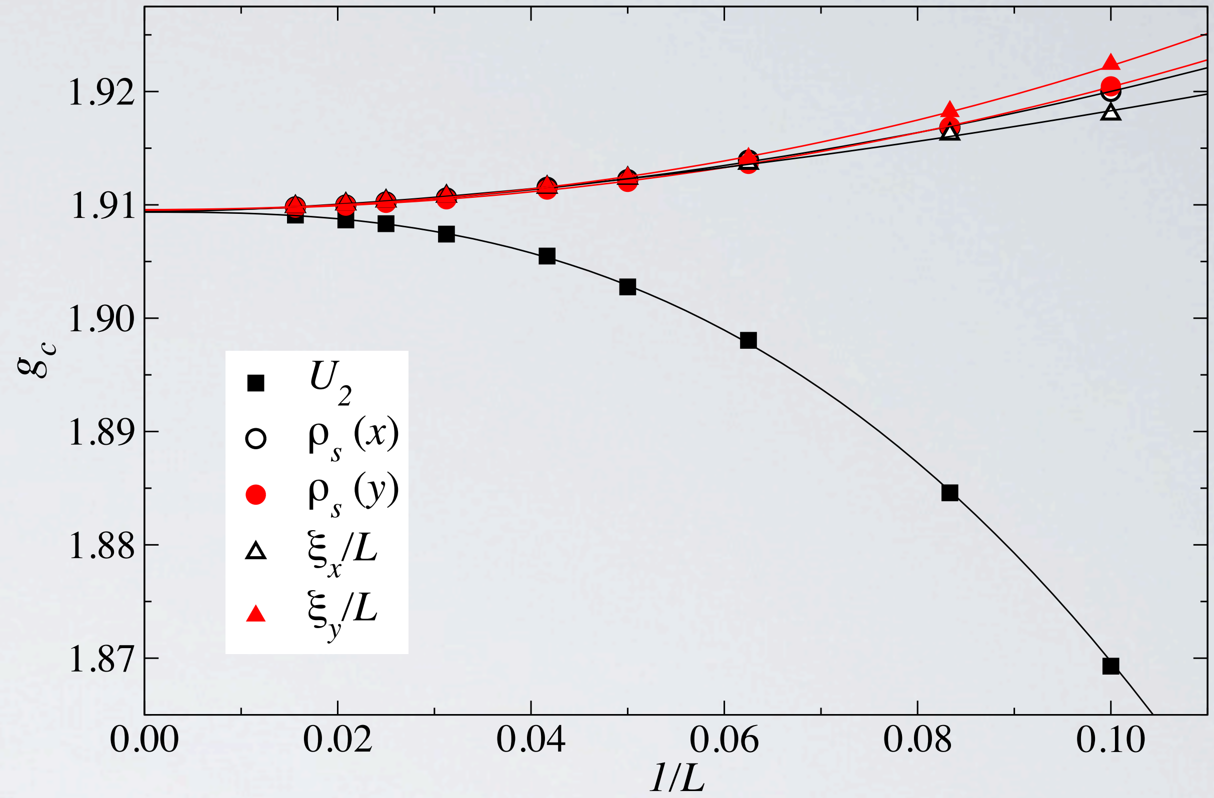




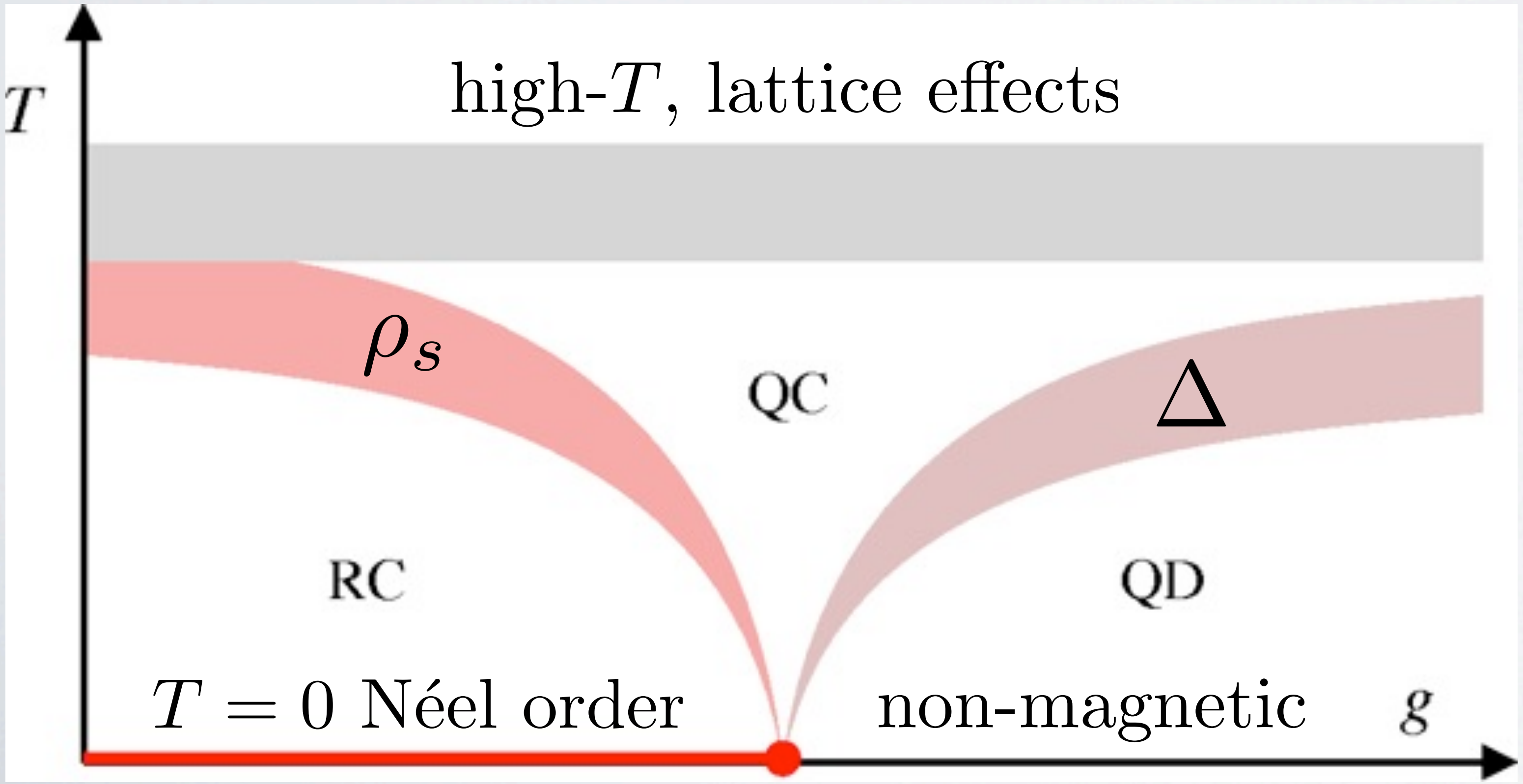
Crossing points drift as the system size is increased
- extrapolations necessary
- can use (L,2L) crossing points

