Projector Monte Carlo in the valence-bond basis

(-H)^n projects out the ground state from an arbitrary state

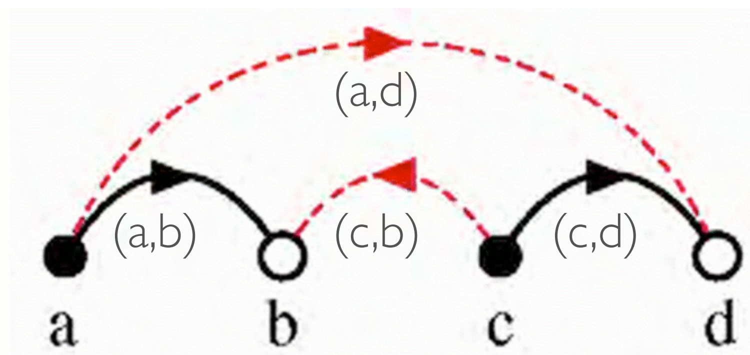
$$(-H)^n|\Psi\rangle = (-H)^n \sum_i c_i|i\rangle \to c_0(-E_0)^n|0\rangle$$

S=1/2 Heisenberg model

$$H = \sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j = -\sum_{\langle i,j\rangle} H_{ij}, \qquad H_{ij} = (\tfrac{1}{4} - \vec{S}_i \cdot \vec{S}_j)$$

Project with string of bond operators

$$\sum_{\{H_{ij}\}} \prod_{p=1}^{n} H_{i(p)j(p)}|\Psi\rangle \to r|0\rangle$$



A B A B

$$(i,j) = (|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)/\sqrt{2}$$

Action of bond operators

$$H_{ab}|...(a,b)...(c,d)...\rangle = |...(a,b)...(c,d)...\rangle$$

$$H_{bc}|...(a,b)...(c,d)...\rangle = \frac{1}{2}|...(c,b)...(a,d)...\rangle$$

Simple reconfiguration of bonds (or no change; diagonal)

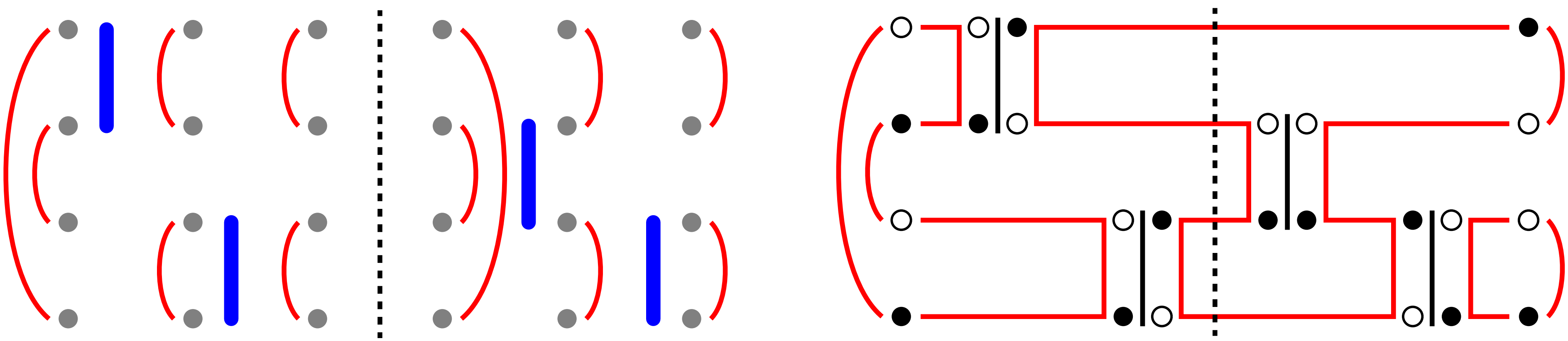
- no minus signs for A→B bond ‘direction’ convention
- sign problem does appear for frustrated systems

Loop updates in the valence-bond basis

Put the spins back in a way compatible with the valence bonds

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

and sample in a combined space of spins and bonds



Loop updates similar to those in finite-T SSE method

- good valence-bond trial wave functions can be used
  - faster convergence vs number of operators in string

- sample spins (and possibly also the edge bonds)
  - but measure "in the middle" using the propagated valence bonds
  - spin-rotationally invariant loop-based estimators

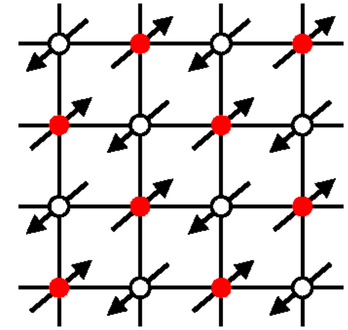
T → 0 limit can be taken with SSE

- but VB projection can be faster; only singlet sector, k=0

Results for 2D Heisenberg model

Sublattice magnetization

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



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

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

Quantum Monte Carlo

- finite-size calculations
- statistical errors
- no other approximations
- extrapolation to infinite size

Reger & Young (world-line) 1988

$$m_s = 0.30(2)$$

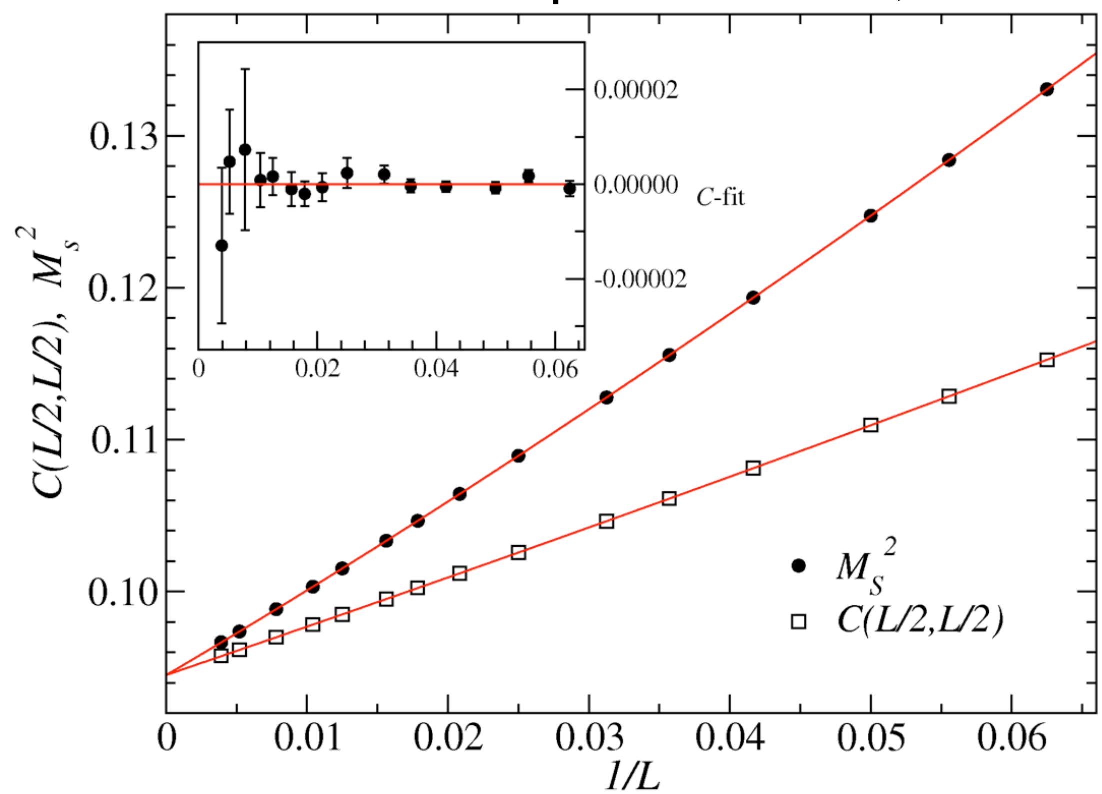
$$\approx 60\ \%\ \text{of classical value}$$

AWS & HG Evertz, PRE 2010

- Valence-bond projector

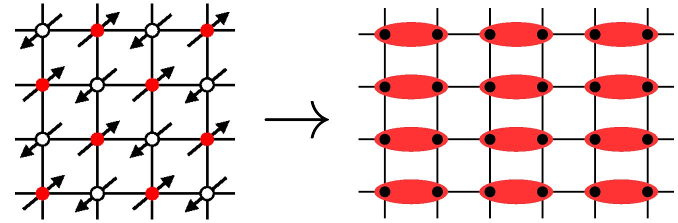
$$m_s = 0.30743(1)$$

L×L lattices up to 256×256, T→0

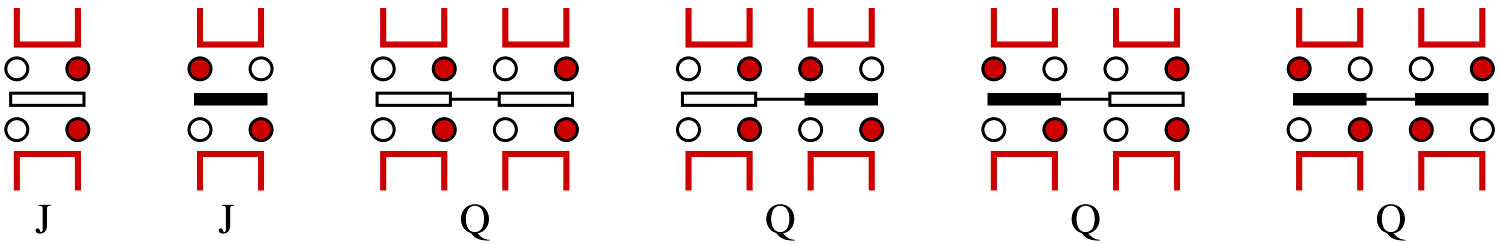


SSE and projector methods can be easily generalized for J-Q models

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

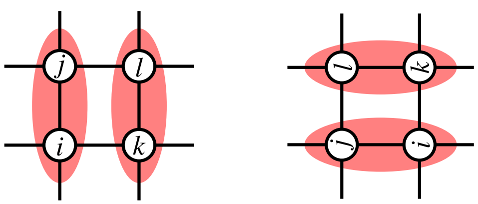


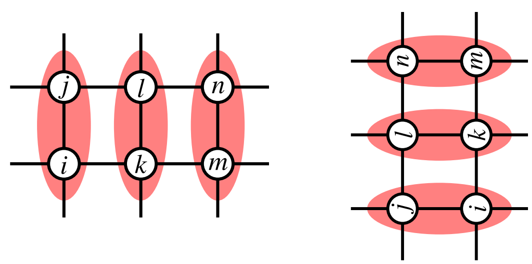
J- and Q-vertices, loops enter and exit at the individual 2-spin diagonal and off-diagonal parts



