TOPMAT, CEA Saclay, June 12, 2018

Exploring Novel Quantum Phase Transitions with J-Q models (2D)

Anders W Sandvik
Institute of Physics, Chinese Academy of Sciences, Beijing
and Boston University

Part I

Symmetry-enhanced first-order transition between an AFM and a Z_2 VBS

Part II

AFM to random-singlet transition in the presence of disorder

SIMONS FOUNDATION

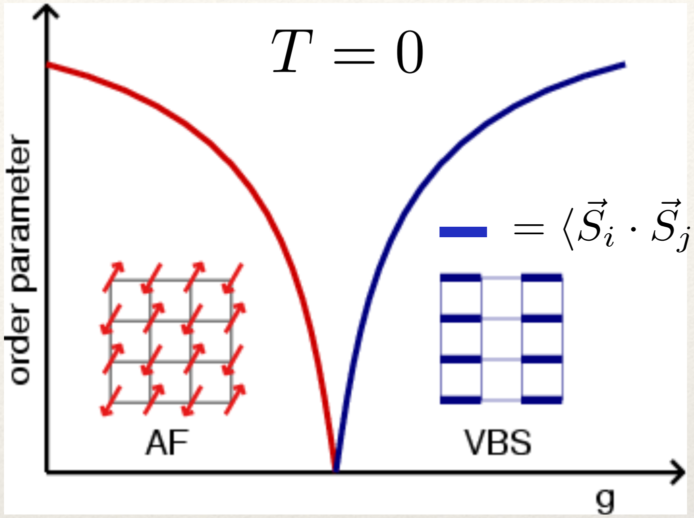
BOSTON UNIVERSITY

Broader context: deconfined quantum criticality

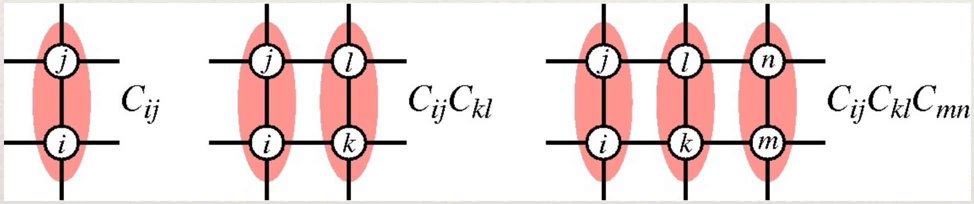
Senthil, Vishwanath, Balents, Sachdev, Fisher (Science 2004)
(+ many previous works; Read & Sachdev, Sachdev & Murthy, Motrunich & Vishwanath….)

Continuous AF - VBS transition at T=0

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



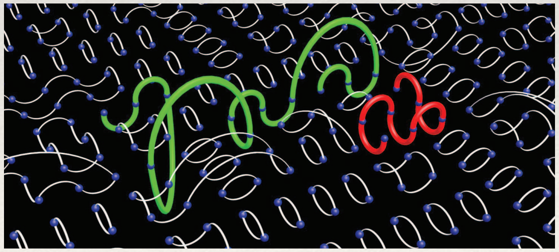
Numerical (QMC) tests using J-Q models



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

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

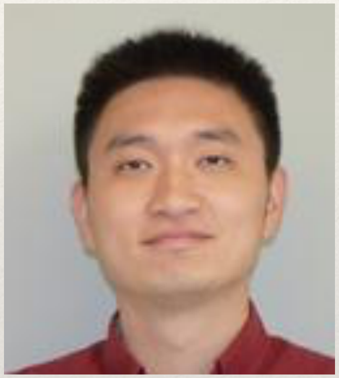
$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q \sum_{\langle ijkl \rangle} C_{ij} C_{kl}$$



- **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)]

Symmetry Enhanced First-Order Phase Transition in a 2D Quantum Antiferromagnet

in collaboration with
Bowen Zhao and Phil Weinberg (BU)



- Experimental motivation: Plaquette singlet solid (PSS) in $SrCu_2(BO_3)_2$
- J-Q model to mimic aspects of the Shastry-Sutherland model
- Simulation results; unusual AFM-PSS first-order transition
- Emergent O(4) symmetry

arXiv:1804.07115

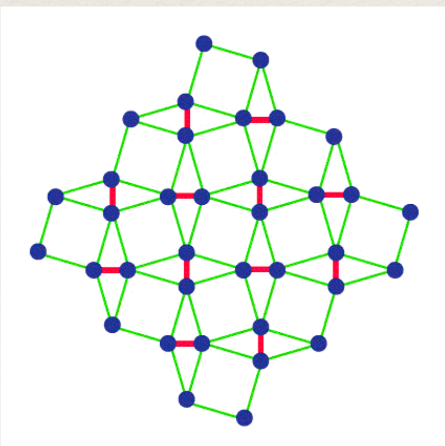
nature physics

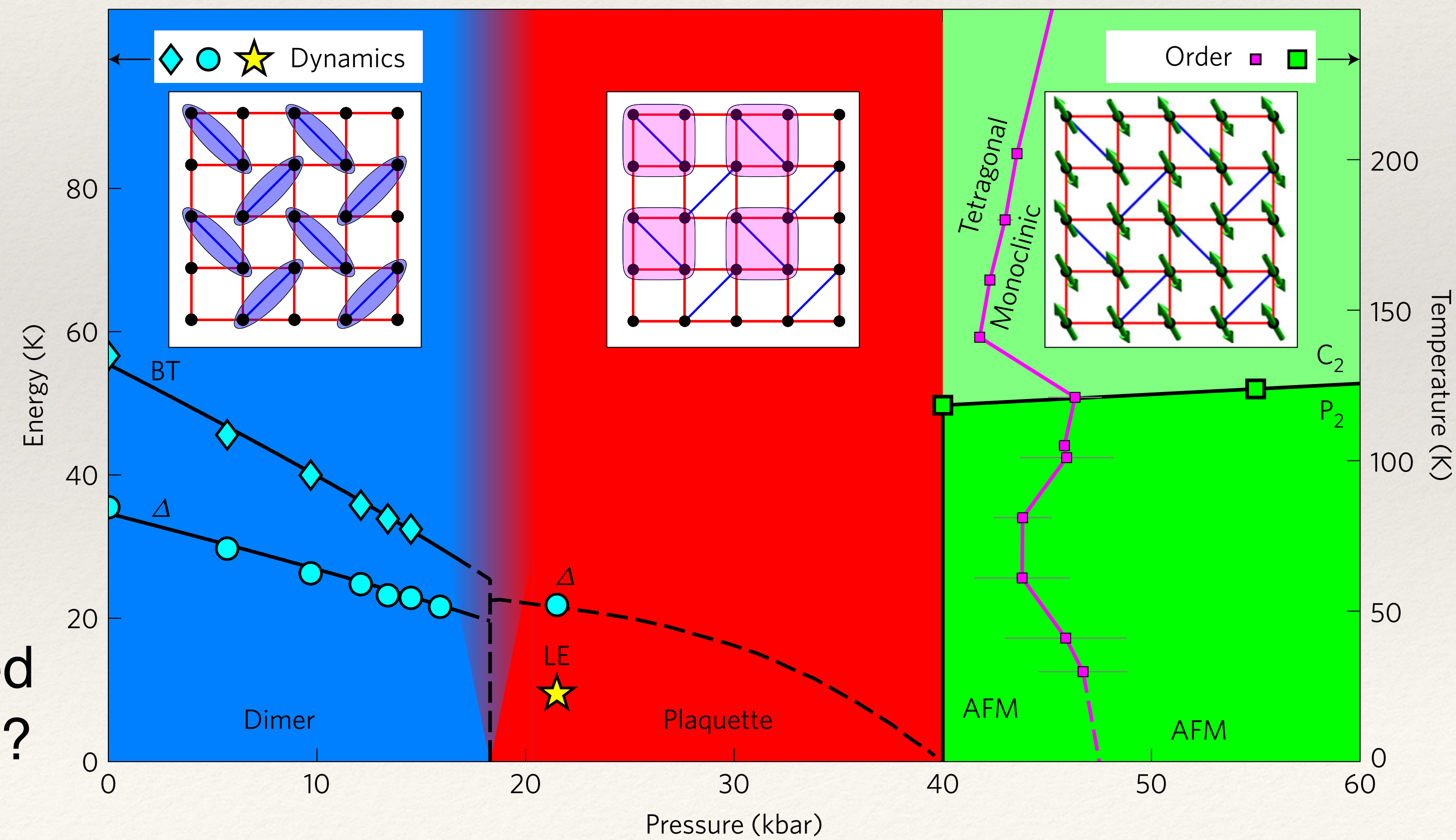
LETTERS

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]

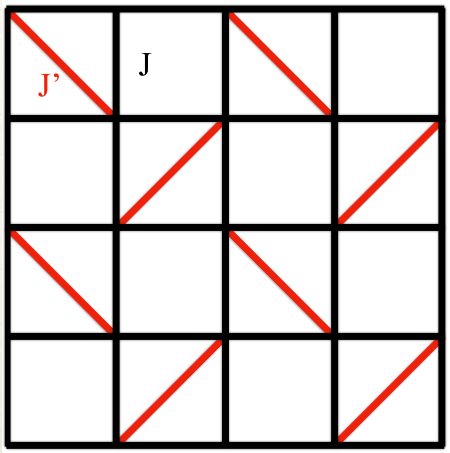


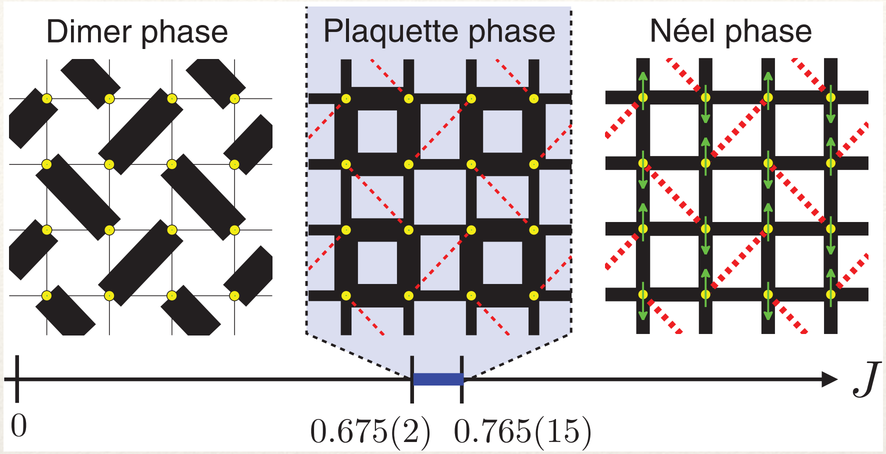


Is the Plaquette-AFM transition a deconfined quantum critical point?

Shastry-Sutherland (SS) model

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

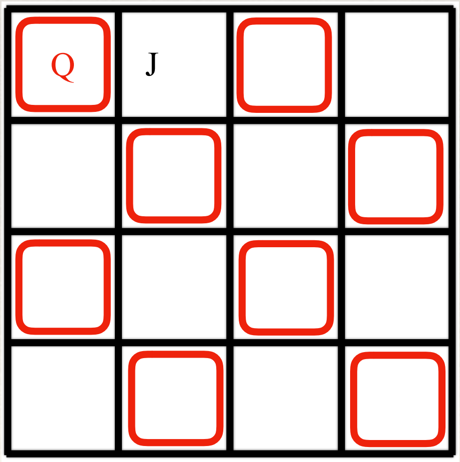




Corboz & Mila
PRB 2013

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

Checker-board J-Q (CBJQ) model



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

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

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

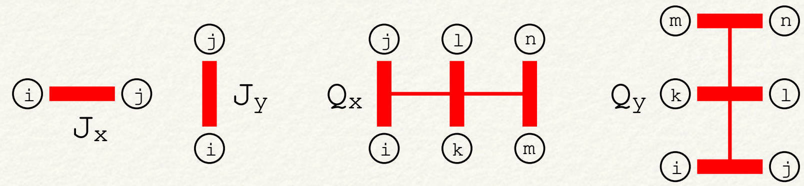
Do we get a PSS phase, and what kind of phase transition?

