Algorithms in Lattice Gauge Theory and Spin Systems
IACS, Kolkata, Jan 27 - Feb 1, 2020

III. Applications

Anders W Sandvik

Finite-size scaling at critical points
- general method illustrated by 2D Ising model

Examples
- scaling corrections in dimerized Heisenberg models
- quantum phase transition in $TlCuCl_3$ (3d dimerized Heisenberg)
- deconfined quantum criticality (J-Q models)
- emergent symmetries
- detecting deconfined spinons in spectral functions
- plaquett-solid state in $SrCu_2(BO_3)_2$; unusual first-order transition
- random-singlet state in the presence of disorder

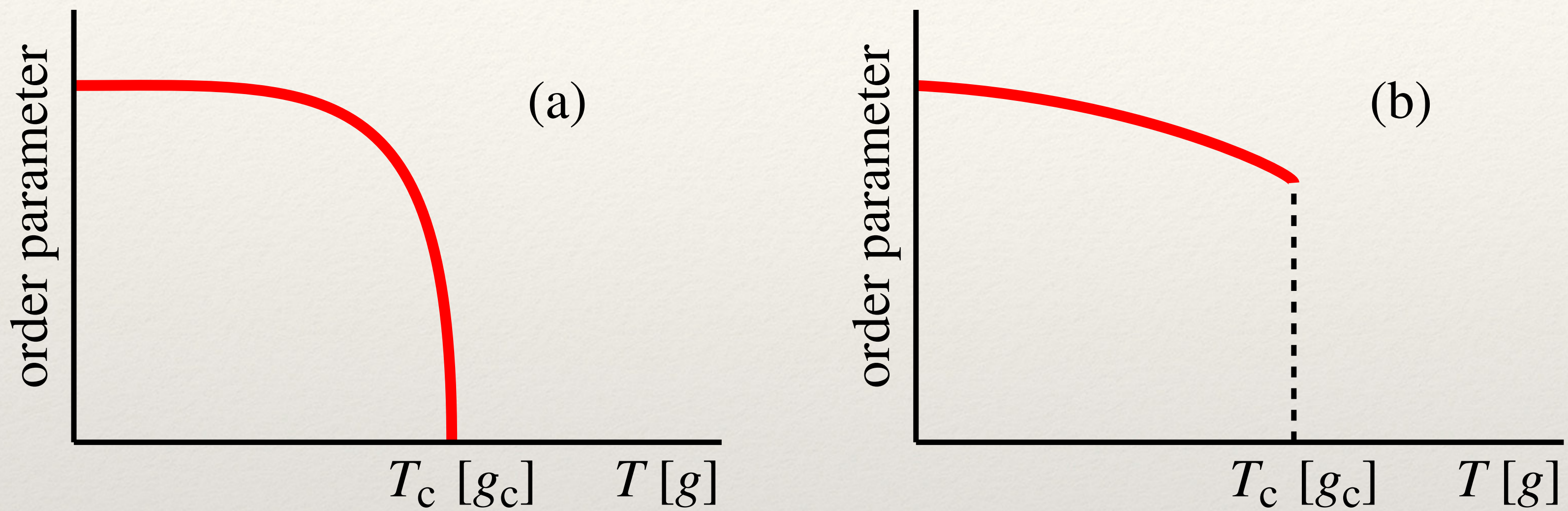
Classical and quantum phase transitions

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 $\xi \sim |T-T_c|^{-\nu}$

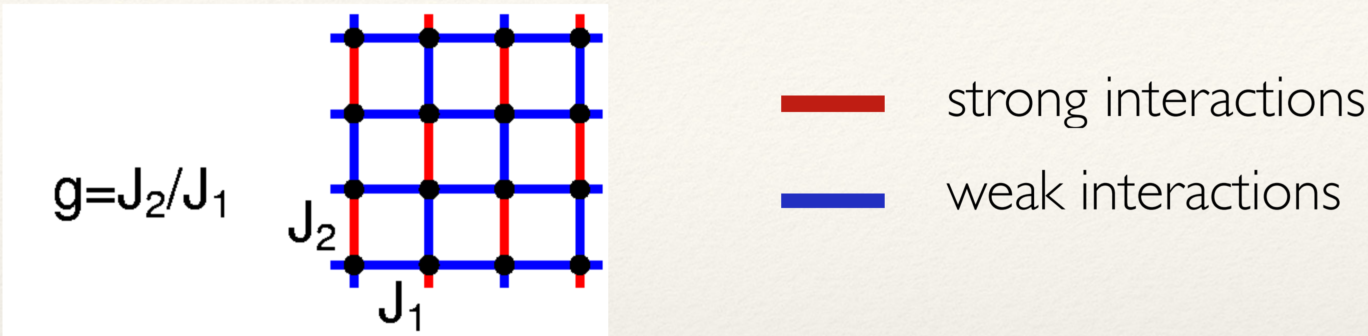
There are many similarities between classical and quantum transitions
- and also important differences

The quantum phases (ground states) can also be highly non-trivial
- even with rather simple lattice models

Example: Néel-paramagnetic quantum phase transition

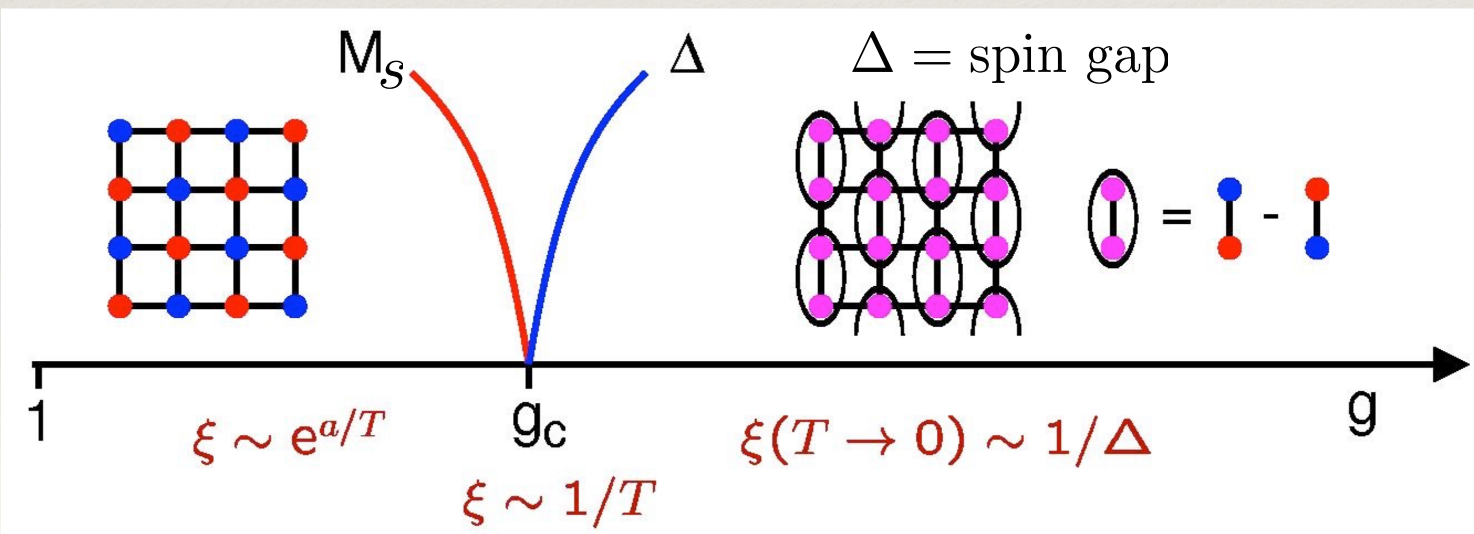
Dimerized S=1/2 Heisenberg models

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



Singlet formation on strong bonds ➙ Néel - quantum-paramagnetic transition

Ground state (T=0) phases

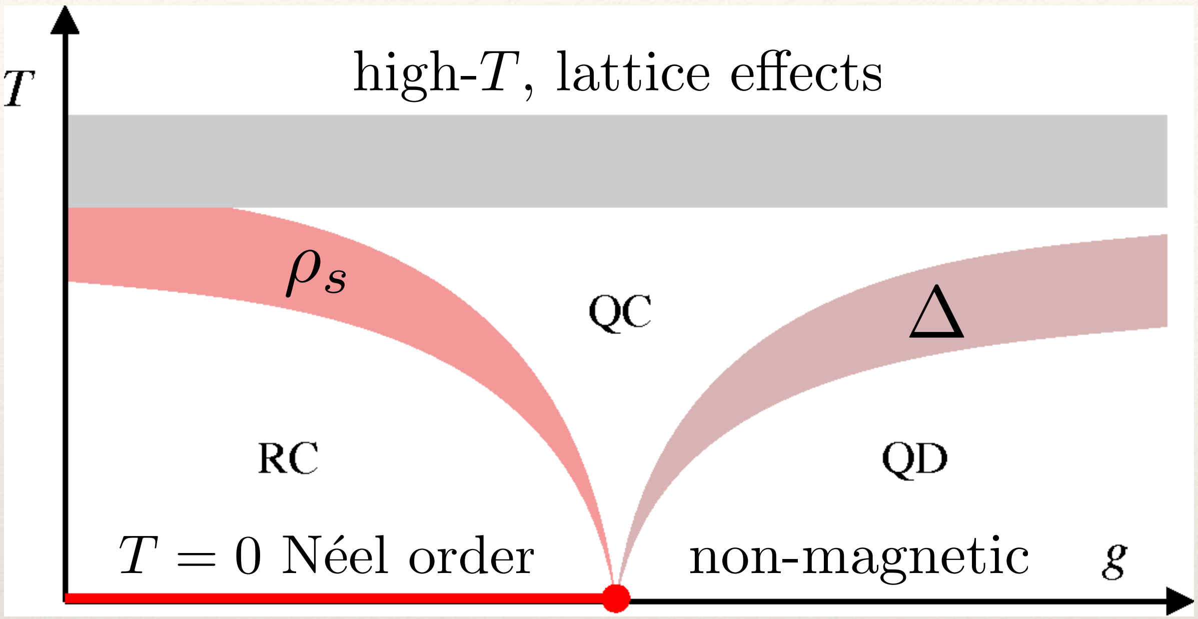


⇒ 3D classical Heisenberg (O3) universality class; QMC confirmed

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

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)

Quantum phase transition (T=0) can be unusual - 'beyond Landau'

QMC used to test existing theories, discover new physics,…

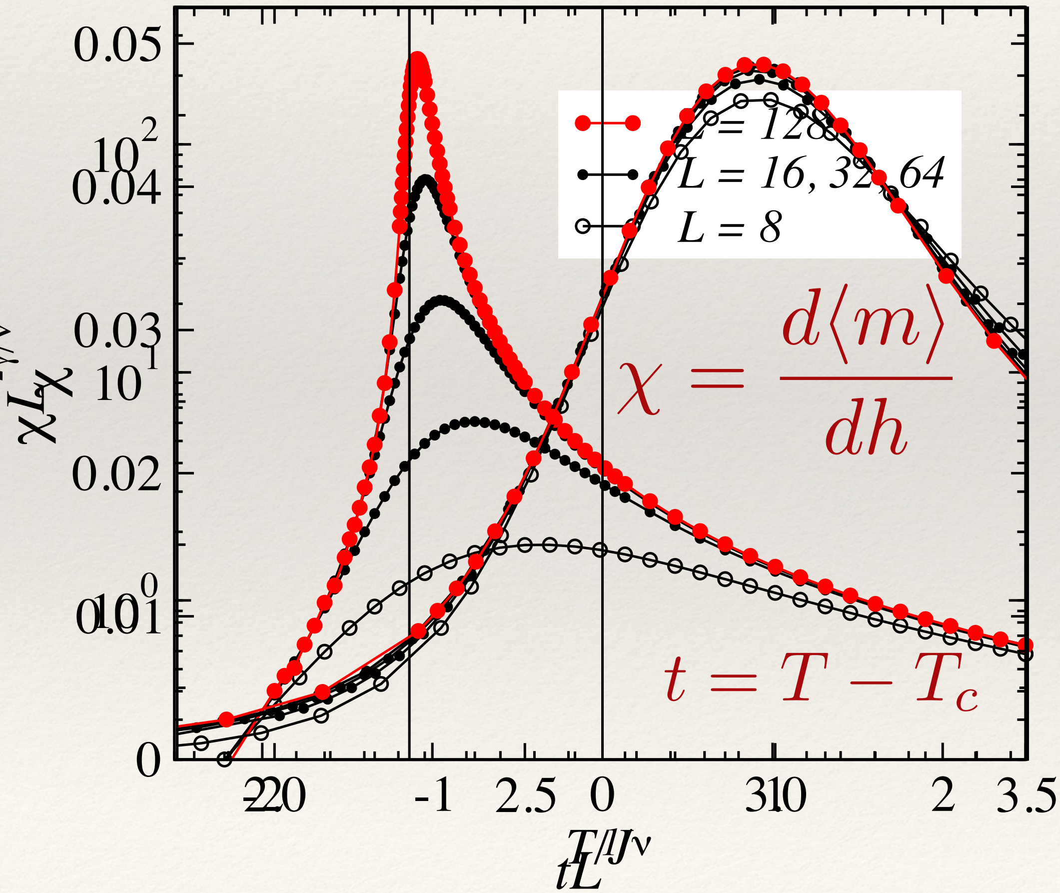
Phase transitions - Finite-size scaling

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 **ξ→L**: $A(T \approx T_c, L) \propto L^{-\kappa/\nu}$

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



2D Ising universality class

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

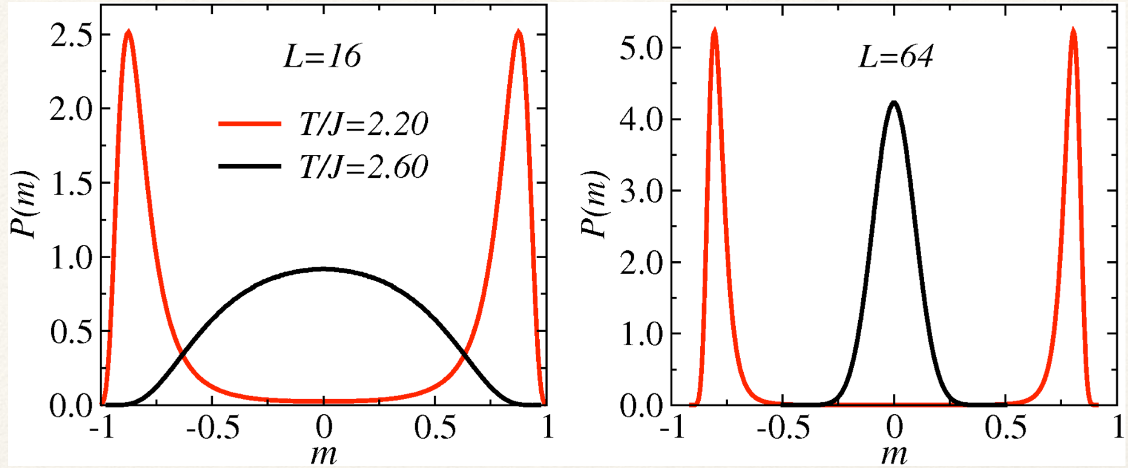
Critical T known

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

When these are not known, treat as fitting parameters - or extract in other way

Binder ratios and cumulants

order parameter distribution



Consider the dimensionless ratio

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

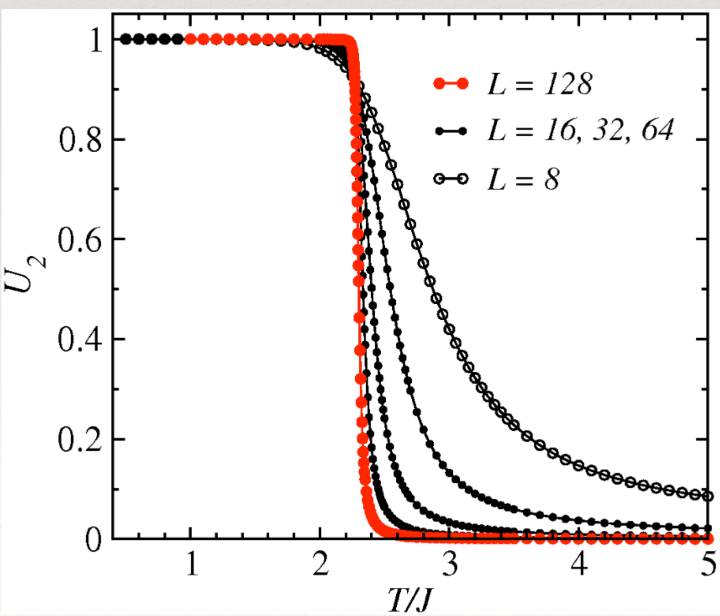
We know R_2 exactly for $N \to \infty$

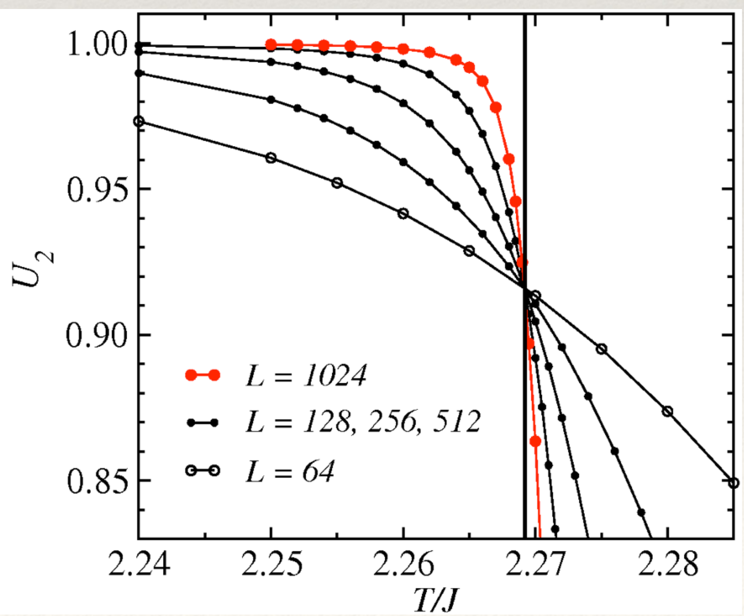
- **for $T<T_c$:** $P(m) \to \delta(m-m^*)+\delta(m+m^*)$
  m^*=|peak m-value|. **$R_2 \to 1$**
- **for $T>T_c$:** $P(m) \to \exp[-m^2/a(N)]$
  $a(N) \sim N^{-1}$ **$R_2 \to 3$** (Gaussian integrals)

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

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

2D Ising model; MC results



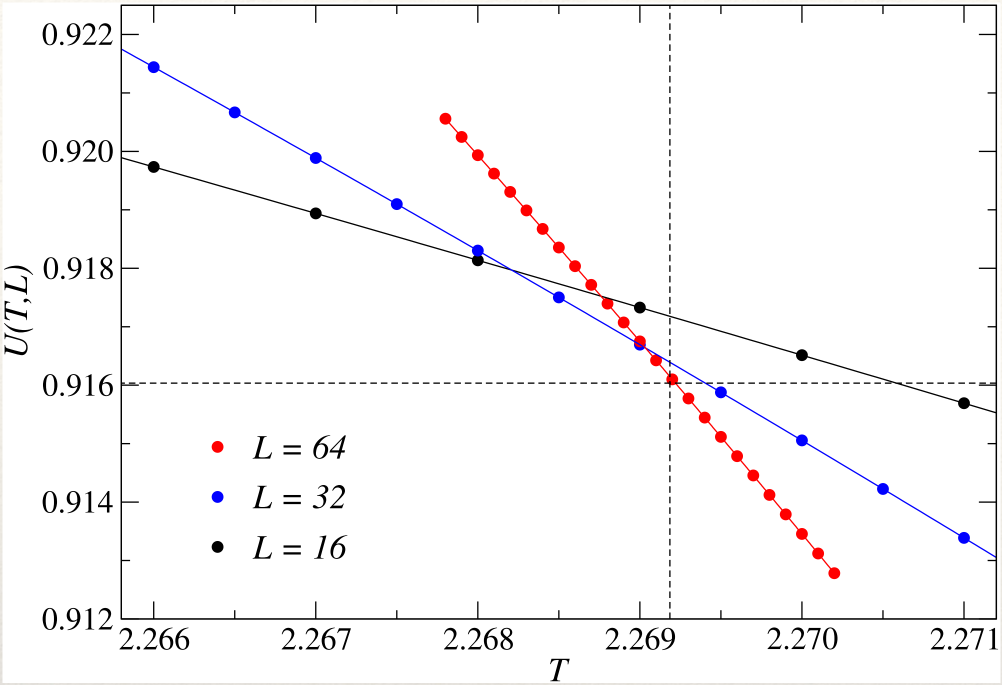


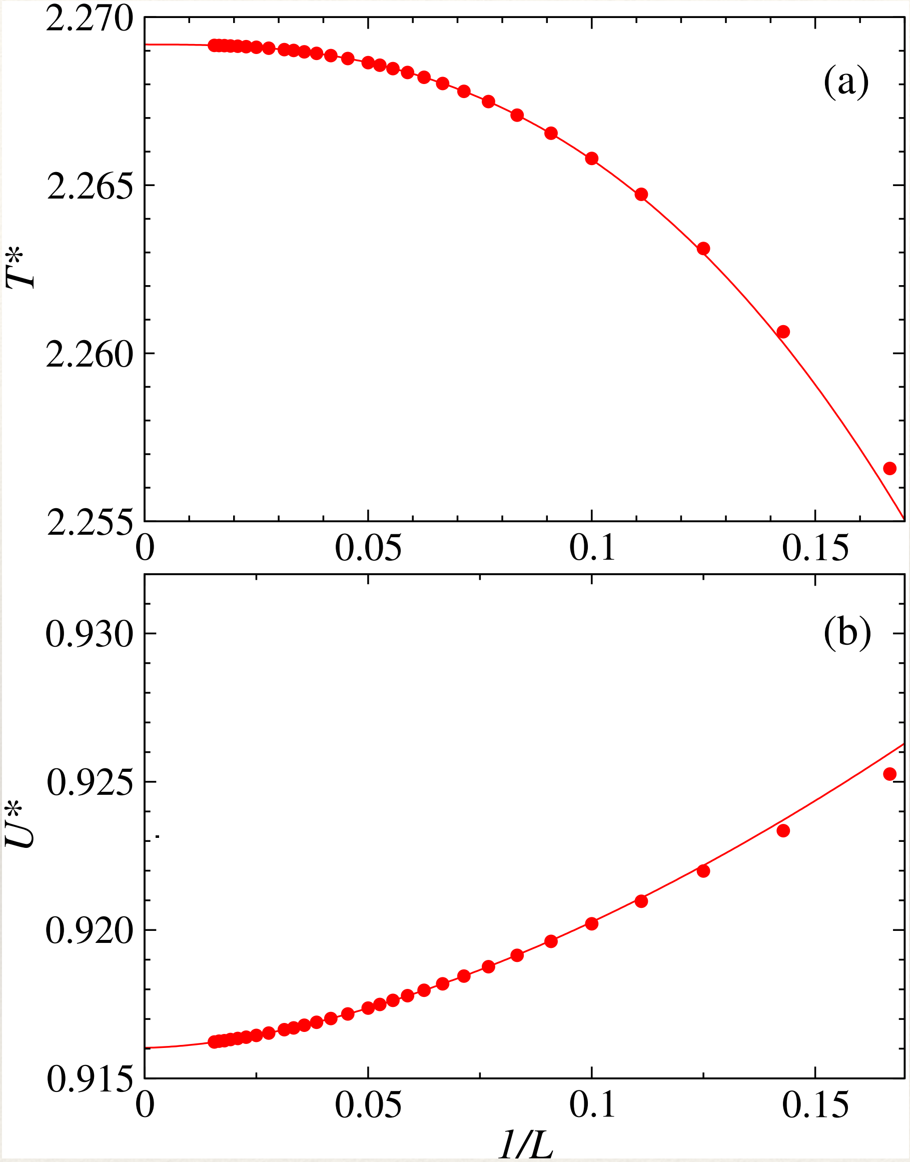
Curves for different L asymptotically cross each other at T_c