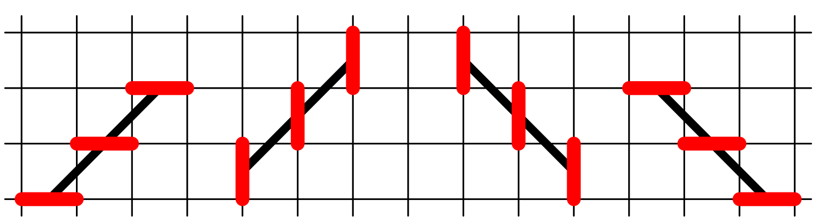
The 1D J-Q model has critical-dimerized transition of exactly the same SU(2) WZW class as in the J_1-J_2 Heisenberg chain [Patil, Katz, Sandvik, PRB (2018)]

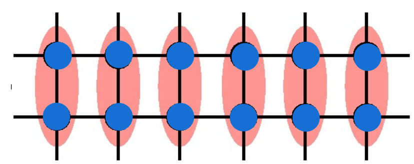
2D J-Q models with first-order and continuous (or almost continuous) transitions (deconfined quantum criticality) can be constructed





Continuous or weak first-order transitions





first-order transitions

Combine different Q terms to tune from weak 1st-order (continuous?) to strongly 1st-order

Parts III & IV combined

Finite-size scaling (“phenomenological RG”)

extracting critical exponents (scaling dimensions)

Deconfined quantum criticality in J-Q models

Phase transition in the J-Q_2 model

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

SSE QMC with T~1/L

Order parameters:

AFM: staggered magnetization

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

VBS: dimer order parameter

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

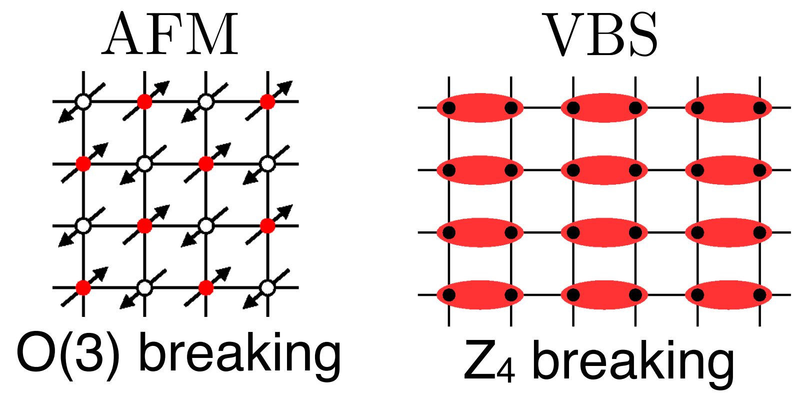
$$D_y = \frac{1}{N} \sum_{i=1}^{N} (-1)^{y_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}}$$

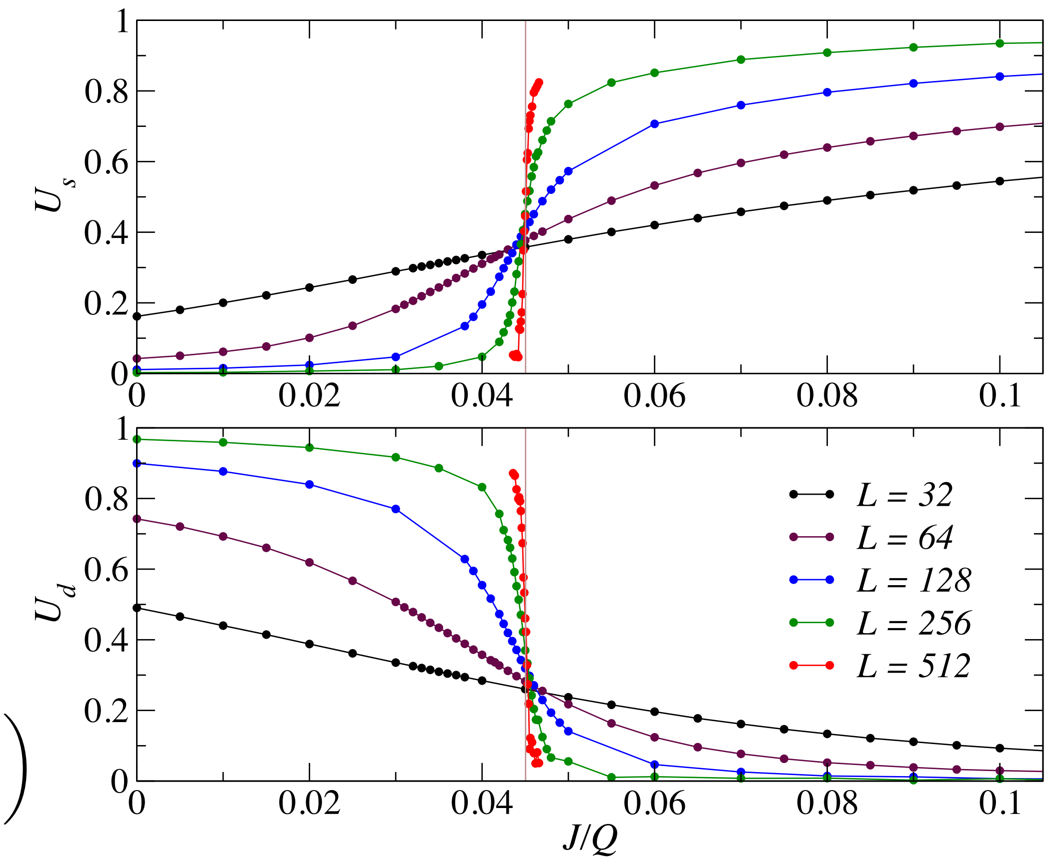
Binder cumulants:

$$U_s = \frac{5}{2}\left(1 - \frac{1}{3}\frac{\langle M_z^4 \rangle}{\langle M_z^2 \rangle^2}\right) \quad U_d = 2\left(1 - \frac{1}{2}\frac{\langle D^4 \rangle}{\langle D^2 \rangle^2}\right)$$

$U_s \to 1$, $U_d \to 0$ in AFM phase
$U_s \to 0$, $U_d \to 1$ in VBS phase

Crossing-point analysis
- simultaneous, continuous(?) transition





Competing scenario:
- weak first-order transition
- non-unitary CFT (“walking”)

Phase transitions - Finite-size scaling

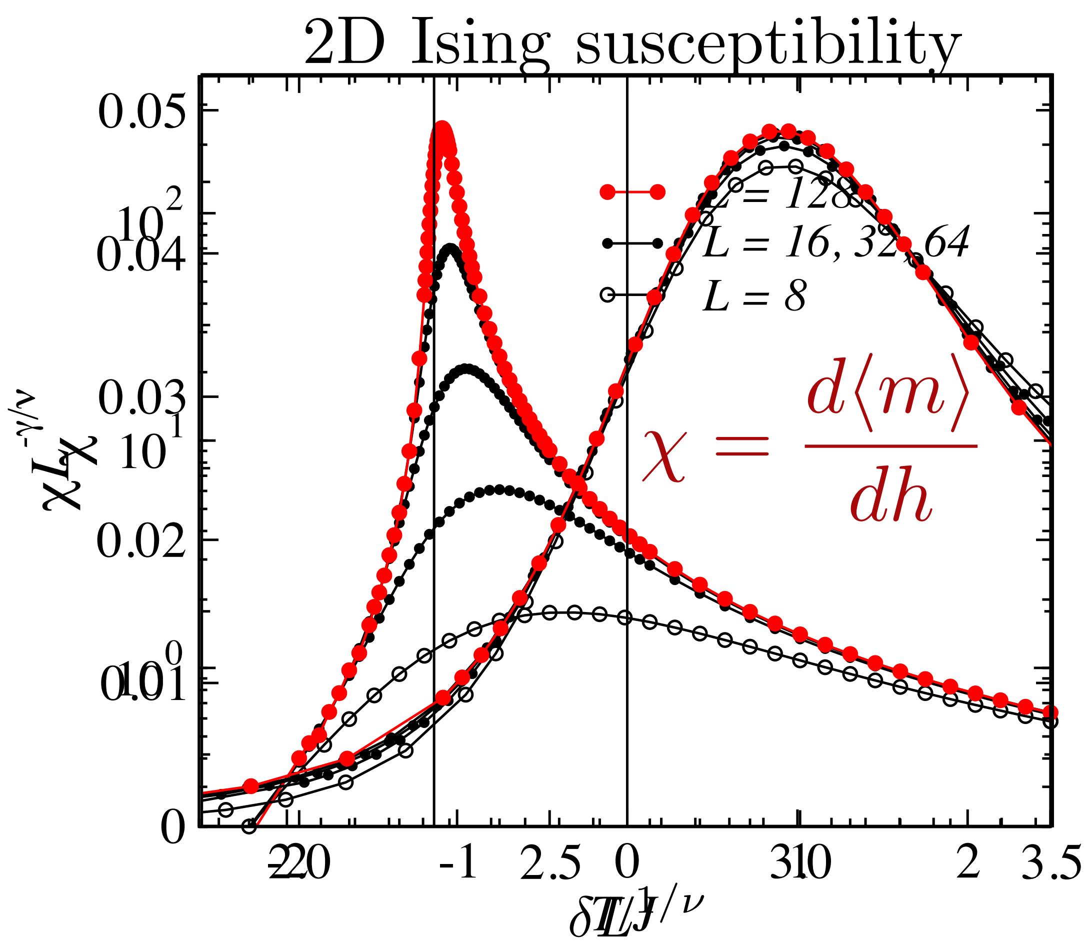
Consider classical transitions first

Correlation length divergent for $T \to T_c$ $\quad \xi \propto |\delta|^{-\nu}, \quad \delta = T - T_c$

Other singular quantity: $A(L \to \infty) \propto |\delta|^{\kappa} \propto \xi^{-\kappa/\nu}$

For **L-dependence** at T_c just let **$\xi \to L$**: $A(T \approx T_c, L) \propto L^{-\kappa/\nu}$

Close to critical point: $A(L,T) = L^{-\kappa/\nu} g(\xi/L) = L^{-\kappa/\nu} f(\delta L^{1/\nu})$



$\mathbf{f(x)}$ **analytic for** $\mathbf{x \to 0}$

$\mathbf{f(x \to \infty) \propto x^{\kappa}}$

2D Ising universality class

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

Critical T also known

$$T_c = 2/\ln(1+\sqrt{2}) \approx 2.2692$$

When exponents and T_c are not known, treat as fitting parameters - or extract in other way