Detection of bond/plaquette order

Dimer order parameter

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

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



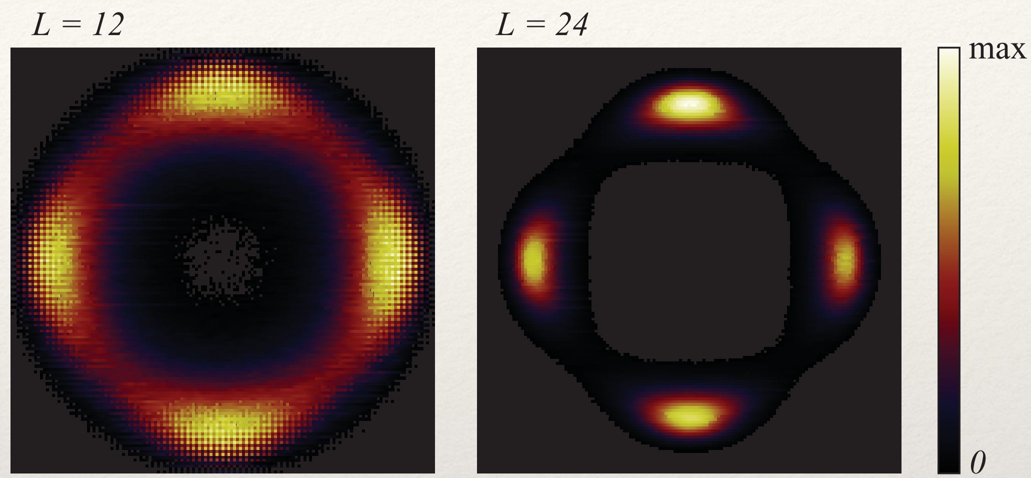
J-Q_3 model

J_x=J_y, Q_x=Q_y

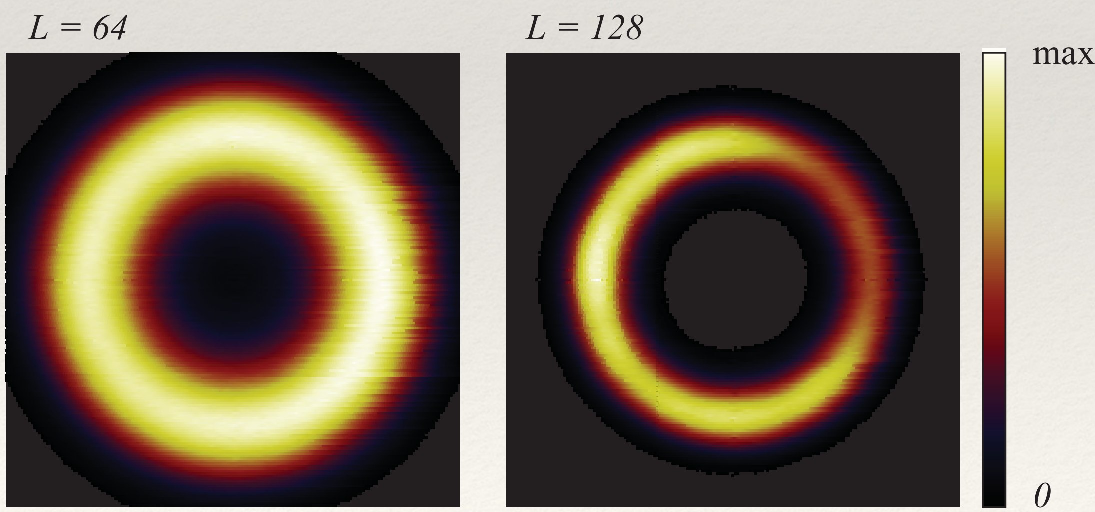
Lou, Sandvik, Kawashima, PRB (2009), Sandvik, PRB (2012)

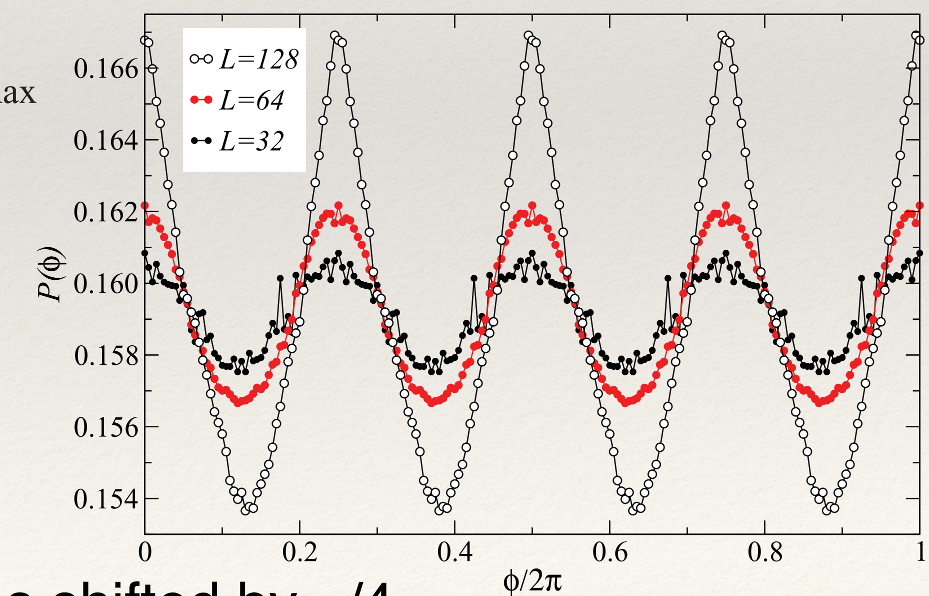
Collect histograms P(D_x,D_y) with valence-bond basis QMC

Strong columnar VBS when J/Q_3=0



J-Q_2 model with J/Q_2=0
- weak columnar VBS

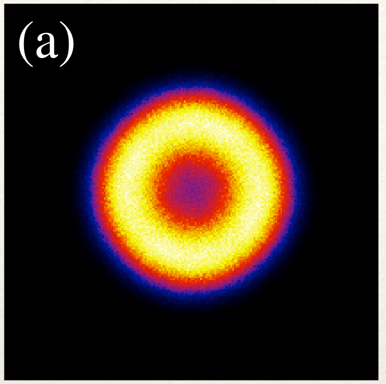




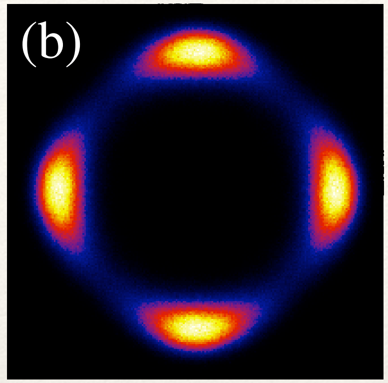
Plaquette singlet solid will have maximums shifted by $\pi/4$

Emergent symmetries at quantum critical points

- Symmetries that are not apparent in a system's Hamiltonian
- Only seen (emerge) at low energy, large length scales



near-critical VBS



VBS

Emergent U(1) symmetry of the VBS at the deconfined quantum-critical point

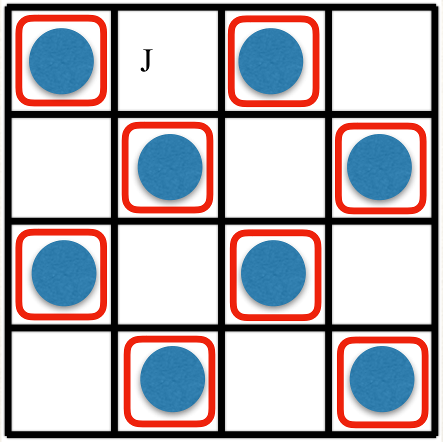
Even higher symmetries proposed in some scenarios
- SO(5) symmetry for deconfined criticality in SU(2) spin systems
- O(4) symmetry in U(1) (planar) spin systems

Discussed recently, e.g., by
- Wang, Nahum, Metlitski, Xu, Senthil, PRX 2017
- Qin, He, You, Xu, Sen, Sandvik, Xu, Meng, PRX 2017

Emergent symmetries may also be manifested approximately at weak first-order transitions (close to critical points with emergent symmetries or approximate such symmetries); Wang et al. PRX 2017
- how close do we have to be?

Plaquette-Singlet Solid state in the CBJQ model

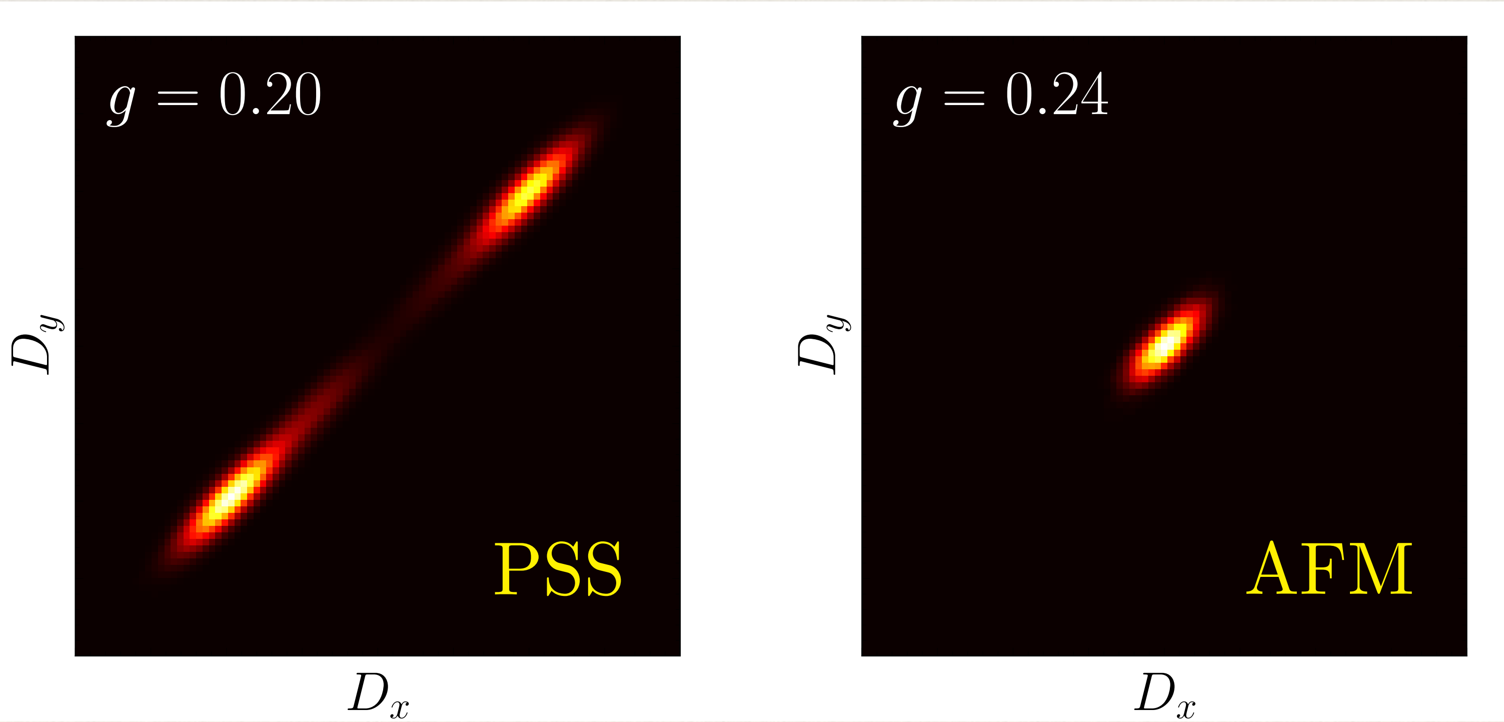
The lattice and interactions are compatible with
- 4 fold degenerate columnar VBS
- 2-fold degenerate PSS state



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 $P(D_x,D_y)$



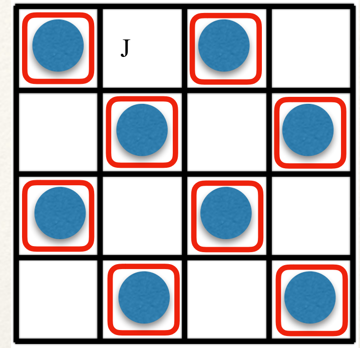
We find 2-fold PSS order for small g=J/Q

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:

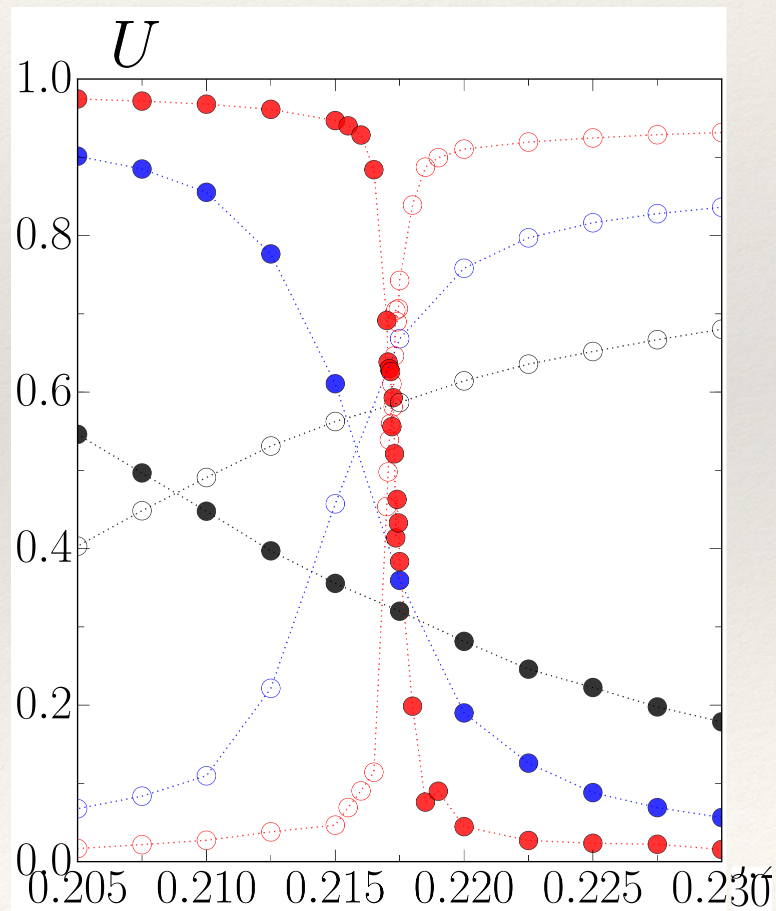
$$U_s = \frac{5}{2}\left(1 - \frac{\langle m_s^4\rangle}{3\langle m_s^2\rangle^2}\right) \quad U_p = \frac{3}{2}\left(1 - \frac{\langle m_p^4\rangle}{3\langle m_p^2\rangle^2}\right)$$