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

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

⇒ scaling corrections in crossings

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

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

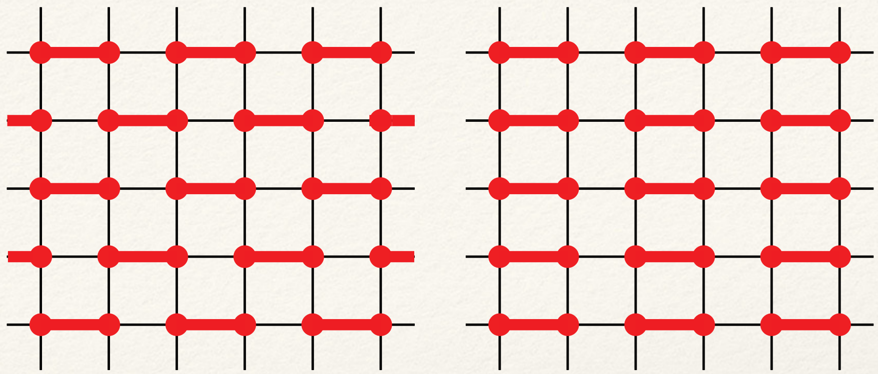
Use correction with free exponent

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

Case with more significant corrections

- common at quantum critical points

S=1/2 Heisenberg model with
- columnar dimers (CDM)
- staggered dimers (SDM)



The SDM has been controversial
- O(3) or new universality class
- strange scaling behaviors

PHYSICAL REVIEW LETTERS **121**, 117202 (2018)

Anomalous Quantum-Critical Scaling Corrections in Two-Dimensional Antiferromagnets

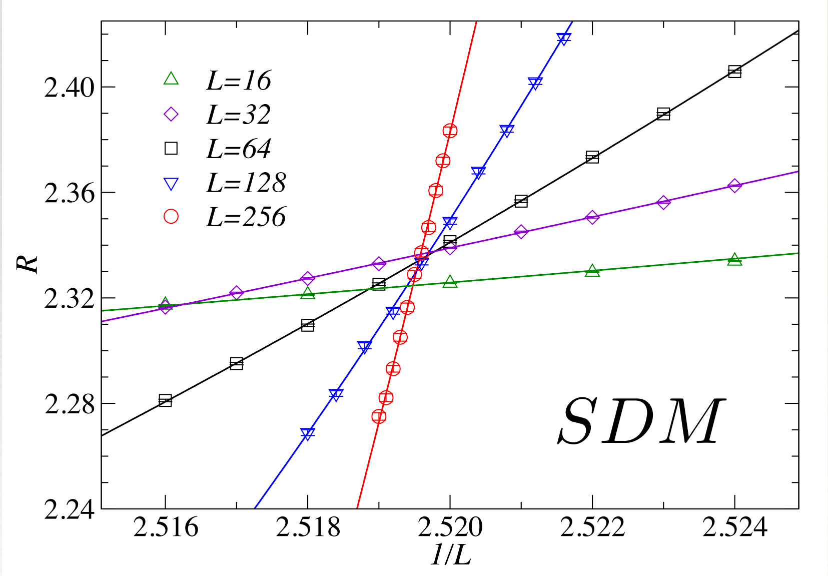
Nvsen Ma,[1,2,3] Phillip Weinberg,[3] Hui Shao,[4,3] Wenan Guo,[5,4] Dao-Xin Yao,[1,*] and Anders W. Sandvik[3,2,†]

Analyze critical behavior with two scaling corrections taken into account

$$O(g,L) = f[(g-g_c)L^{1/\nu}, \lambda_1 L^{-\omega_1}, \lambda_2 L^{-\omega_2}, \cdots]$$

Taylor expand, analyze crossing points for different dimensionless quantities

Compare CDM and SDM behaviors

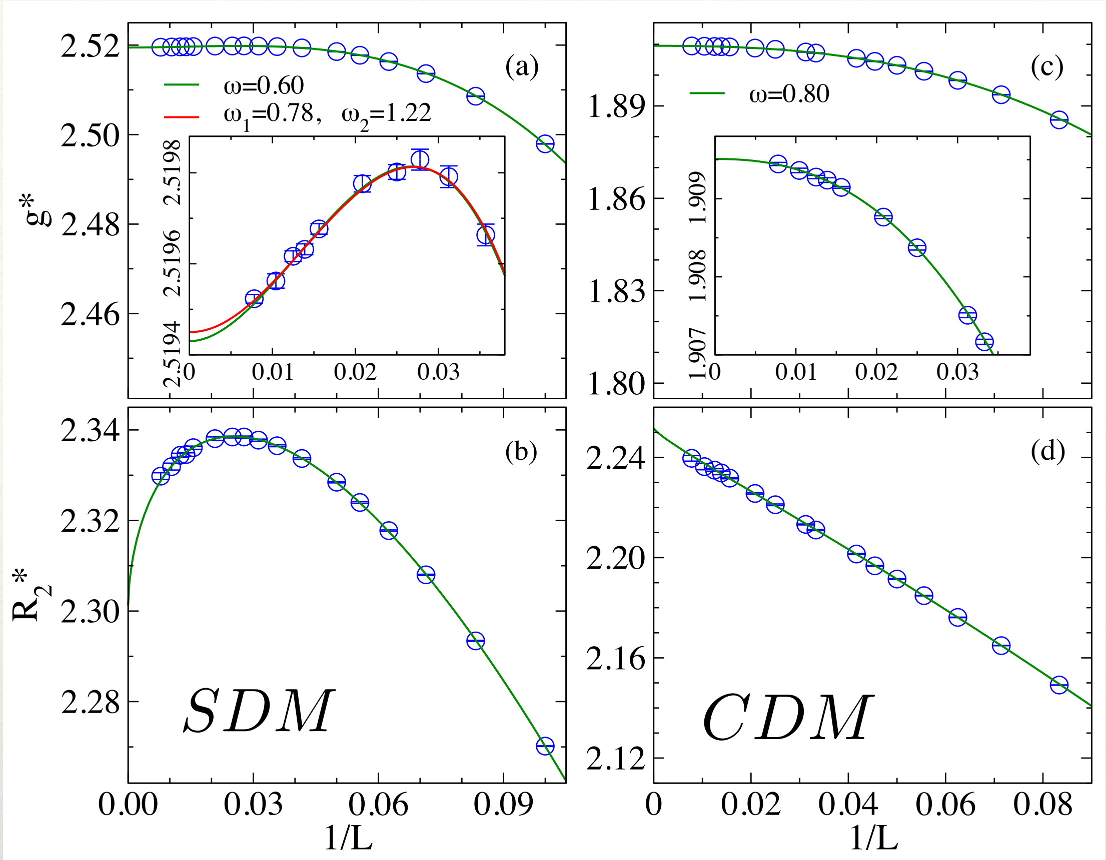


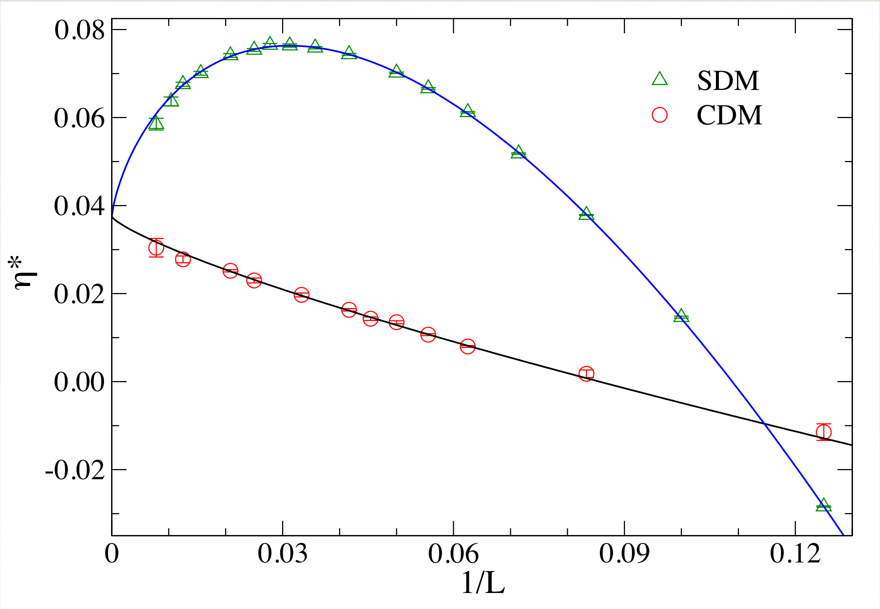
Leading-order cross-point shifts

$$g^*(L) = g_c + aL^{-\omega_1 - 1/\nu},$$

$$O^*(L) = O_c + bL^{-\omega_1},$$

- Works for CDM, $\omega_1 \approx 0.78$
- Two corrections needed for SDM
  $\omega_1 \approx 0.78$, $\omega_2 \approx 1.25$
- Fits within theory where the SDM field theory needs a new term (Fritz et al, PRB 2012)





Order parameter at the critical point

$$\langle m^2 \rangle_c \propto L^{-(1+\eta)}(1 + b_1 L^{-\omega_1} + b_2 L^{-\omega_2} + \ldots)$$

$$\eta^*(L) = \ln[\langle m^2(L)\rangle_c / \langle m^2(2L)\rangle_c] / \ln(2) - 1$$

$$\eta^*(L) = \eta + c_1 L^{-\omega_1} + c_2 L^{-\omega_2} + \ldots.$$

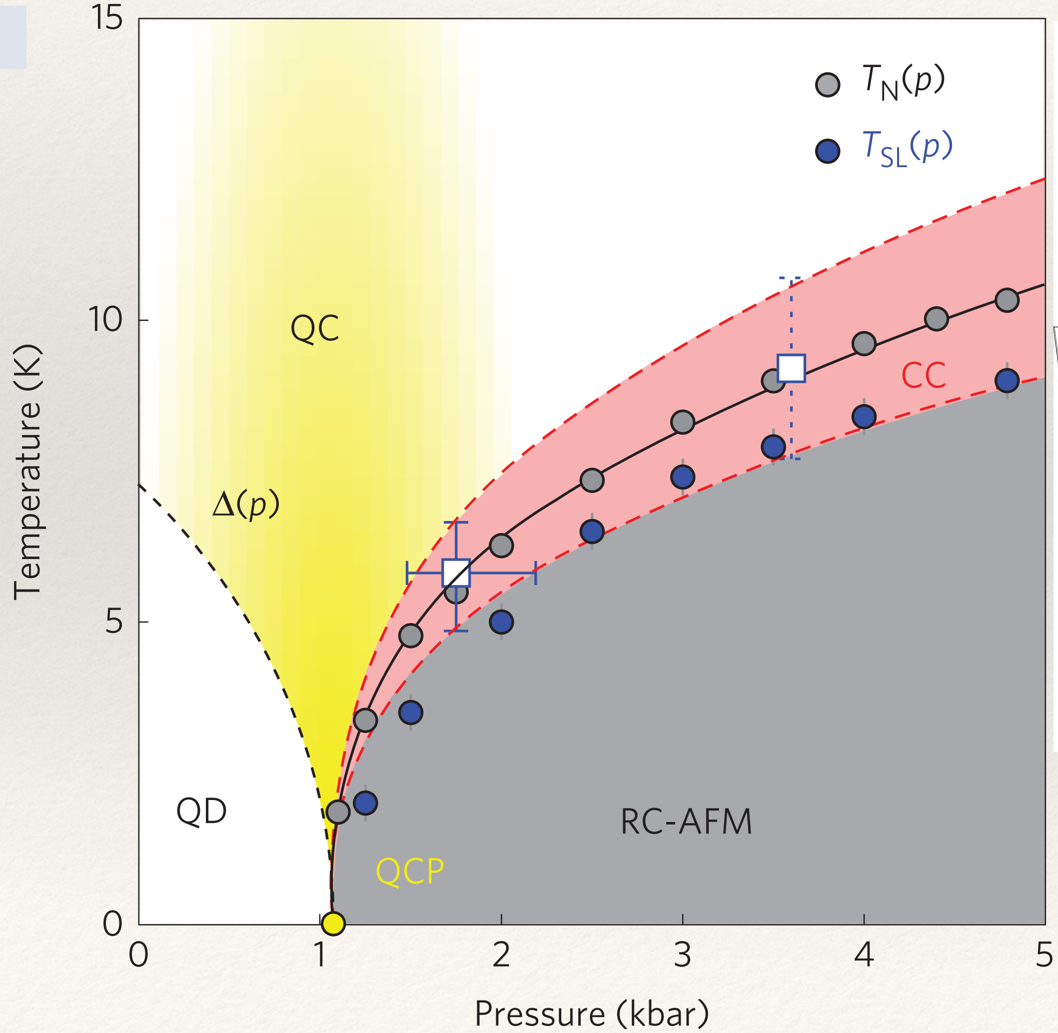
nature physics
ARTICLES
PUBLISHED ONLINE: 6 APRIL 2014 | DOI: 10.1038/NPHYS2902

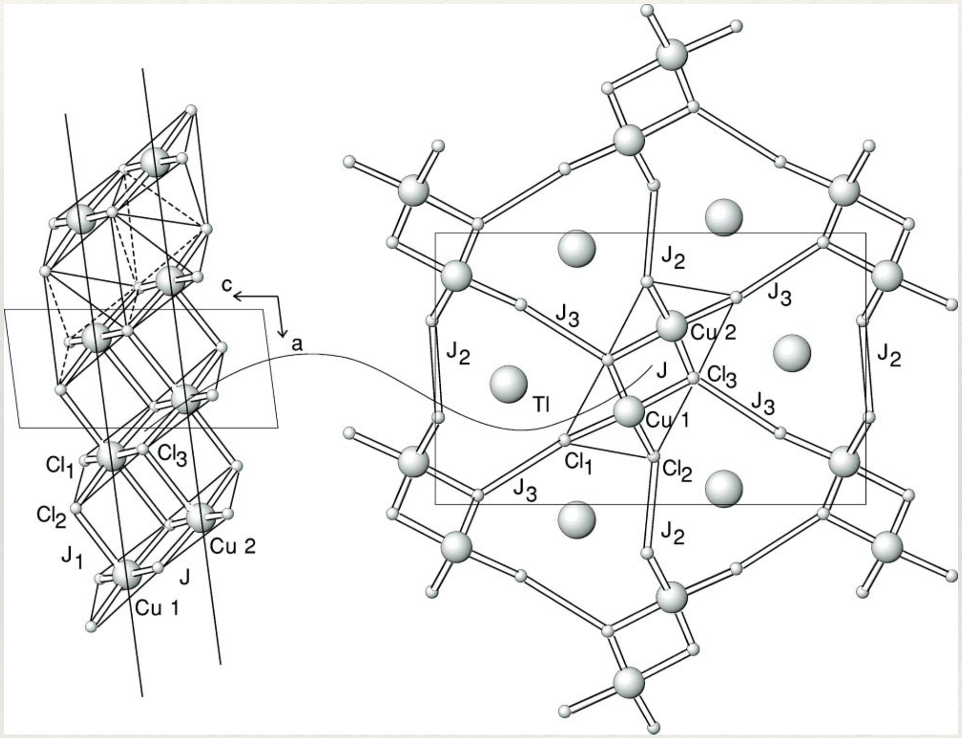
$TlCuCl_3$

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



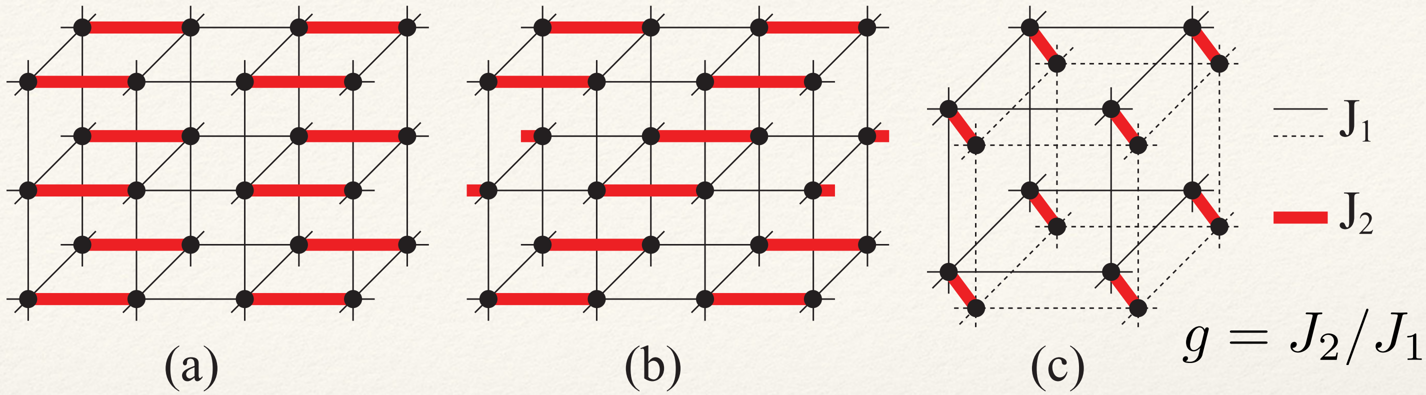


From: M Matsumoto, B Normand, TM Rice, M Sigrist, PRB (2004)

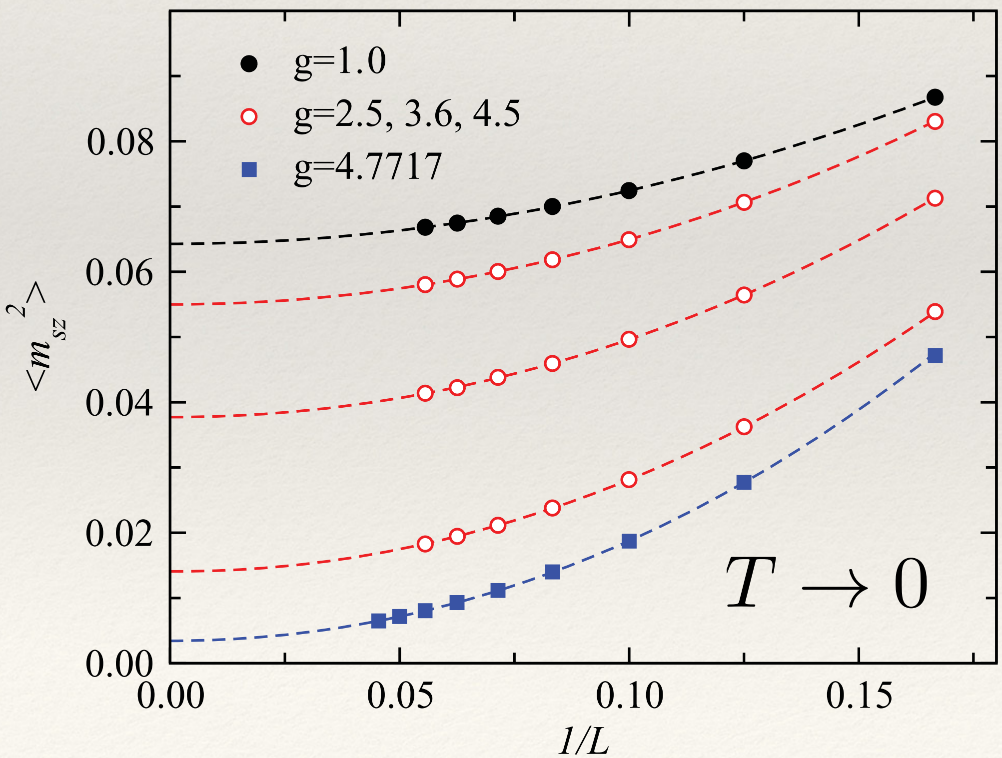
Universality of the Neel temperature in 3D dimerized systems?