Binder ratios and cumulants

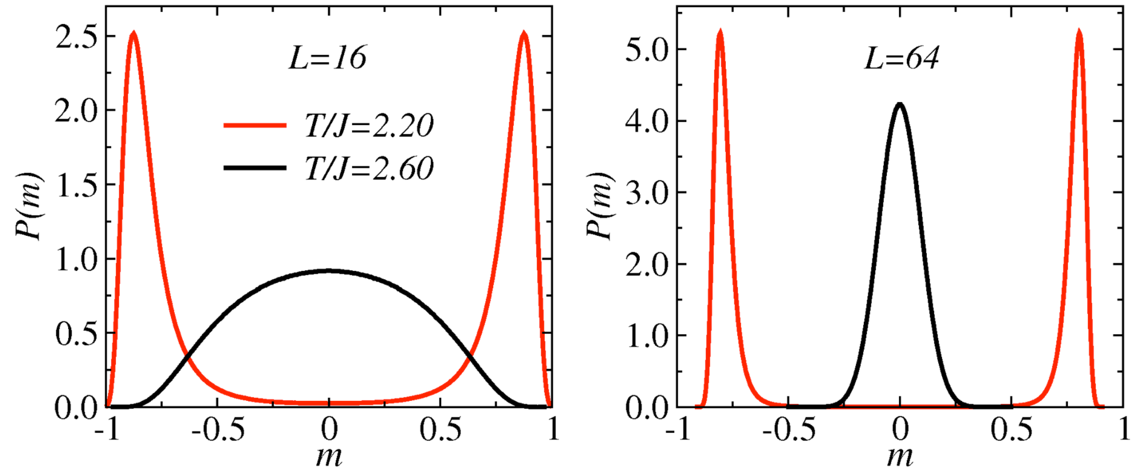
Consider the **dimensionless** ratio

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

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

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

order parameter distribution

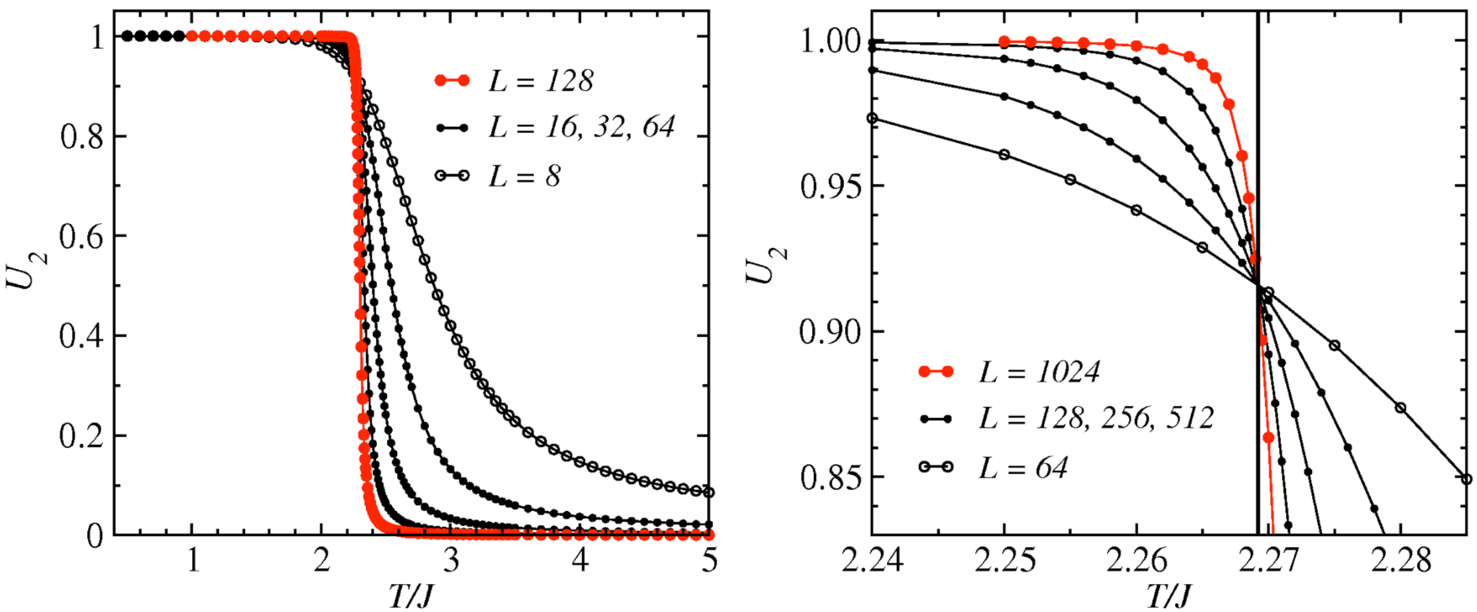


- **for $T>T_c$:** $P(m) \to \exp[-m^2/a(N)]$
  $a(N) \sim N^{-1}$ $\mathbf{R_2 \to 3}$ (Gaussian integrals)

The **Binder cumulant** is defined as (n-component order parameter; n=1 for Ising)

$$U_2 = \frac{n+2}{2}\left(1 - \frac{n}{n+2} R_2\right) \to \begin{cases} 1, & T < T_c \\ 0, & T > T_c \end{cases}$$

2D Ising model; MC results

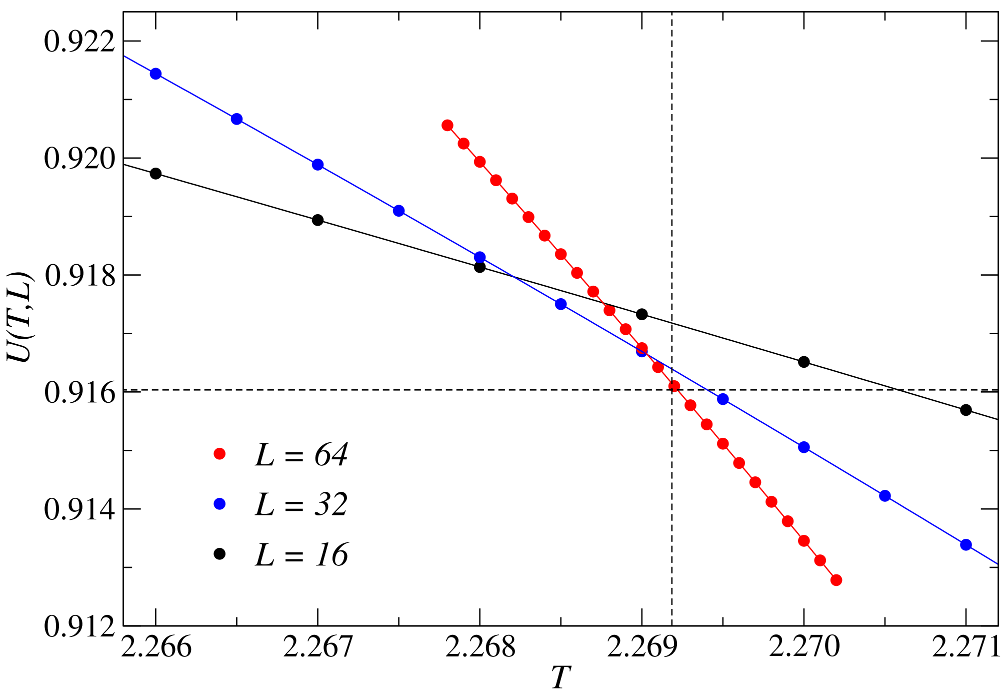


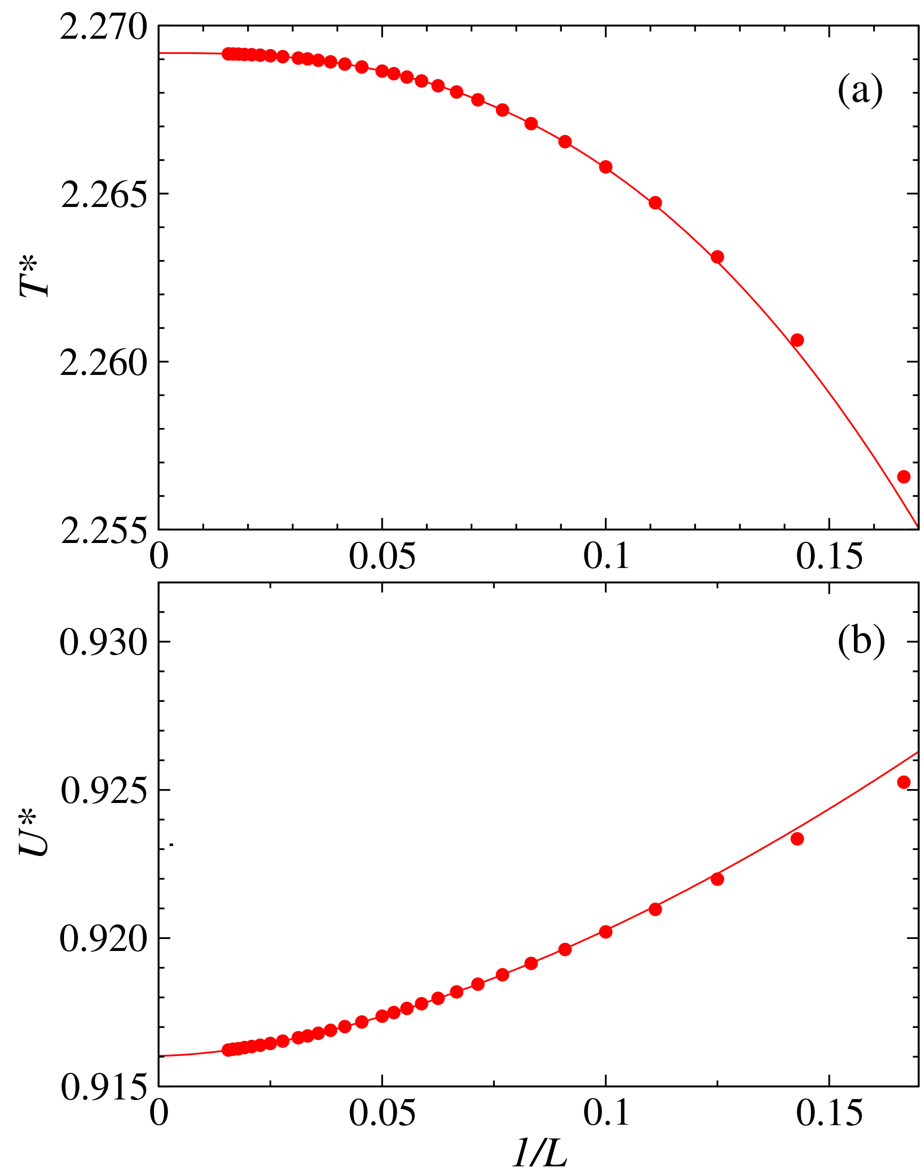
Curves for different L asymptotically cross each other at T_c

Extrapolate crossing for sizes L and 2L to infinite size

- converges faster than single-size T_c defs.

Systematic crossing-point analysis (2D Ising)





Drift in (L,2L) crossing points

$$U = U(\delta L^{1/\nu}, L^{-\omega_1}, L^{-\omega_2}, \ldots)$$

$\Rightarrow$ scaling corrections in crossings

$\sim L^{-(1/\nu+\omega)}$ for $T^* \rightarrow T_c$

$\sim L^{-\omega}$ for $U^* \rightarrow U(T_c)$

Use correction with free exponent

Fit with L_{min}=12: T_c=2.2691855(5). Correct: T_c=2.2691853...