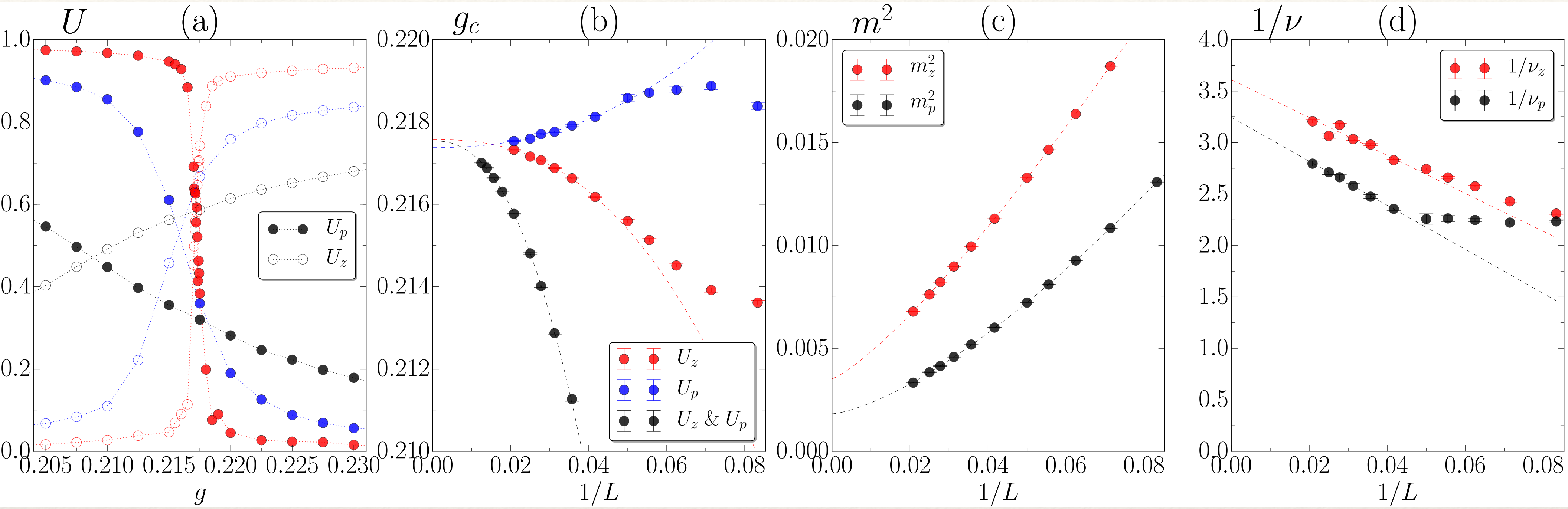
Expectation:
$U_s \to 1$, $U_p \to 0$ in AFM phase
$U_s \to 0$, $U_p \to 1$ in PSS phase

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

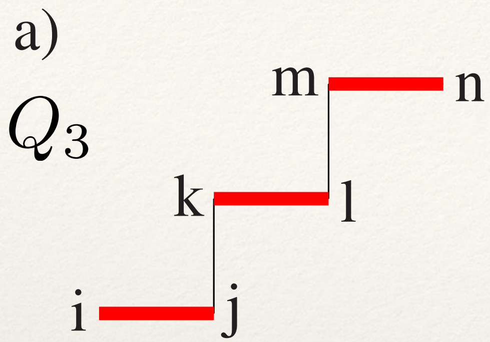
$$\frac{1}{\nu_{sp}} = \frac{1}{\ln(b)} \ln \left[\frac{dU_{sp}(g, bL)/dg}{dU_{sp}(g, L)/dg} \right]_{g=g_c(L)}$$

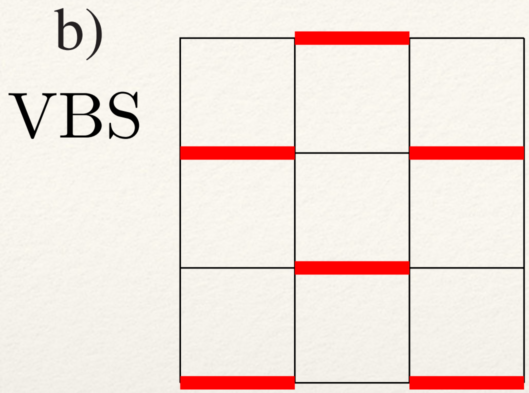
Both exponent extrapolate to values > d+1 = 3; first-order behavior

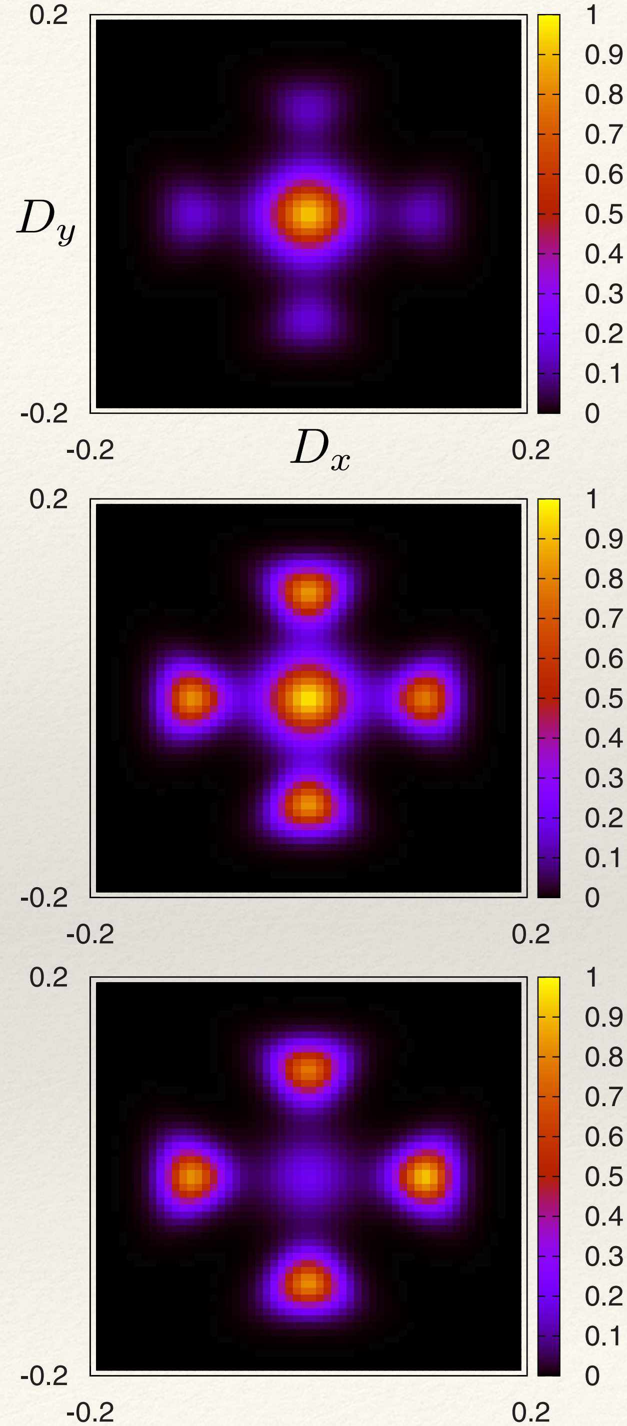
Why are there no negative Binder peaks?

Conventional first-order case

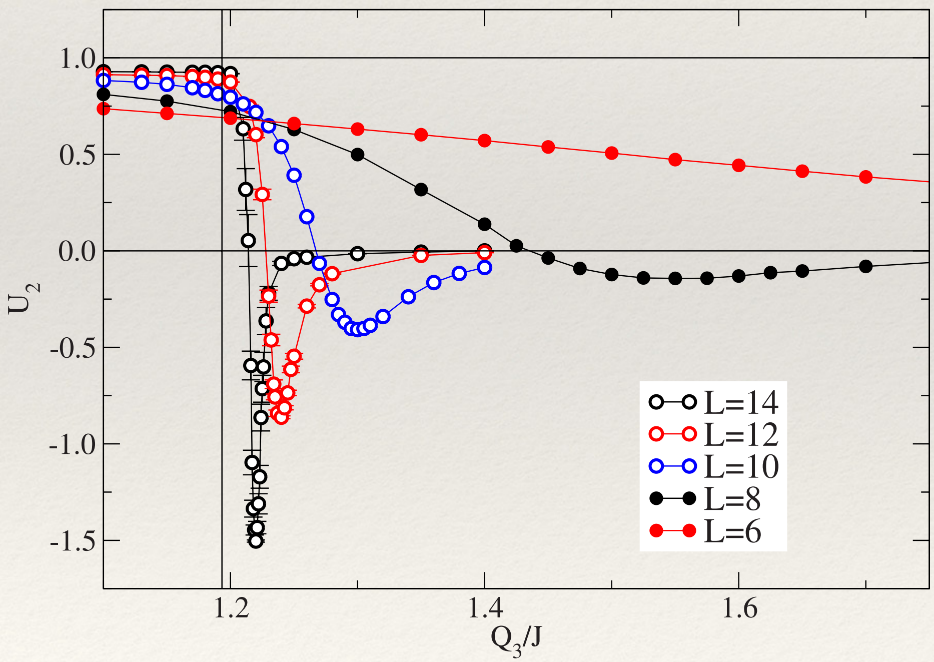
Staircase J-Q_3 model [Sen, Sandvik, PRB 2010]







Binder cumulant of AFM order parameter



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

CBJQ model seems unusual

Do we know any phase transition with similar characteristics?

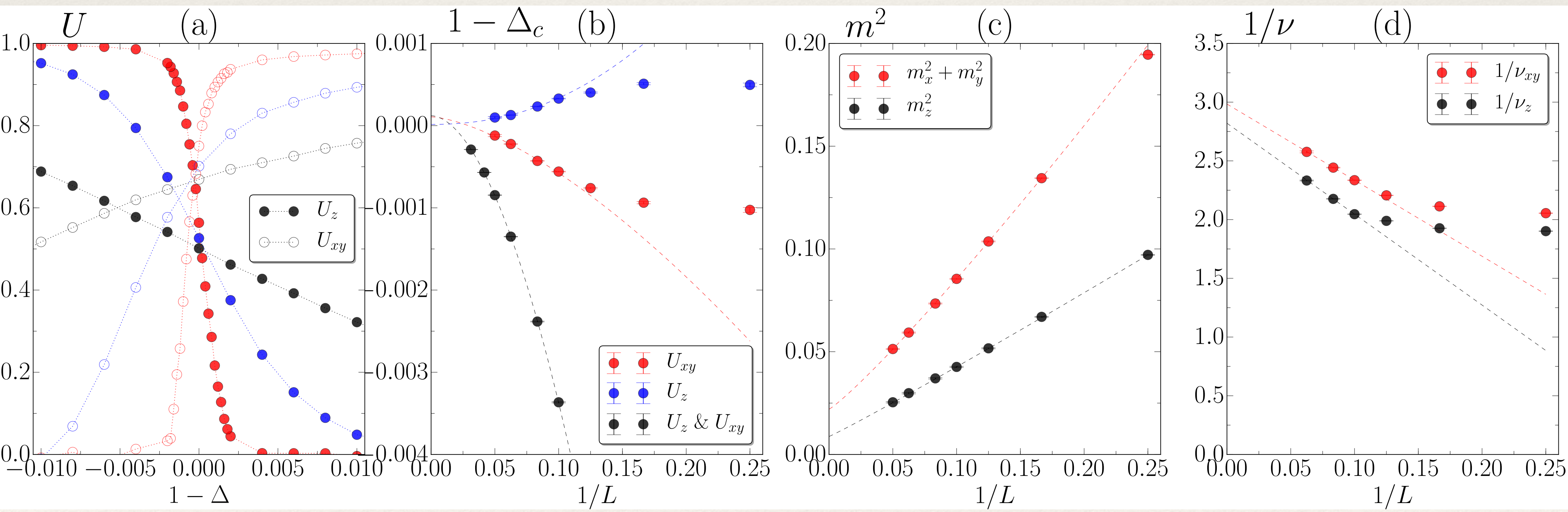
Yes: 3D O(N) models with N=3,4,5,… in their ordered states ($T < T_c$)

