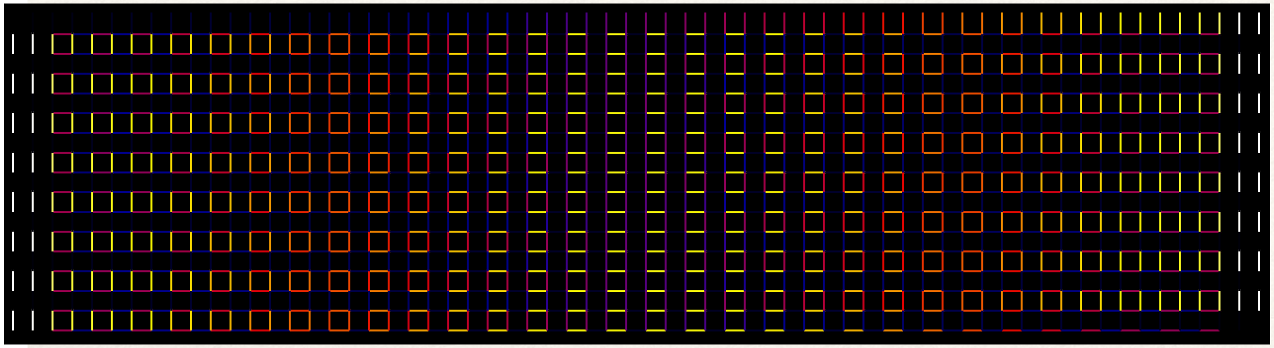
Domain walls in the VBS

Domain walls can be induced by boundary conditions



H. Shao, W. Guo, A. W. Sandvik, PRB and J. Phys. Conf. (2015) Science (2016)

Close to a DQCP, the thickness of the domain wall grows according to the U(1) length scale: $\xi' \propto \xi^{\nu'/\nu}$