Correlation-length exponent

Consider some generic critical observable A

$$A(L,t) = L^{-\kappa/\nu} f(\delta L^{1/\nu}) \;\rightarrow\; A(L,t)L^{\kappa/\nu} = f(\delta L^{1/\nu})$$

Let us take the derivative wrt δ

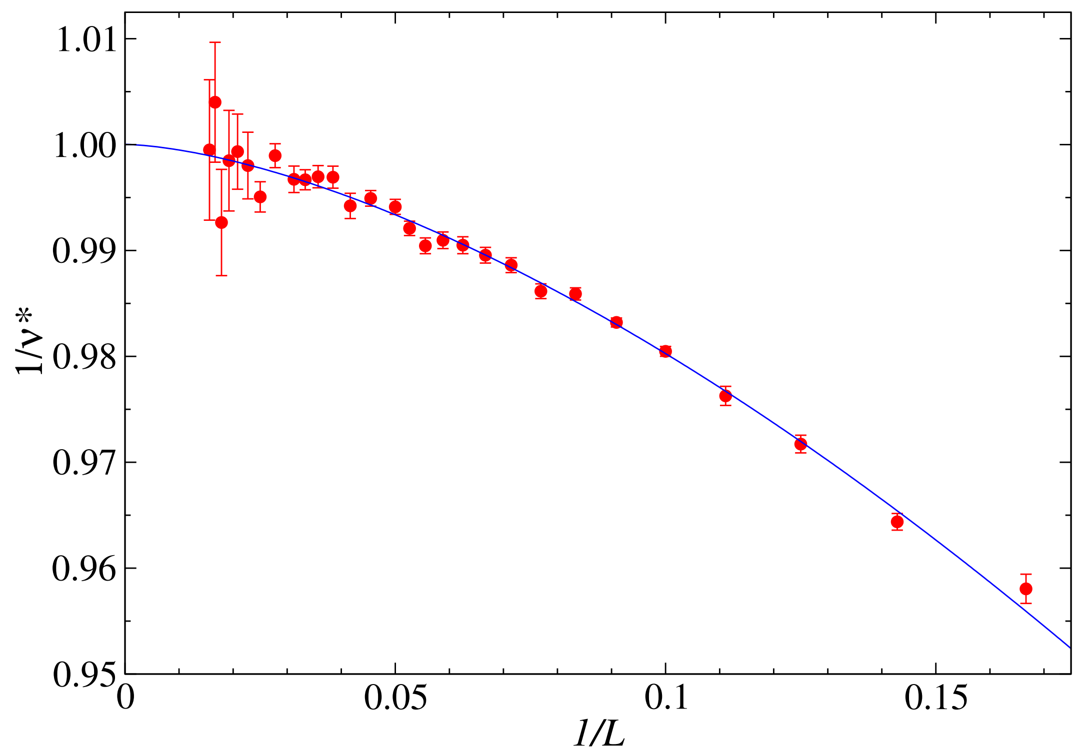
$$\frac{df(\delta L^{1/\nu})}{d\delta} = L^{1/\nu} f'(\delta L^{1/\nu}) \quad \rightarrow \frac{d(AL^{\kappa/\nu})}{d\delta} \propto L^{1/\nu} \quad (\delta = 0)$$

The Binder cumulant is dimensionless

$$U = U(\delta L^{1/\nu}, L^{-\omega_1}, L^{-\omega_2}, \ldots)$$

$$\frac{1}{\ln(2)} \ln\left(\frac{U'(2L)}{U'(L)}\right) \rightarrow \frac{1}{\nu}$$

Test for 2D Ising (ν=1)



Note:
The 2D Ising model has unusually small scaling corrections (ω=2)

Typically ω<1, much more difficult to extrapolate and get correct exponents

Relevant and irrelevant perturbations of a critical point

Critical correlation function of some lattice operator (assume CFT)

$$\langle O(\vec{r}_1)O(\vec{r}_2)\rangle = \sum_i a_i r^{-2\Delta_i}$$

The scaling dimensions Δ_i correspond to the spectrum of 'orthogonal operators' (continuum fields) contained in the lattice operator *O*

- Loosely speaking, we say that the smallest Δ_i is the scaling dimension of *O*

Consider a **critical Hamiltonian H_0** and add some perturbation hM

$$H = H_0 + h\sum_i m_i = hM \;\; (\equiv hNm = hL^d m)$$

RG description of effects of hM at a critical point. Free energy density:

$$f_s(t,h,L) = L^{-d}F_s(tL^{1/\nu}, hL^y)$$

Taylor expand at t=0: $f_s^h \propto hL^{y-d}$

From derivative of $f(h) = -TL^{-d}\ln[Z(h)]$

$$f_s^h = h\langle m\rangle \propto hL^{-\Delta}$$

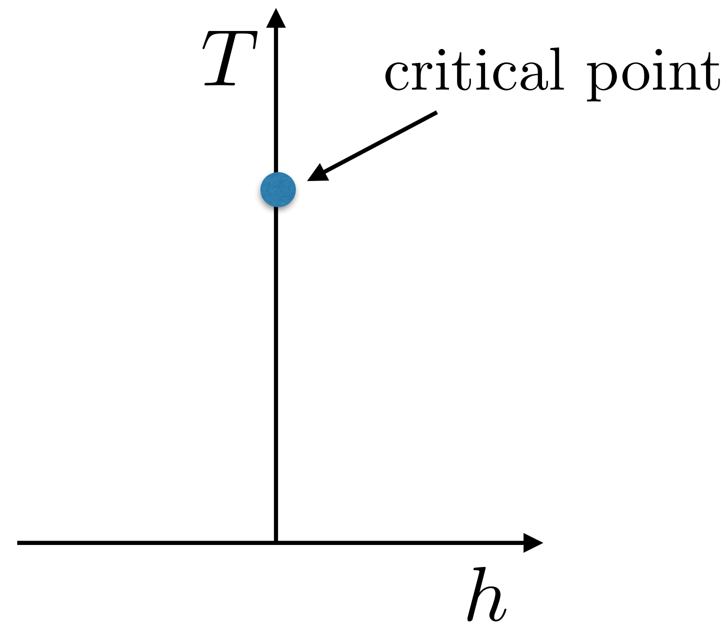
$$\boxed{\rightarrow \; y = d - \Delta}$$

y = scaling dimension of h

- The effect of the perturbation grows with L (it is relevant) only if y>0
- Irrelevant perturbation if y<0 (the critical point stays the same)
- A relevant perturbation causes the system to flow to a different fix point

Symmetric and symmetry-breaking fields

Example: classical Ising model
- competition between energy and entropy



At h=0, T tunes to the critical point
- the 'thermal field' is $t=T-T_c$

Changing T changes the prefactor of E in

$$\mathrm{e}^{-E(\sigma)/T}$$

- E is the operator conjugate to T

$$\langle E(r)E(0) \sim r^{-2\Delta_0}, \quad \Delta_0 = d - 1/\nu$$

Set t=0, tune the magnetic field; E → E+hM
- h ≠ 0 breaks the Z_2 symmetry of the model; relevant but not symmetric

$$\langle M(r)M(0) \sim r^{-2\Delta_M}, \quad \Delta_M = d - 1/\nu_M$$

The exponent Δ_M is related to the exponent we call η

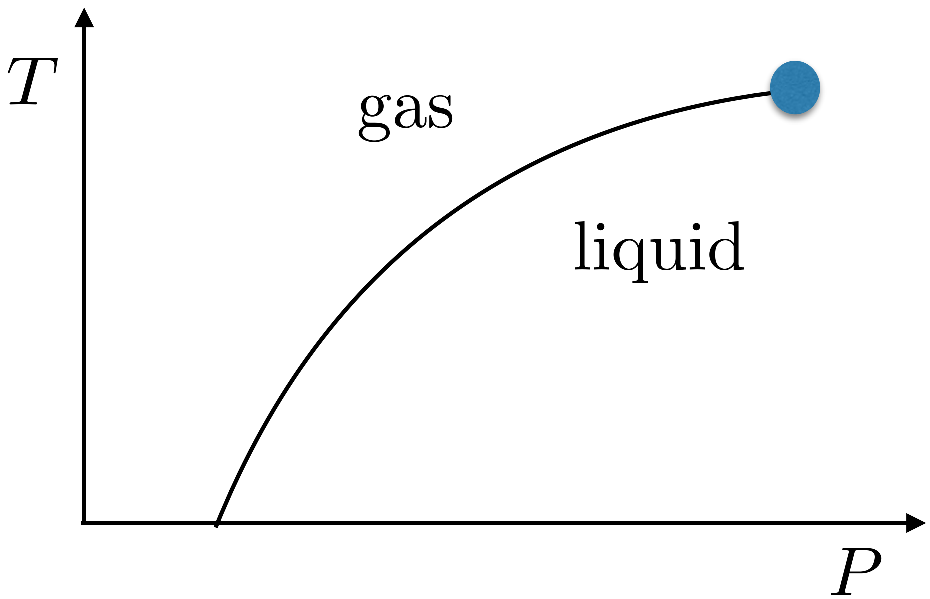
$$\langle M(r)M(0) \sim r^{-(d-2+\eta)} \qquad \Delta_M = (d-2+\eta)/2$$

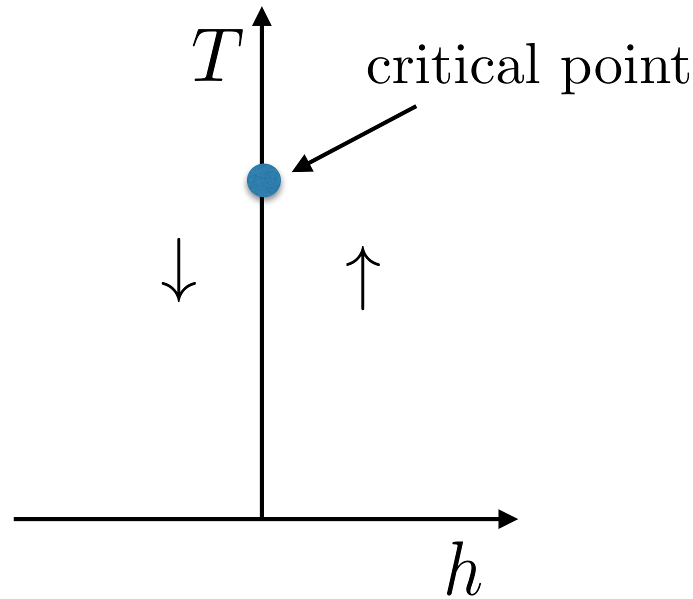
Normally critical points have one relevant symmetric field
- multi-critical points have more than one

Gas-liquid transition

Maps to Ising model even though no apparent Ising (Z_2) symmetry

Order parameter is density (m ~ deviation from mean density at transition)





Tuning the relevant field corresponds to moving tangentially to the coexistence curve from the critical point (not so easy)

Tuning the symmetry-breaking field corresponds to moving perpendicularly to the coexistence curve

Moving along some generic path gives a mix of the two scaling dimensions in correlation functions; one eventually dominates

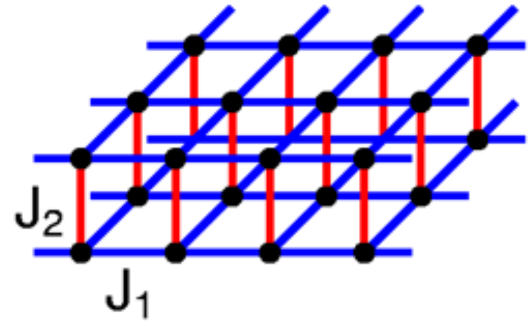
In spin models we often have an explicit symmetry (e.g., zero field, like Ising)