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

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

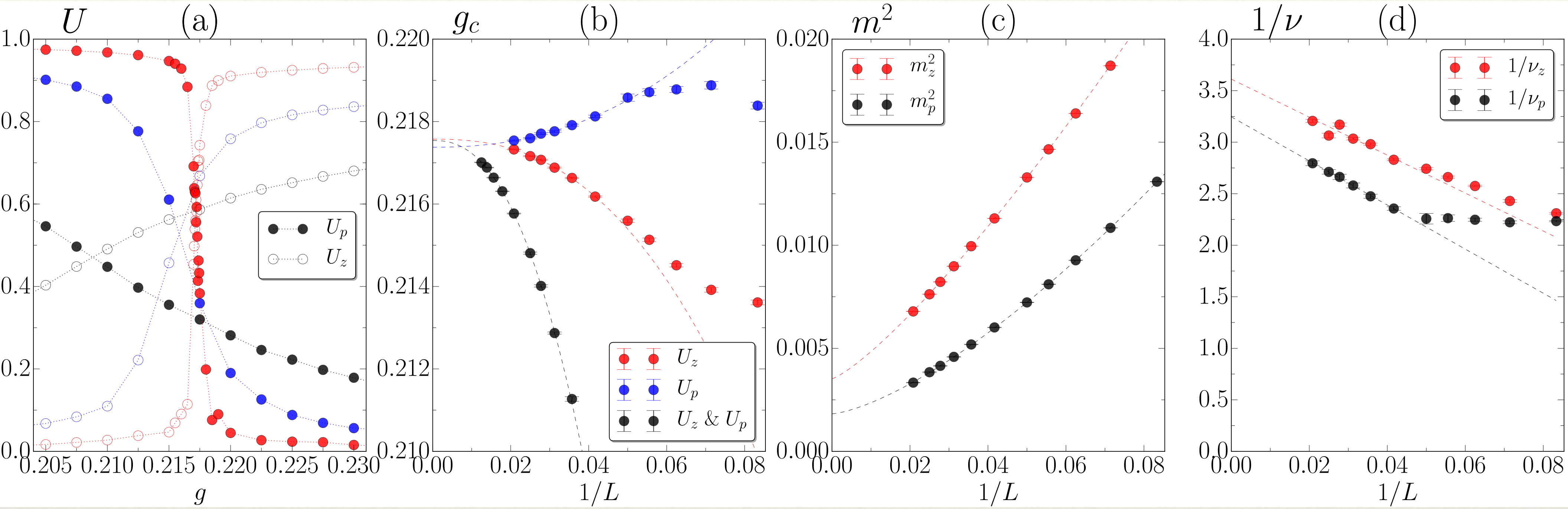
Symmetry changes vs Δ: O(2) for $\Delta<1$, O(3) for $\Delta=1$, Z_2 for $\Delta>1$

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

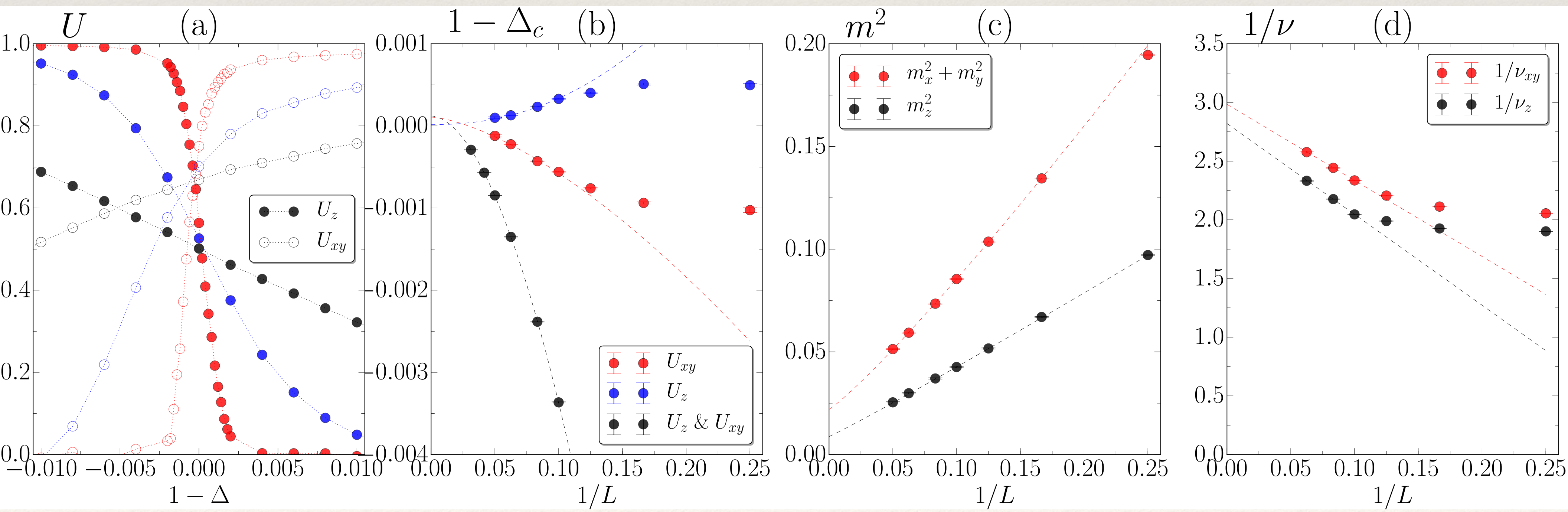


Very similar behaviors as CBJQ model!

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



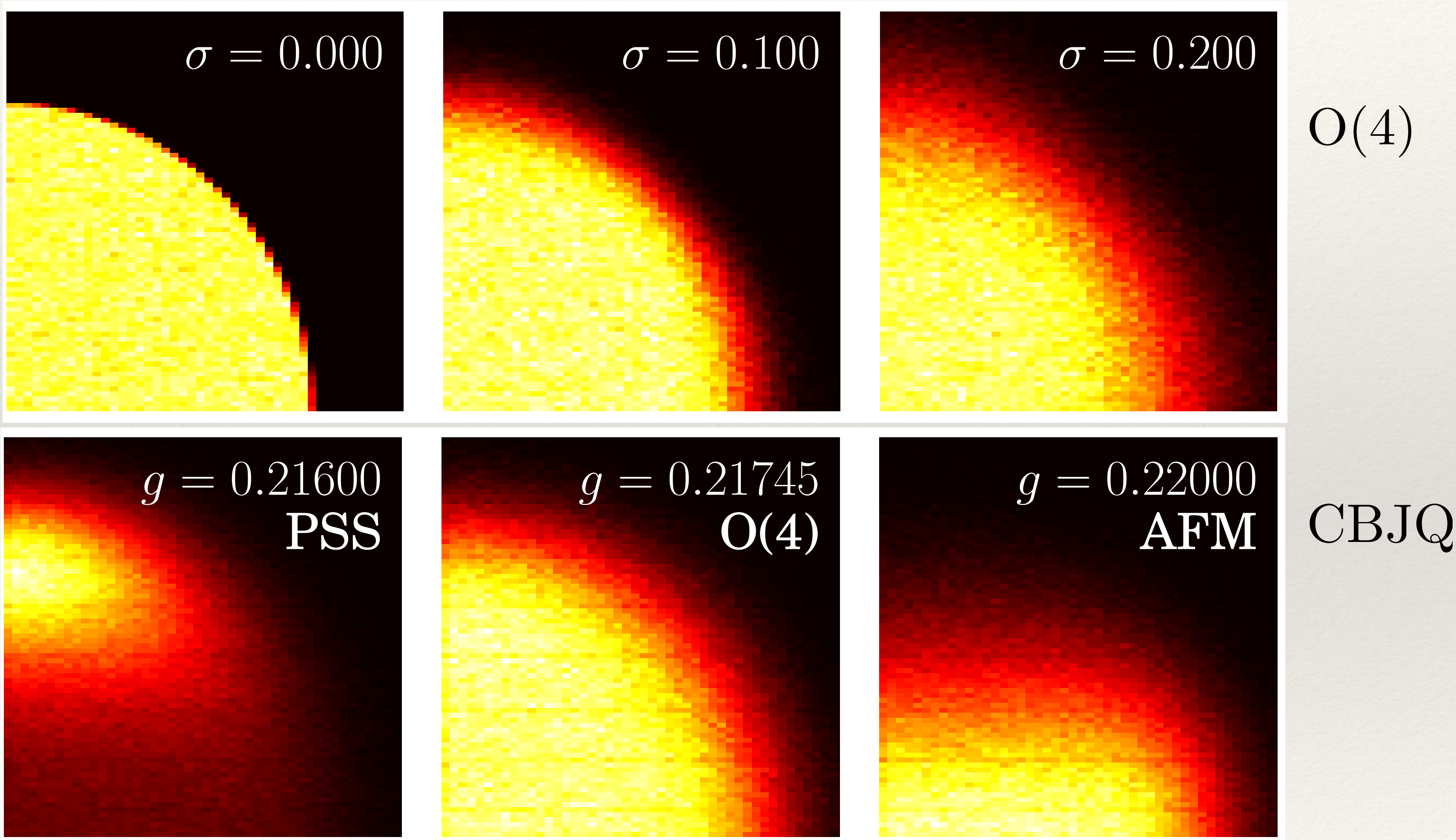
U
(a)
U_p
U_z
g
g_c
(b)
U_z
U_p
U_z & U_p
$1/L$
m^2
(c)
m_z^2
m_p^2
$1/L$
$1/\nu$
(d)
$1/\nu_z$
$1/\nu_p$
$1/L$



U
(a)
U_z
U_{xy}
$1-\Delta$
$1-\Delta_c$
(b)
U_{xy}
U_z
U_z & U_{xy}
$1/L$
m^2
(c)
$m_x^2+m_y^2$
m_z^2
$1/L$
$1/\nu$
(d)
$1/\nu_{xy}$
$1/\nu_z$
$1/L$

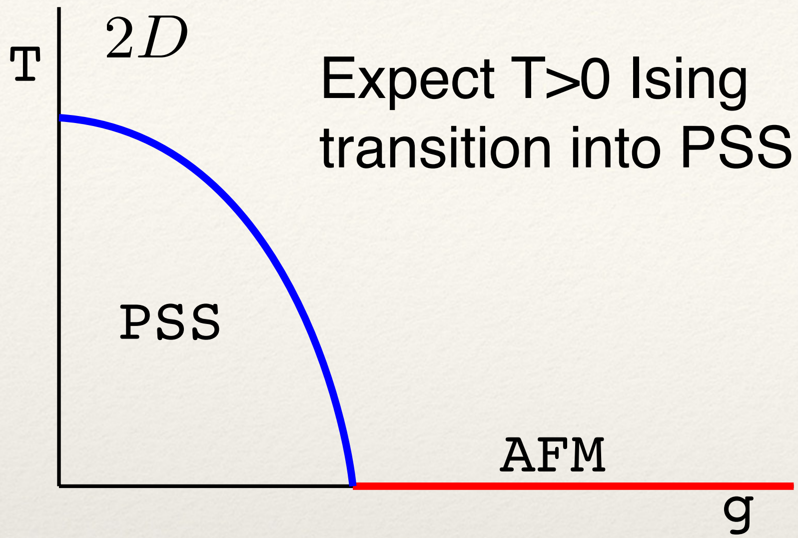
Detecting O(4) symmetry in the CBJQ model