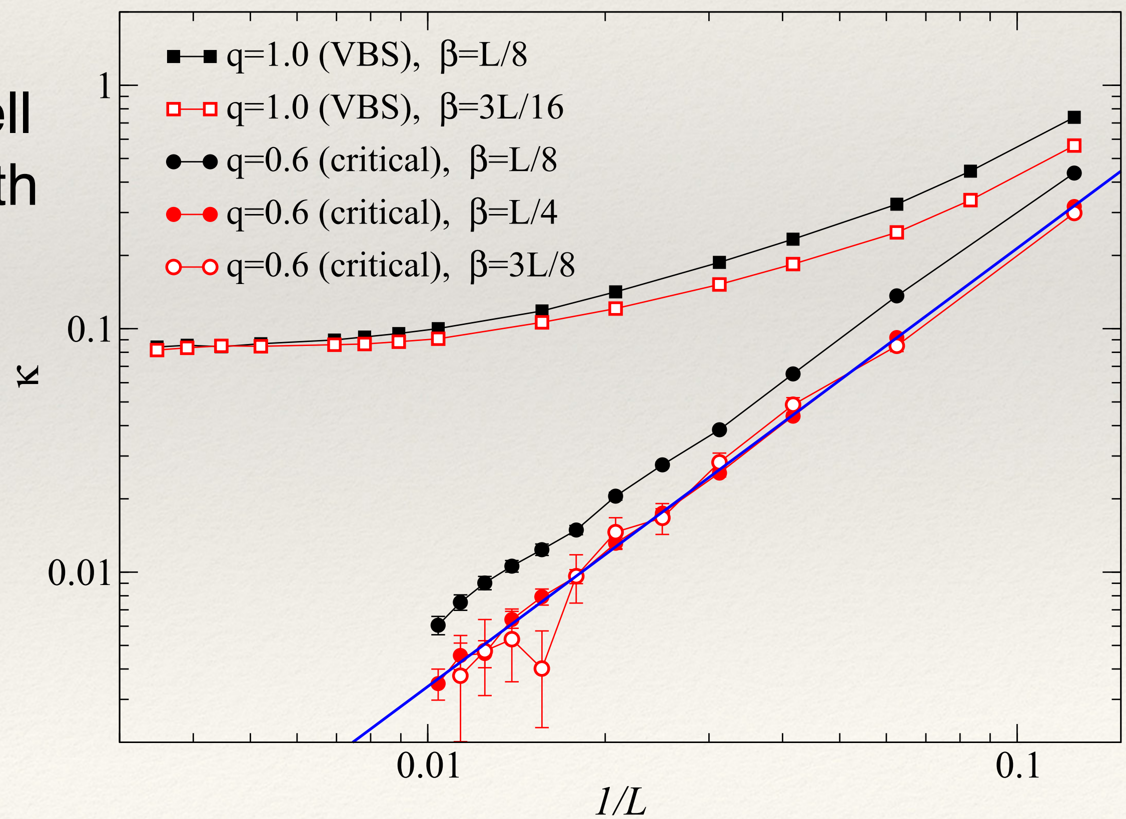
Domain wall fluctuates

- the total energy increase is well defined and can be studied with QMC

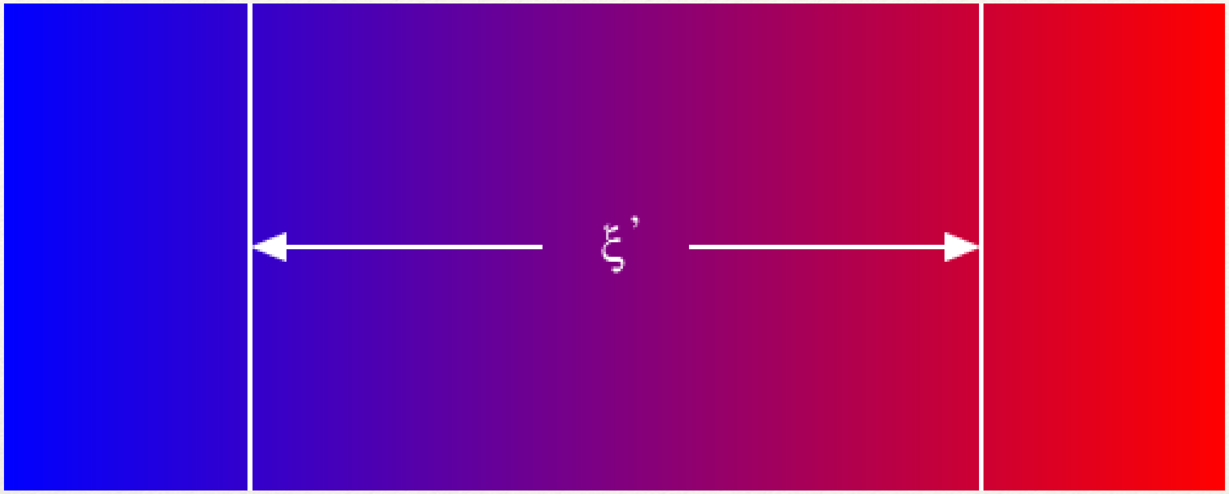
Define energy density

$$\kappa = \frac{\Delta E_0}{L^{d-1}}$$

What do we expect for a critical system?