Quantum system: d → d + z (dynamic exponent), z=1 for CFT

Example: O(3) transition in 2+1 dimensions (2D quantum, d=3)

Bilayer Heisenberg model

$$H = J_1 \sum_{a=1,2} \sum_{\langle ij \rangle} \boldsymbol{S}_{a,i} \cdot \boldsymbol{S}_{a,j} + J_2 \sum_{i=1}^{N} \boldsymbol{S}_{1,i} \cdot \boldsymbol{S}_{2,i}$$

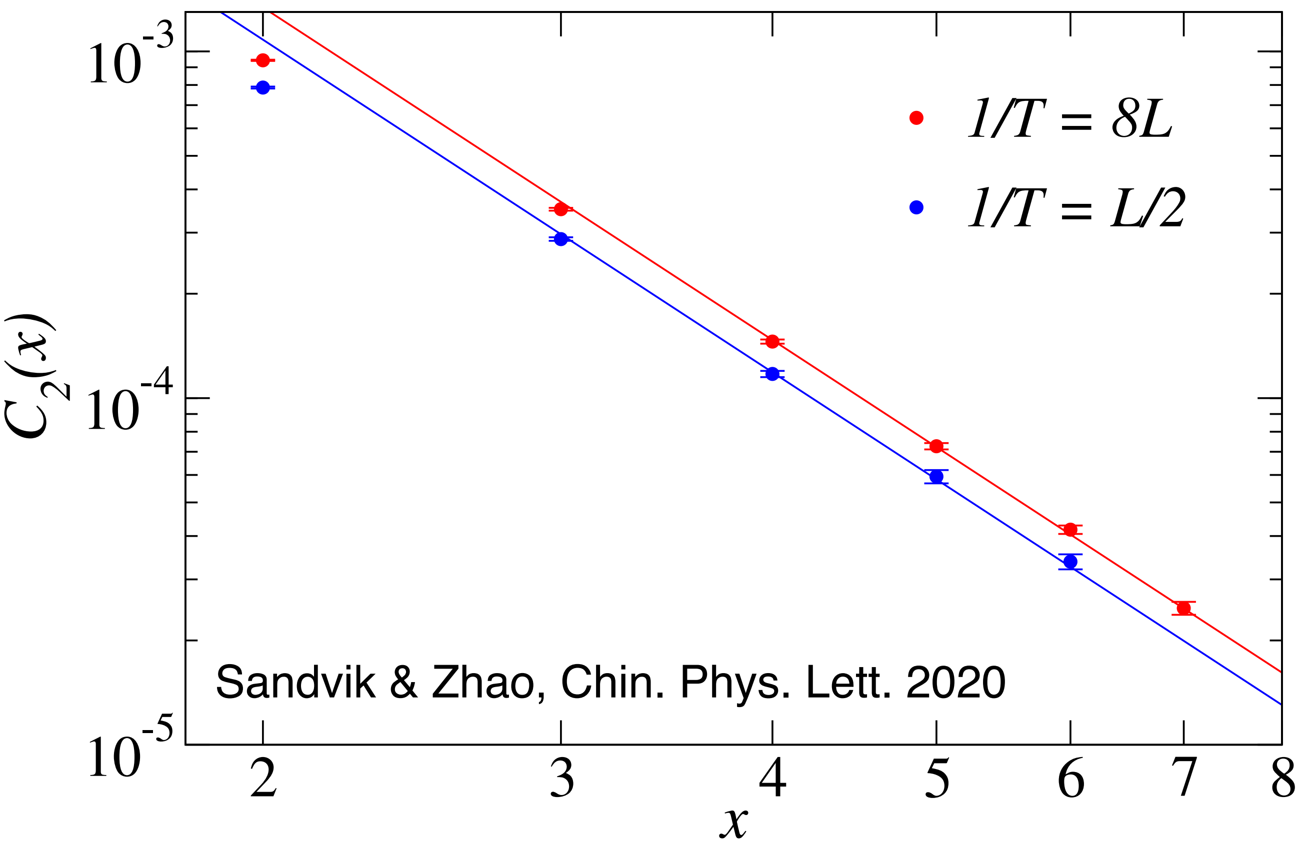


$g = J_2/J_1$

Critical at $J_2/J_1 \approx 2.5202$

The J_1 and J_2 terms are both relevant (no entropy at T=0)
- changing one of them takes us away from the critical point

dimer (inter-plane, J_2) correlations at g_c



$$\boxed{\rightarrow \ y = d - \Delta}$$

$2\Delta \approx 3.188 \rightarrow y \approx 1.406$

- consistent with known $1/\nu$

This is the only relevant symmetric operator at this transition

Corresponds to the classical ‘thermal field’

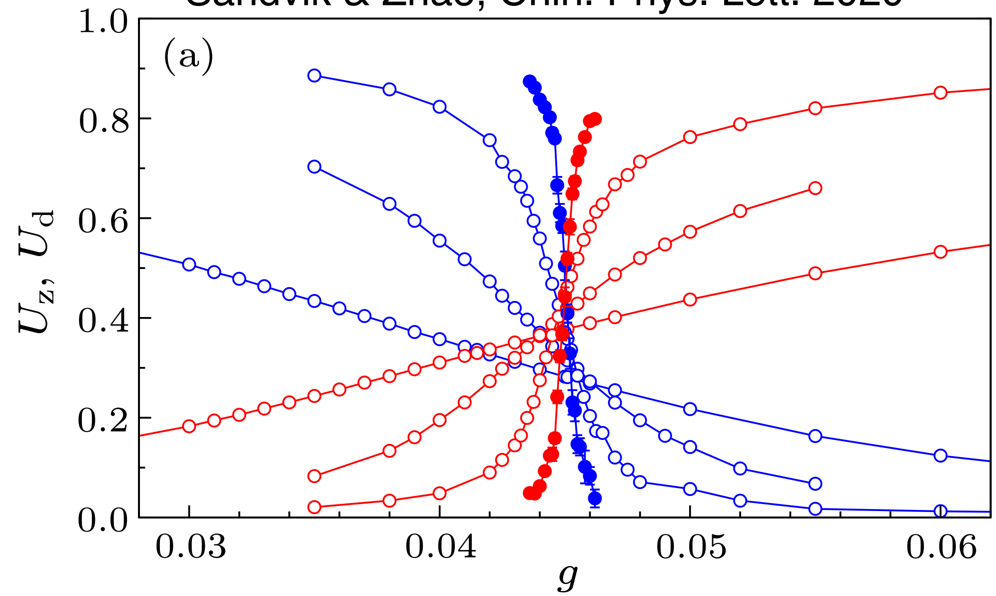
J-Q model (J-Q_2)

Binder cumulants give critical point
- slopes used to define $1/\nu$

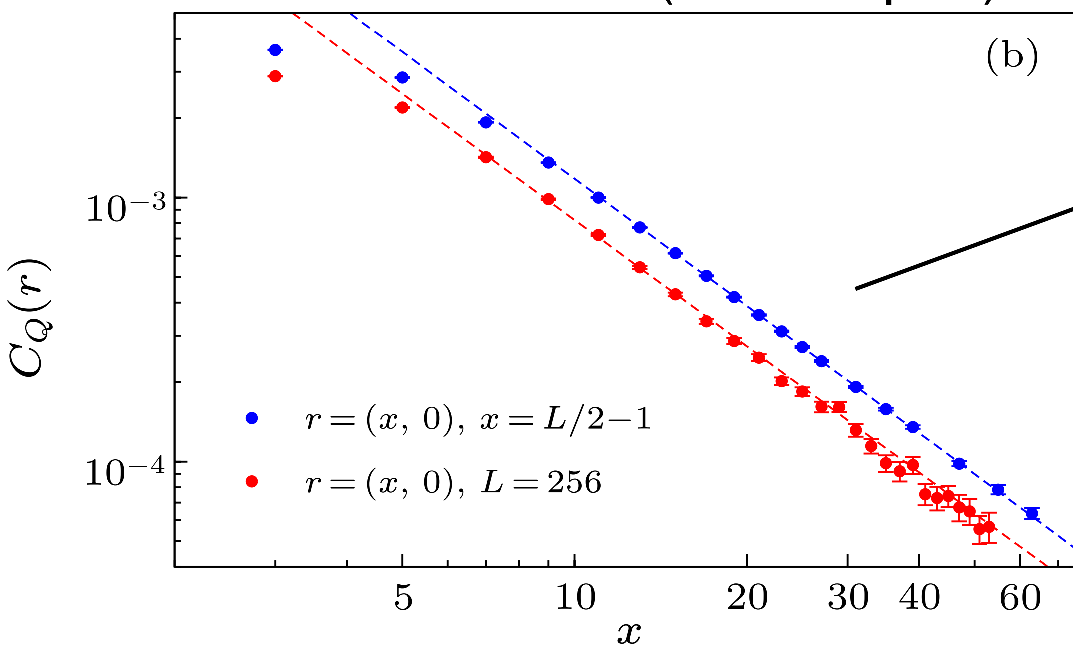
$$\frac{1}{\ln(2)} \ln\left(\frac{U'(2L)}{U'(L)}\right) \rightarrow \frac{1}{\nu}$$

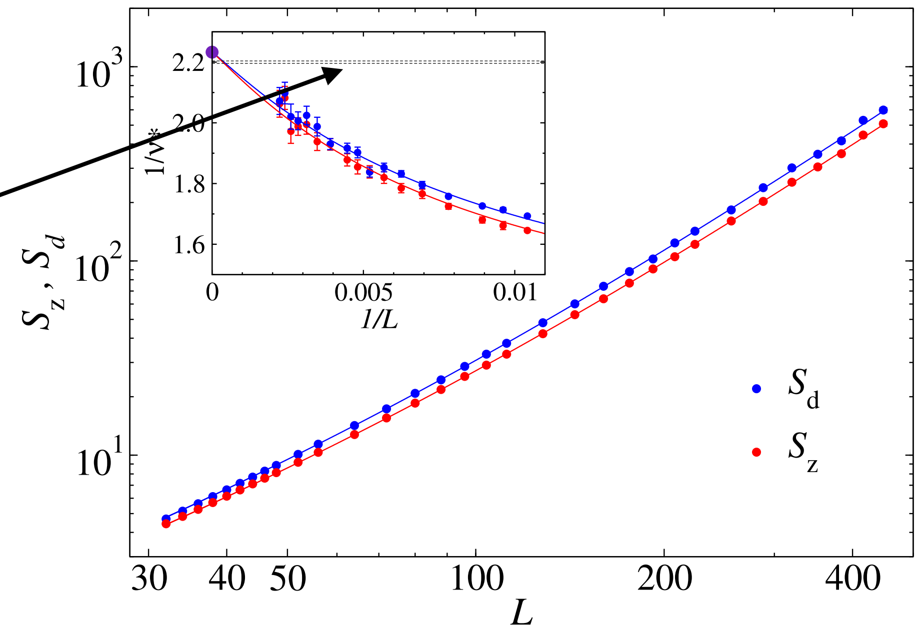
We can also calculate correlations of the relevant J and Q terms in H