- 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

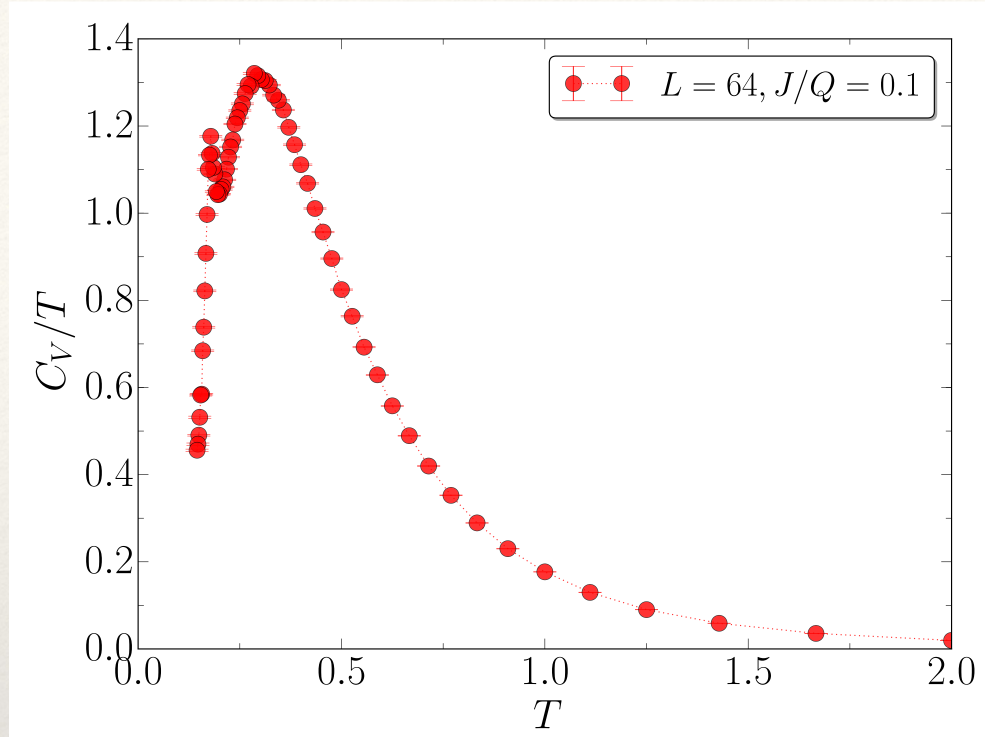


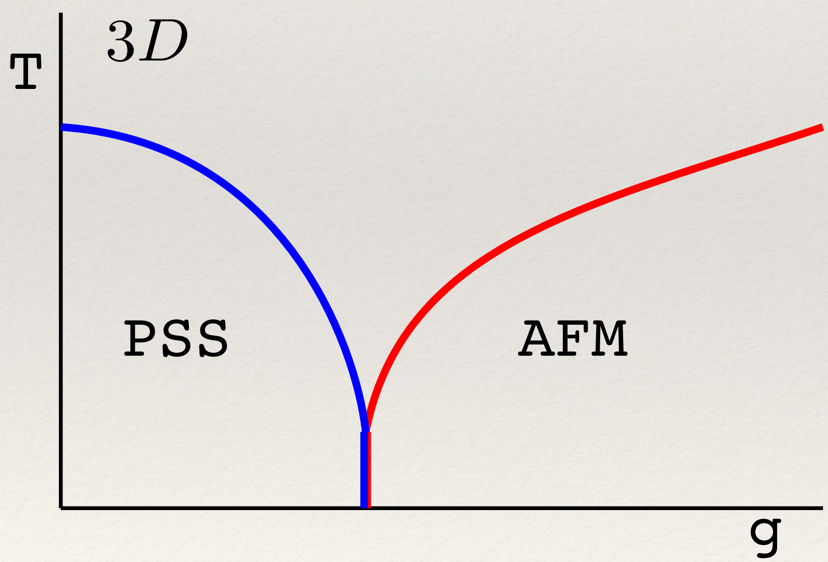
- Appears that there is an O(4) point (the transition point)
- No sign of conventional AFM, PSS coexistence

T>0 phase diagram and specific heat



Expect T>0 Ising transition into PSS





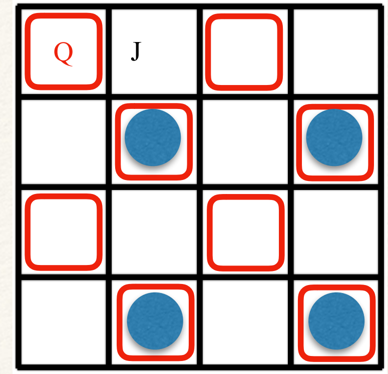
Entropy change small at T>0 transition

- 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?

Same behavior expected in $SrCu_2(BO_3)_2$

Conclusions



CBJQ model with weak first-order AFM-PSS transition

- new type of symmetry-enhanced first-order transition
- more precise tests of symmetry underway
- may be approximate symmetry, but large length-scale

Related on classical 3D loop models (Serna, Nahum, arXiv:1805.03759)
- Z_2 deformation of Z_4 gives near-O(4) symmetry close to dqcp

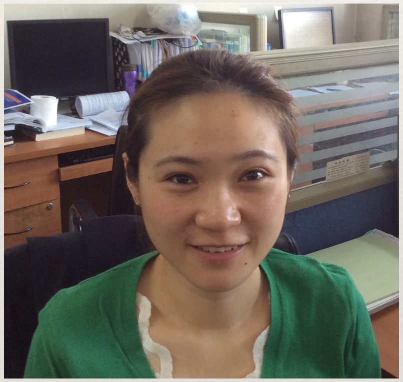
Future theoretical/computational steps:
Connection to deconfined quantum criticality?

- extended model with Q_A and Q_B (on “black” and “white” squares)
- regular J-Q model when $Q_A = Q_B$
- how does the discontinuity vanish when $Q_A \rightarrow Q_B$?
- weak 3D couplings between layers (quasi-2D)
- etc….

Experiments on $SrCu_2(BO_3)_2$
- in progress at IOP, Beijing (specific heat under high pressure)

Random-Singlet Phase in the 2D Disordered J-Q model

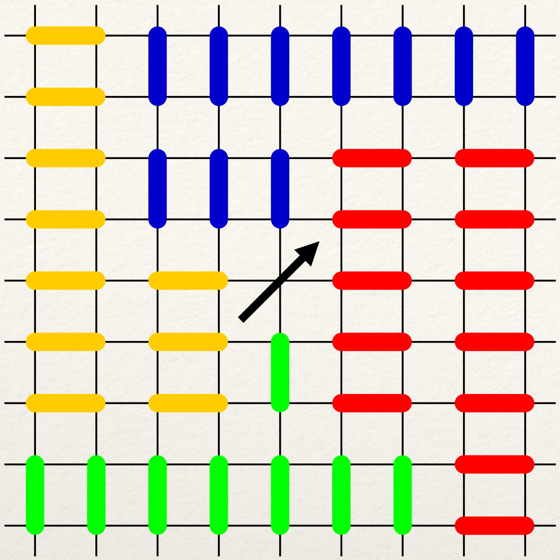
in collaboration with
Lu Liu (Beijing Normal University)
Hui Shao (Beijing CSRC and BU)
Yu-Cheng Lin (NCCU, Taipei, Taiwan)
Wenan Guo (Beijing Normal University)

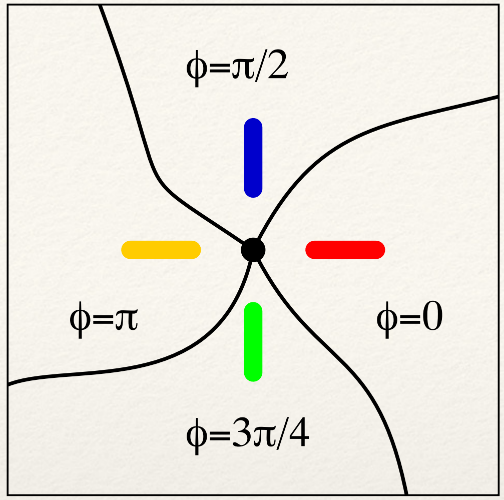



- Theoretical motivation: VBS and DQCP in the presence of disorder
- Experimental motivation: Spin Liquids with disorder
- QMC evidence for random singlet (RS) phase
- properties of the RS phase and nature of AFM-RS transition

arXiv:1804.06108

Localized spinons in a disordered square-lattice VBS





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

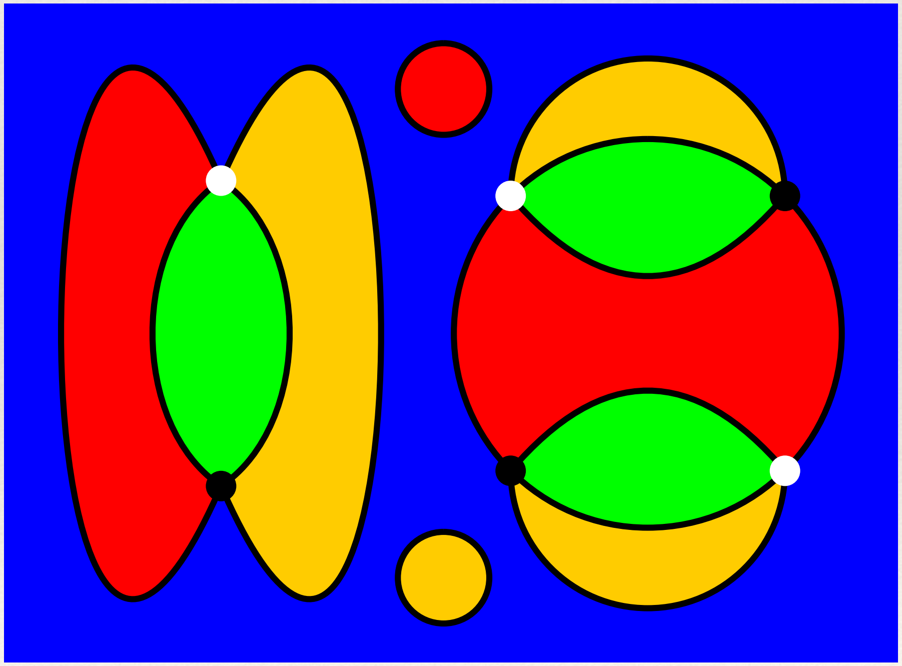
Spinons will form in pairs

What kind of magnetic state forms from interacting spinons?

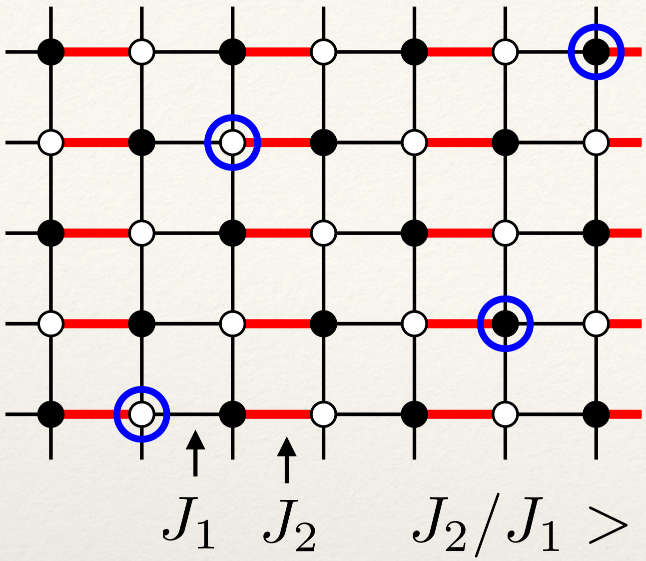
1D: RS state forms generically

2D: Controversial

- Our work: RS appears to be stable
- Kimchi, Nahum, Senthil, arXiv:1710.06860: Weak AFM order

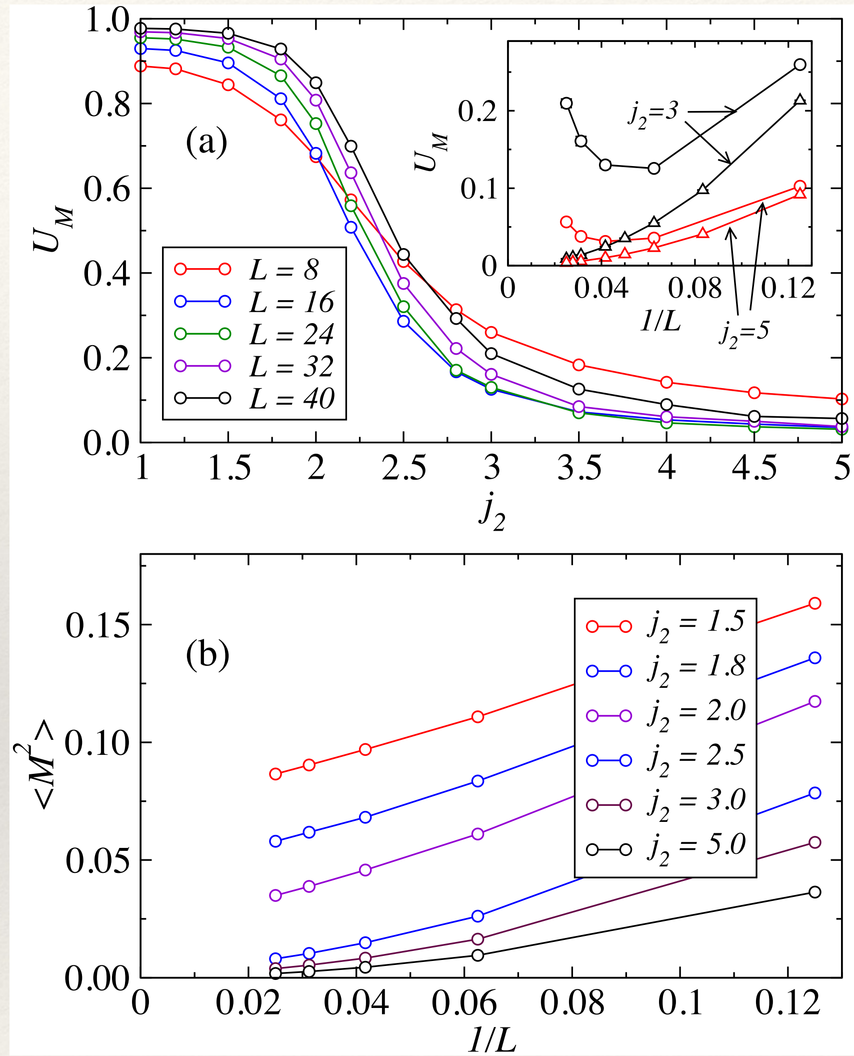


Simpler system: site diluted Heisenberg dimer system



$J_2/J_1 > 1.91$

T=0 projector QMC results
- Binder cumulant, sublattice magn.



Unpaired 'dangling spin' moments form in gapped host system

Effective bipartite interactions

Moments form weak AFM order

Is this the faith of the spinons in the square-lattice disordered VBS?