Domain walls in classical critical systems



In conventional systems

ξ' = ξ

Free-energy density

$$\kappa = \frac{\Delta F_s}{L^{d-1}} \propto \frac{1}{\xi^{d+z-1}}$$

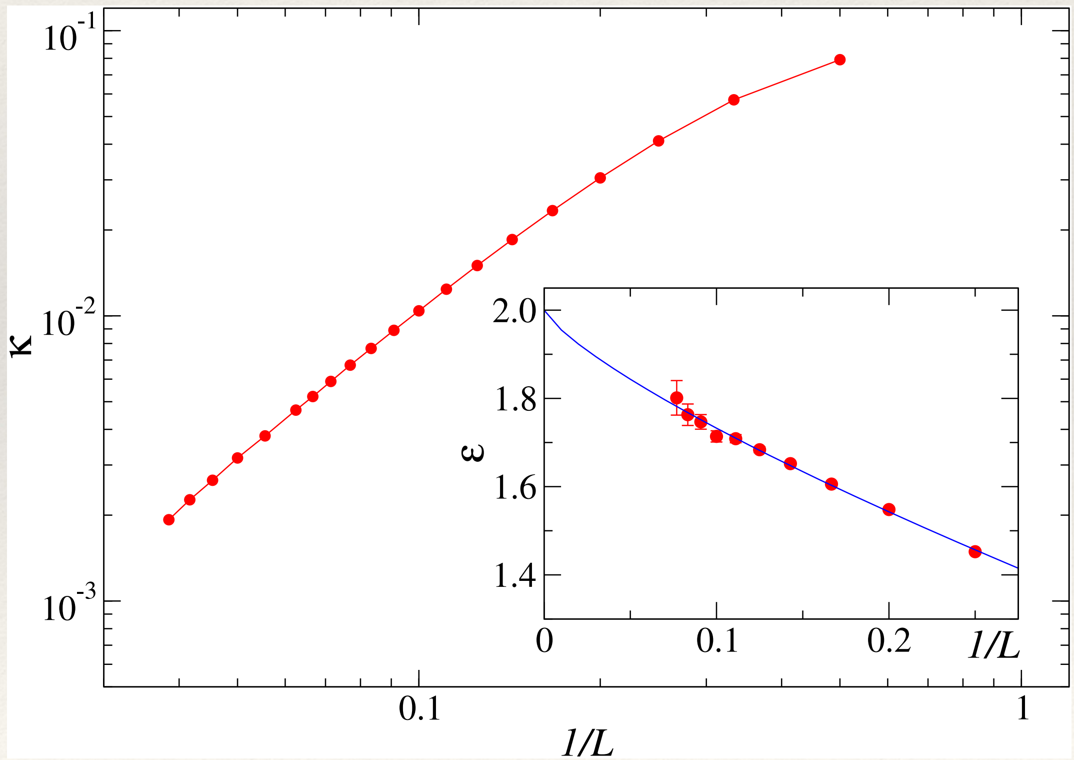
$$\kappa(L) \propto L^{-(d+z-1)}$$

Scaling from (L,2L) pairs

$$\kappa \sim L^{-\epsilon}$$

$$\epsilon = \ln[\kappa(L)/\kappa(2L)]/\ln(2) \to$$

$$d + z - 1 = 3 + 0 - 1 = 2$$

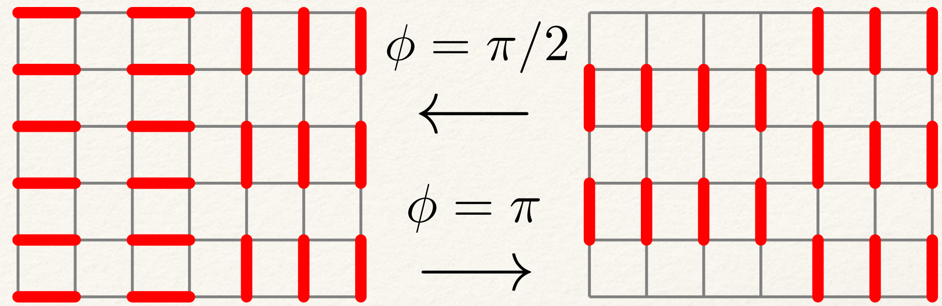


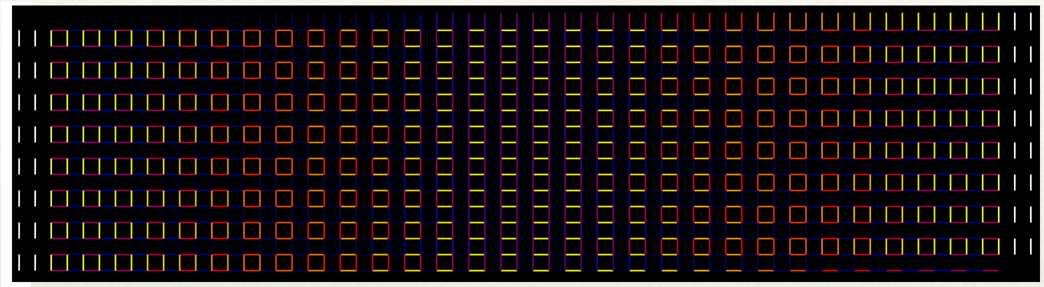
Expected behavior confirmed

Domain walls in critical J-Q_3 model

Two kinds of VBS domain walls can be imposed in open-boundary systems

- π wall splits into two π/2 walls





Energy density can be shown to be (Senthil et al.)