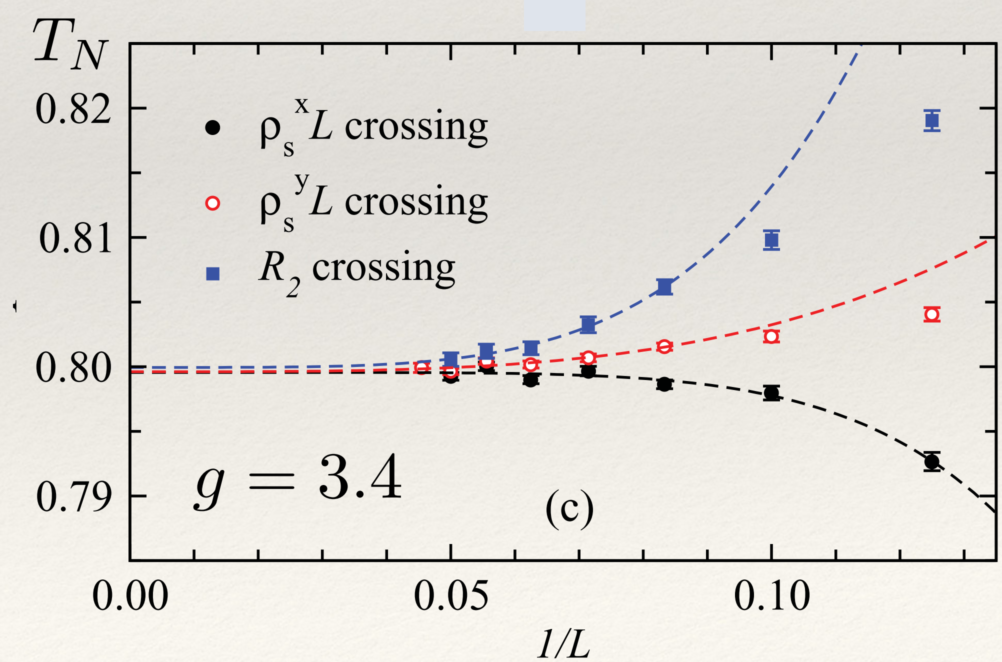
[S. Jin, AWS, PRB2012]

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



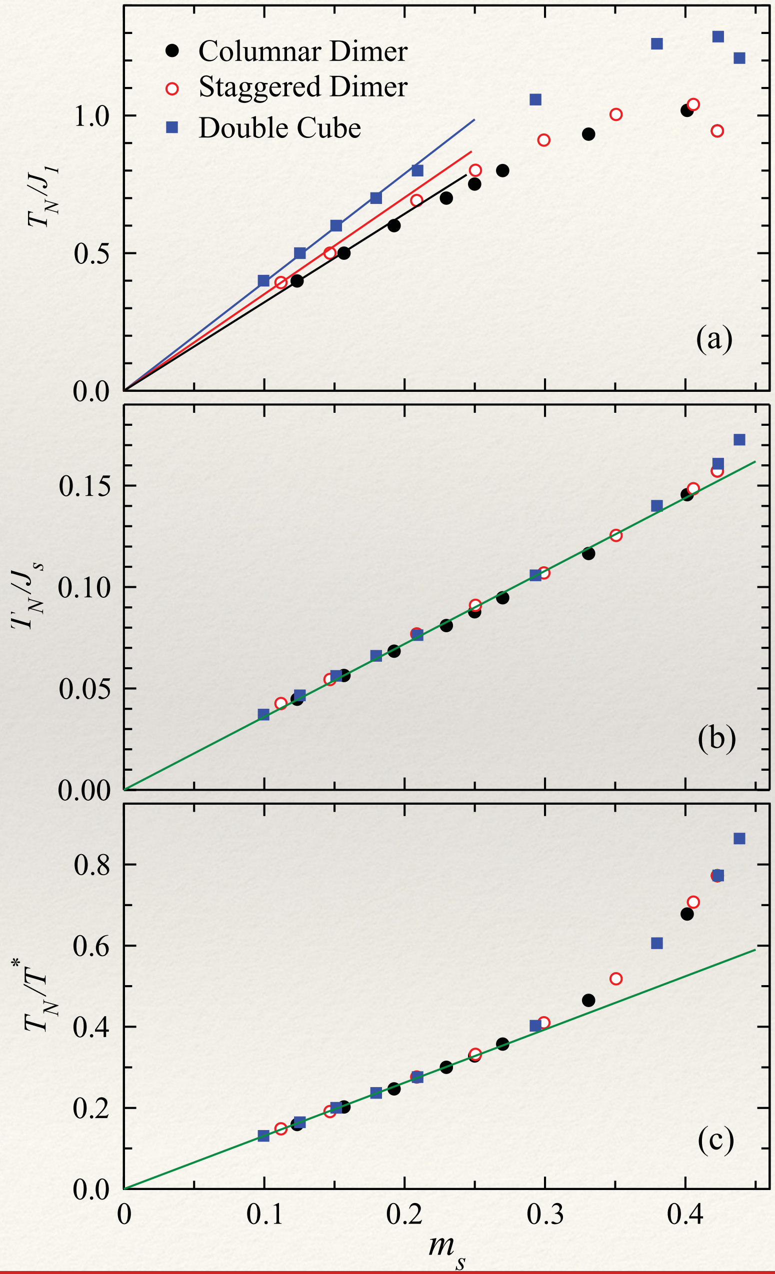
Example: Columnar dimers





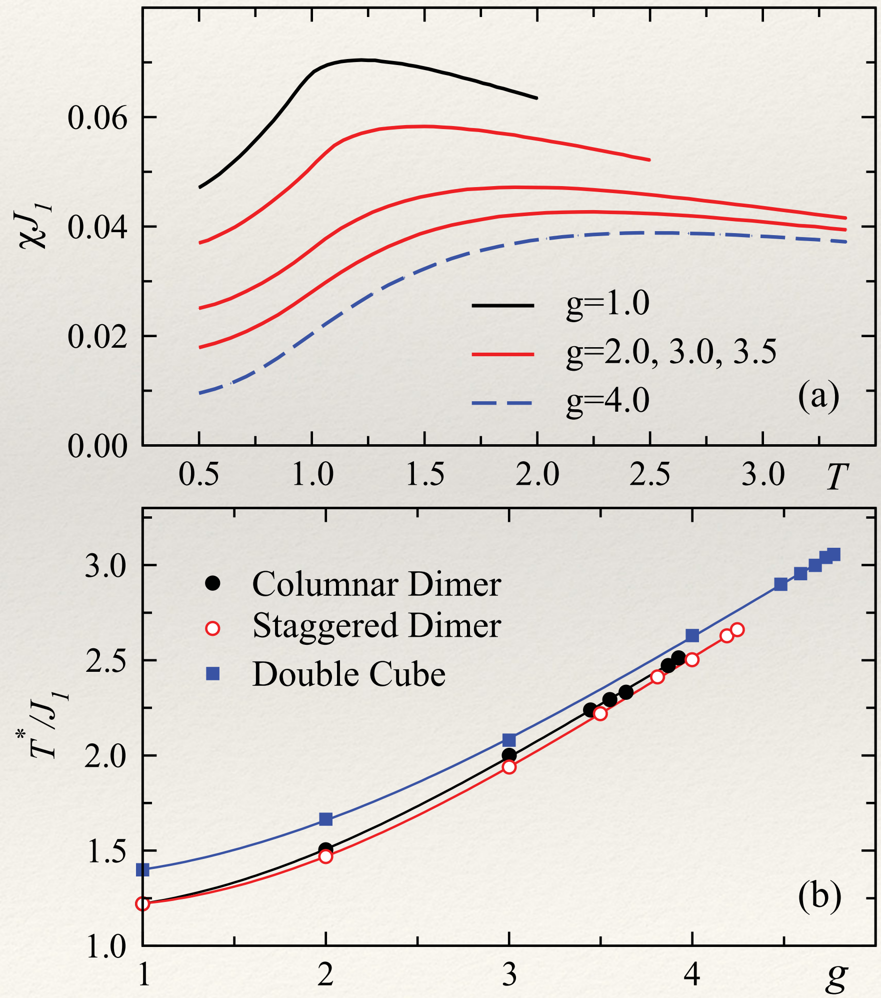
Couplings vs pressure not known experimentally

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



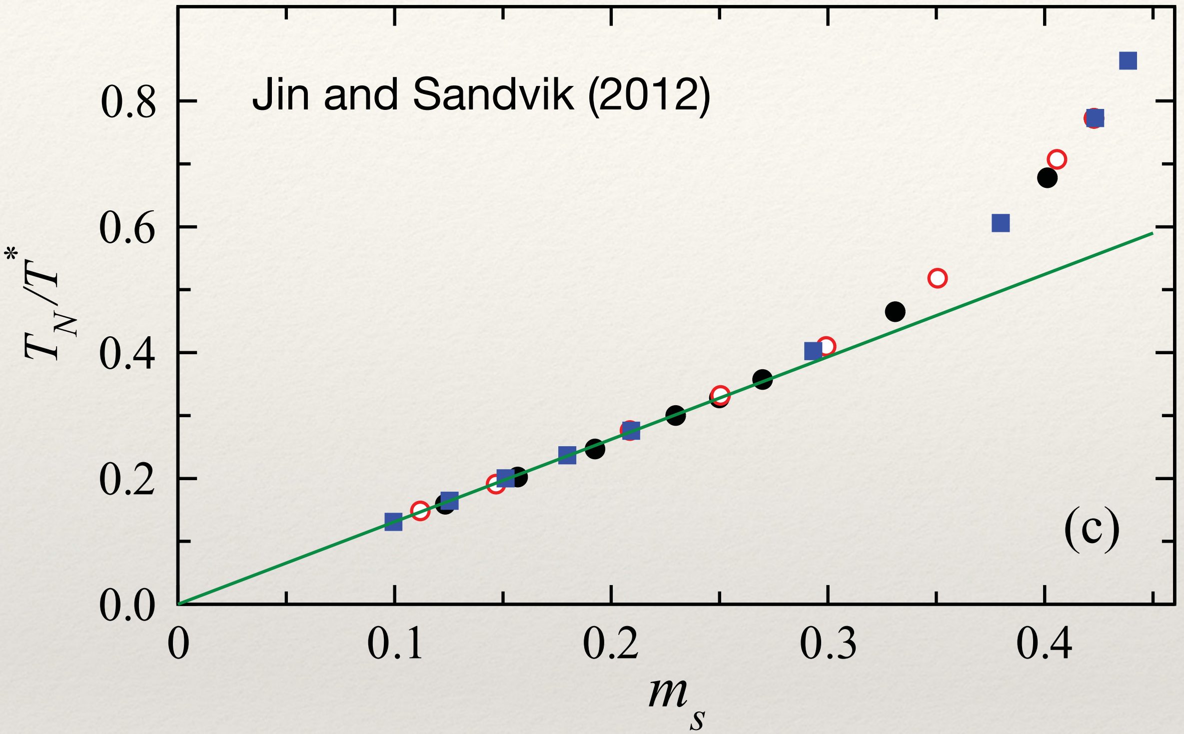
Three normalizations

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

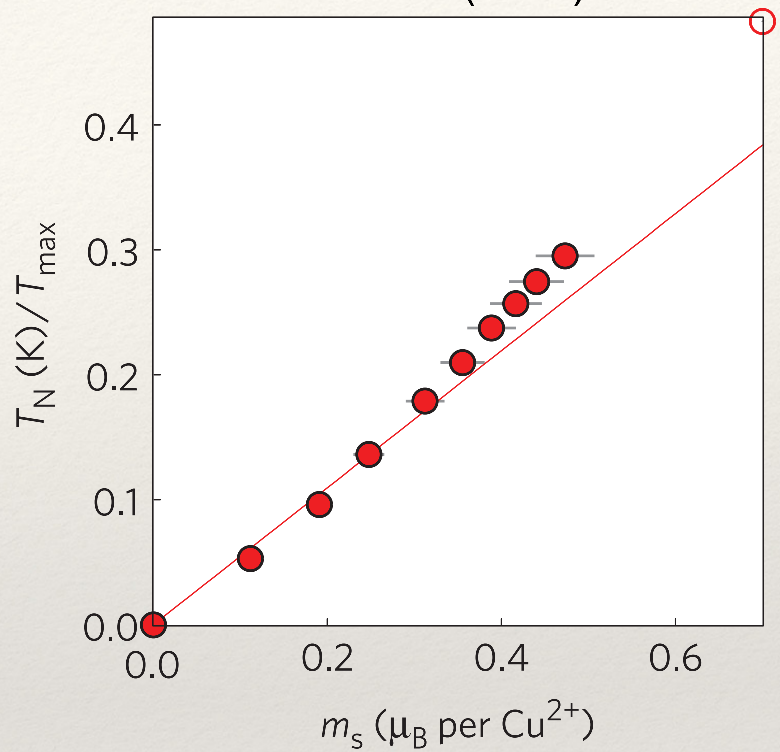


T* normalization is accessible experimentally

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



Merchant et al (2014)



Same features observed in models and experiment

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

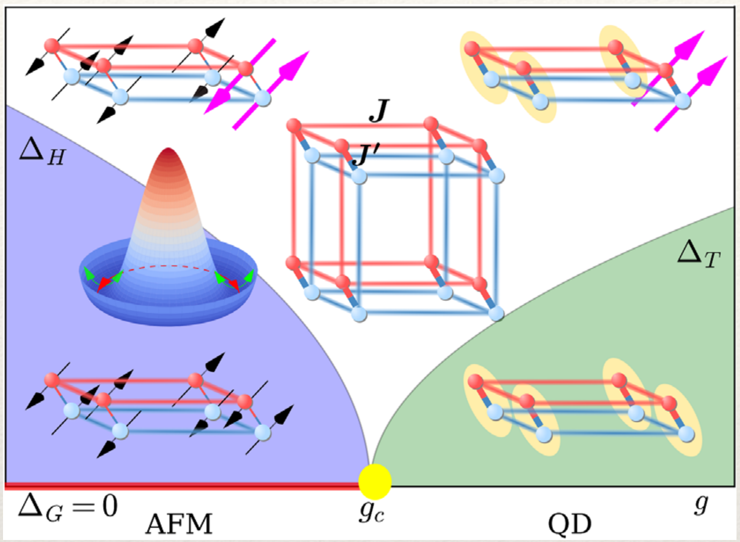
More recent works to study log corrections, dynamics,….

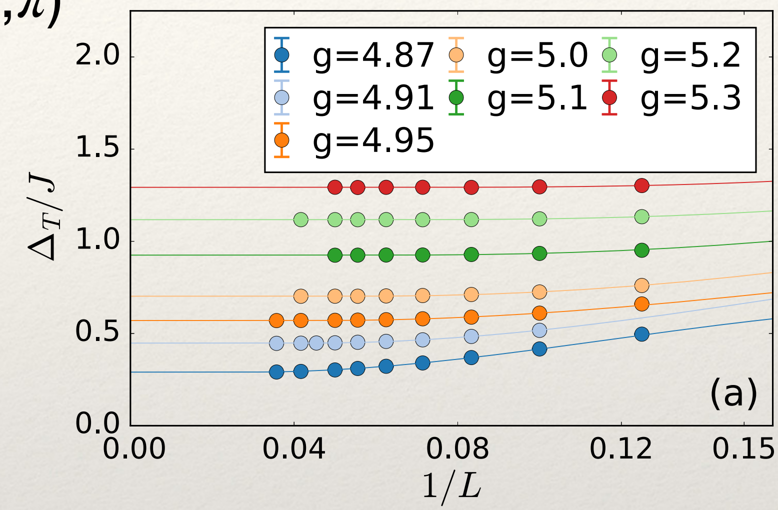
Qin, Normand, Sandvik, Meng, PRB 2015, PRL 2017

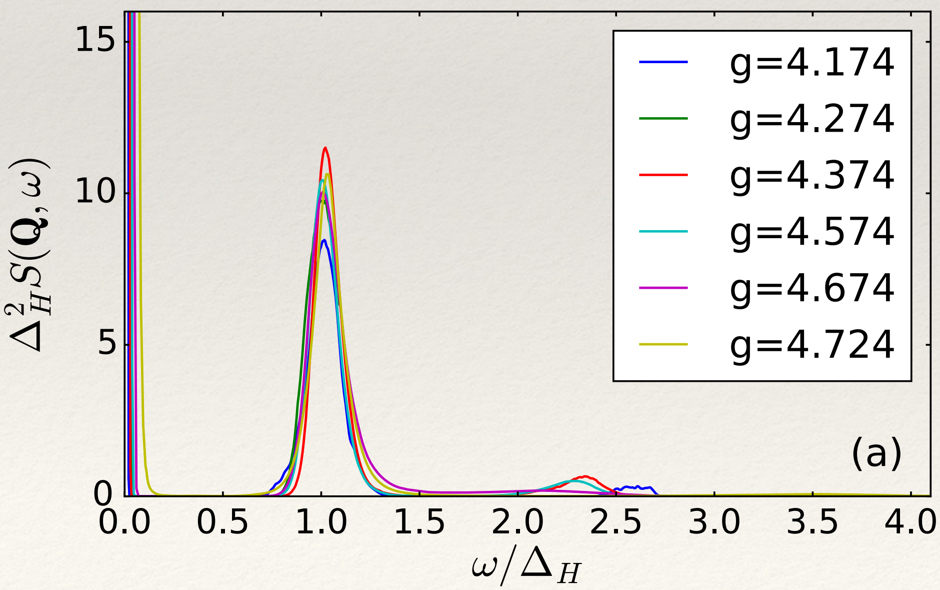
Amplitude Mode in Three-Dimensional Dimerized Antiferromagnets

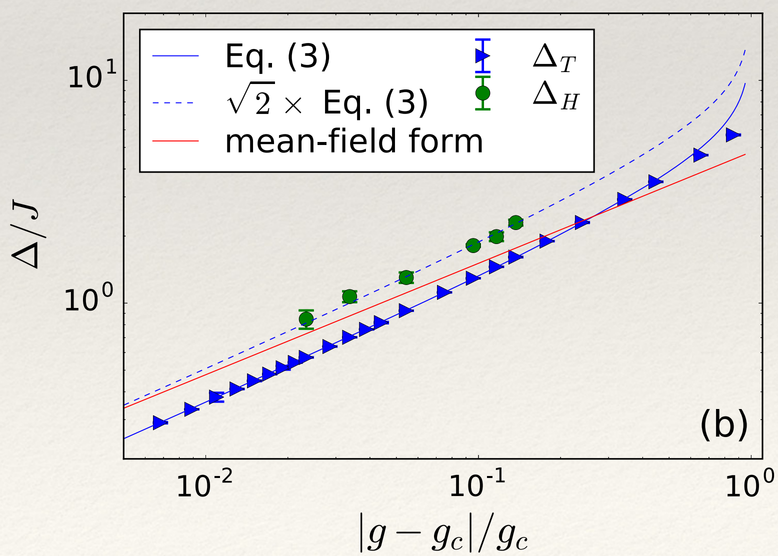
Yan Qi Qin,[1] B. Normand,[2] Anders W. Sandvik,[3] and Zi Yang Meng[1]

SSE and SAC used to study scaling of the "Higgs" mode in the "double cube" Q=(π,π,π,π)







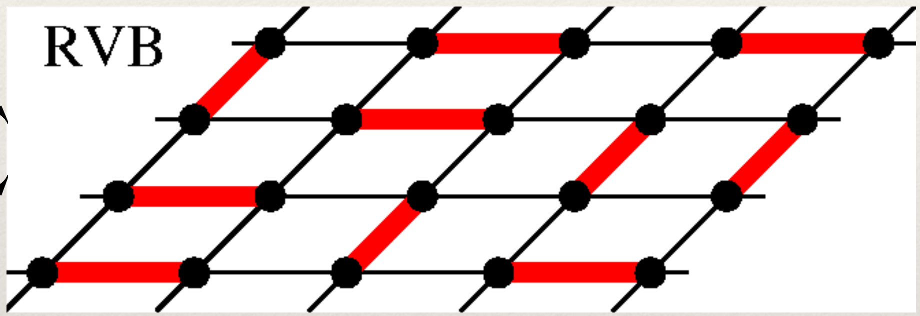


More complex non-magnetic states; systems with 1 spin per unit cell

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

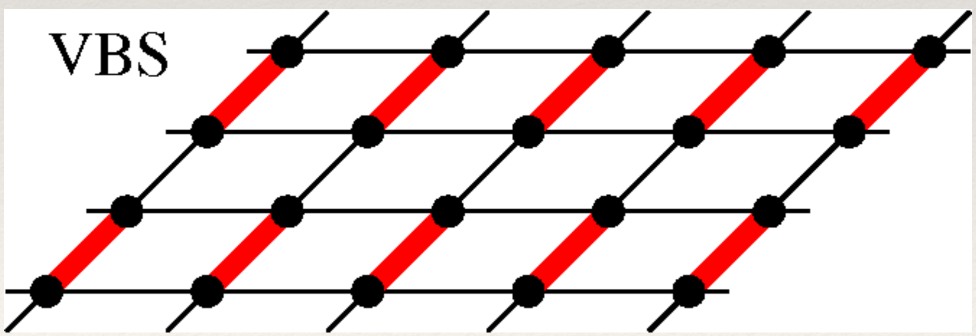
- **highly non-trivial non-magnetic ground states are possible, e.g.,**
  - ➡ resonating valence-bond (RVB) spin liquid
  - ➡ valence-bond solid (VBS)

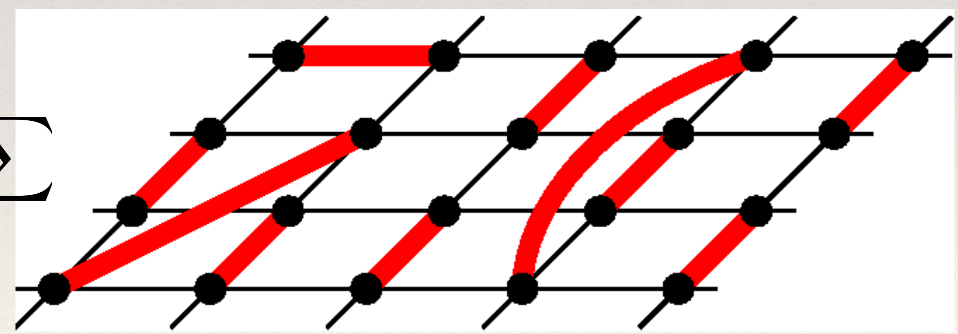
Non-magnetic states often have natural descriptions with **valence bonds**

$\sum$ 

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

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



$\sum$ 

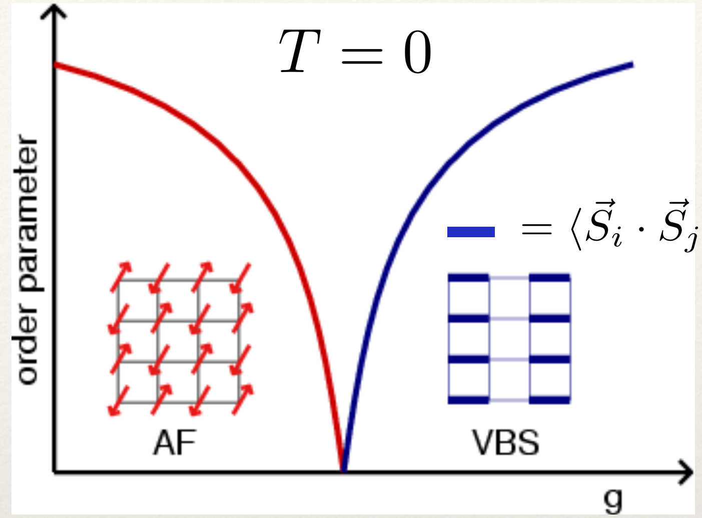
- non-magnetic states dominated by short bonds

Deconfined quantum criticality

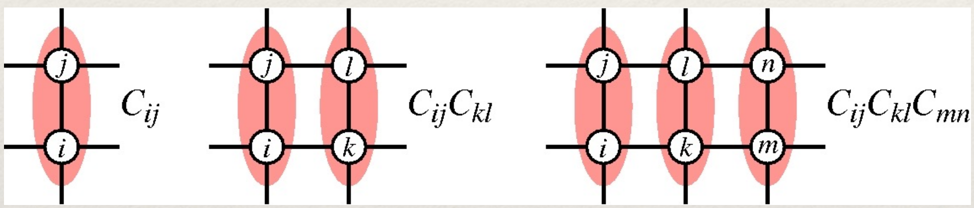
Senthil, Vishwanath, Balents, Sachdev, Fisher (Science 2004)
(+ many previous works; Read & Sachdev, Sachdev & Murthy, Motrunich & Vishwanath….)