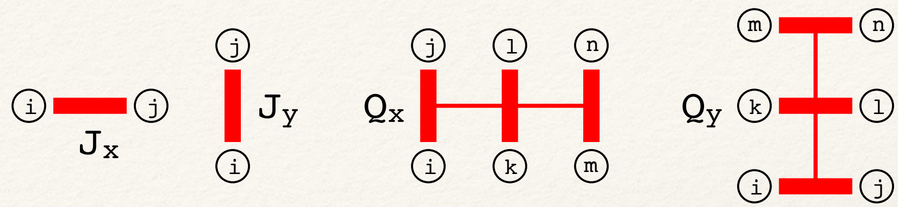
Kimchi, Nahum, Senthil: Most likely, yes
- frustrated interactions required to induce RS state (unstable to spin glass?)

Our conclusion: AFM-RS transition and RS phase in the J-Q model

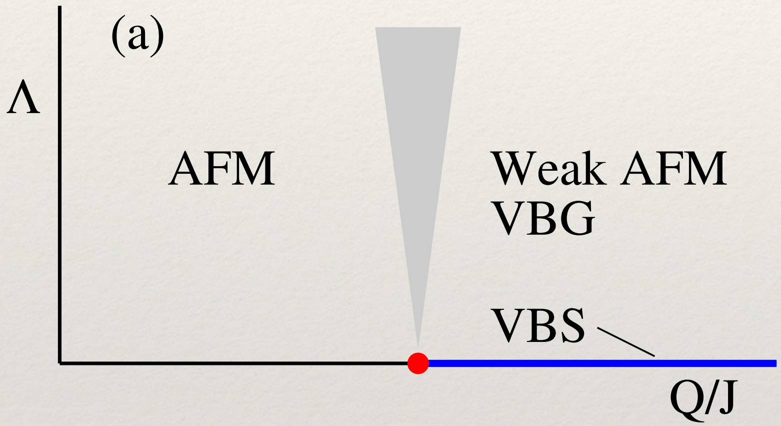
Models, schematic phase diagrams

2D square-lattice J-Q_3 model with site dilution, or random J or random Q

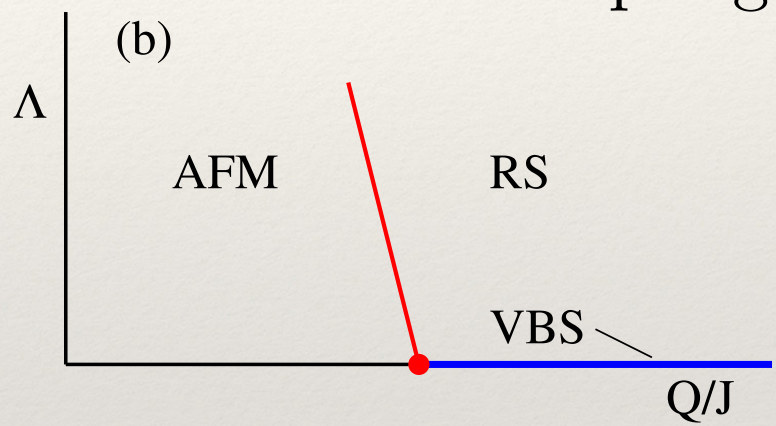
$$H = -J\sum_{\langle ij\rangle} P_{ij} - Q\sum_{\langle ijklmn\rangle} P_{ij}P_{kl}P_{mn}$$



site dilution



random couplings



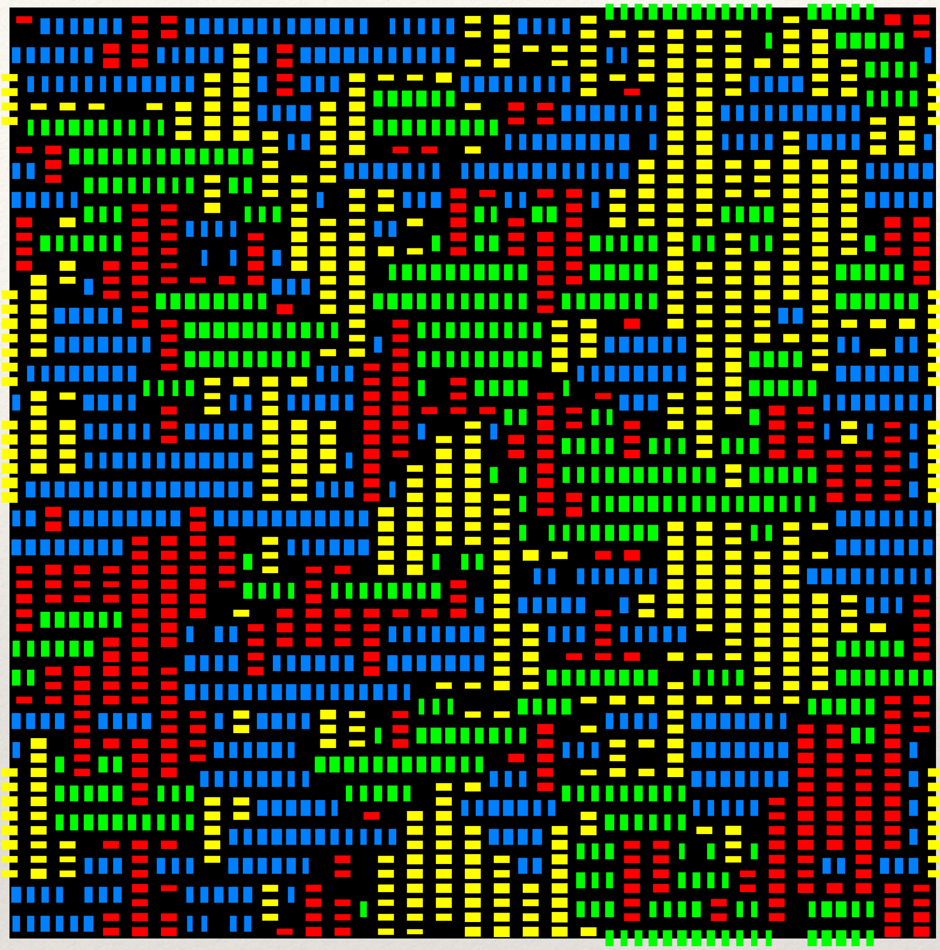
Λ = disorder strength

- definition depends on model
- Λ not varied systematically here
- schematic phase diagrams inferred from examples

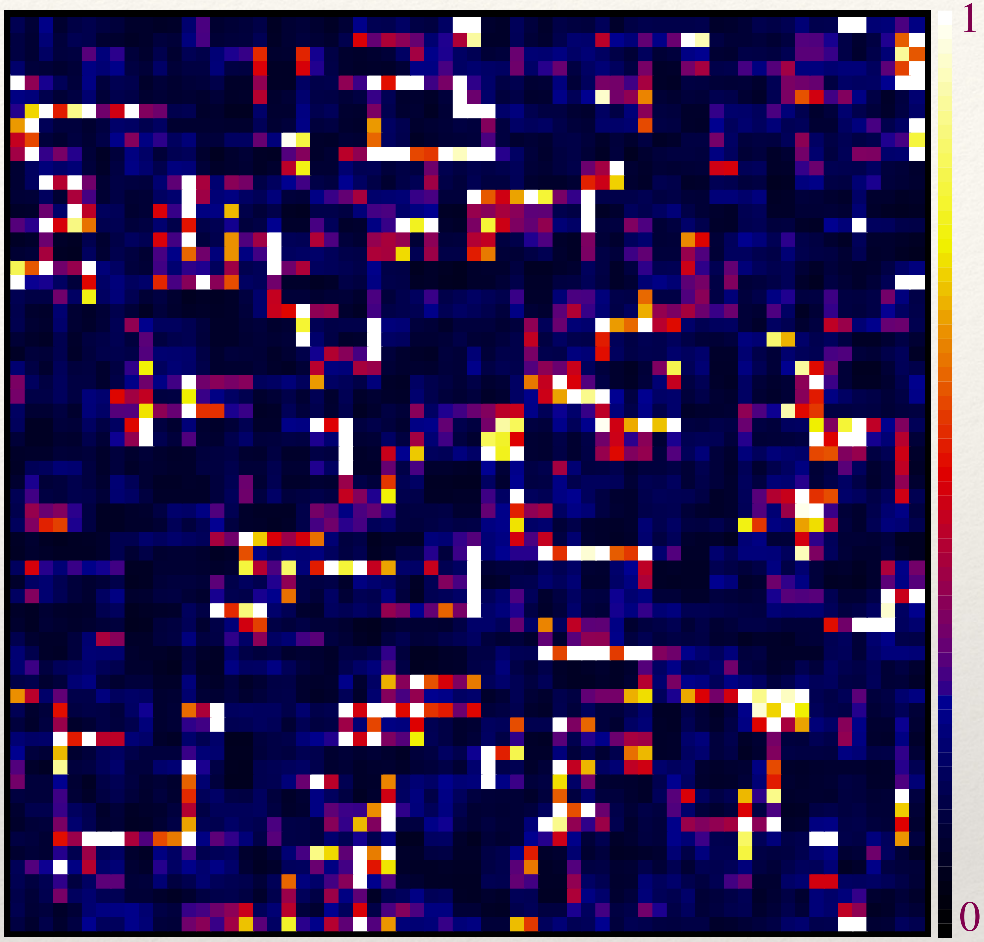
T=0 and T>0 QMC calculations

- existence of RS phase
- properties of RS phase
- nature of AFM-RS transition

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



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



Local susceptibility (normalized)

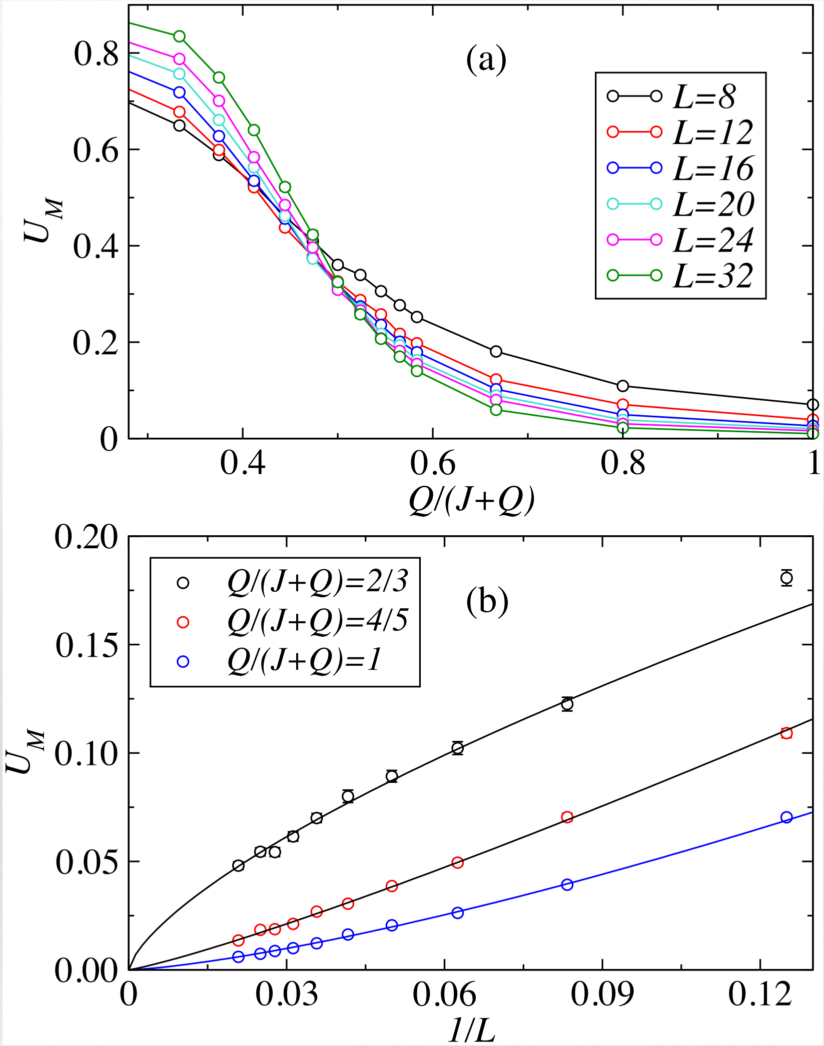
$$\chi_{\mathrm{loc}}(\mathbf{r}) = \int_0^{1/T} d\tau \langle S^z_{\mathbf{r}}(\tau) S^z_{\mathbf{r}}(0)\rangle$$