Sandvik & Zhao, Chin. Phys. Lett. 2020



Q-Q correlations (uniform part)





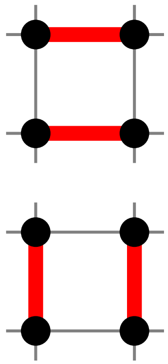
Mutual consistency between two ways of calculating $1/\nu$: $\nu = 0.455 \pm 0.002$
- at the very least, the model is extremely close to a critical point
- but violates a CFT bound: $\nu > 0.52\ldots$

Multi-Critical DQCP Scenario

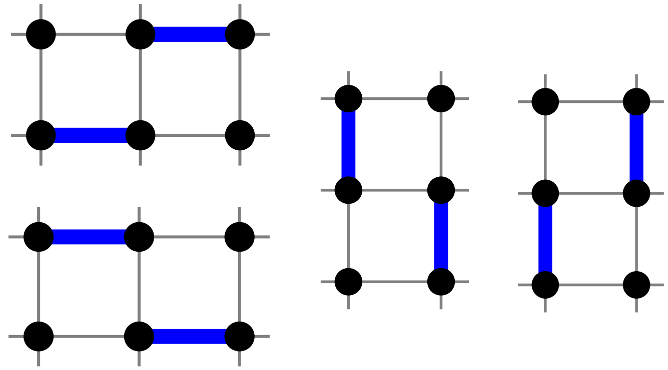
Zhao, Takahashi, Sandvik, PRL 2020

Identified a second symmetric relevant operator

Q



Z



summed over all lattice positions

Compute scaling dimension of the Z perturbation in the critical J-Q model

$$H(\delta) = H_c + \delta Z$$

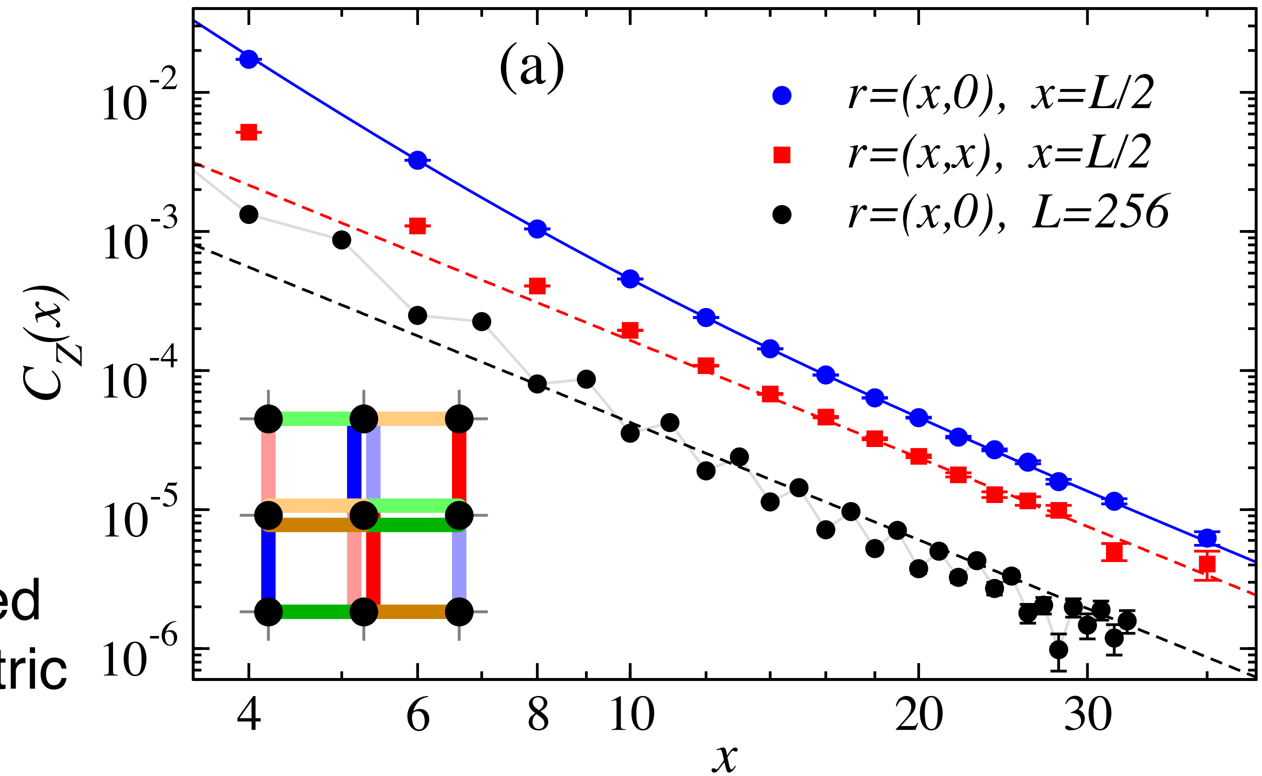
ZZ Correlations decay with a power corresponding to

$\Delta_Z \approx$ 1.40

different from

$\Delta_Q \approx$ 0.8

Bootstrap bound assumed a single relevant symmetric operator



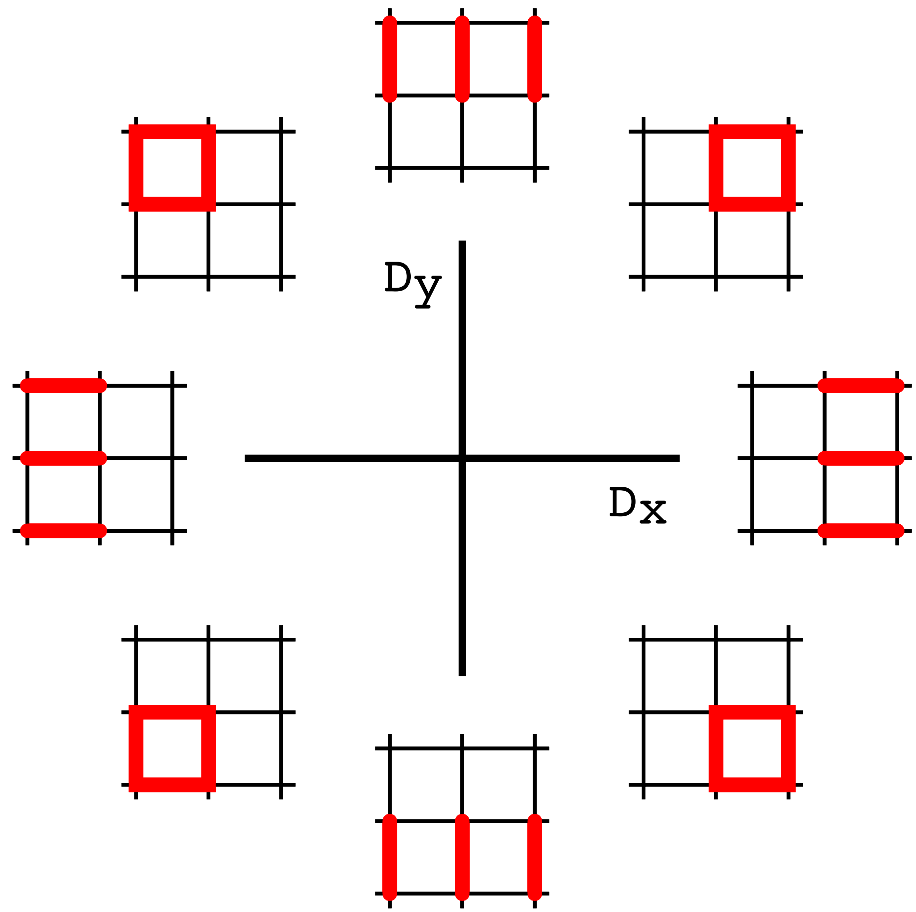
Multi-critical scenario goes beyond original DQC proposal

VBS order parameter: emergent U(1) symmetry

Dimer order parameter

$$D_x = \frac{1}{N}\sum_{x,y}(-1)^x \mathbf{S}_{x,y}\cdot\mathbf{S}_{x+1,y}$$

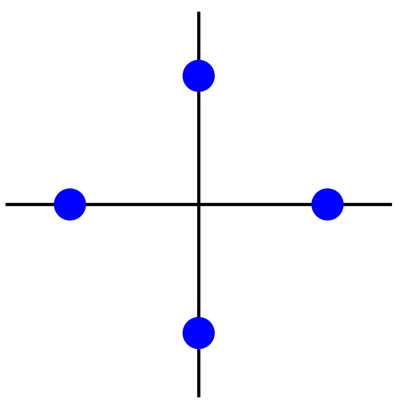
$$D_y = \frac{1}{N}\sum_{x,y}(-1)^y \mathbf{S}_{x,y}\cdot\mathbf{S}_{x,y+1}$$



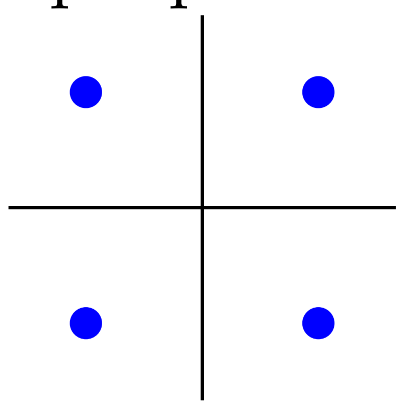
Collect histograms $P(D_x,D_y)$ with valence-bond basis QMC

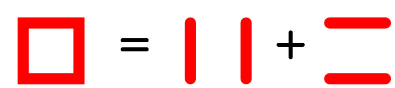
Two possible types of order patterns distinguished by histograms

columnar



plaquette

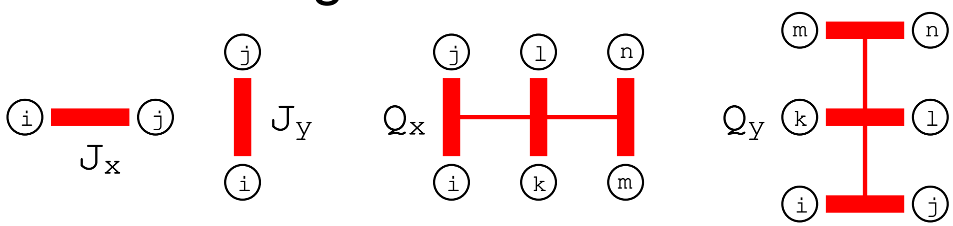




Finite-size fluctuations
- amplitude
- angular

Emergent U(1) symmetry of columnar VBS order

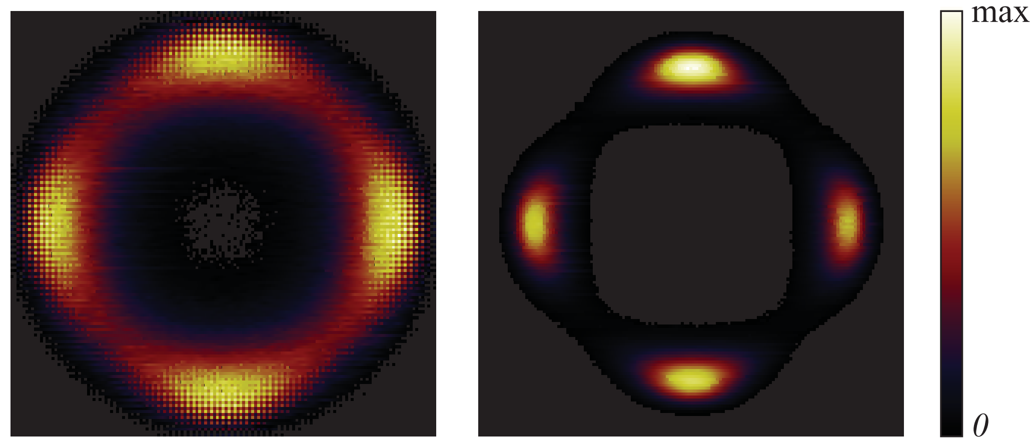
Realize stronger VBS order with J-Q_3 model