Continuous AF - VBS transition at T=0

- would be violation of Landau rule
- first-order would normally be expected
- role of topological defects



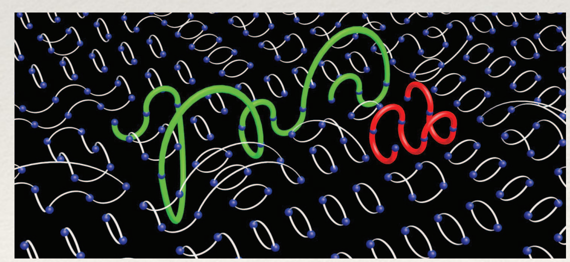
Numerical (QMC) tests using J-Q models



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

The "J-Q" model with two projectors is (Sandvik, PRL 2007)

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



- **Has Néel-VBS transition, appears to be continuous**
- **Not a realistic microscopic model for materials**
- **"Designer Hamiltonian" for VBS physics and AF-VBS transition**

- **Unusual scaling properties** [Shao, Guo, Sandvik (Science 2016)]

Phase transition in the J-Q model

Staggered magnetization

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

Dimer order parameter (D_x,D_y)

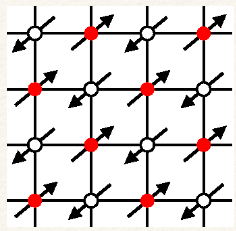
$$D_x = \frac{1}{N}\sum_{i=1}^{N}(-1)^{x_i}\mathbf{S}_i\cdot\mathbf{S}_{i+\hat{x}}$$

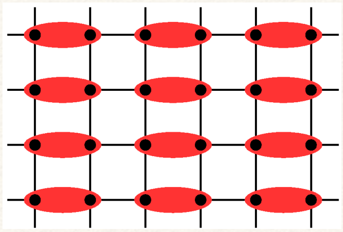
$$D_y = \frac{1}{N}\sum_{i=1}^{N}(-1)^{y_i}\mathbf{S}_i\cdot\mathbf{S}_{i+\hat{y}}$$

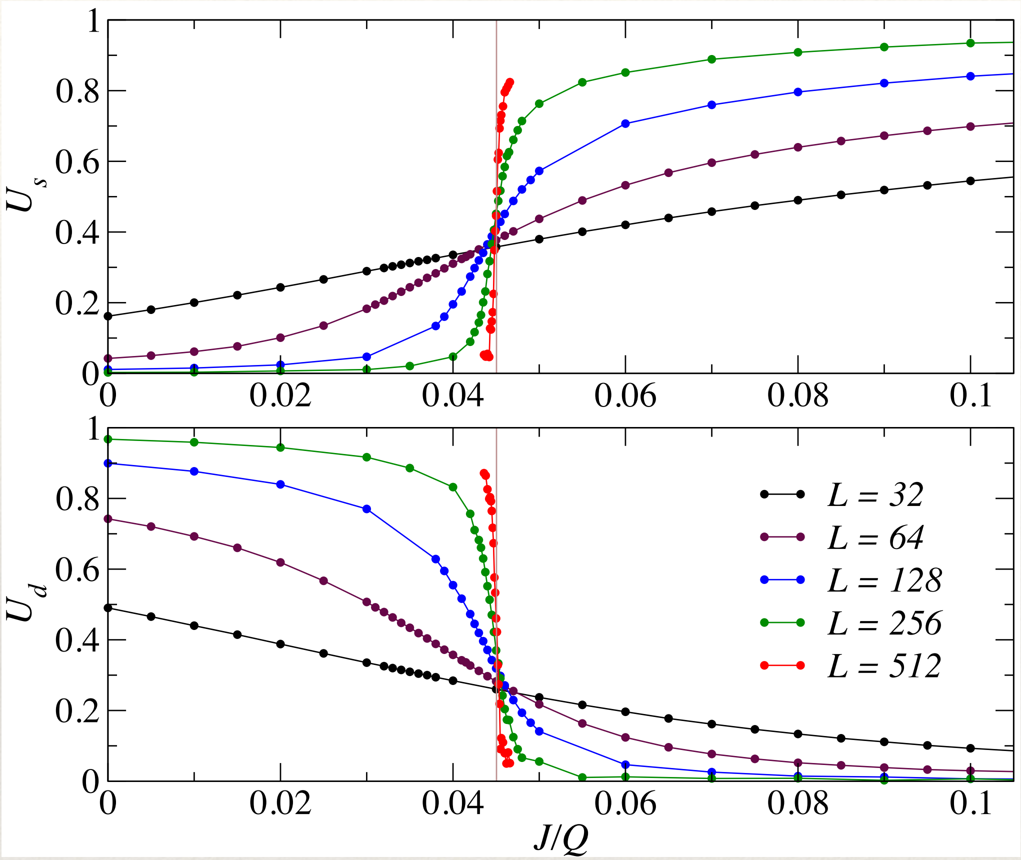
Binder cumulants:

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

$$U_d = 2\left(1 - \frac{1}{2}\frac{\langle D^4\rangle}{\langle D^2\rangle^2}\right)$$







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

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

Behaviors of crossing points → exponents

Phenomenological two-length scaling

[Shao, Guo, Sandvik (Science 2016)]

Competing scenario:

- weak first-order transition
- non-unitary conformal field theory

Exponent ν: crossing-point analysis

H. Shao, W. Guo, A. W. Sandvik (Science 2016)

Binder ratio of the AF order parameter

$$R_1 = \frac{\langle m_{sz}^2 \rangle}{\langle |m_{sz}| \rangle^2}$$

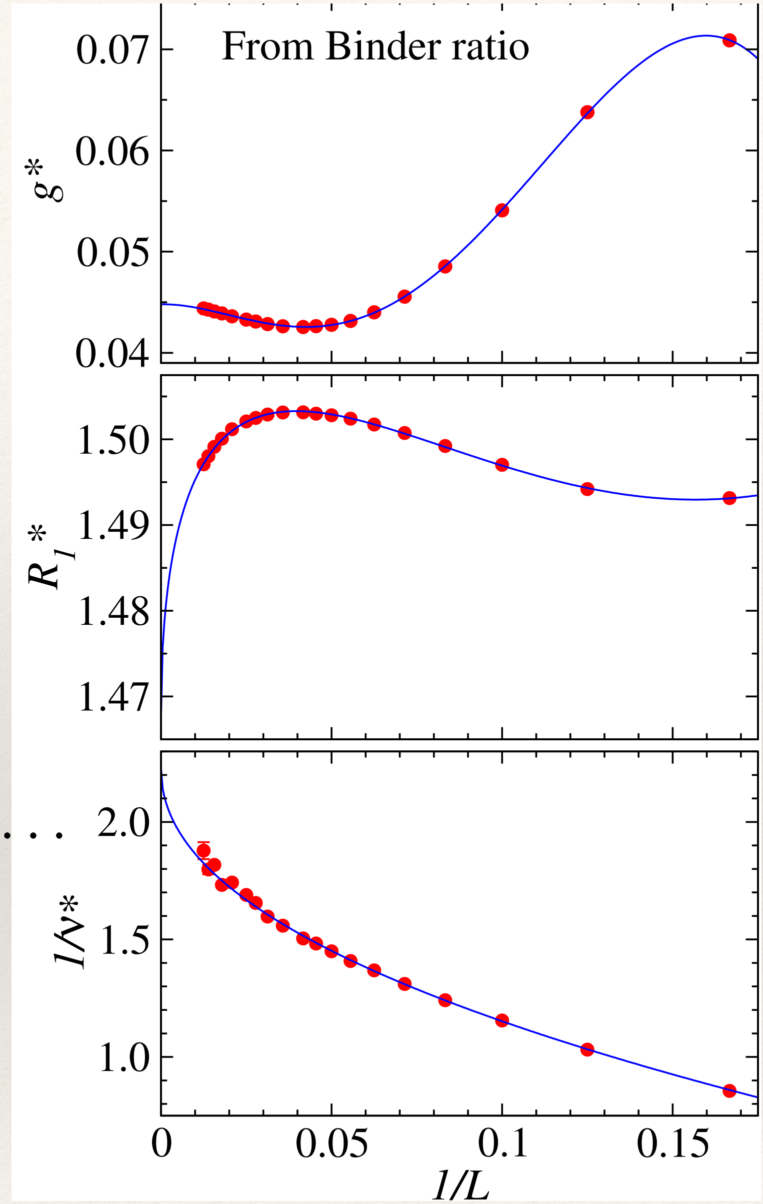
- **Crossing of $R_1(g,L)$, $R_1(g,rL)$**, g=J/Q, g*(L), analyze size dependence (using r=2)

$$g^*(L) = g_c + aL^{-(1/\nu+\omega)} + \ldots$$

$$R_1^*(L) = R_{1c} + aL^{-\omega} + \ldots$$

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

$$s(g, L) = dR_1(g, L)/dg \quad \text{(slope)}$$



- Small correction exponent; ω ≈ 0.5
- ν = 0.45 +/- 0.01

No sign of first-order transition (then ν ≥1/3 in finite-size scaling)

The VBS order parameter

Dimer order parameter

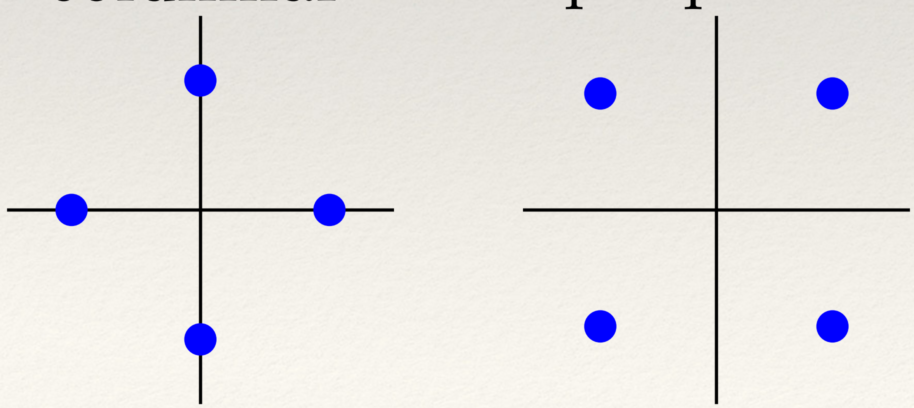
$$D_x = \frac{1}{N}\sum_{x,y}(-1)^x \mathbf{S}_{x,y}\cdot\mathbf{S}_{x+1,y}$$

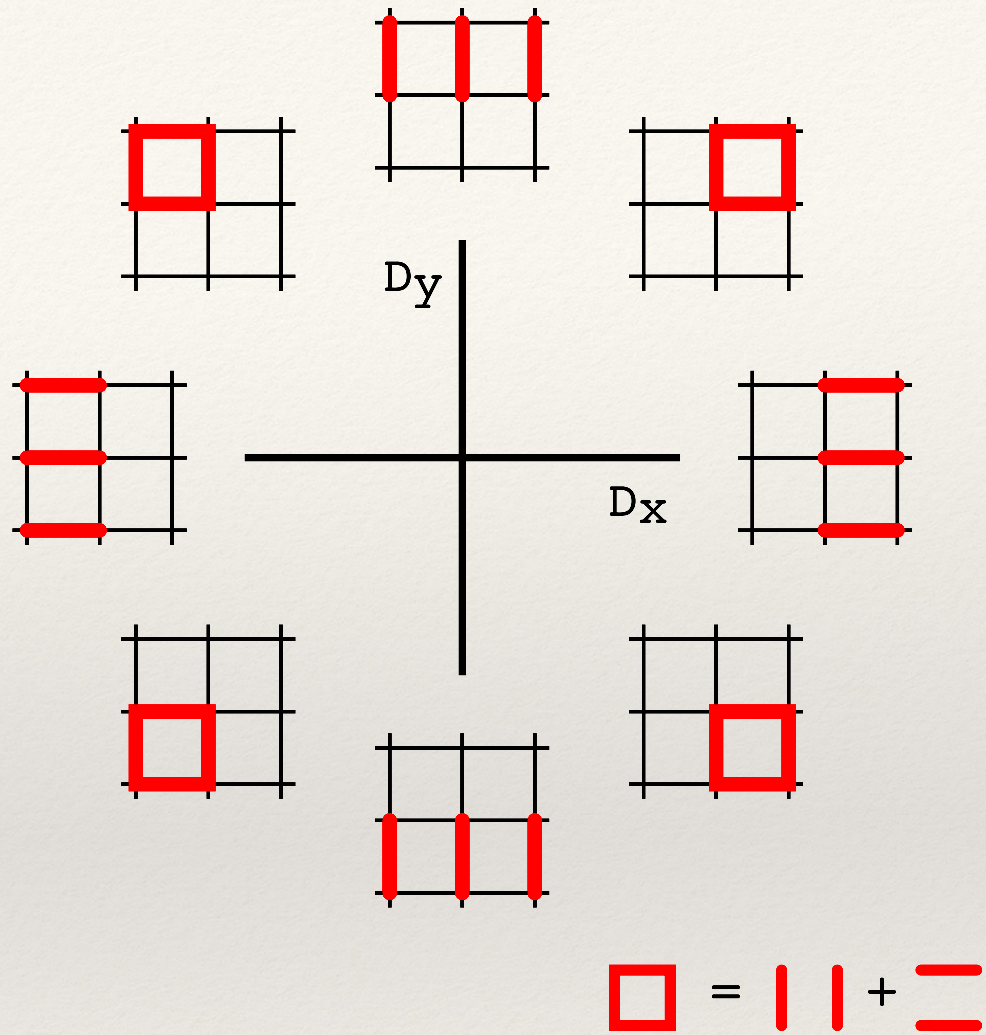
$$D_y = \frac{1}{N}\sum_{x,y}(-1)^y \mathbf{S}_{x,y}\cdot\mathbf{S}_{x,y+1}$$

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

Two possible types of order patterns distinguished by histograms

columnar plaquette

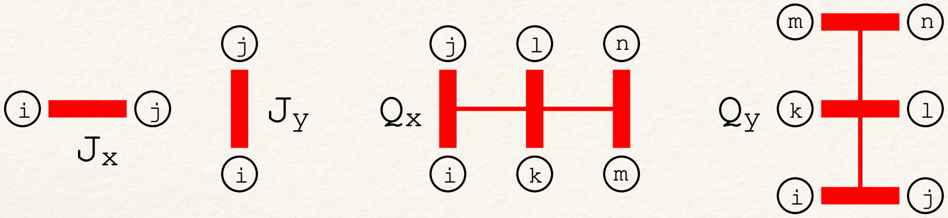




Finite-size fluctuations
- amplitude
- angular

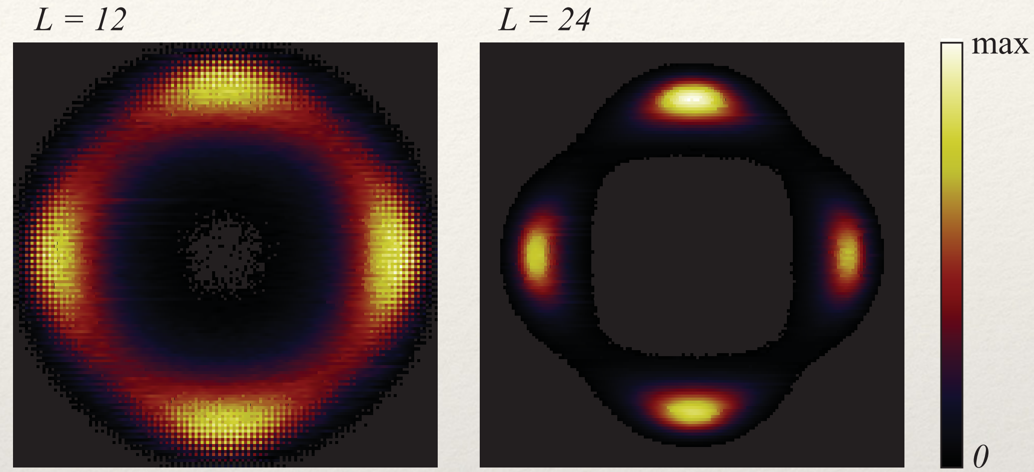
Emergent U(1) symmetry of columnar VBS order

Realize stronger VBS order with J-Q_3 model



J-Q_3 model
$J_x=J_y$, $Q_x=Q_y$

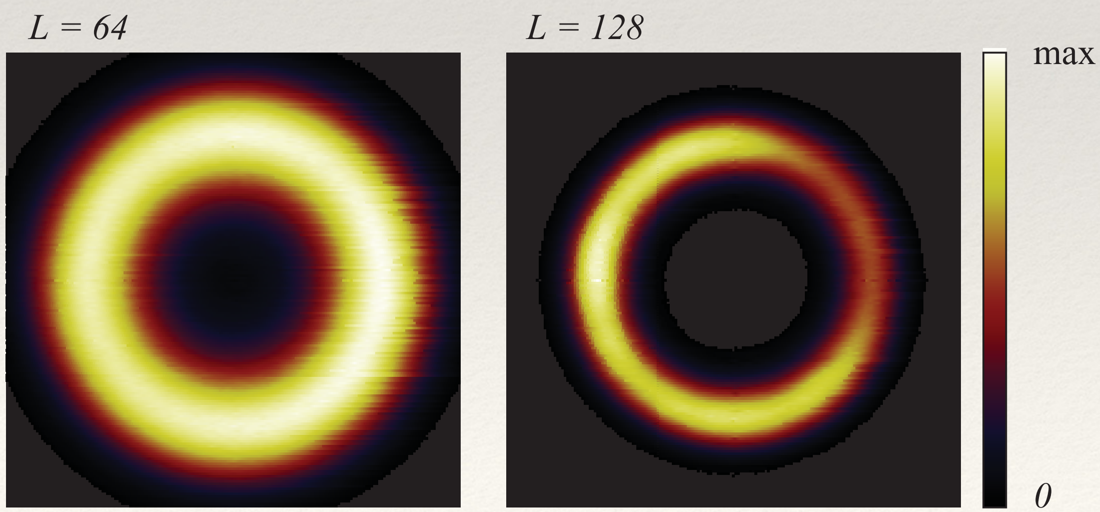
Lou, Sandvik, Kawashima, PRB (2009),
Sandvik, PRB (2012)

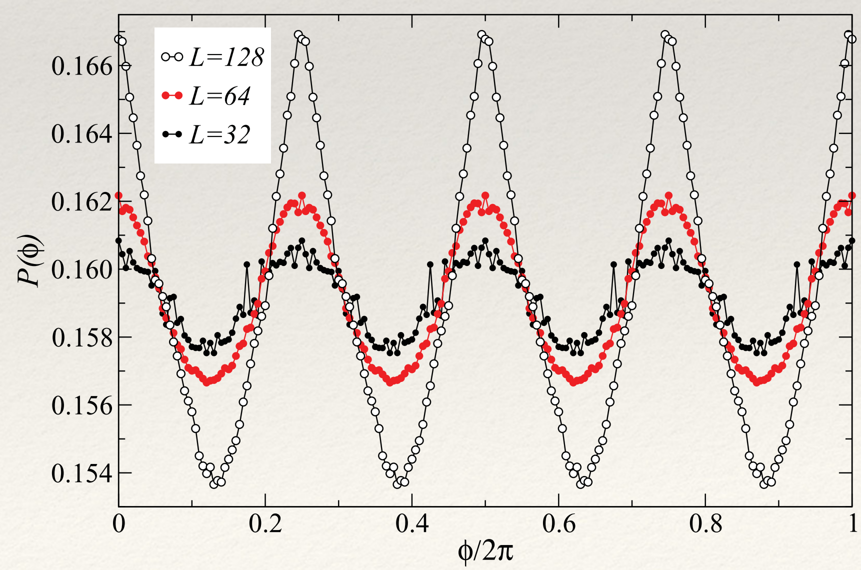


Strong columnar VBS when J/Q_3=0

J-Q_2 model with J/Q_2=0

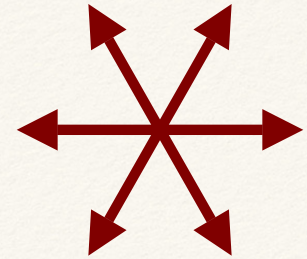
- weak columnar VBS
- very large angular fluctuations
- emergent U(1) symmetry





Analogy: Emergent U(1) in classical 3D XY model

$$H = -J \sum_{\langle ij \rangle} \cos(\Theta_i - \Theta_j) - h \sum_i \cos q\Theta_i$$



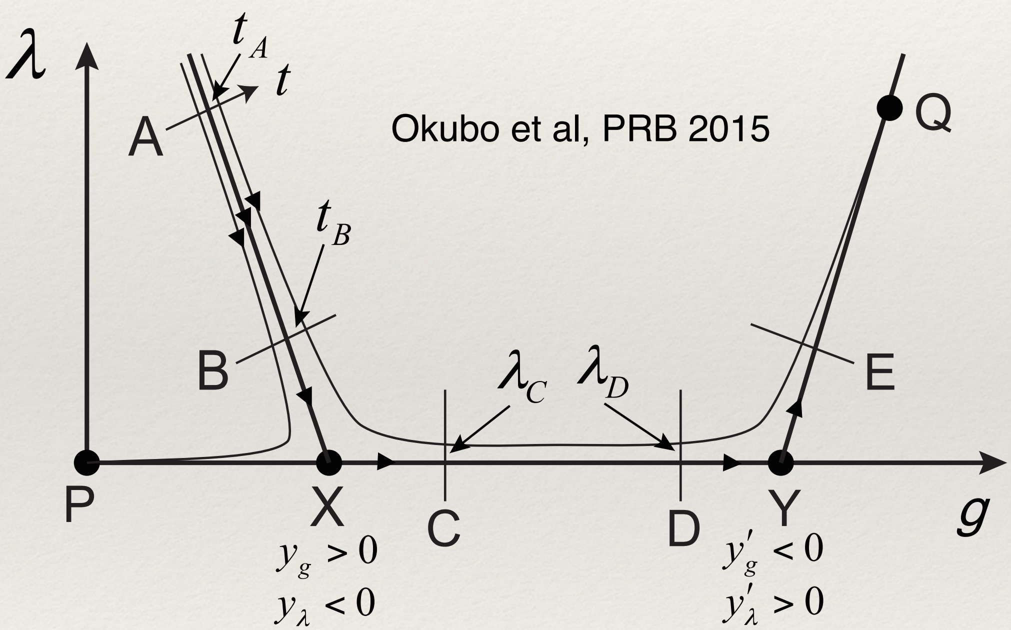
$q = 6$

Dangerously irrelevant perturbation

- irrelevant at T_c, relevant for $T<T_c$
- correlation length $\xi \propto (g-g_c)^{-\nu}$ and emergent U(1) length $\xi' \propto (g-g_c)^{-\nu'}$

Jose, Kadanoff, Kirkpatrick, Nelson, PRB 1977

$\nu' > \nu$



Clock models

Fixed points:

P = paramagnet

X = 3D XY critical point

Y = XY symmetry breaking

Q = Z_q symmetry breaking

Cross-over from XY ordering to Z_q ordering at length scale ξ'_q

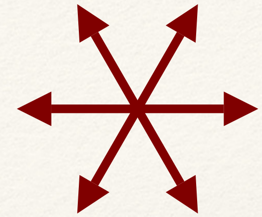
RG flows can be observed in MC simulations

“phenomenological renormalization”

MC simulations of classical 3D clock model

$$H = -J\sum_{\langle ij\rangle}\cos(\Theta_i - \Theta_j) - h\sum_i \cos q\Theta_i$$ (soft clock model)

$$H = -J\sum_{\langle ij\rangle}\cos(\Theta_i - \Theta_j)$$ q clock angles (hard clock model)

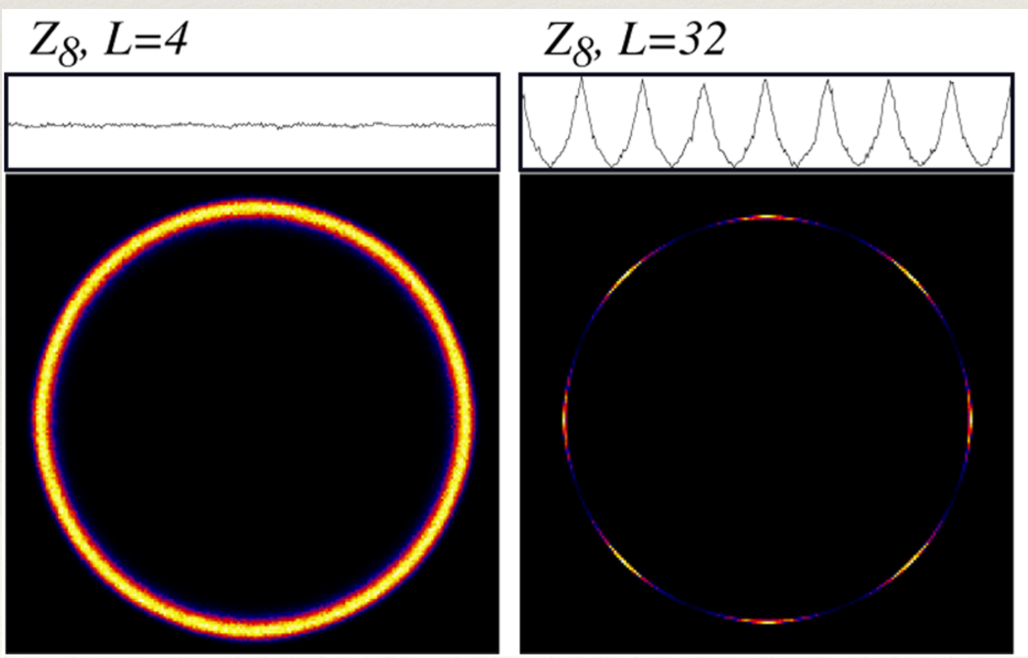


$q = 6$

Standard order parameter **(m_x,m_y)**

$$m_x = \frac{1}{N}\sum_{i=1}^{N}\cos(\Theta_i) \qquad m_y = \frac{1}{N}\sum_{i=1}^{N}\sin(\Theta_i) \quad \rightarrow \quad \text{global angle } \theta$$