Mechanism of RS state formation

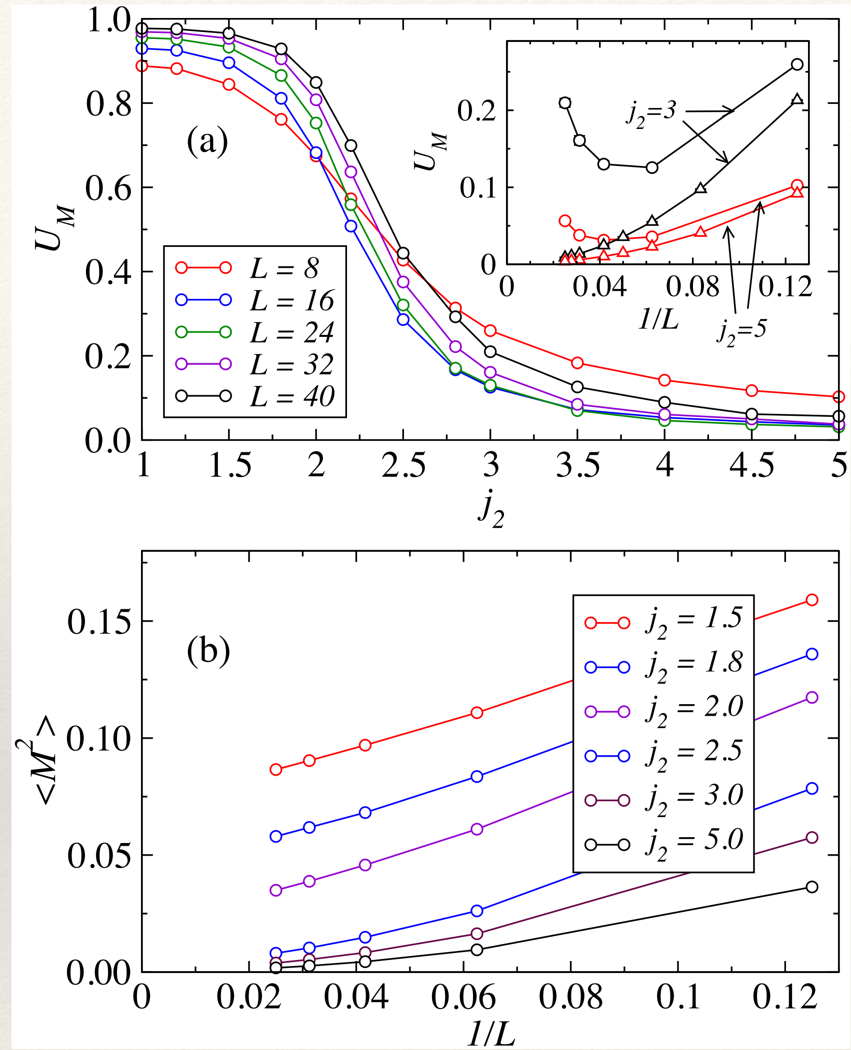
- spinons appear in pairs (not random distribution of spinons)
- domain walls mediate spinon-spinon interactions
- pairing avoids AFM order, instead power-law correlations

AFM order parameter in the disordered VBS

random Q



diluted J_1-J_2



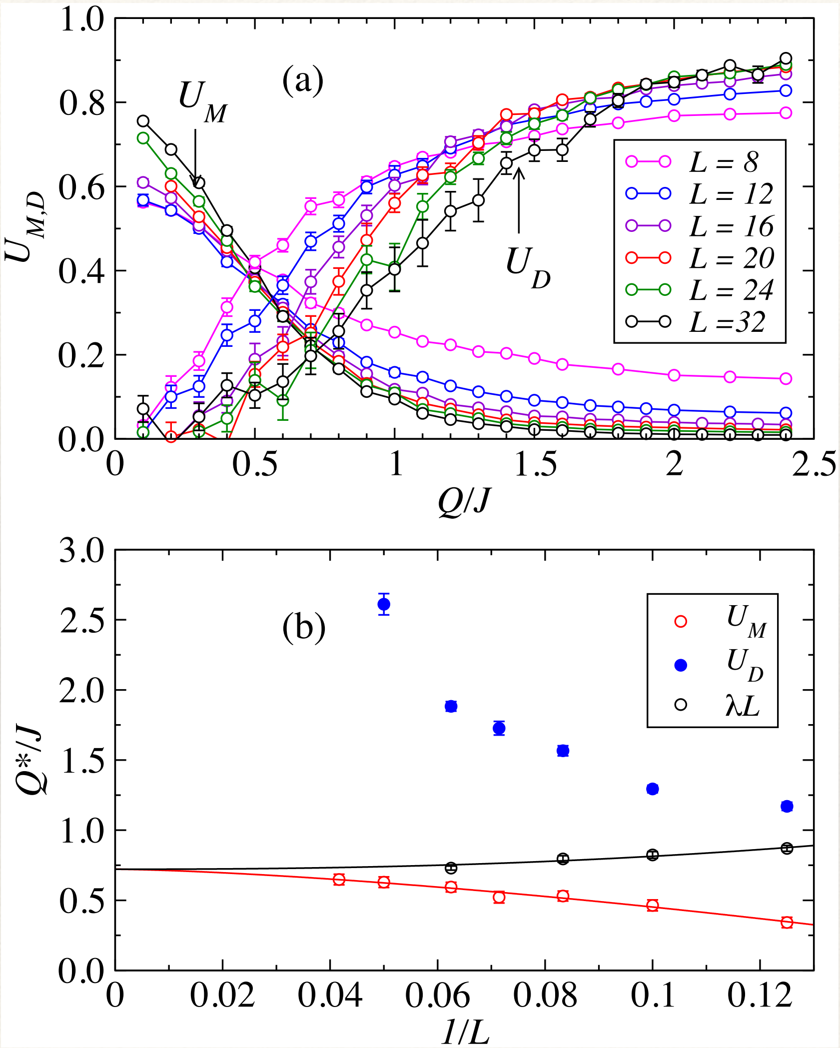
Behavior suggests no AFM order in the random Q model for large Q

- qualitatively different from diluted systems (convergent cross points)
- suggests an RS phase

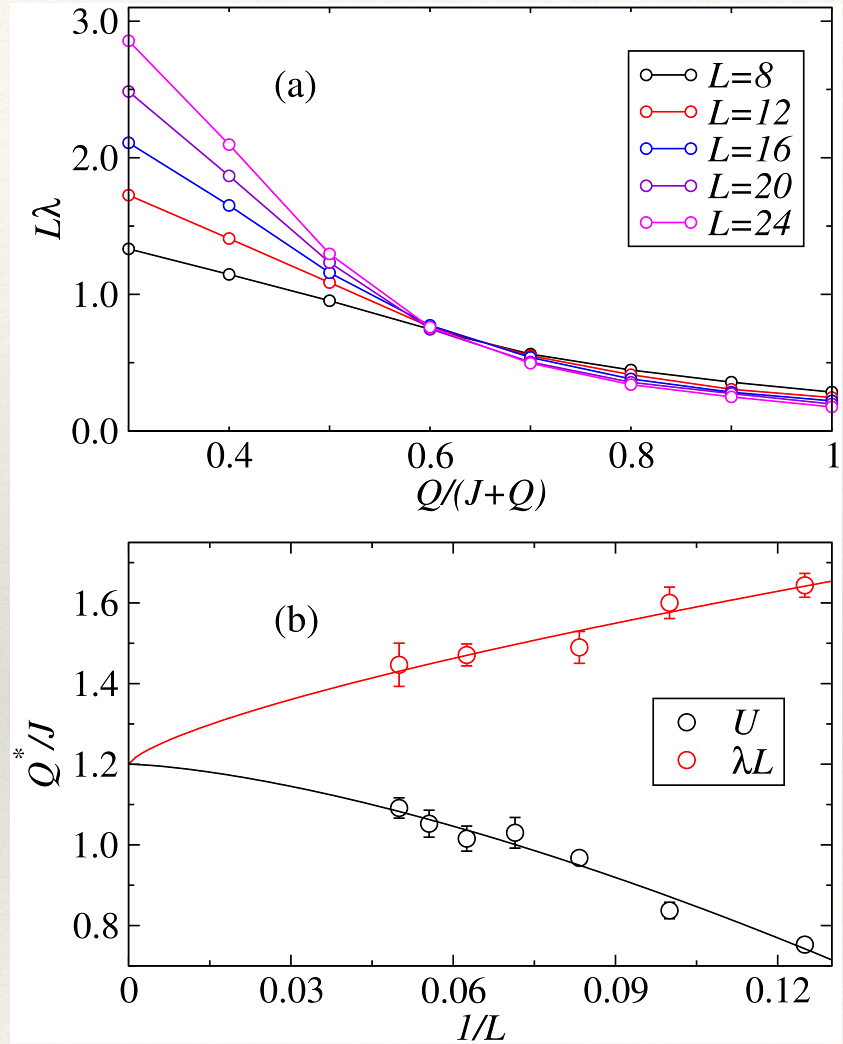
AFM-RS quantum phase transition

Transition point Q*(L) detected by AFM cumulant and string-length crossings

random J



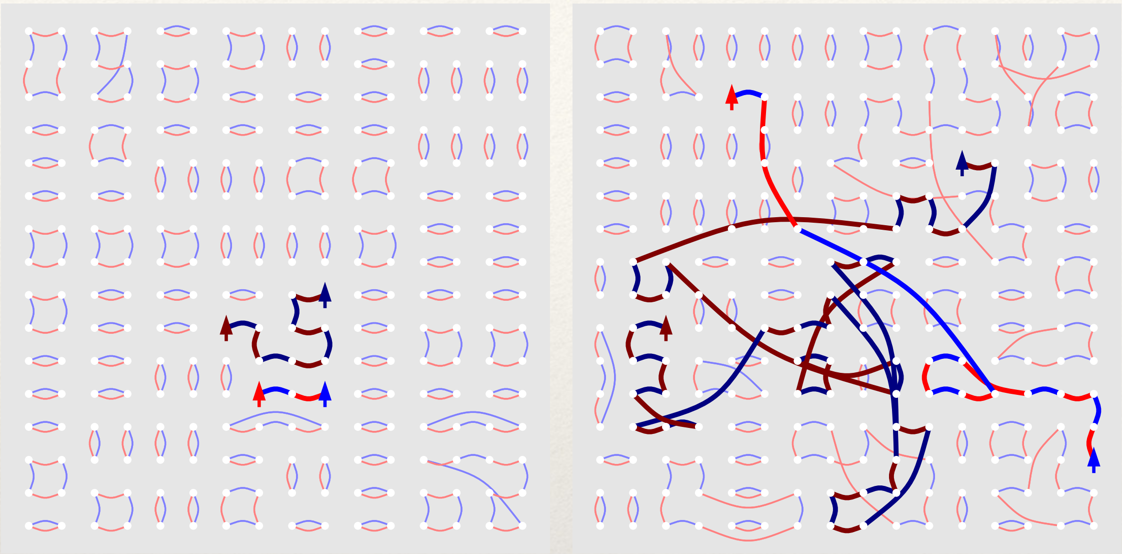
random Q

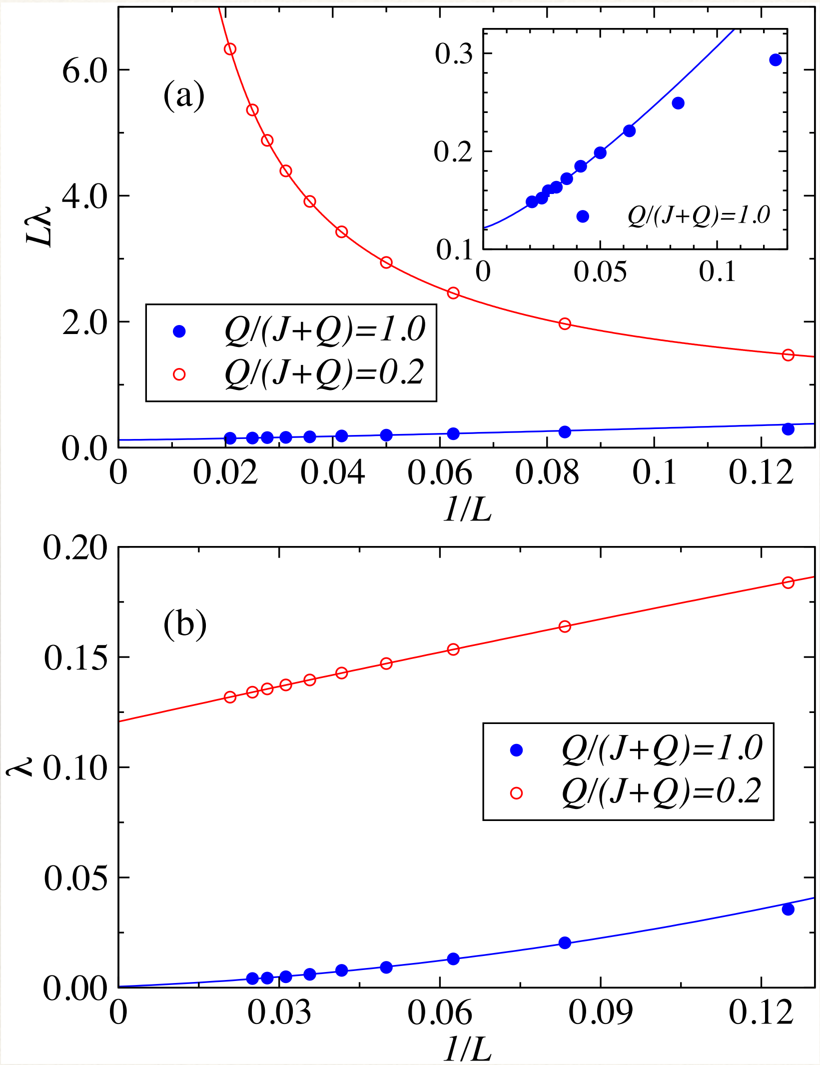


Perfect agreement between the two detection methods

Spinon strings in the valence-bond basis

S=1 state represented by N/2 valence bonds, 2 unpaired (up) spins
- overcompleteness → 2 open strings in transition (overlap) graphs