$$\kappa \sim \xi^{-1}\xi'^{-1}$$

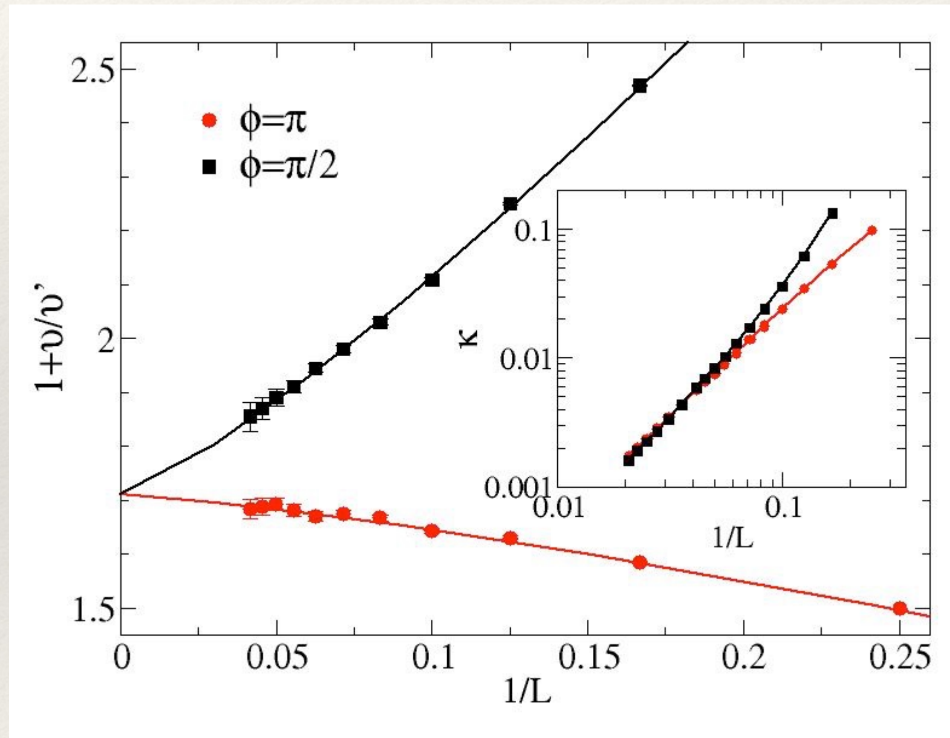
Ambiguity in finite-size scaling:

option 1) $\xi \rightarrow L$, $\xi' \rightarrow L^{\nu'/\nu}$: **$\kappa \sim L^{-(1+\nu'/\nu)}$**

option 2) $\xi \rightarrow L$, $\xi' \rightarrow L$: **$\kappa \sim L^{-2}$**

option 3) $\xi' \rightarrow L$, $\xi \rightarrow L^{\nu/\nu'}$: **$\kappa \sim L^{-(1+\nu/\nu')}$**

$$\ln[\kappa(L)/\kappa(2L)]/\ln(2) \rightarrow 1 + \nu/\nu'$$



Results show option 3 (exponent < 2): $\nu/\nu' \approx 0.715 \pm 0.015$

Two-length scaling hypothesis [Shao, Guo, Sandvik (Science 2016)]

Two divergent lengths tuned by one parameter: $\xi \sim \delta^{-\nu}, \quad \xi' \sim \delta^{-\nu'}$

Finite-size scaling of some quantity A. Thermodynamic limit: $A \propto \delta^{\kappa}$

Conventional scenario

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

When L→∞: $f(\delta L^{1/\nu}, \delta L^{1/\nu'}) \to (\delta L^{1/\nu})^{\kappa}$

Alternative scenario

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

When L→∞: $f(\delta L^{1/\nu}, \delta L^{1/\nu'}) \to (\delta L^{1/\nu'})^{\kappa}$