Probability distribution P(m_x,m_y) shows cross-over from U(1) to Z_q for $T<T_c$



Lou, Balents, Sandvik, PRL 2007

Can be quantified with "angular order parameter":

$$\phi_q = \int_0^{2\pi} d\theta \cos(q\theta) P(\theta)$$

$\varphi_q > 0$ only if q-fold anisotropy

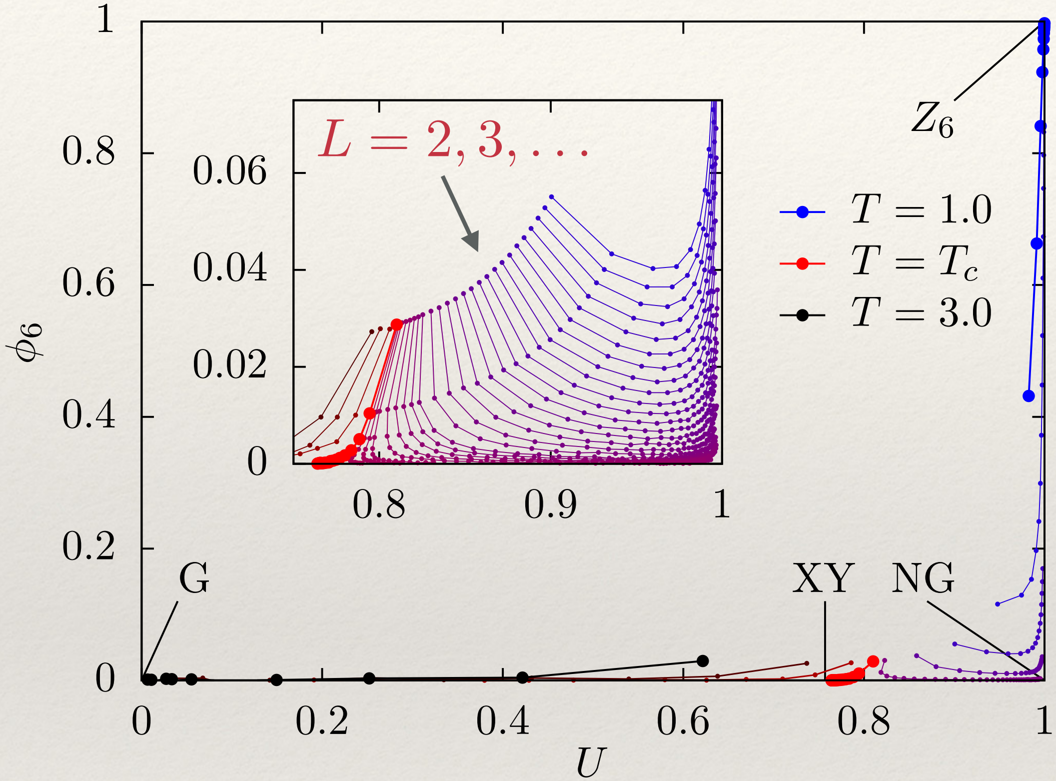
Finite-size scaling of φ_q can be used to extract length scale $\xi' > \xi$ and associated scaling dimension y_q

Angular order parameter φ_q reflects the dangerously irrelevant field

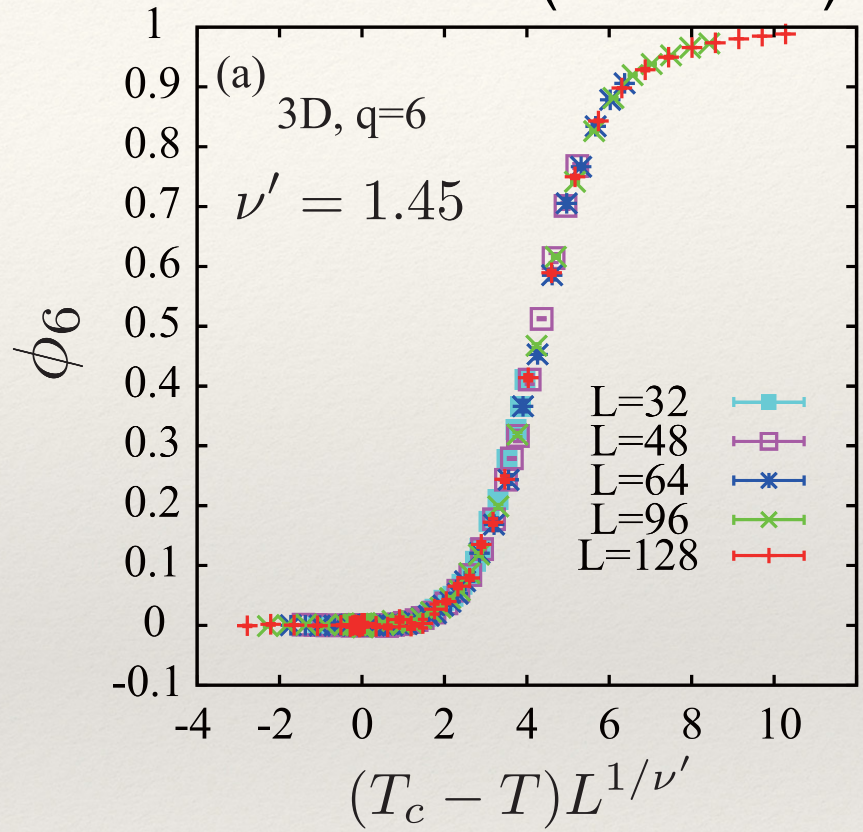
Relevant field accessed through the Binder cumulant: $U_m = 2 - \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}$

MC RG flows in the plane (U_m, φ_q)

[Shao, Guo, Sandvik, arXiv:1905.13640]



Okubo et al. (PRB 2015)

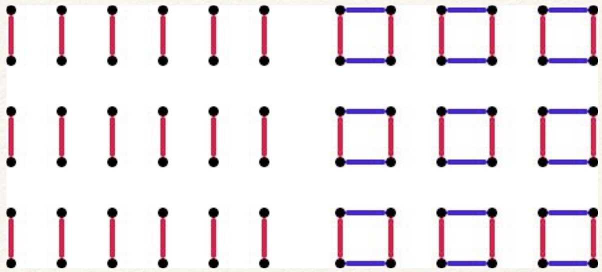


Entire RG flow can be explained by phenomenological scaling function with two relevant arguments:

$$\phi_q = L^{y_q} \Phi(tL^{1/\nu}, tL^{1/\nu'_q})$$

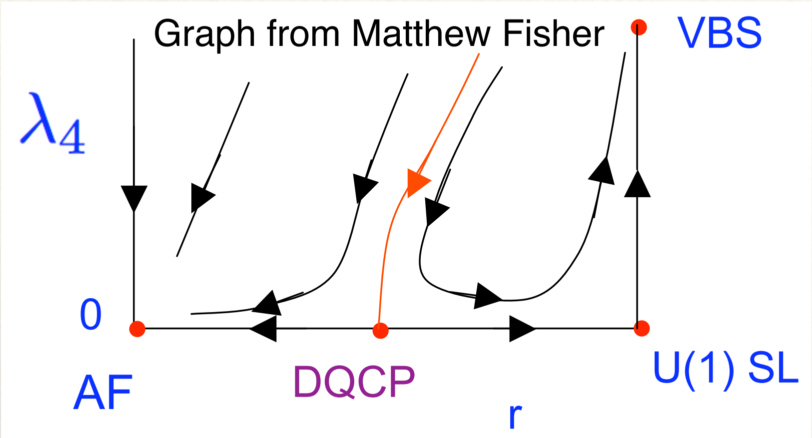
The exponent ν' can be directly extracted from φ_q when it is large - follows from scaling function

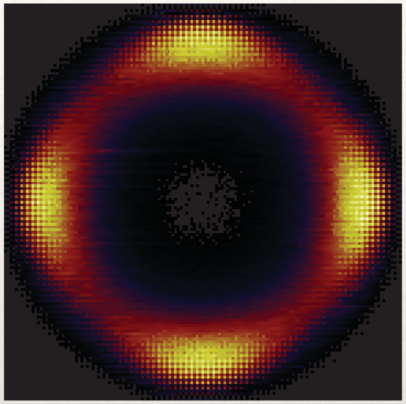
DQCP: In the field theory the VBS corresponds to condensation of topological defects (quadrupoled monopoles on square lattice)

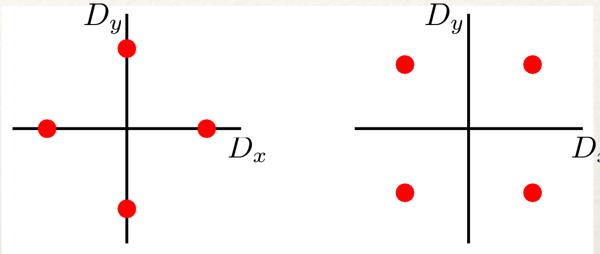


Analogy with 3D clock models: The topological defects should be dangerously irrelevant

Fugacity of topological defects λ_4

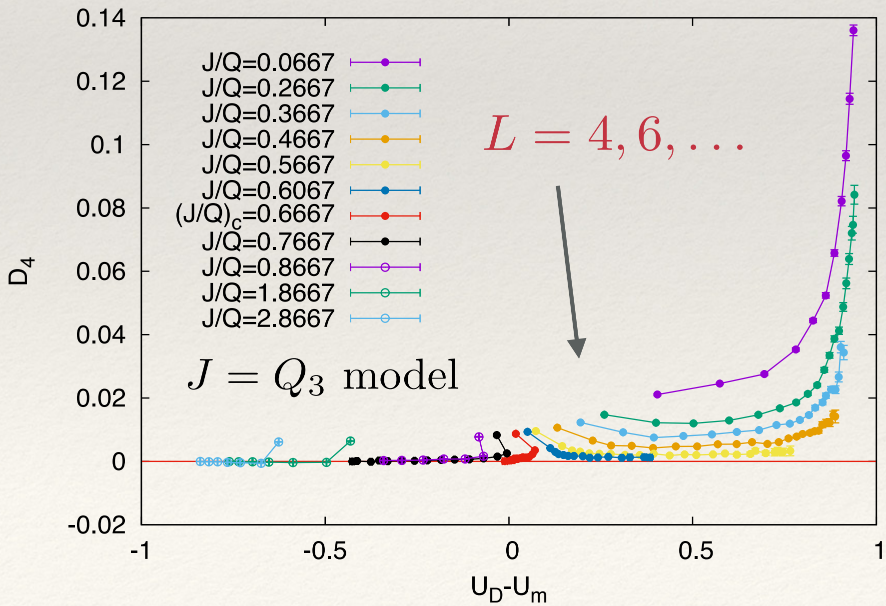


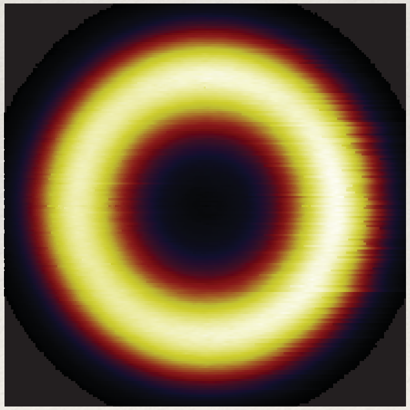




Ratio ν/ν' plays important in finite-size scaling

Shao, Guo, Sandvik (Science 2016)

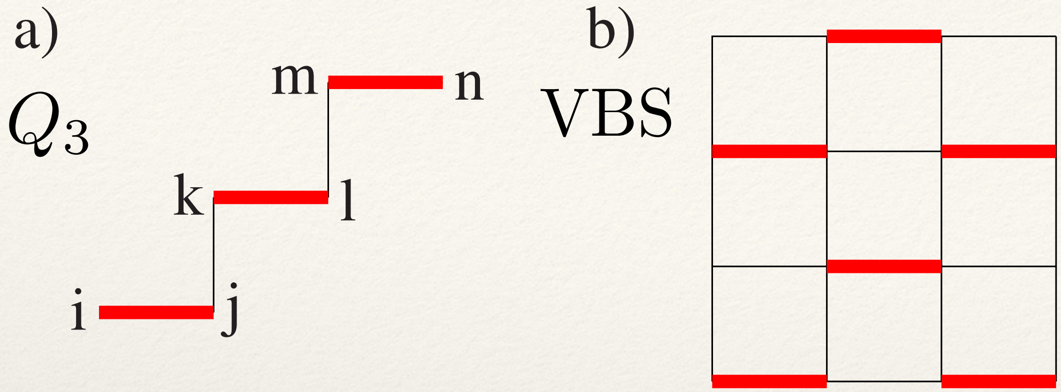




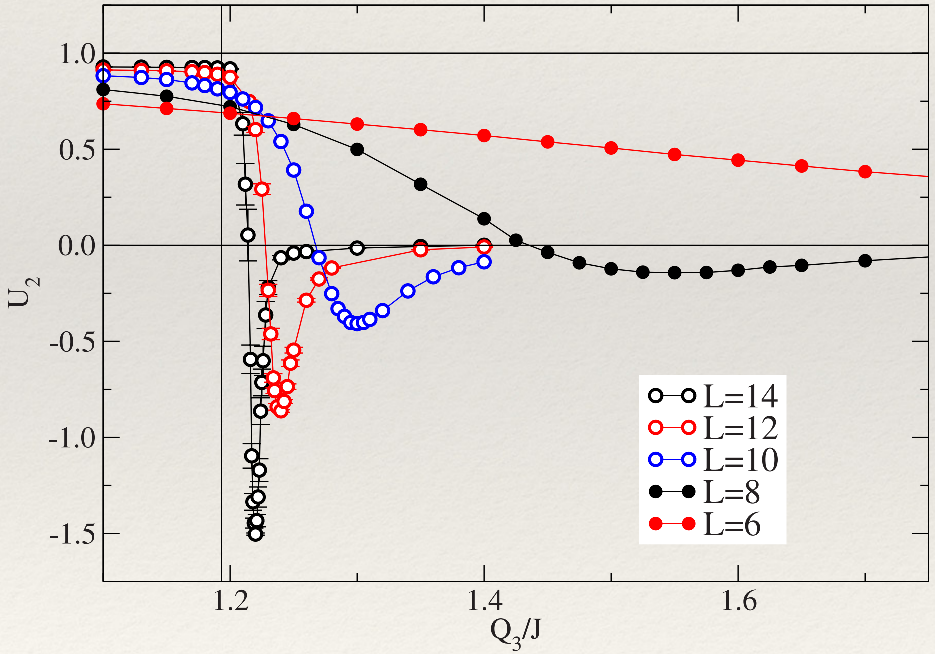
MC RG flows for J-Q_3 model
- work in progress

Conventional first-order transition

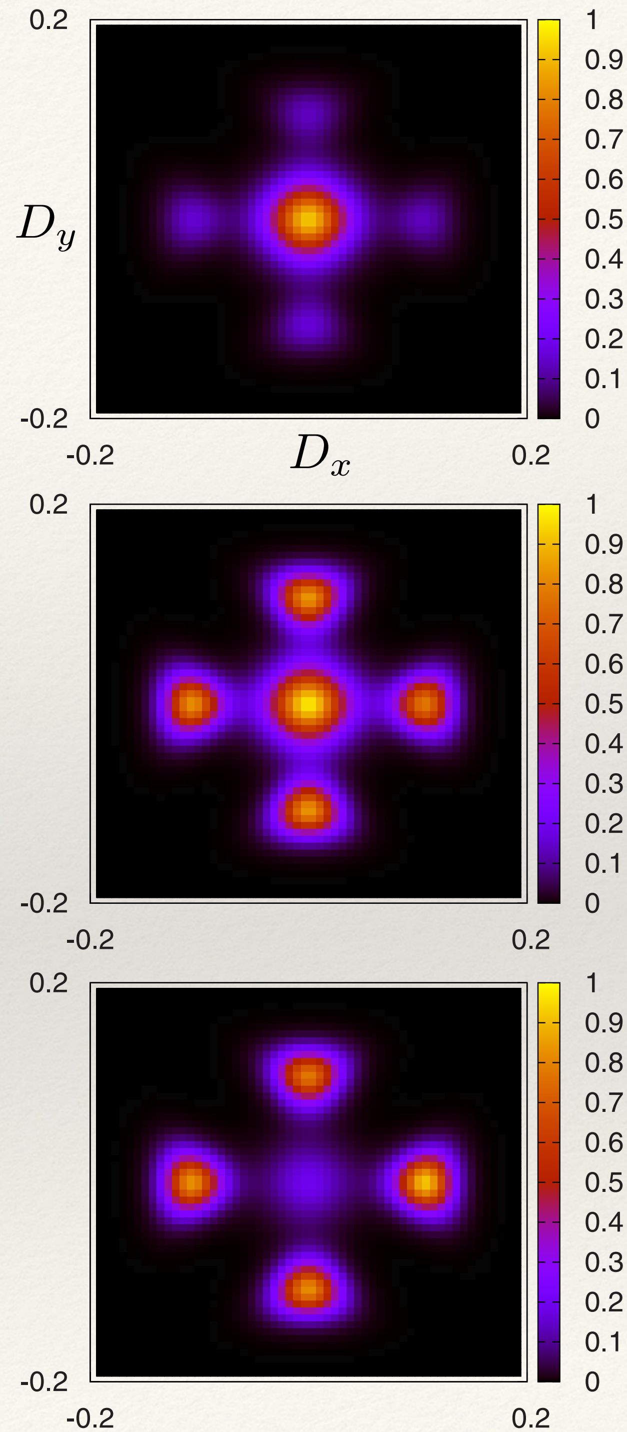
Staircase J-Q_3 model [Sen, Sandvik, PRB 2010]



Binder cumulant of AFM order parameter



Negative Cumulant peak is a sign of phase coexistence; first-order transition



No emergent symmetry seen in $P(D_x,D_y)$

Dynamic signatures of deconfined quantum criticality

PHYSICAL REVIEW B **98**, 174421 (2018)

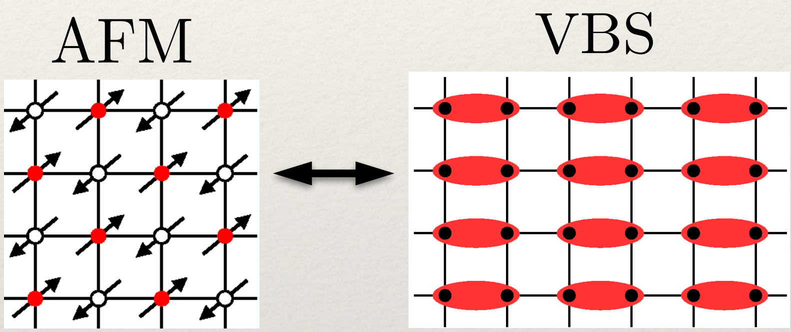
Editors' Suggestion

Dynamical signature of fractionalization at a deconfined quantum critical point

Nvsen Ma,[1] Guang-Yu Sun,[1,2] Yi-Zhuang You,[3,4] Cenke Xu,[5] Ashvin Vishwanath,[3] Anders W. Sandvik,[1,6] and Zi Yang Meng[1,7,8]

Planar J-Q model: $H_{\rm JQ} = -J\sum_{\langle ij\rangle}\left(P_{ij} + \Delta S_i^z S_j^z\right) - Q\sum_{\langle ijklmn\rangle} P_{ij}P_{kl}P_{mn}$

Spin structure factor S(q,ω)

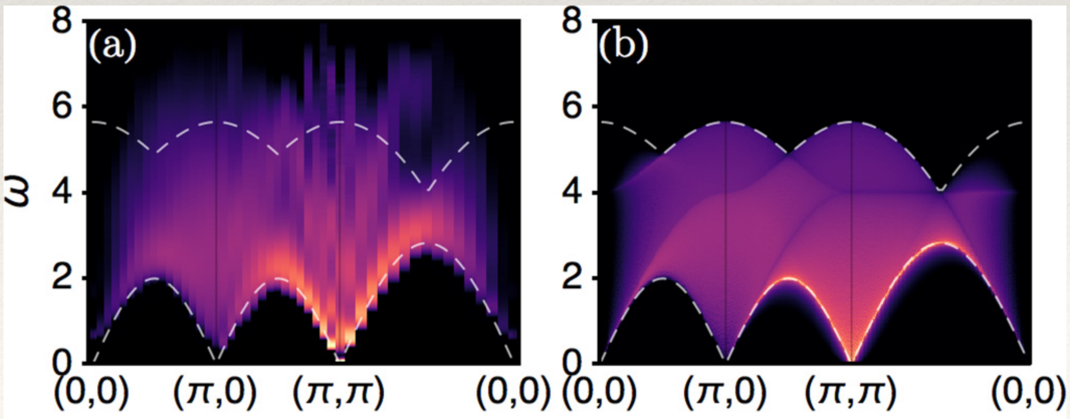


Close to critical point:
Good agreement with mean-field fermionic parton theory (π-flux)

$$\boldsymbol{S}_i = \frac{1}{2} f_i^\dagger \boldsymbol{\sigma} f_i$$

$$H_{\rm MF} = \sum_i \mathrm{i}(f_{i+\hat{x}}^\dagger f_i + (-)^x f_{i+\hat{y}}^\dagger f_i) + \mathrm{H.c.}$$

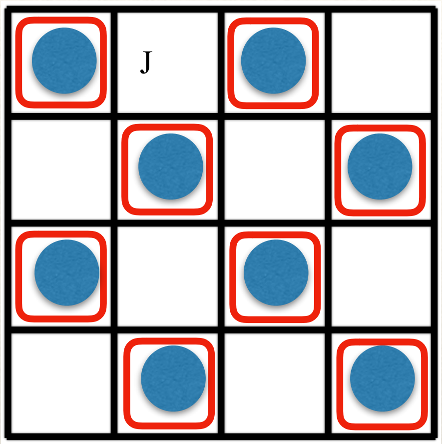
$$\epsilon_{\boldsymbol{k}} = 2(\sin^2(k_x) + \sin^2(k_y))^{1/2}$$

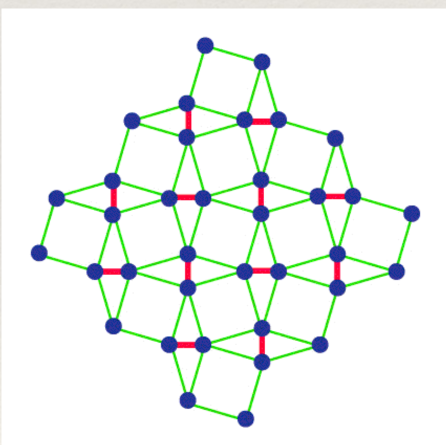


Deconfinment manifest on large length scales close to the phase transition

Connection to experiments: Checker-board J-Q model

Plaquette-singlet solid (PSS) state
- 2-fold degenerate





Is the PSS-AFM transition a deconfined quantum critical point?