The string fraction λ~constant in AFM state
- Anderson S=1 quantum rotor state (extended, not particle-like state)

λ~1/N=1/L^2 in clean VBS state
- bound spinons → triplon (particle)

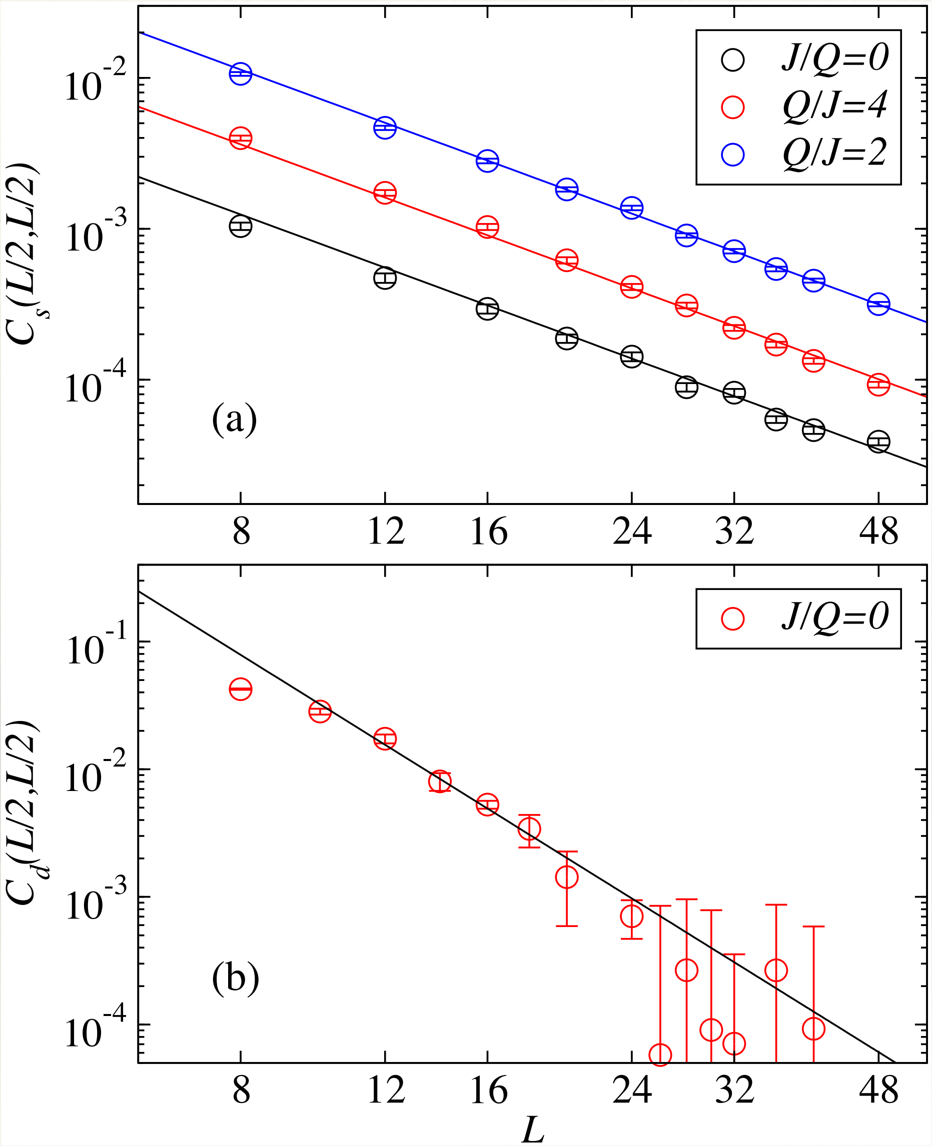
In the disordered VBS (random Q or J)
- λ~1/L (empirical property of the RS state)

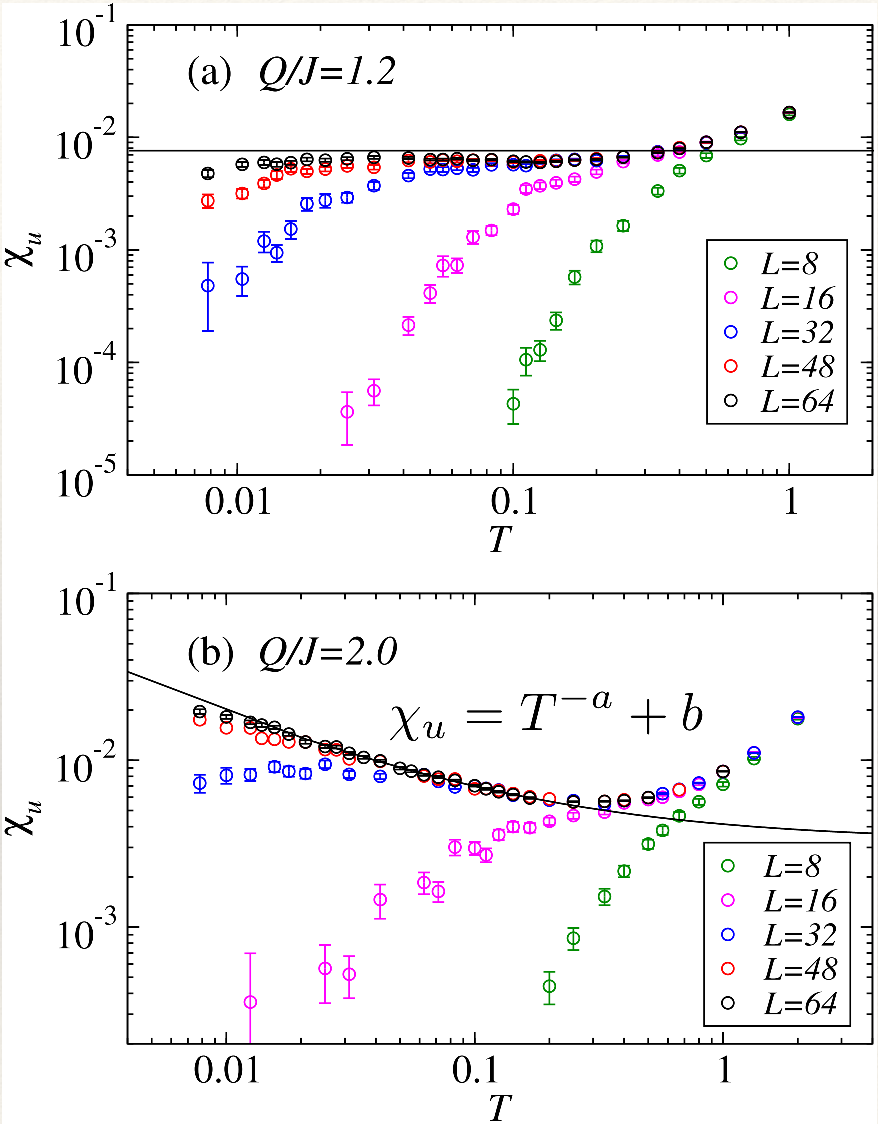
Some properties of the RS phase

spin and dimer correlations

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

dynamic exponent z





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

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

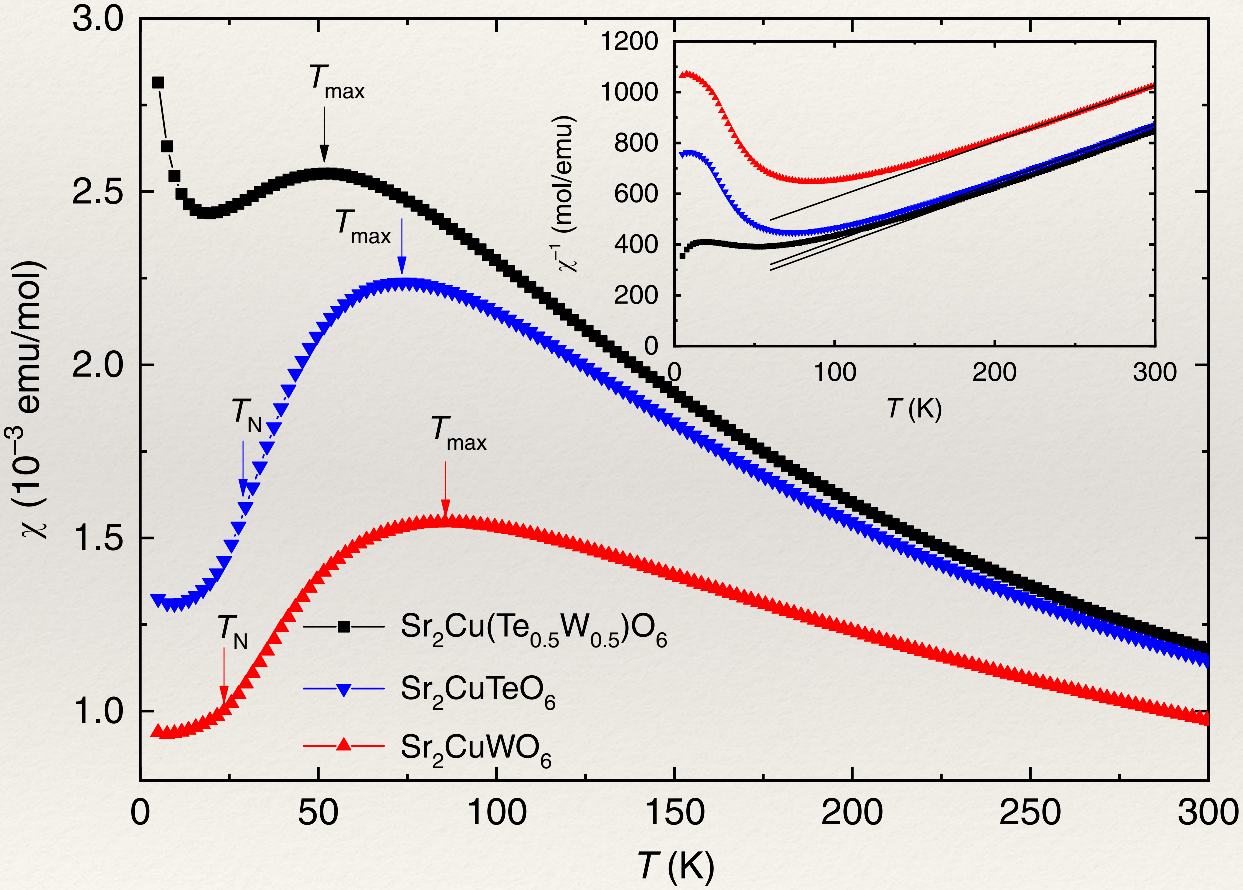
Experiments

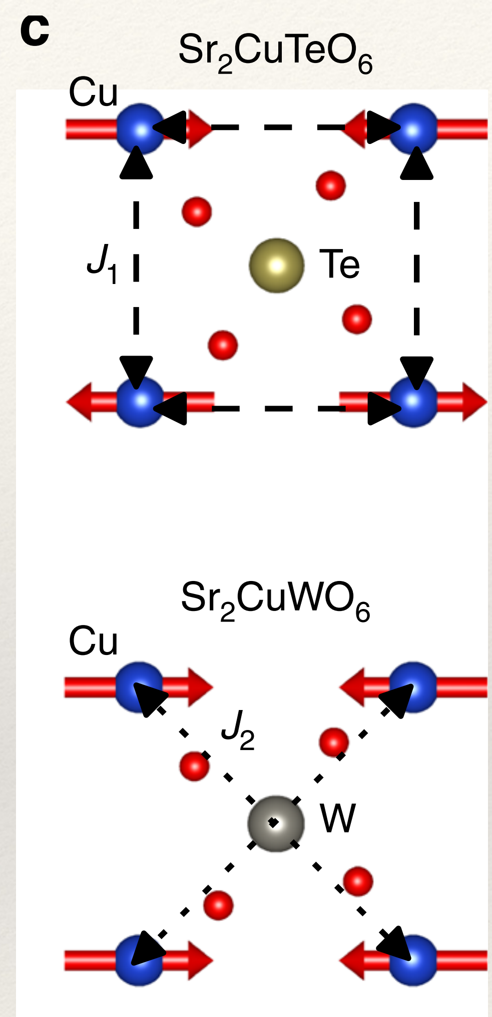
Some ‘disordered spin liquids’ may actually be RS states

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 (exponent?)

Conclusions

Found RS phase in unfrustrated 2D system
- not infinite-randomness fixed point (z is finite)

Is the state stable on very large length scales
- could weak AFM order form?

We can not rigorously exclude weak AFM order
- unlikely, in light of well-characterized AFM-RS critical point
- the spinon size diverges at the critical point
- the spinon density vanishes at the critical point

The RS phase is likely universal, same as in frustrated systems
- properties can be investigated in great detail with QMC
- comparisons with experiments possible, e.g., varying z

Future work
- further characterize the RS phase (incl dynamics)
- realizations in other models