Equivalent view: At the critical point: $A = \xi^{-\kappa/\nu}$

Replace ξ by L: $A = L^{-\kappa/\nu}$ or, replace ξ' by L, ξ by $L^{\nu/\nu'}$: $A = L^{-\kappa/\nu'}$

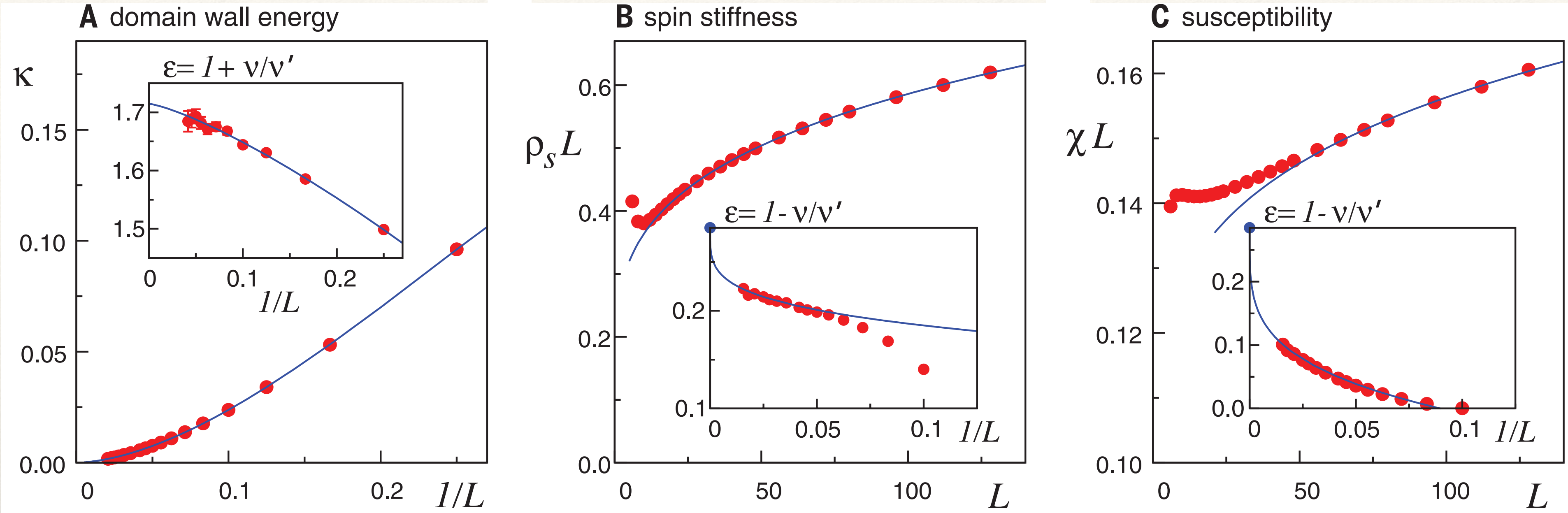
Example: Spin stiffness: κ=ν(z+d-2). At criticality:

$\rho_s \propto L^{-(z+d-2)}$ or $\rho_s \propto L^{-(z+d-2)\nu/\nu'}$

The first scenario has so far been implicitly assumed

- can the drifts be explained using $\nu \approx 0.45$, $\nu/\nu' \approx 0.7$?