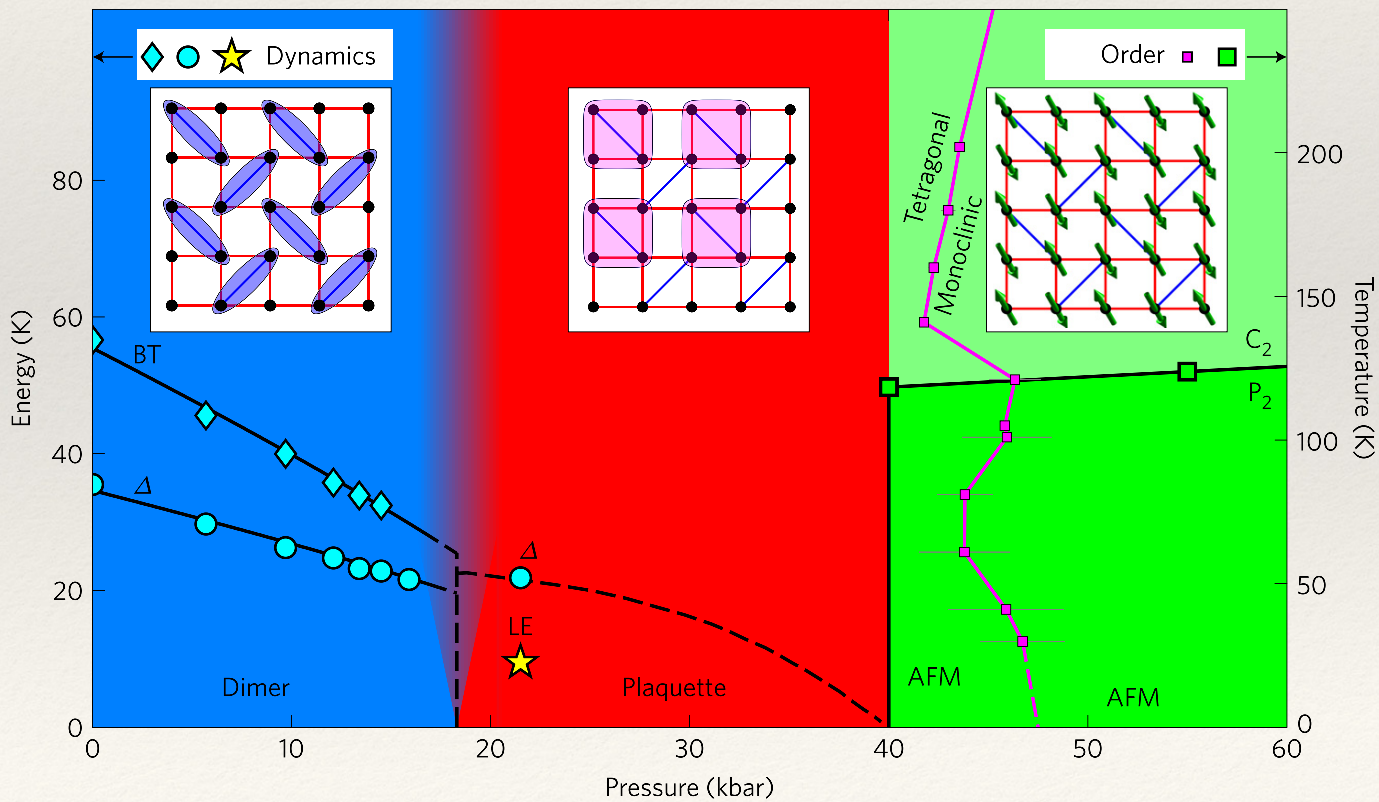
nature physics

LETTERS

PUBLISHED ONLINE: 17 JULY 2017 | DOI: 10.1038/NPHYS4190

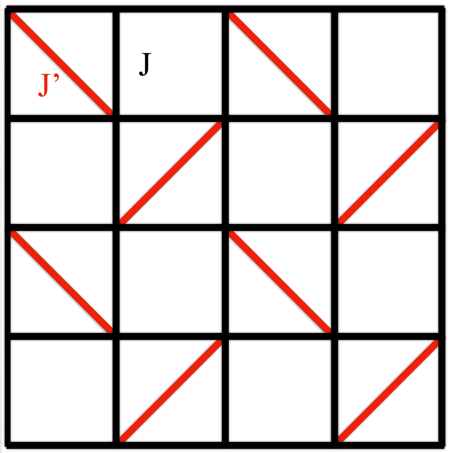
4-spin plaquette singlet state in the Shastry–Sutherland compound $SrCu_2(BO_3)_2$

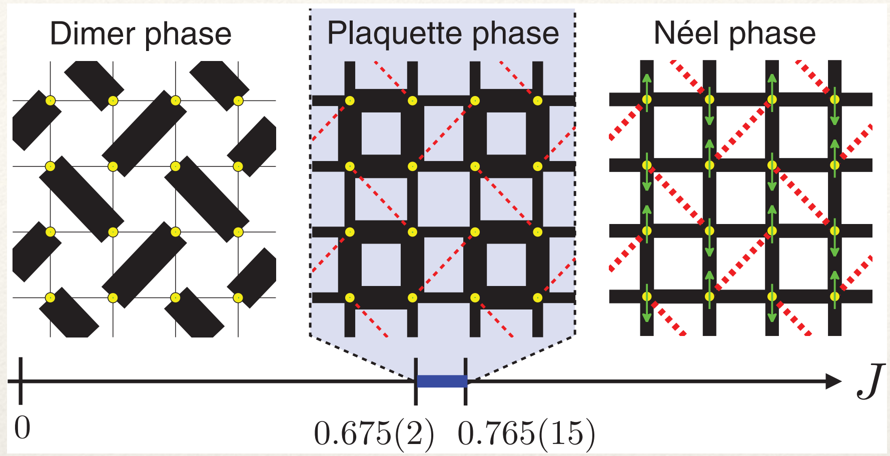
M. E. Zayed[1,2,3*], Ch. Rüegg[2,4,5], J. Larrea J.[1,6], A. M. Läuchli[7], C. Panagopoulos[8,9], S. S. Saxena[8], M. Ellerby[5], D. F. McMorrow[5], Th. Strässle[2], S. Klotz[10], G. Hamel[10], R. A. Sadykov[11,12], V. Pomjakushin[2], M. Boehm[13], M. Jiménez-Ruiz[13], A. Schneidewind[14], E. Pomjakushina[15], M. Stingaciu[15], K. Conder[15] and H. M. Rønnow[1]



Shastry-Sutherland (SS) model

PSS state known in the SS model (tensor network, iPEPS, calculations)



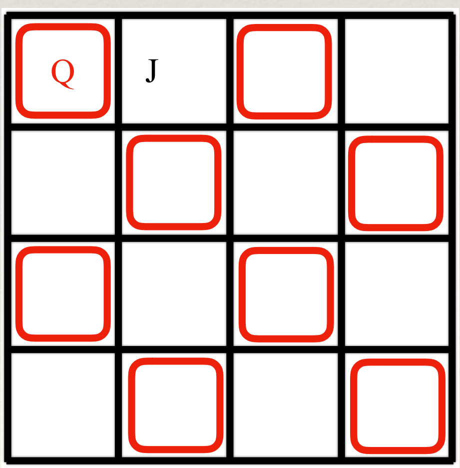


Corboz & Mila
PRB 2013

Weak first-order transition from Neel to plaquette phase was found

Checker-board J-Q (CBJQ) model

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



To study AFM-PSS transition in detail with QMC
- replace frustrated bonds by 4-spin Q terms

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

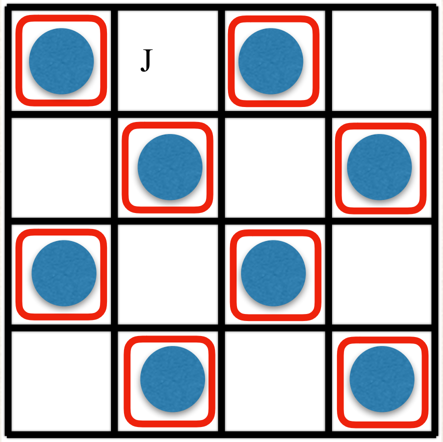
$$P_{ij} = \frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j$$

Do we get a PSS phase, and what kind of phase transition?

Plaquette-Singlet Solid state in the CBJQ model

Zhao, Weinberg, AWS, Nature Physics 2019

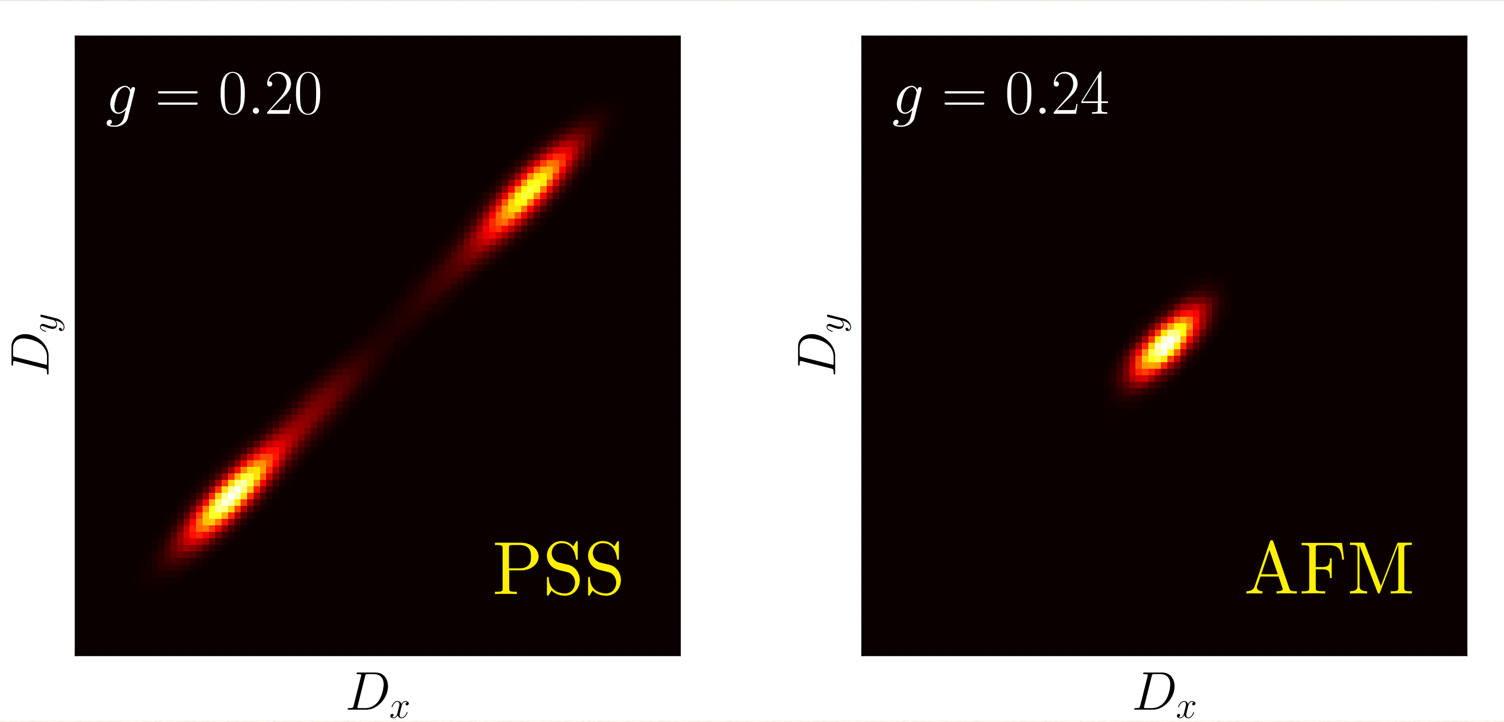
The lattice and interactions are compatible with
- 4 fold degenerate columnar VBS
- 2-fold degenerate PSS state



Both can be detected using the dimer order parameter

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

With valence-bond QMC, collect $P(D_x,D_y)$

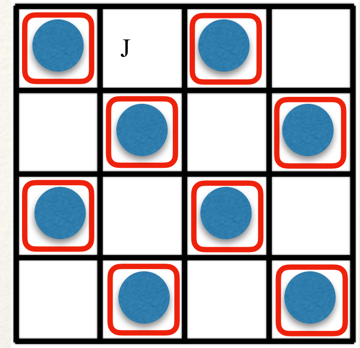


We find 2-fold PSS order for small g=J/Q

AFM-PSS quantum phase transition

Define order parameters with z-spin components in SSE QMC

$$m_s = \frac{1}{N}\sum_{\mathbf{r}} \phi(\mathbf{r}) S^z(\mathbf{r}), \quad m_p = \frac{2}{N}\sum_{\mathbf{q}} \theta(\mathbf{q}) P^z(\mathbf{q})$$



$$P^z(\mathbf{q}) = S^z(\mathbf{q}) S^z(\mathbf{q}+\hat{x}) S^z(\mathbf{q}+\hat{y}) S^z(\mathbf{q}+\hat{x}+\hat{y})$$

Binder cumulants:

$$U_s = \frac{5}{2}\left(1 - \frac{\langle m_s^4\rangle}{3\langle m_s^2\rangle^2}\right) \quad U_p = 2\left(1 - \frac{1}{2}\frac{\langle m_p^4\rangle}{\langle m_p^2\rangle^2}\right)$$

Expectation:

$U_s \to 1$, $U_p \to 0$ in AFM phase

$U_s \to 0$, $U_p \to 1$ in PSS phase

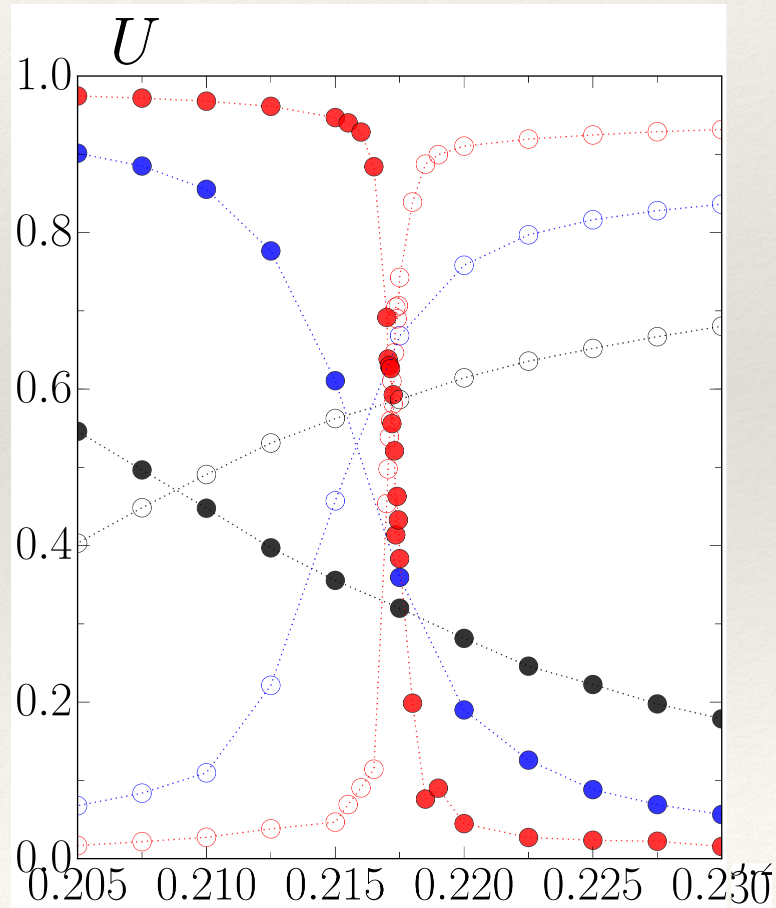
Crossing points used to analyze the transition

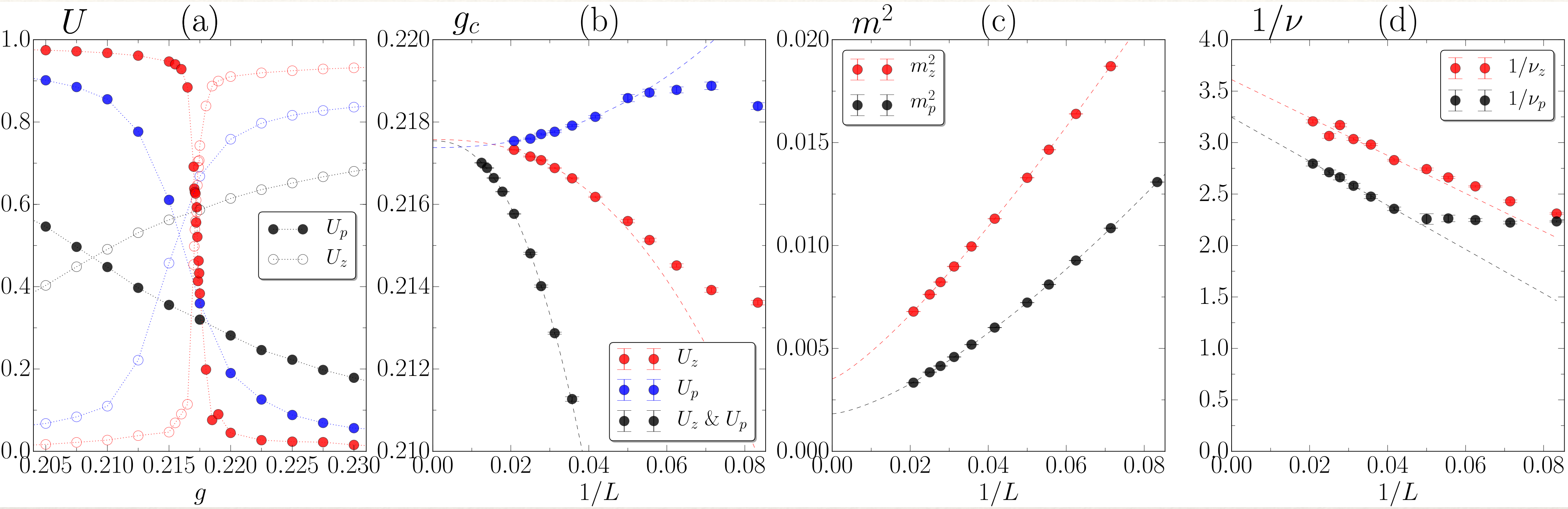
No negative peaks in U - continuous transition?

● p, ○ s, $L = 24$

● p, ○ s, $L = 48$

● p, ○ s, $L = 96$





Finite-size scaling behaviors show

- single AFM-PSS transition at g_c = 0.2175(1)
- coexistence of non-vanishing orders at g_c → **first-order transition**

Analysis of slopes of U gives correlation-length exponent

$$\frac{1}{\nu_{sp}} = \frac{1}{\ln(b)} \ln\left[\frac{dU_{sp}(g,bL)/dg}{dU_{sp}(g,L)/dg}\right]_{g=g_c(L)}$$

Both exponent extrapolate to values > d+1 = 3; first-order behavior

Why are there no negative Binder peaks?

Do we know any phase transition with similar characteristics?

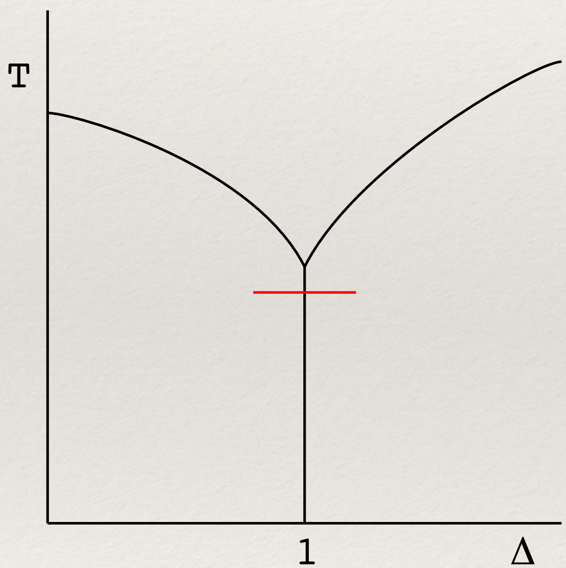
Yes: 3D O(N) models with N=3,4,5,… in their ordered states (T < T_c)

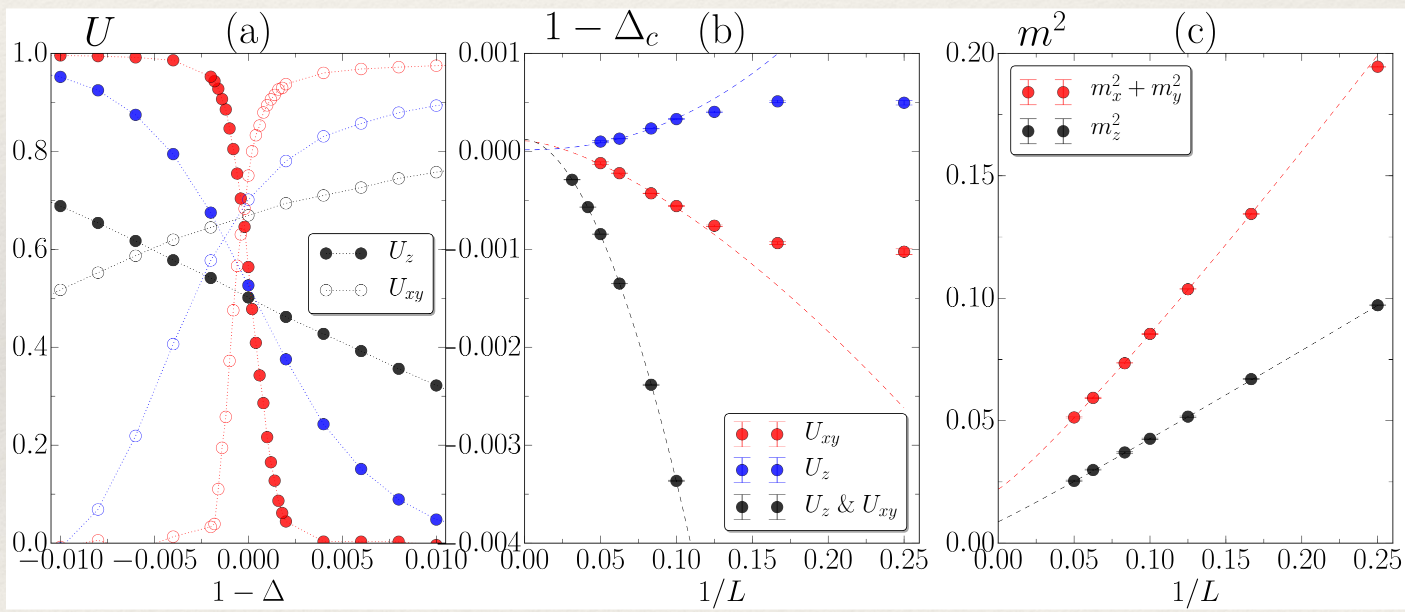
Example: **Classical 3D O(3) (Heisenberg) model** with tunable anisotropy

$$H = -\sum_{\langle ij \rangle} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \Delta \sigma_i^z \sigma_j^z)$$

Symmetry changes vs Δ: O(2) for $\Delta<1$, O(3) for $\Delta=1$, Z_2 for $\Delta>1$

For T<T_c, analyze xy and z order parameters and Binder cumulants





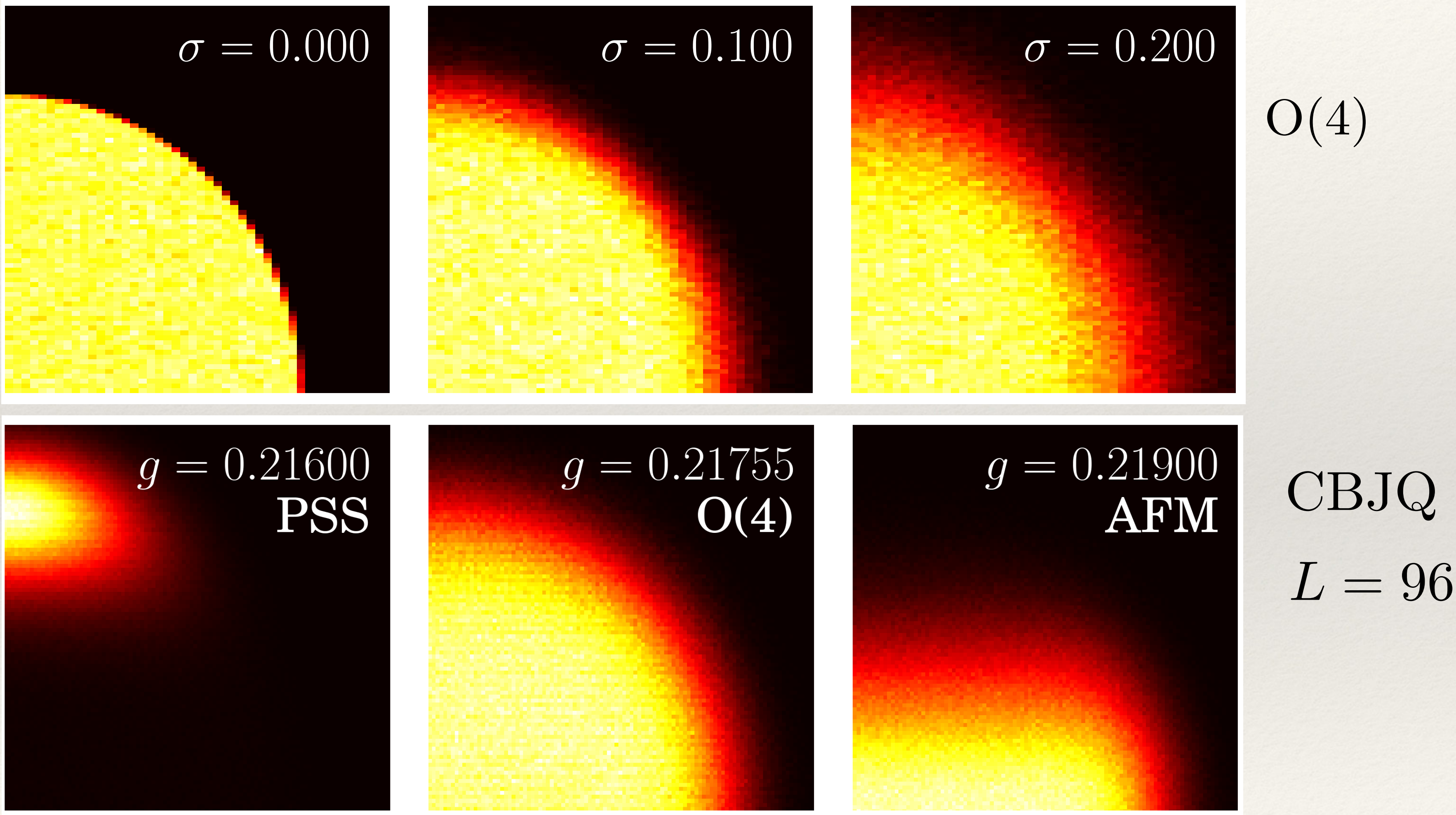
Very similar behaviors as CBJQ model!