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

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



What's special with quantum-criticality?
- large T>0 quantum-critical fan where T is the only relevant energy scale
- physical quantities expect power laws governed by the T=0 critical point



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

Making connections with quantum field theory

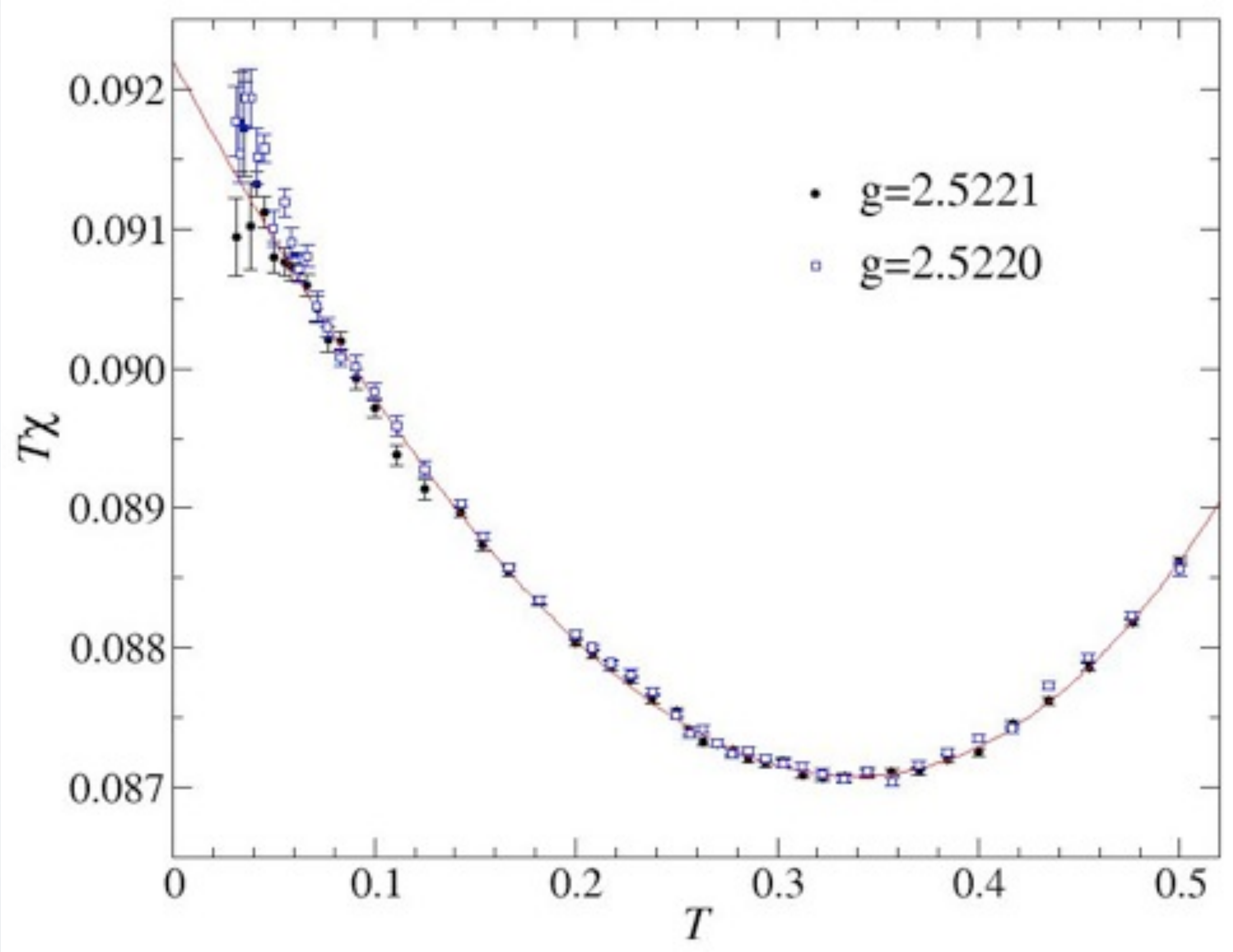
Low-energy properties described by the (2+1)-dimensional nonlinear σ-model
- Chakravarty, Halperin, Nelson (1989), Chubukov, Sachdev, Ye (1994)