Tests of second length scale scenario



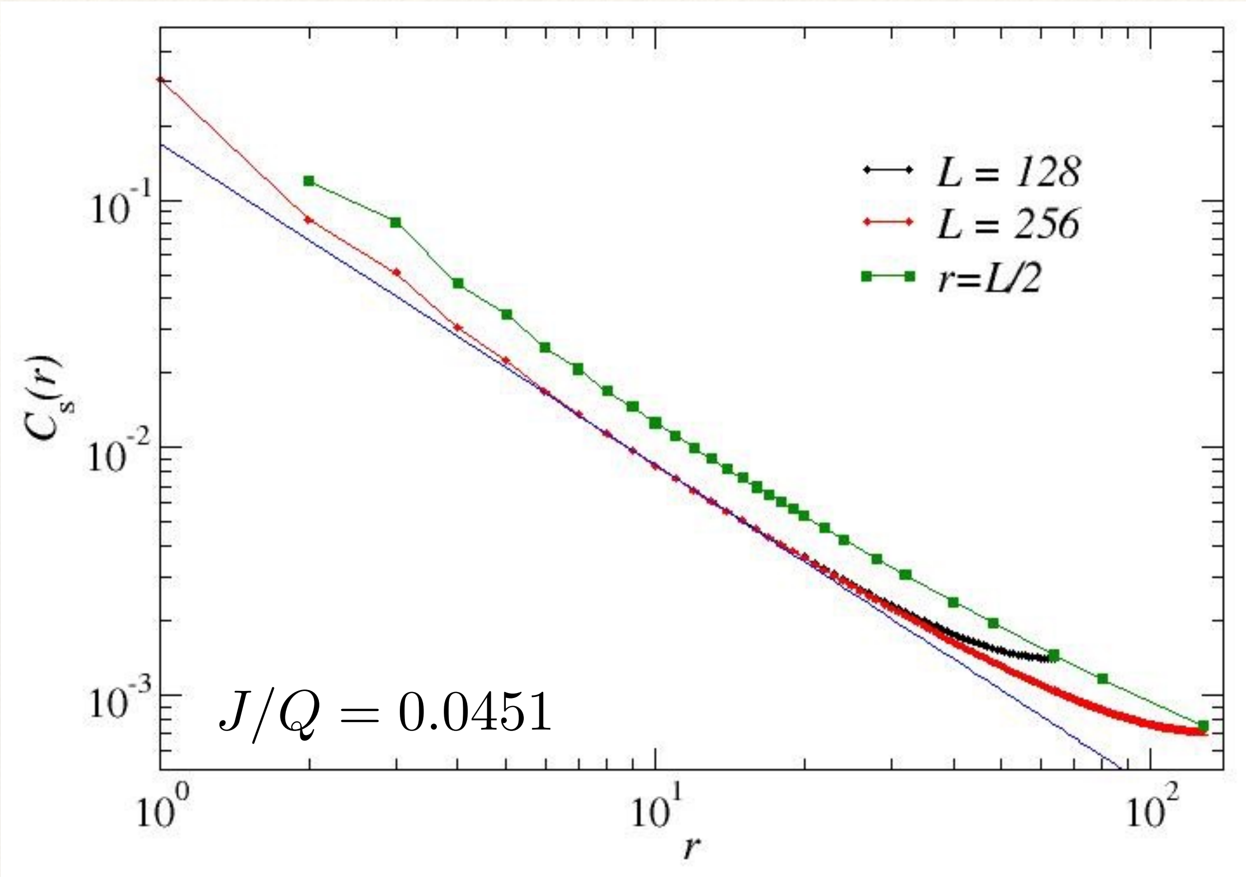
The second length scale must exist also in the AFM state!

- Candidate: the (π,0) triplet mode may scale as $\delta^{\nu'}$

Critical correlation functions, conventional view

For r<<L (d=2,z=1), $C(r) \propto r^{-(1+\eta)}$ For any r,L: $C(r,L) = r^{-(1+\eta)} f(r/L)$

$$r \to L : f(r/L) \to (r/L)^{1+\eta}, \quad C(r \sim L) \propto L^{-(1+\eta)}$$



The behavior at r=L/2 seems to violate the conventional form; slower than expected decay for large L

New scenario:

$$L \to L^{\nu/\nu'}$$

$$C(r \sim L) \propto L^{-(1+\eta)\nu/\nu'}$$

J-Q model, spin correlation (T=0): $\eta \approx 0.3$ from r<<L behavior

- agrees with 3D loop model (Nahum et al., PRX 2015)
- some uncertainty because r not very large

Is there emergent SO(5) symmetry?