But no point of obvious higher symmetry vs g in the CBJQ model…

Proposal: O(3) AFM and Z_2 PSS orders form emergent O(4) vector

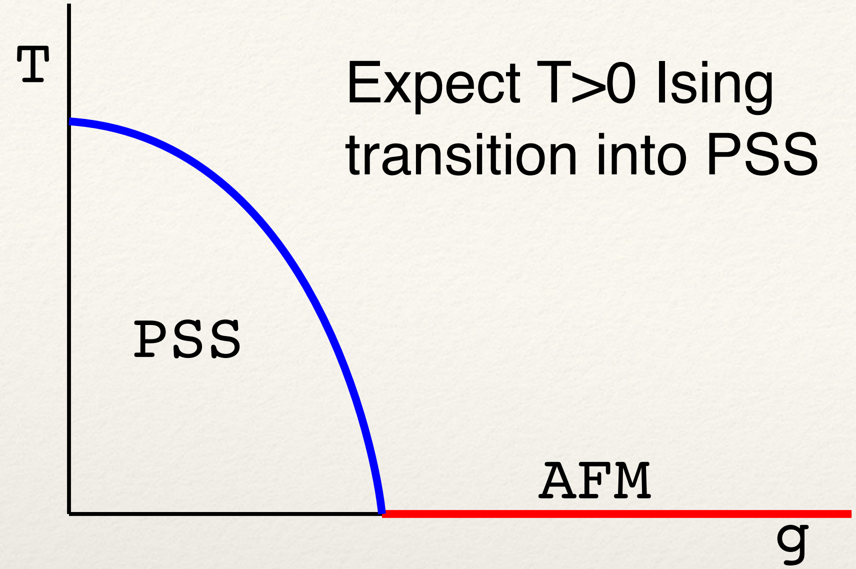
Detecting O(4) symmetry in the CBJQ model

- We know that the AFM component has O(3) symmetry
- Need to check only PSS order and one AFM component; $P(m_z, m_p)$
- O(4) projected down to a plane - constant density within circle
- Radius fluctuates because of finite size



- Appears that there is an O(4) point (the transition point)
- No sign of conventional AFM, PSS coexistence

Manifestation of O(4) in T>0 phase diagram



Expect T>0 Ising transition into PSS

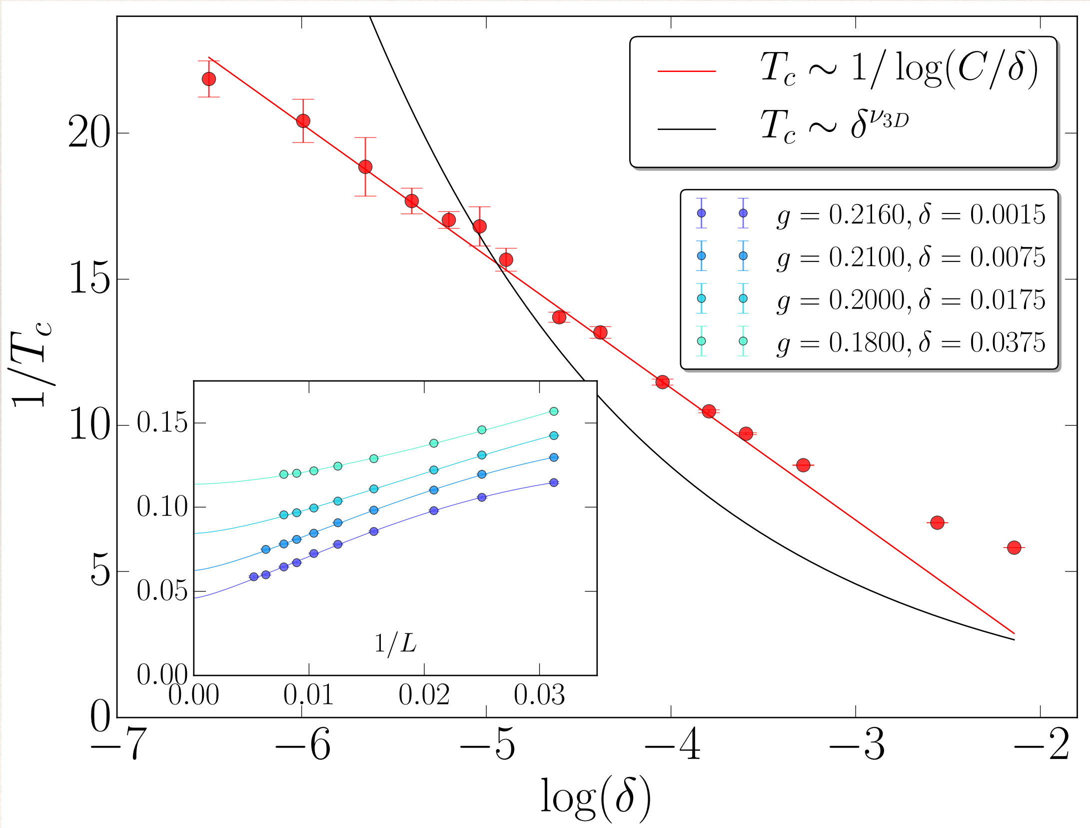
At a conventional continuous transition we should have:

$$T_c \propto (|g - g_c|)^{\nu_{3D}}$$

- cut off at low T_c if the transition is eventually first-order

When approaching an O(N) point we expect (RG analysis by Irkhin, Katanin, PRB 1998):

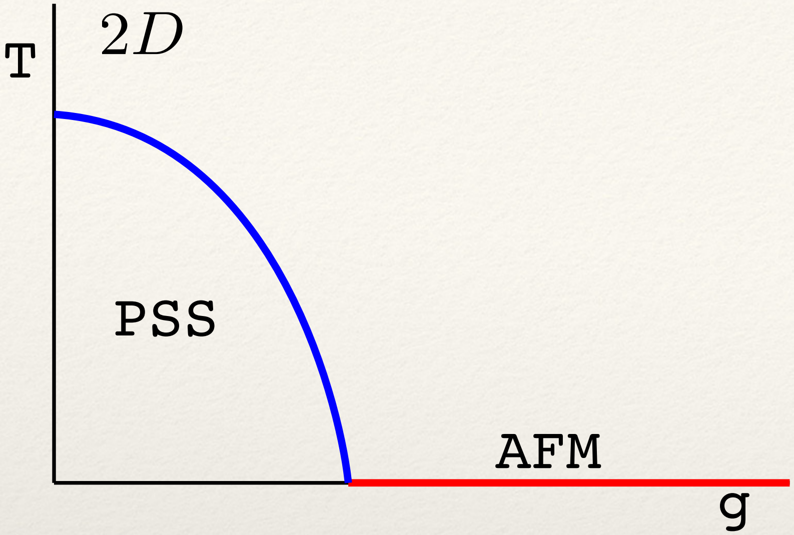
$$T_c \propto \frac{1}{\ln(C/|g - g_c|)}$$

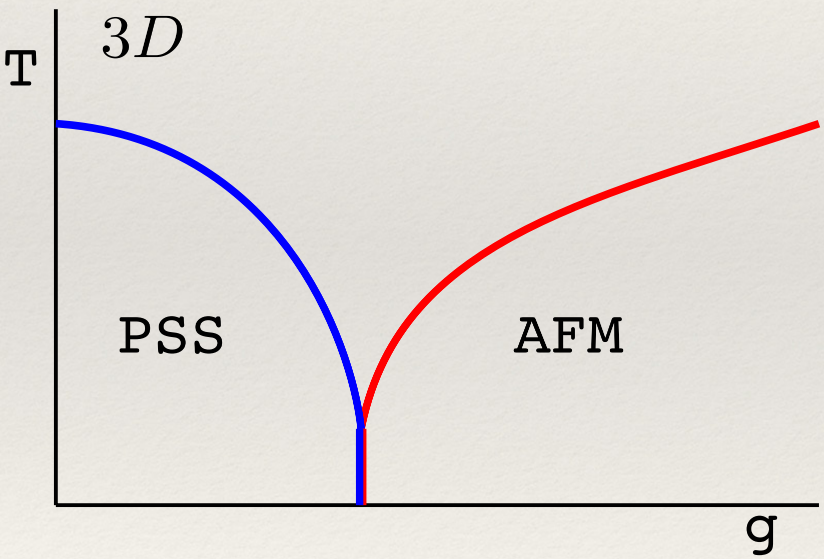


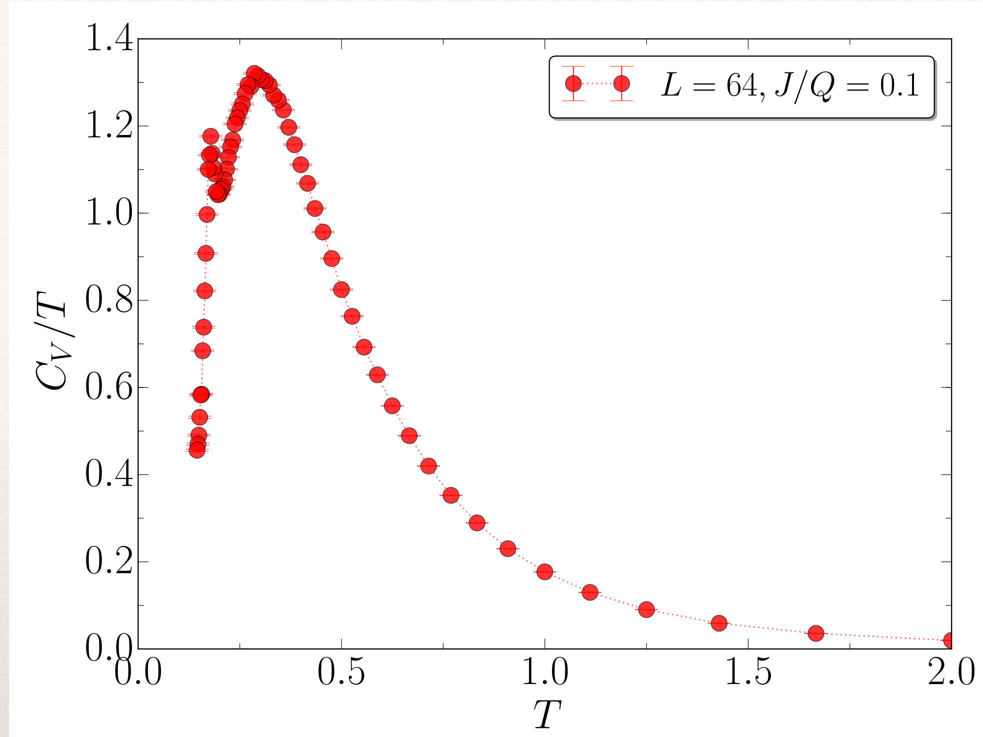
Results support the log form

manifestation of O(4) symmetry in physical observable

Specific heat, 3D T>0 phase diagram







Entropy change small at T>0 transition

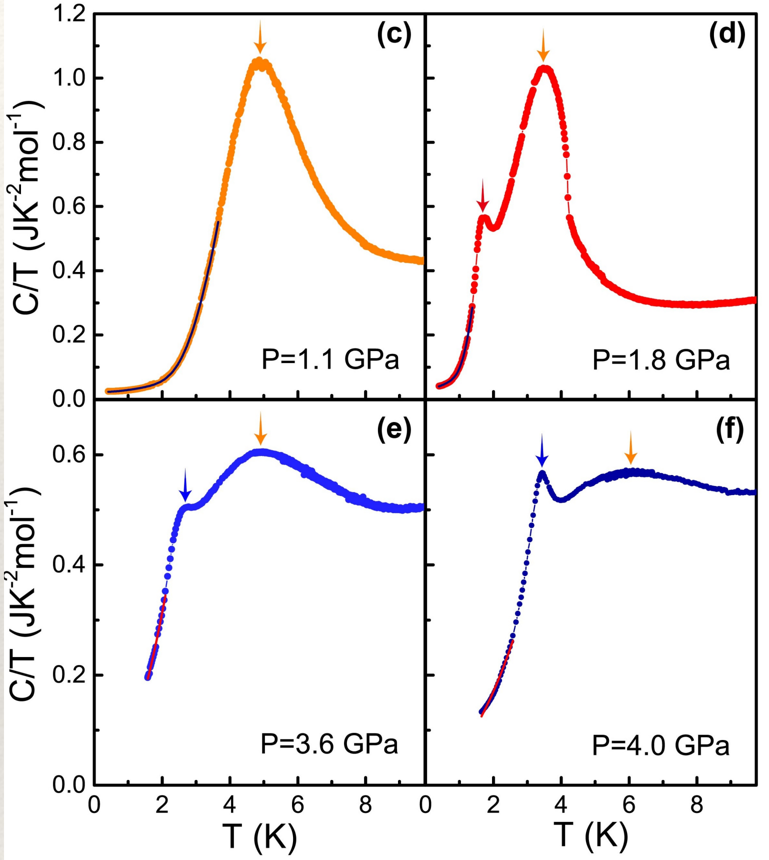
- a lot of entropy goes to freezing out higher states on the plaquettes

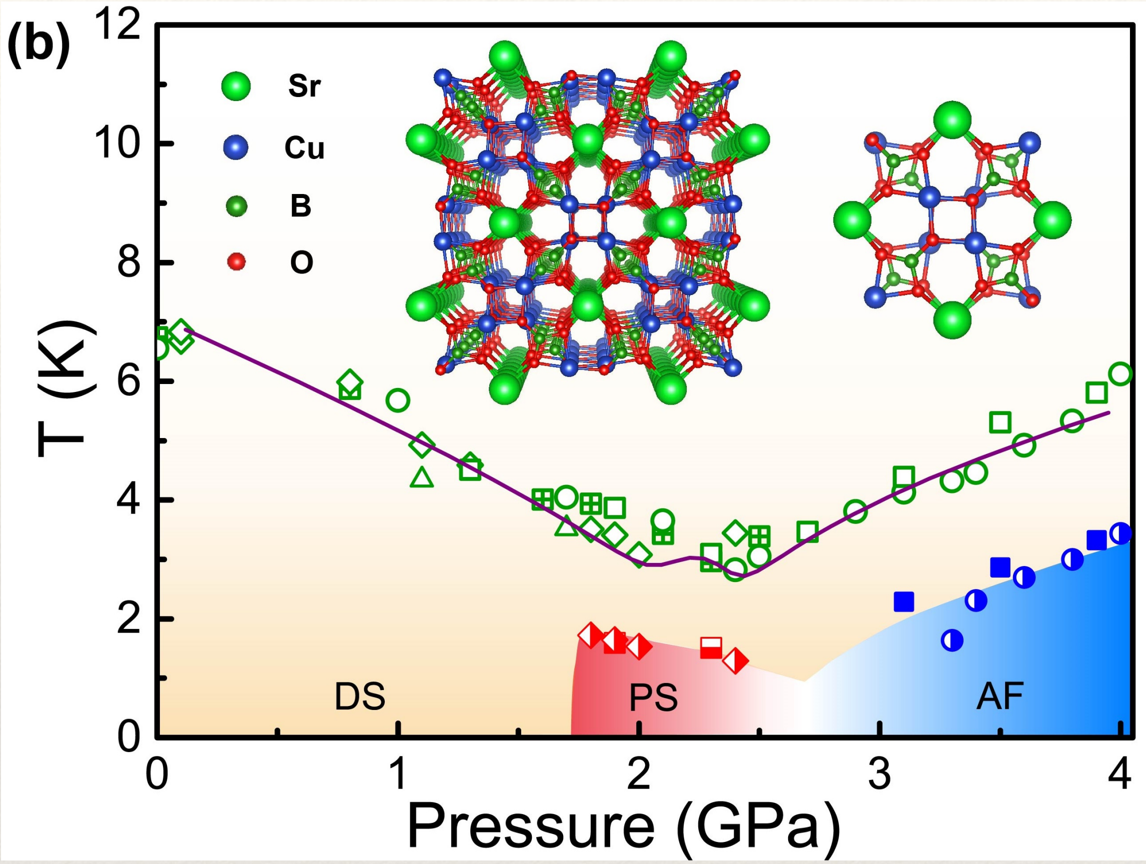
3D effects should cause first-order line
- could there be remnant O(4) above?

Similar behavior in $SrCu_2(BO_3)_2$
- high-pressure, low-T experiments (J. Guo et al., IOP) arXiv:1904.09927

Quantum phases of $SrCu_2(BO_3)_2$ from high-pressure thermodynamics arXiv:1904.09927

Jing Guo,[1] Guangyu Sun,[1,2] Bowen Zhao,[3] Ling Wang,[4] Wenshan Hong,[1,2] Vladimir A. Sidorov,[5] Nvsen Ma,[1] Qi Wu,[1] Shiliang Li,[1,2,6] Zi Yang Meng,[1,7,6,8,*] Anders W. Sandvik,[3,1,†] and Liling Sun[1,2,6,‡]





First (P,T) phase diagram

- PS phase smallar than expected
- new AF phase

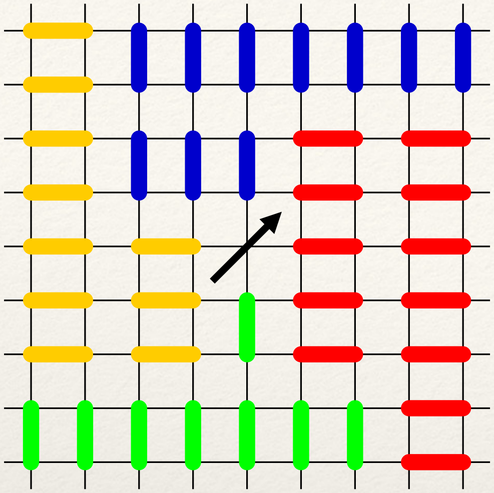
couplings from $T_{hump}(P)$ fit to SS model

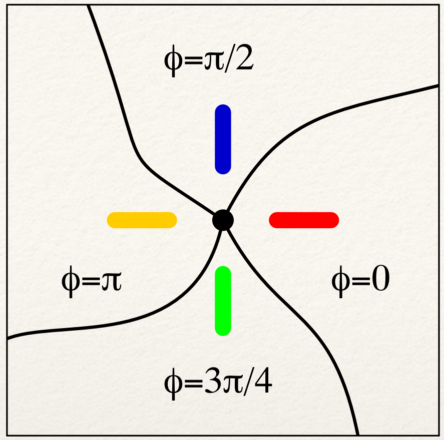
$$J'(P) = [75 - 8.3P/\text{GPa}]\ \text{K}$$

$$J(P) = [46.7 - 3.7P/\text{GPa}]\ \text{K}$$

Random-singlet (RS) state in disordered J-Q model

Lu Liu, Hui Shao, Yu-Cheng Lin, Wenan Guo, AWS (PRX 2018)



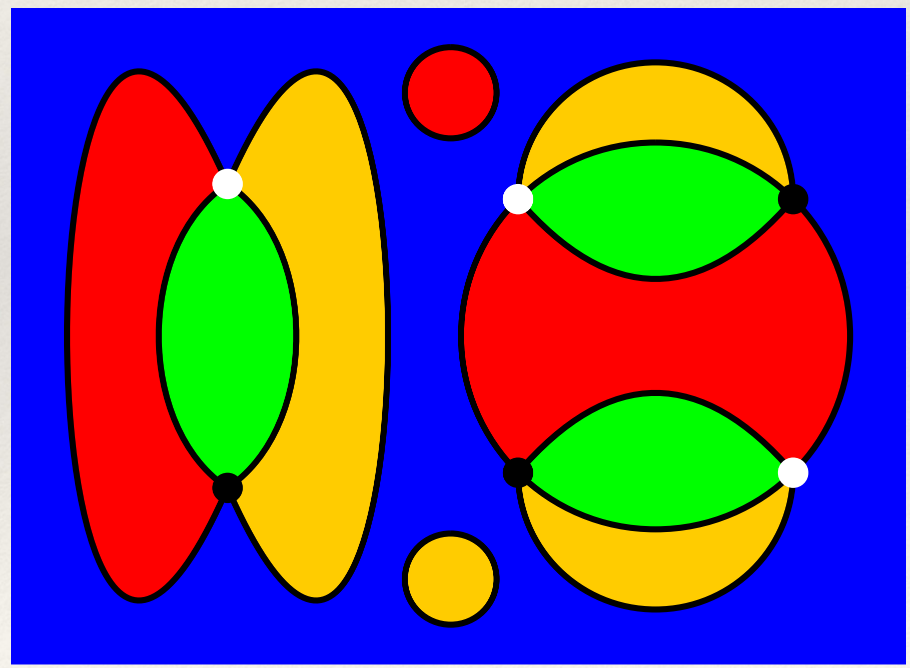


Spinon
nexus of four domain walls, with unpaired spin in the core
(Levin, Senthil, 2004,…)

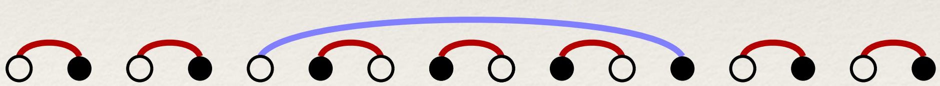
Imry-Ma argument (1D, 2D)
any amount of disorder in a VBS will cause domain formation

What kind of magnetic state forms from the interacting spinons?