J-Q_3 model

$J_x = J_y$, $Q_x = Q_y$

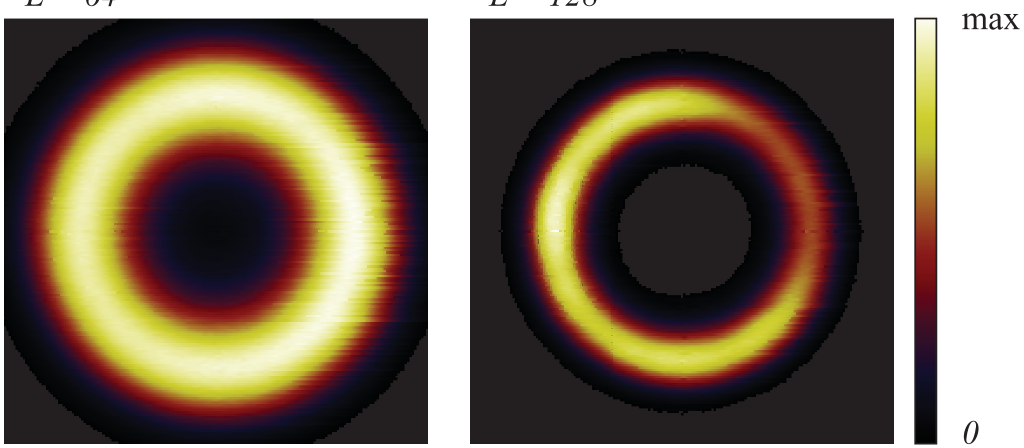
Lou, Sandvik, Kawashima, PRB (2009),
Sandvik, PRB (2012)

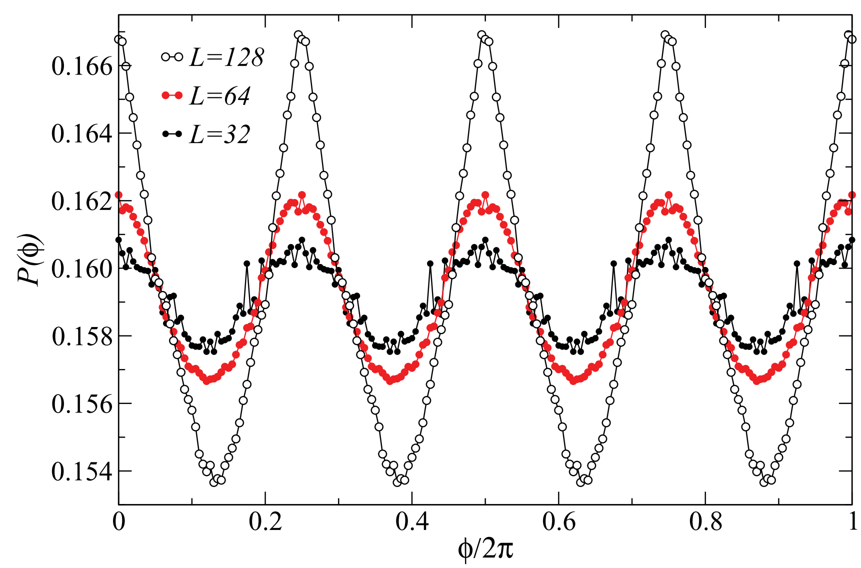


Strong columnar VBS when $J/Q_3=0$

J-Q_2 model with $J/Q_2=0$

- weak columnar VBS
- very large angular fluctuations
- emergent U(1) symmetry





U(1) symmetry emerges on a length scale

$$\Lambda \sim (g-g_c)^{-\nu'} > \xi \sim (g-g_c)^{-\nu}$$

Finite-size scaling: $\nu'/\nu \sim 1.4$ (H. Shao, W. Guo, AWS, Science 2016)

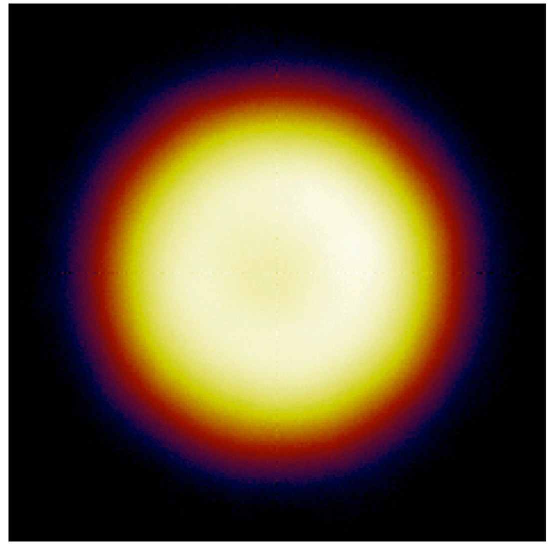
Critical VBS fluctuations

J-Q_2 model

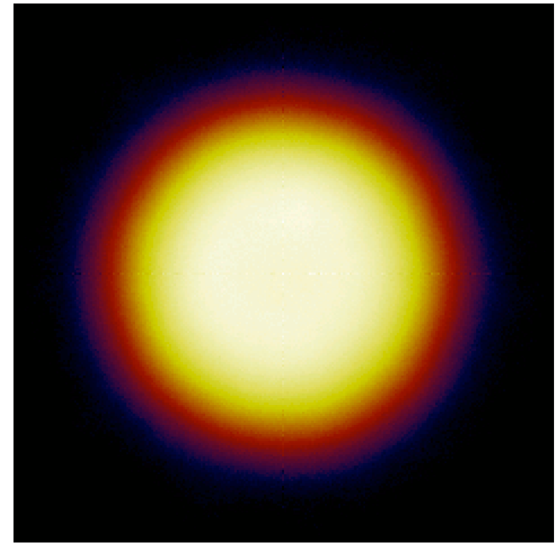
Emergent SO(5) symmetry has also been detected (Nahum et al, PRL 2015)

- emergent U(1) VBS order combined with O(3) AFM order parameter

L=64, J/Q=0.042



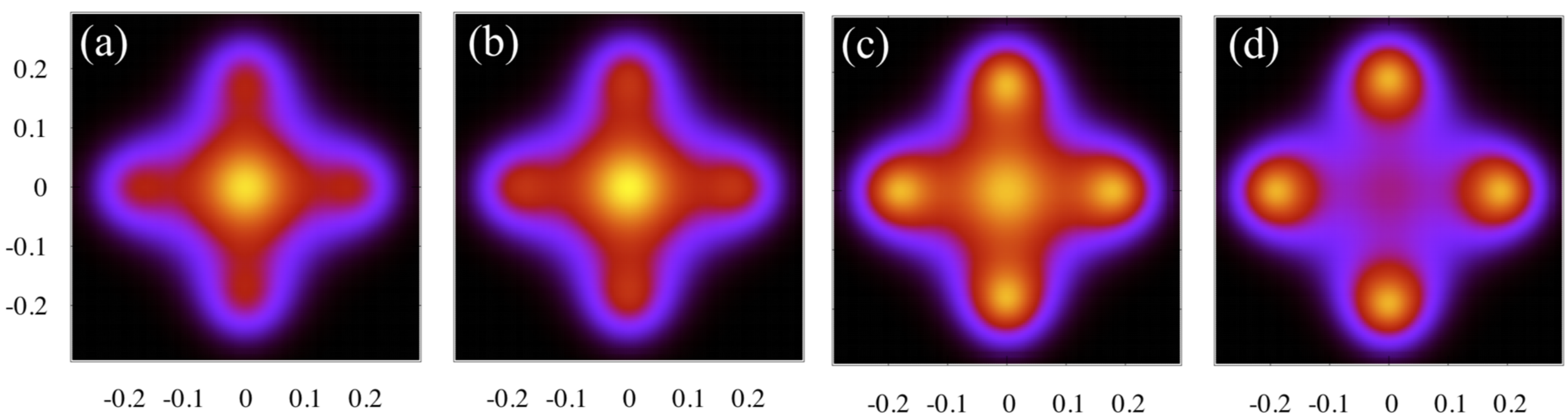
L=64 J/Q=0.043



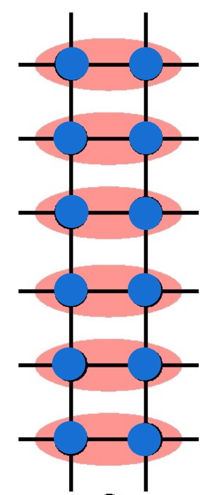
What happens in a columnar J-Q_n model with large n?

- will nucleation of VBS order (first-order transition) happen?