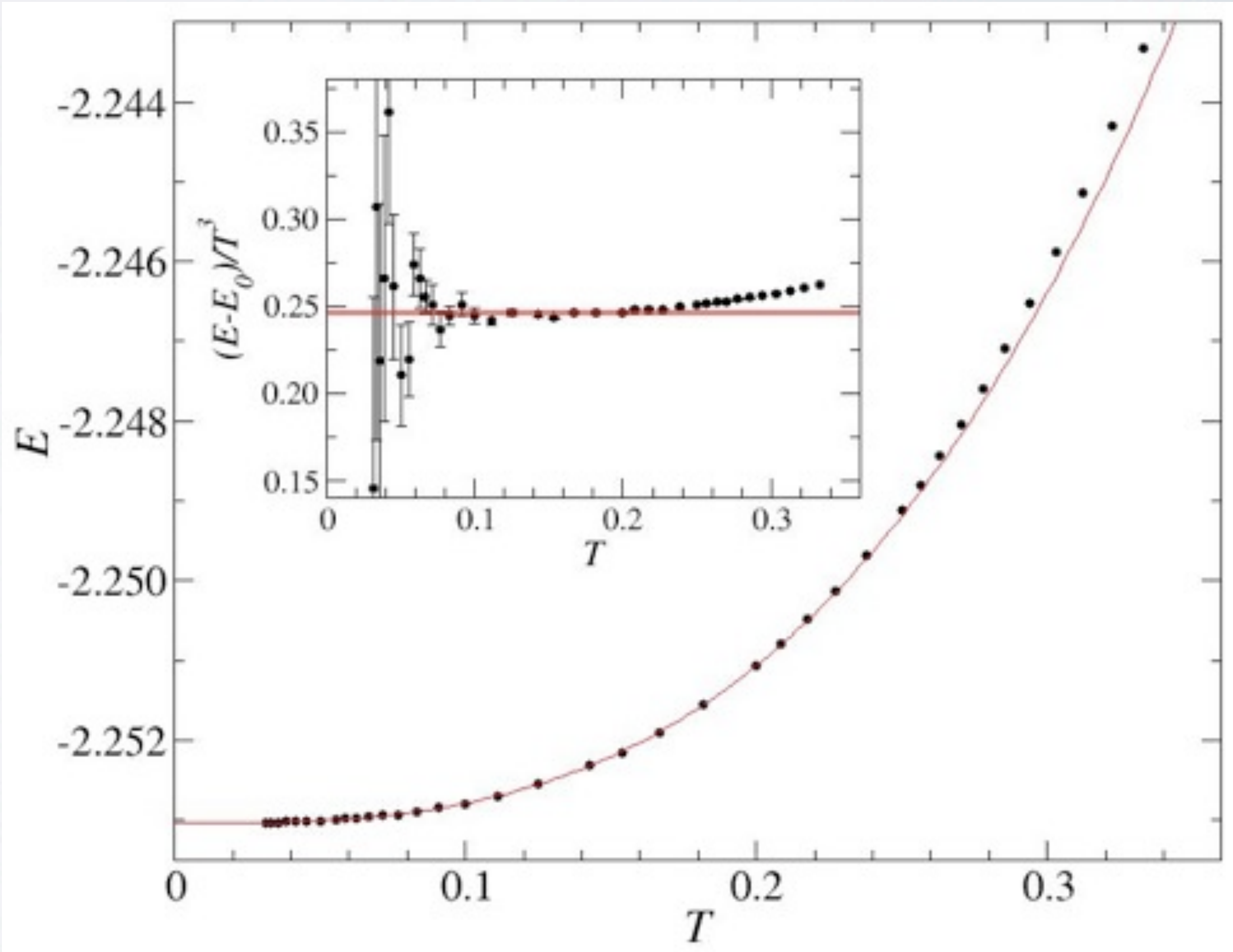
Expand O(3) order-parameter symmetry to O(N), large-N calculations