Spinons will form in pairs

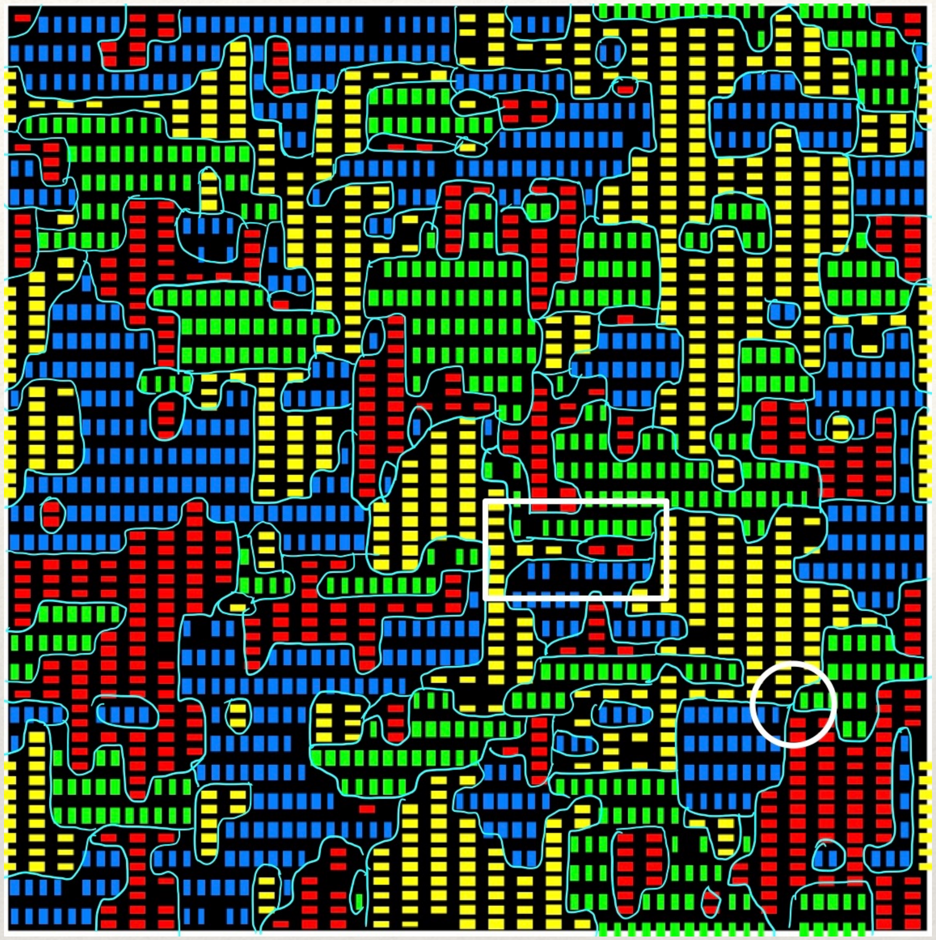


1D: RS state in random S=1/2 chain
- infinite-randomnes fixed point (z=∞)

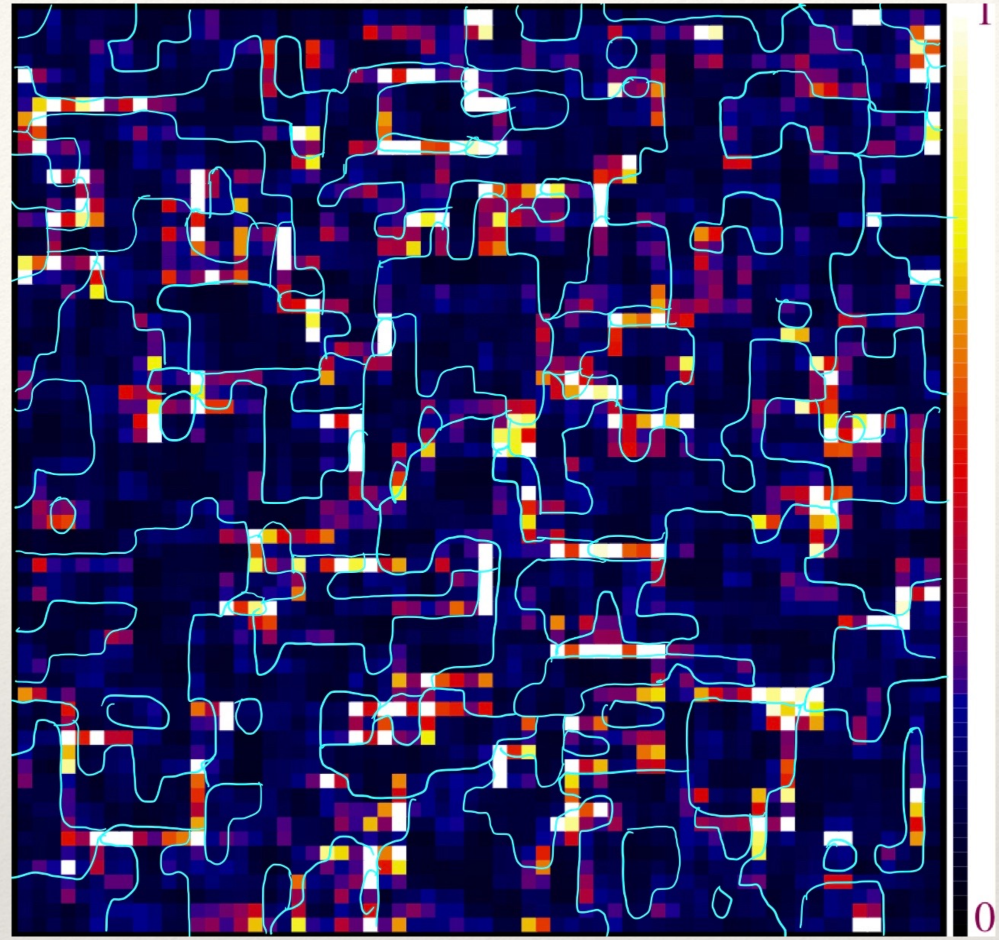


2D: Controversial
- Our work: RS appears to be stable
- Kimchi, Nahum, Senthil, PRX 2018: Likely weak AFM order

Random-Q J-Q model (large Q/J)



Strongest bond at each site
- empty if not strongest for both sites



Local susceptibility (normalized)

$$\chi_{\rm loc}(\mathbf{r}) = \int_0^{1/T} d\tau \langle S^z_{\mathbf{r}}(\tau) S^z_{\mathbf{r}}(0) \rangle$$

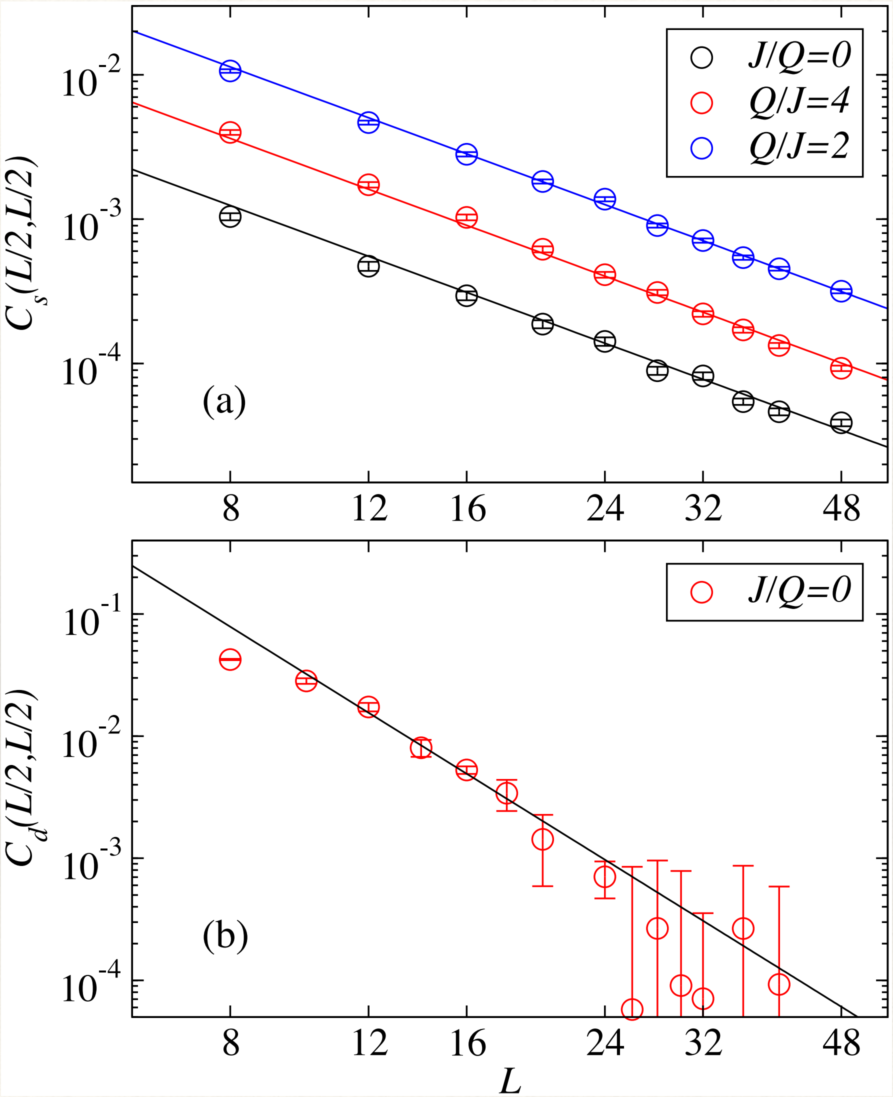
Mechanism of RS state formation

- spinons appear in pairs (not random distribution of spinons)
- domain walls mediate spinon-spinon interactions
- pairing avoids AFM order, instead power-law correlations

Some properties of the RS phase

- bimodal random Q model (J uniform)

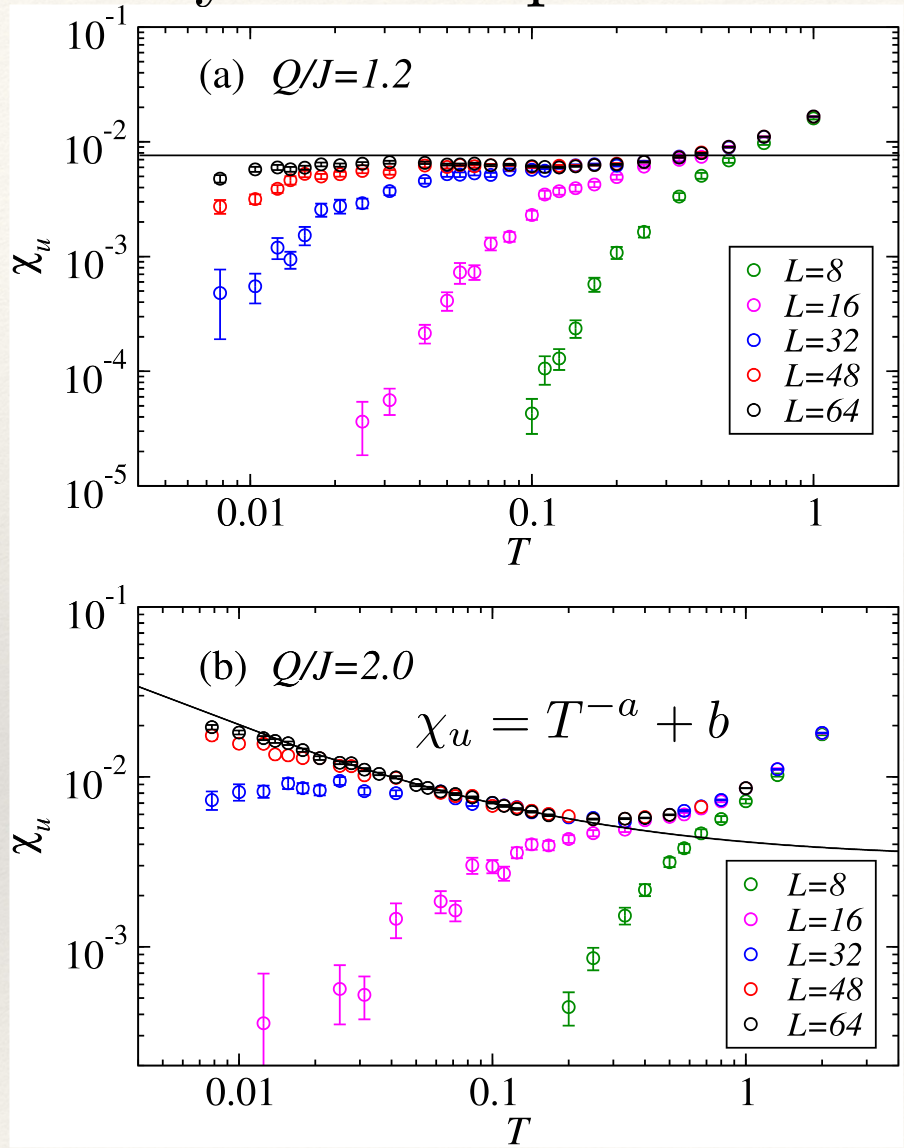
spin and dimer correlations



spin correlations ~$1/r^2$
dimer correlations ~$1/r^4$

$$\chi_u \propto T^{d/z-1}$$

dynamic exponent z



z=d=2 at AFM-RS boundary
z>2 inside RS phase

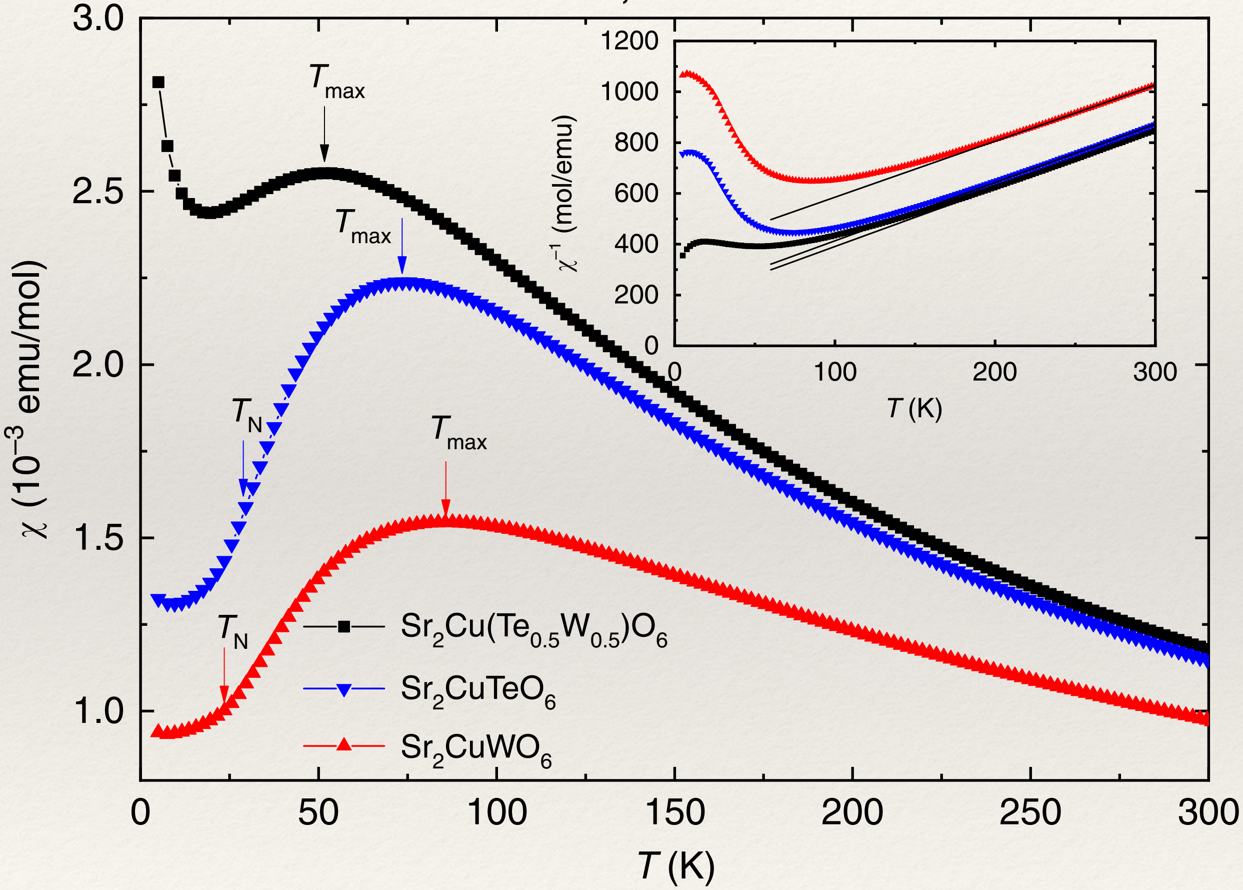
Experiments

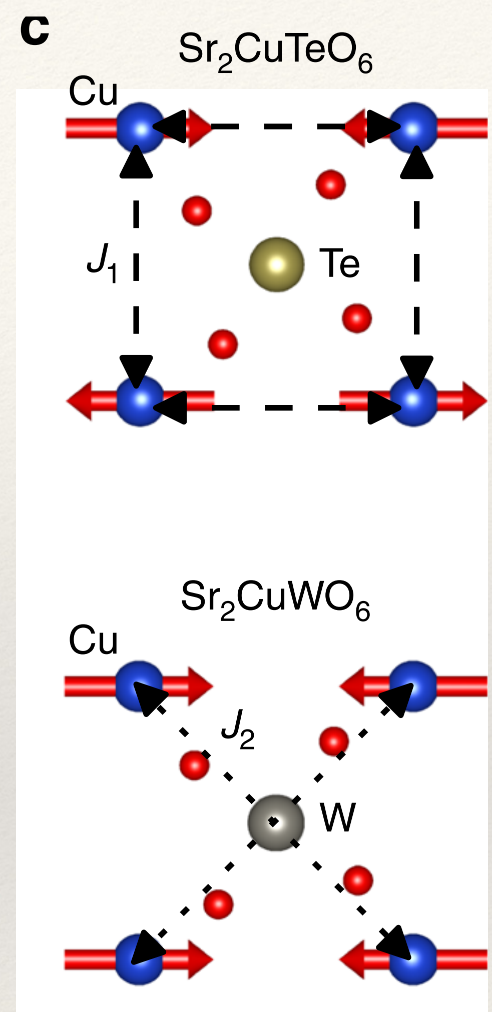
Some 'disordered spin liquids' may actually be RS states

Recent example $Sr_2CuTe_xW_{1-x}O_6$

- square-lattice S=1/2 system with J_1 or J_2 randomly on plaquettes

Mustonen et al, Nature Comm 2018



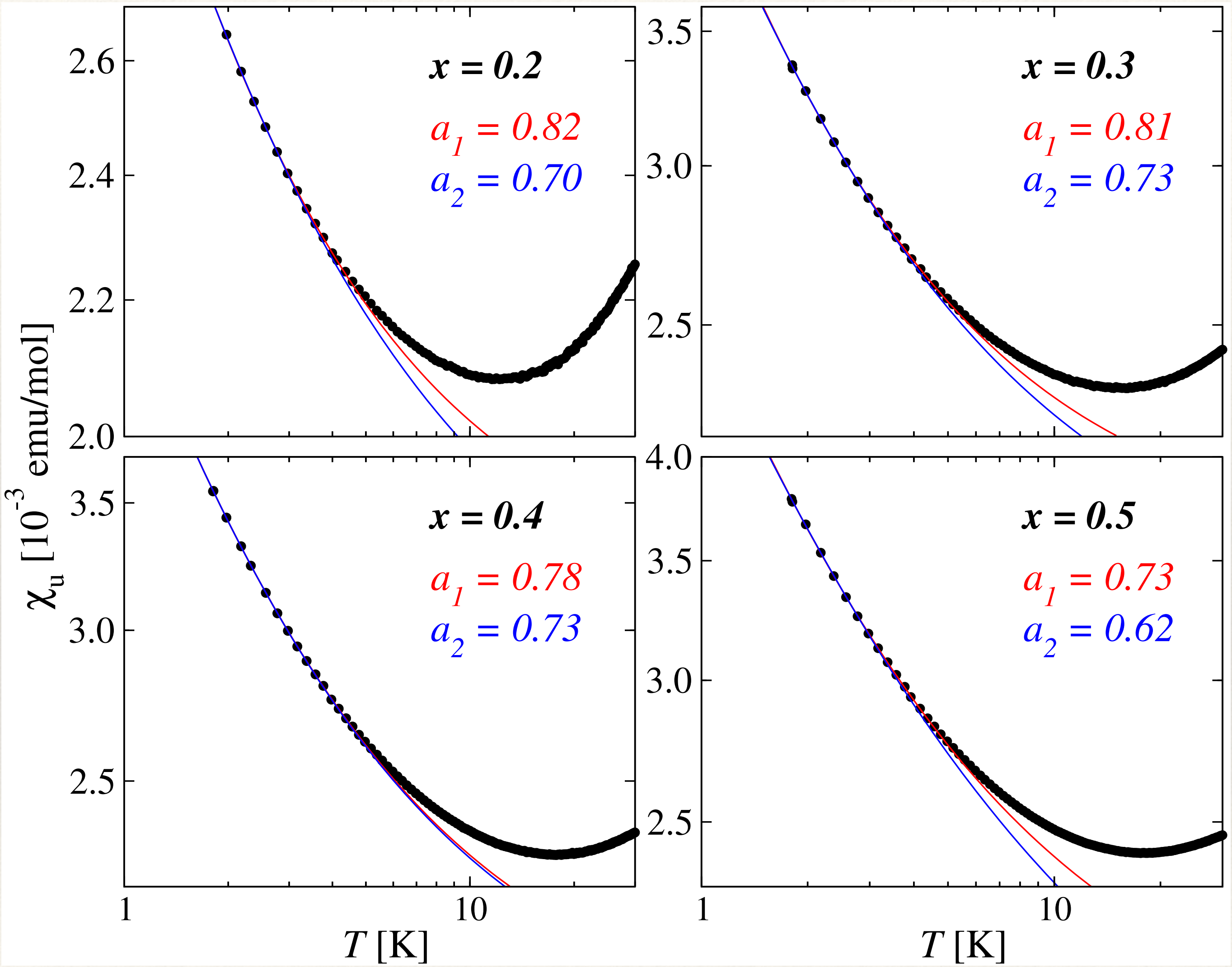


Susceptibility divergence for x=0.5 may be sign of RS

- re-analysis of experimental data shows power slower than 1/T

Analyzing data from Watanabe et al. PRB 98, 054422 (2018)

- fitting to constant + T^{-a}
- use different high-T cutoffs



Indication of slower than Curie divergence; possible RS phase