J-Q_6 model (J. Takahashi, AWS, PRR 2020)



Q_6 interaction

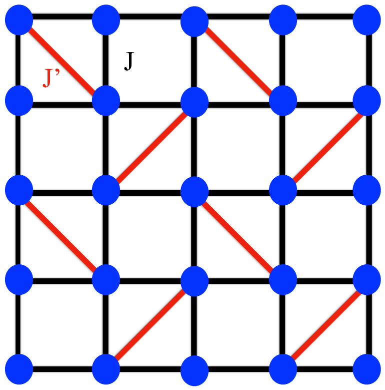


Coexistence between 4-fold degenerate columnar state and AFM

- J-Q_n model has first-order transition above some n (maybe even for n=2)

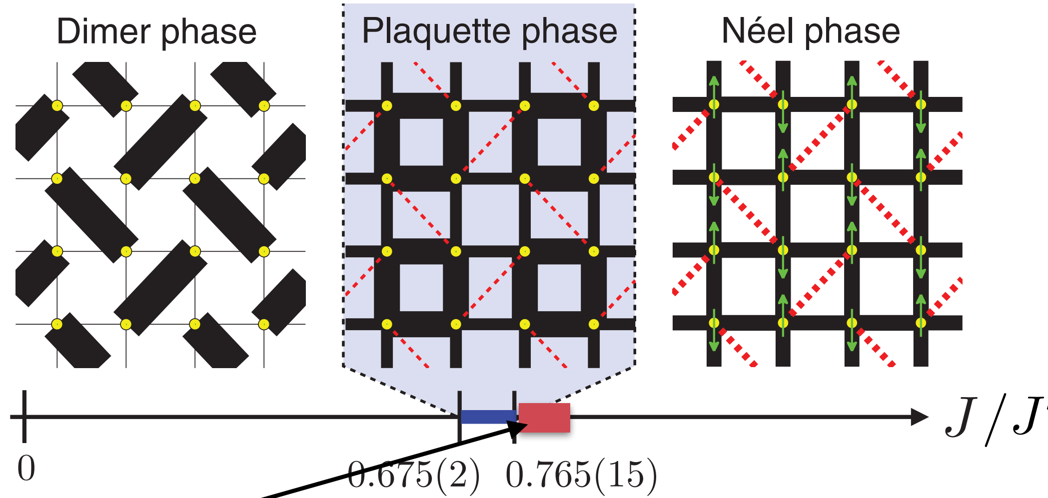
Deformed J-Q model with emergent O(4) symmetry

Recall Shastry-Sutherland model



$$H_{SS} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle ij \rangle'} \mathbf{S}_i \cdot \mathbf{S}_j$$

Corbotz & Mila, 2013i



evidence for gapless spin liquid phase

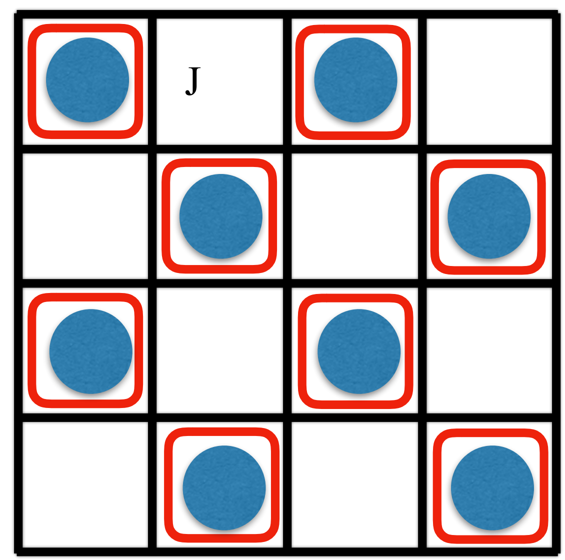
Yang, Wang, Sandvik, PRB 2022
Wang, Zhang, Sandvik, CPL 2022

2D SS model: calculations are challenging

- designer Hamiltonian for PS (Z_2) state?
- also to study PS - AFM transition

2D Checker-board J-Q (CBJQ) model

B. Zhao, P. Weinberg, AWS, Nature Physics 2019



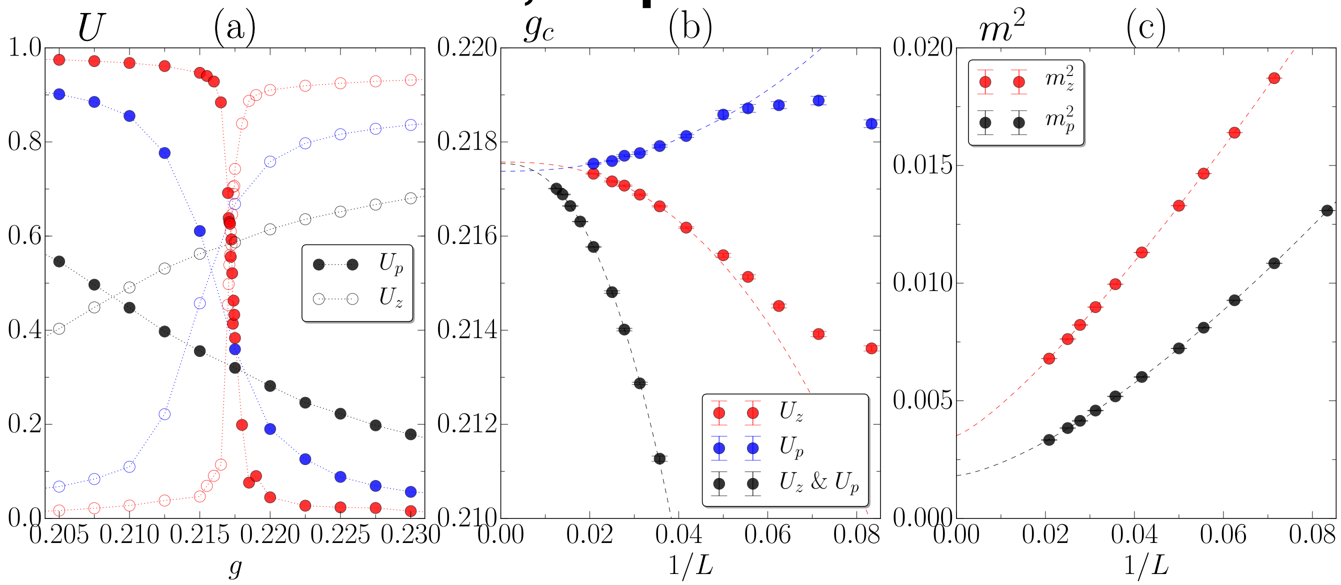
Replace frustrated SS bonds by 4-spin Q terms

$$\mathcal{H} = -J \sum_{\langle ij \rangle} P_{ij} - Q \sum_{ijkl \in \square'} (P_{ij} P_{kl} + P_{ik} P_{jl})$$

Allows 2-fold degenerate PS state - Z_2 symmetry breaking

QMC results vs 1/L, L up to 96

$g = J/Q$



Finite-size scaling

(a) AF-PS transition

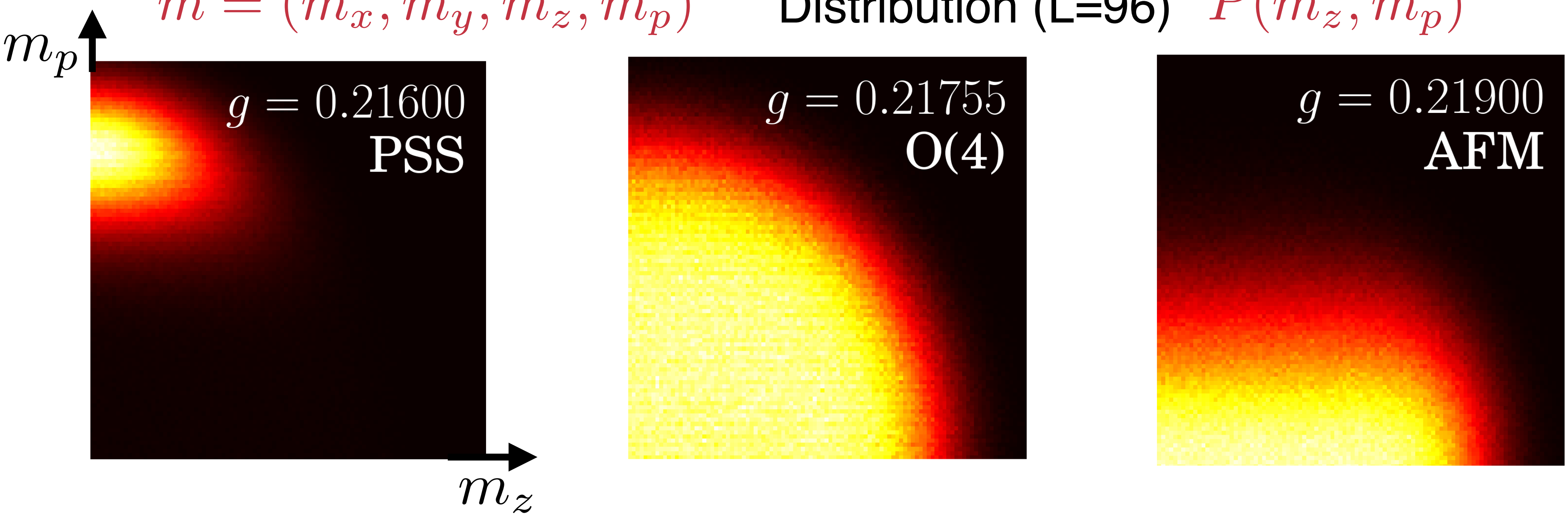
(b) $g_c = 0.2175(1)$

(c) coexisting orders

first-order transition

Emergent O(4) symmetry: Combine AF,PS order parameter

$\vec{m} = (m_x, m_y, m_z, m_p)$ Distribution (L=96) $P(m_z, m_p)$



At transition: order parameter lives on surface of O(4) sphere

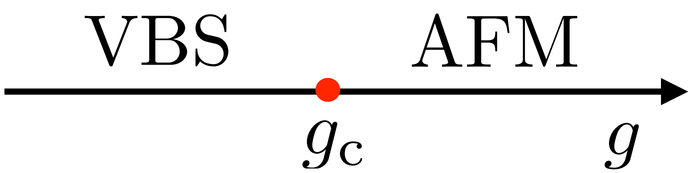
- fluctuating radius due to finite size

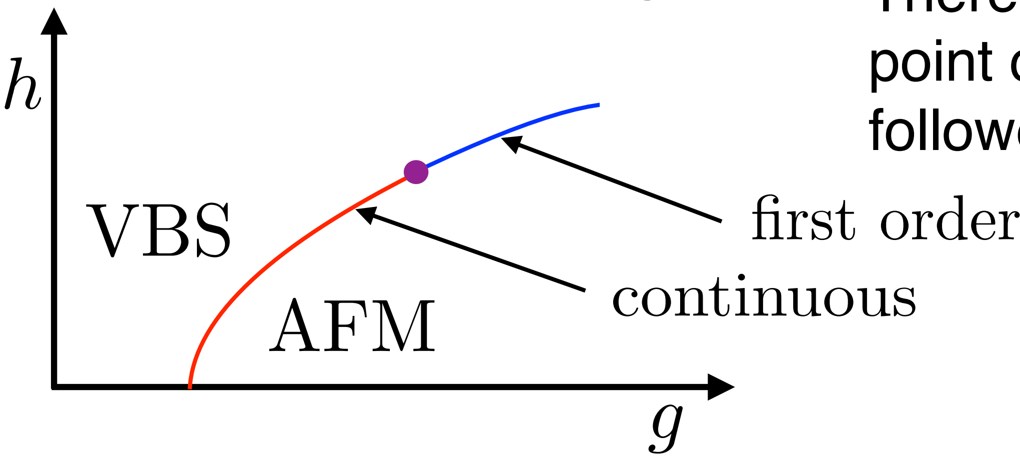
Emergent SO(5) in a different model: J. Takahashi & AWS, PRR 2020

Unified phase diagram for quantum magnets with DQCPs

Original DQCP scenario:
generic transition vs one parameter

B. Zhao, J. Takahashi, Sandvik (PRL 2020)
J. Yang, Sandvik, L. Wang (PRB 2022)





Does not exclude 1st-order transitions

There can be a multi-critical end point of the generic critical line, followed by 1st-order line

The continuous transitions may even be unreachable
- non-unitary CFT
  (Senthil et al. PRX 2017,…)
- but we can at least get close enough to observe critical scaling

Alternative scenario

The DQCP is a fine-tuned multi-critical point

- separating first-order line and a gapless spin-liquid
- g, h are relevant fields at the DQCP, tuned by two parameters in a lattice model