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

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

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

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$TlCuCl_3$

Quantum and classical criticality in a dimerized quantum antiferromagnet

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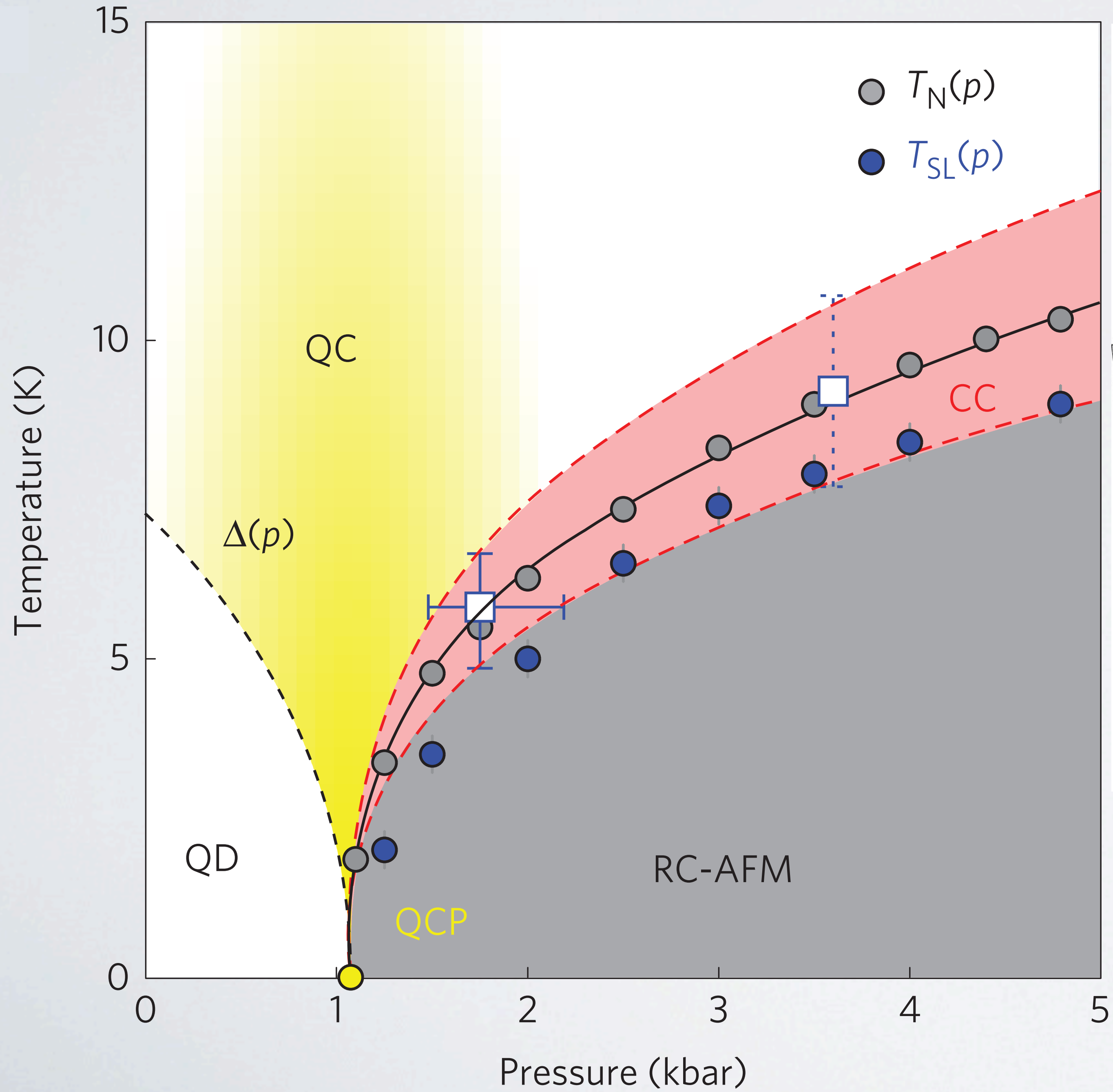
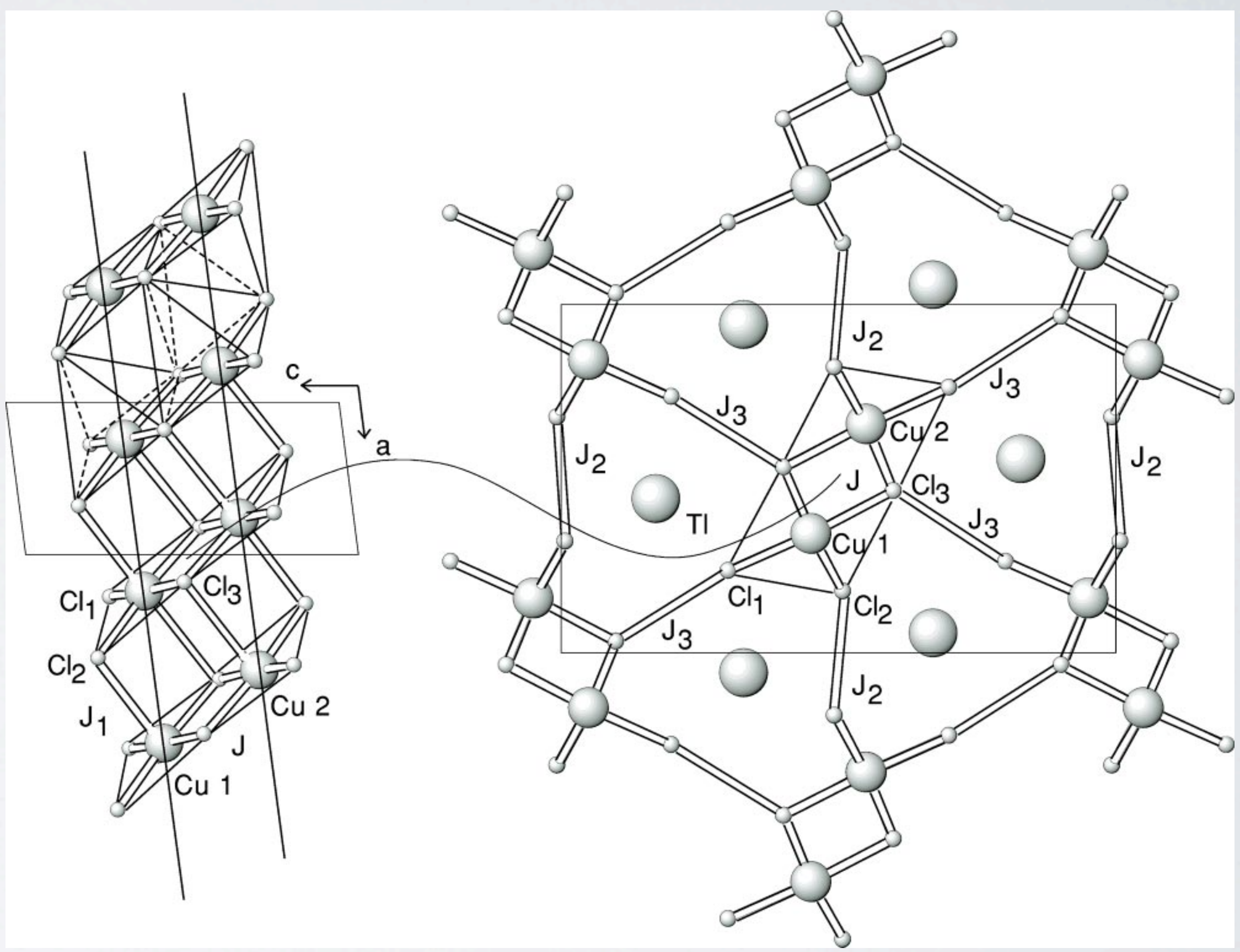
3D Network of dimers
- couplings can be changed by pressure



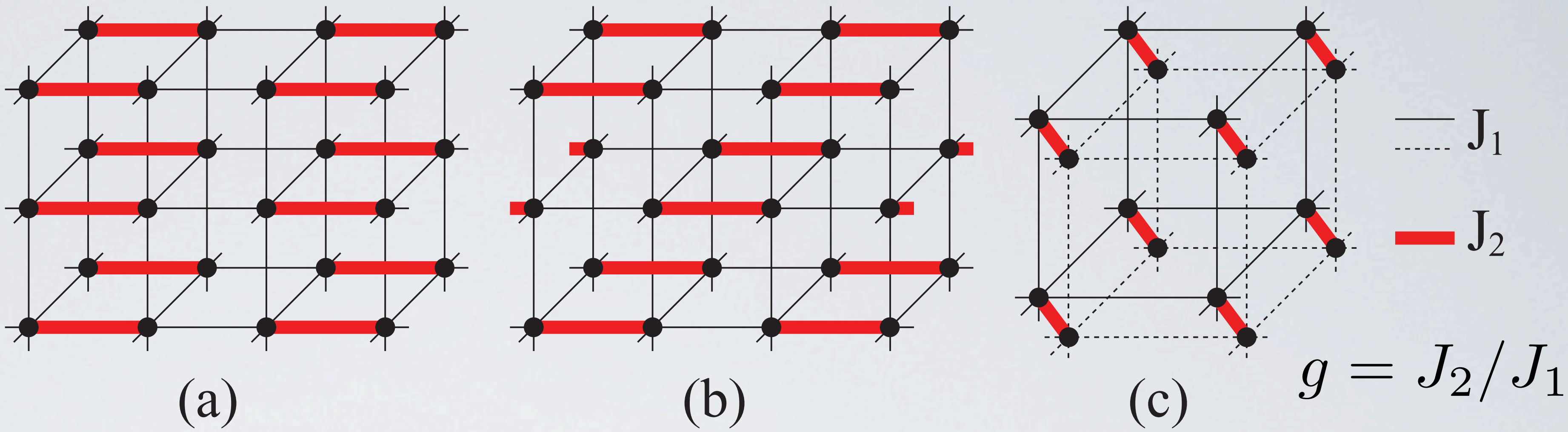


From: M Matsumoto, B Normand, TM Rice, M Sigrist, PRB (2004)

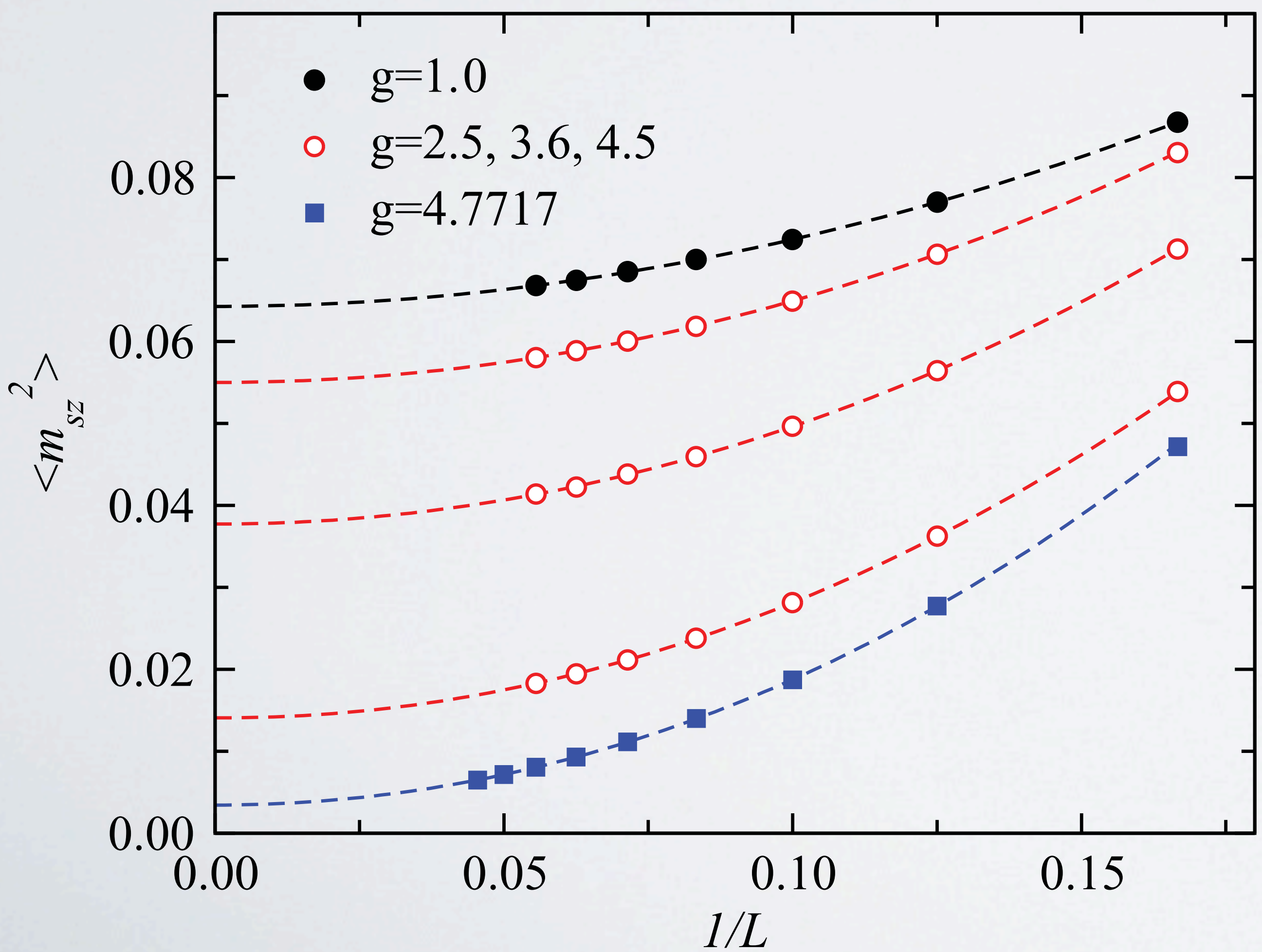
Universality of the Neel temperature in 3D dimerized systems?

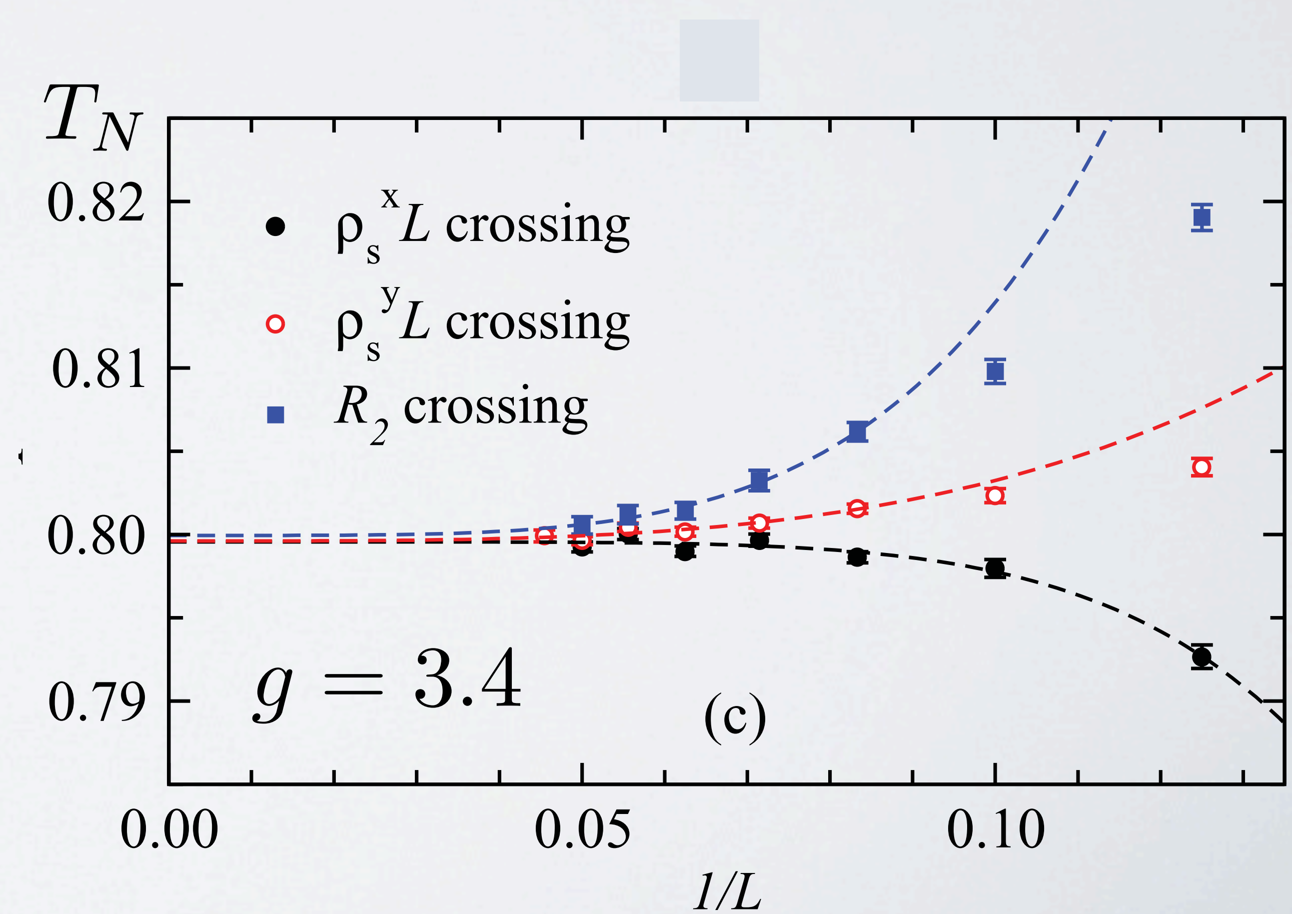
[S. Jin, AWS, PRB2012]

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



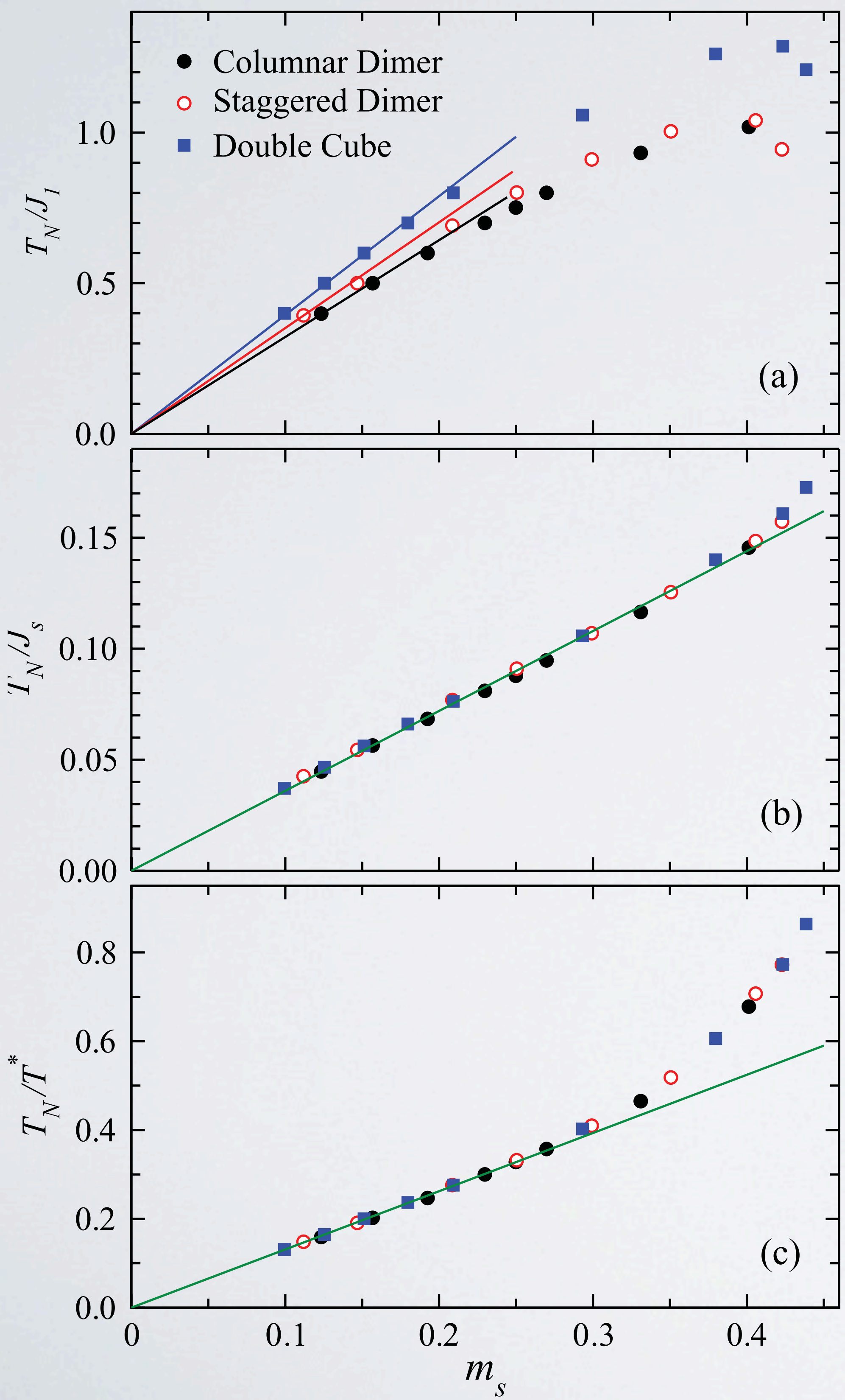
Example: Columnar dimers





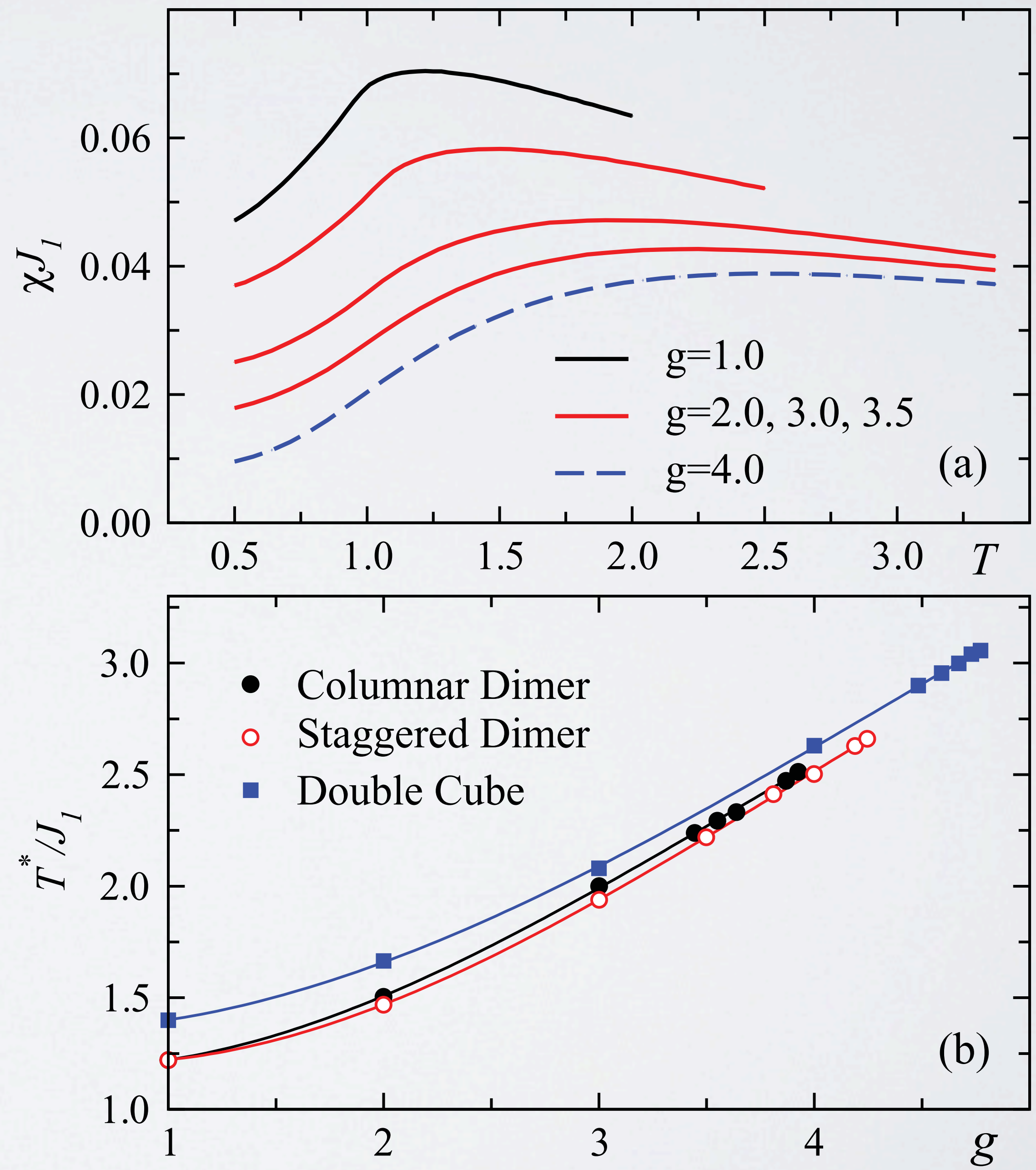
Couplings vs pressure not known experimentally

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



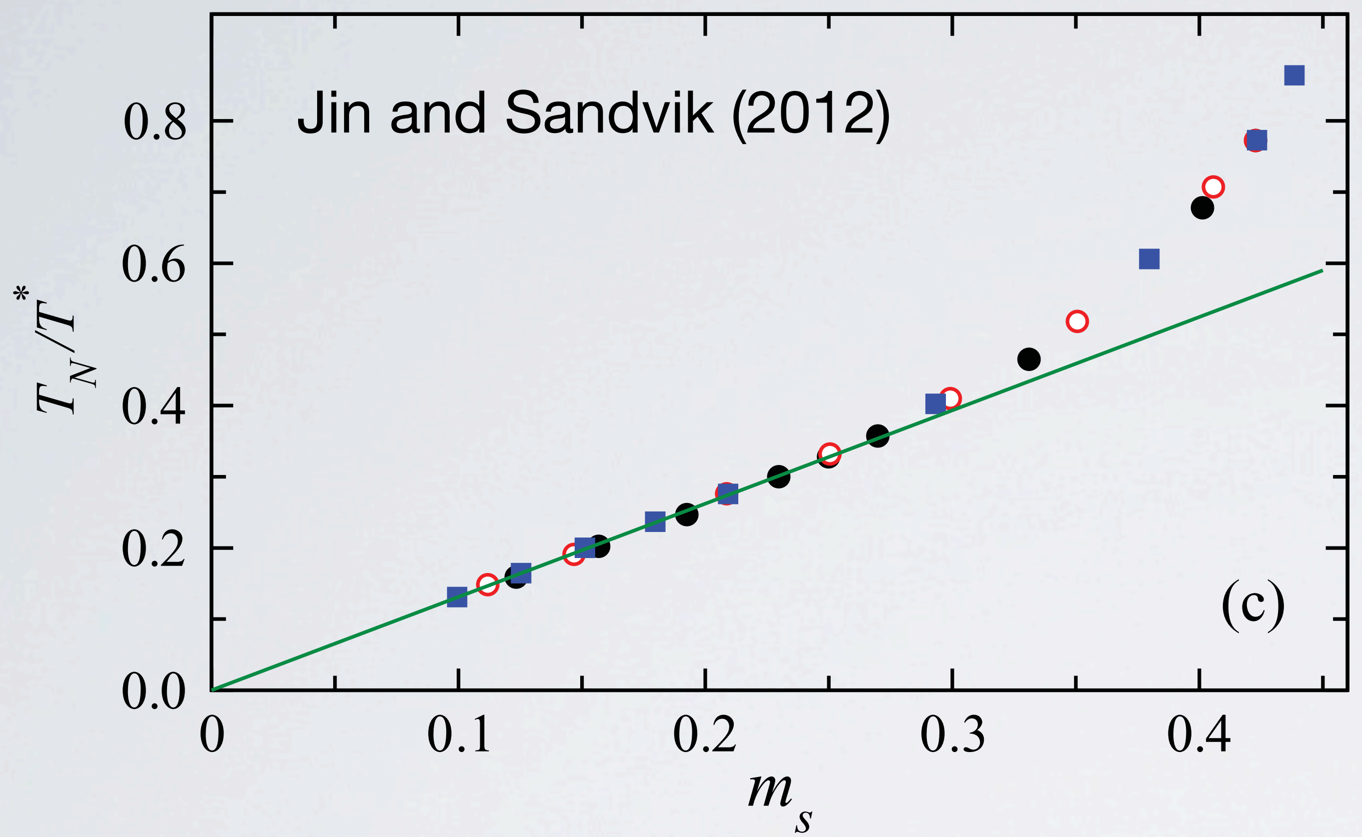
Three normalizations

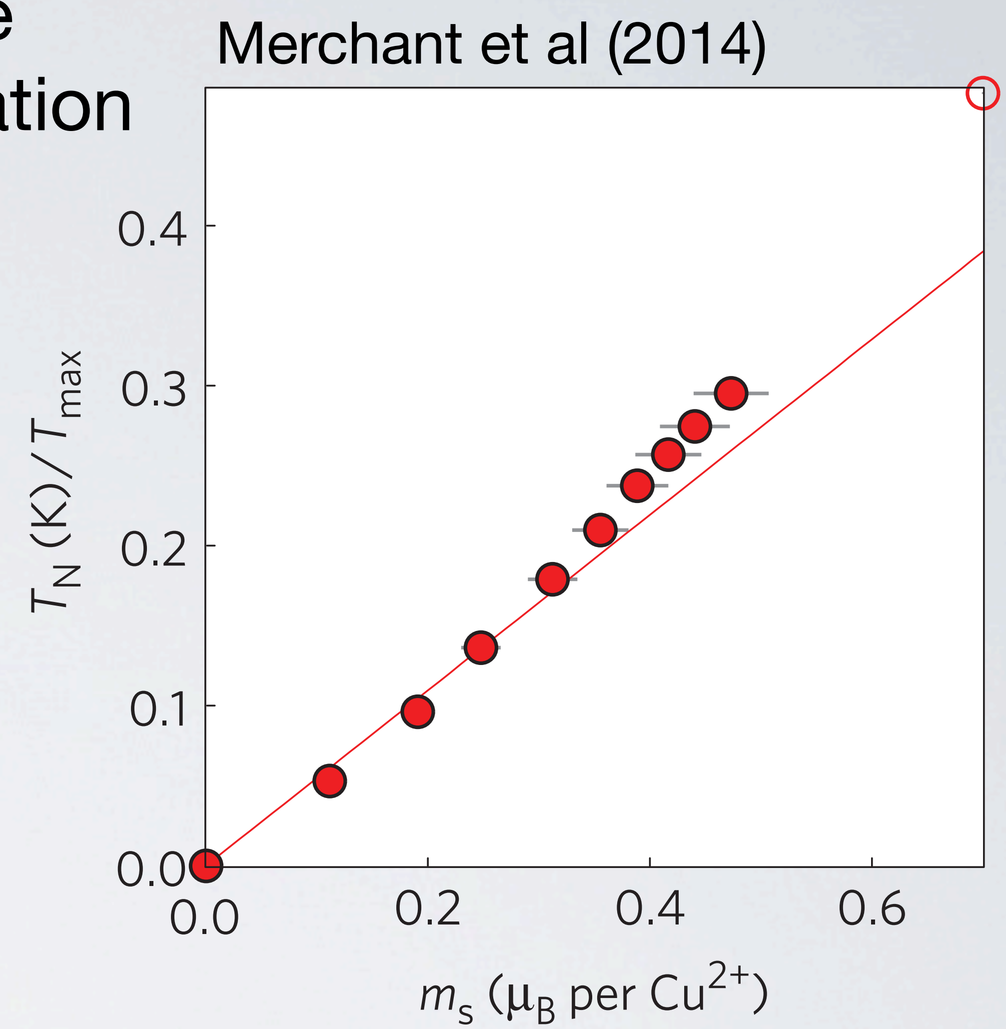
- weaker copling J_1
- sum J_s of couplings per spin
- peak T^* of magnetic susceptibility



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?)