For SU(2) spins, there is a special SO(5) DQCP theory (Senthil, Fisher, 2006)

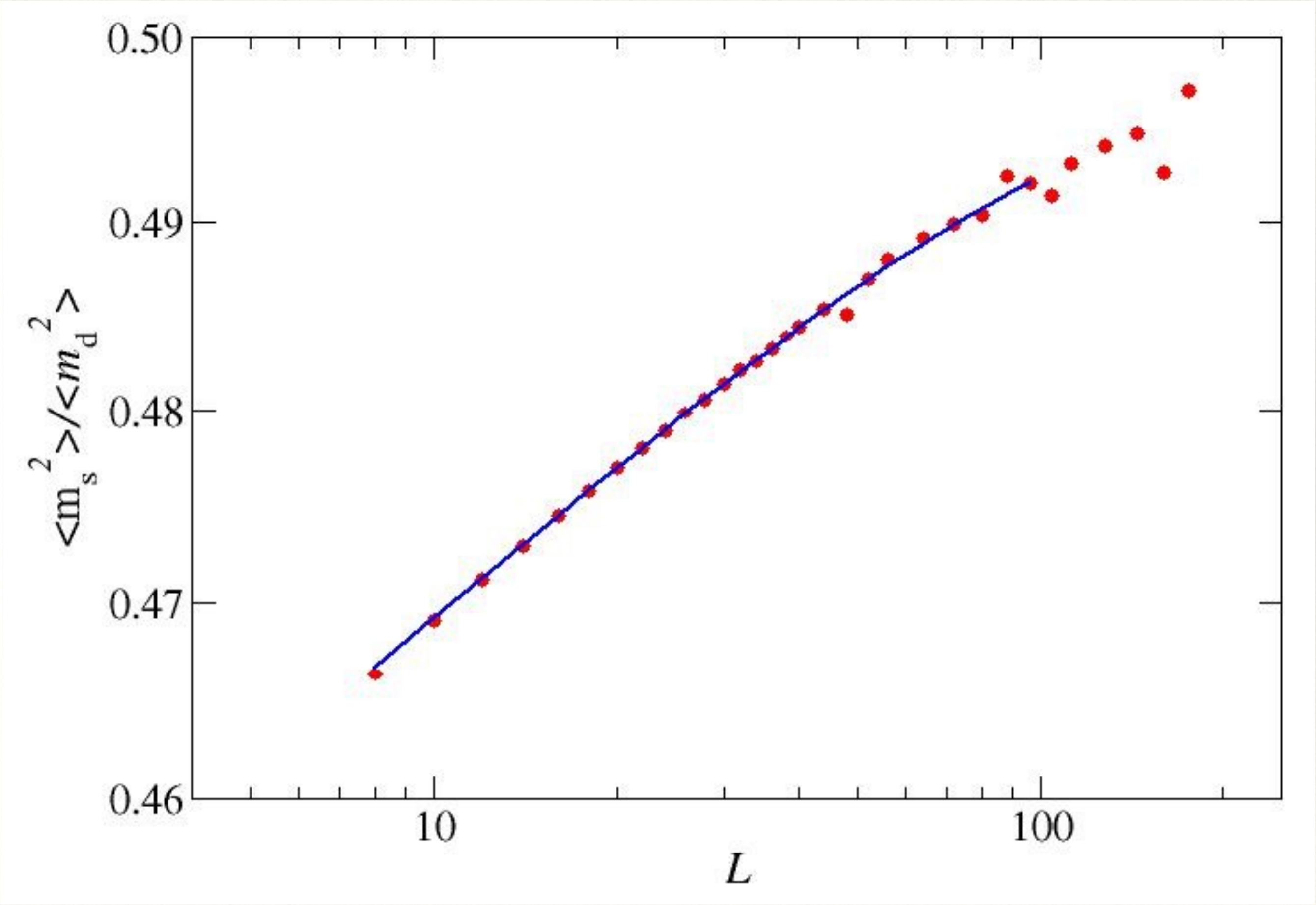
SO(5) symmetry seems to be realized in 3D loop model of DQCP
- Nahum, Chalker,… PRL 2015

First requirement for SO(5): $\eta_s = \eta_d$
- satisfied within error bars (our results and Nahum et al.)

Direct test of $\eta_s = \eta_d$

Finite-size scaling of the ratio of the squared order parameters

Seems to diverge with power ≈ 0.02
- may converge
- not conclusive…



Dynamic signatures of deconfined quantum criticality

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

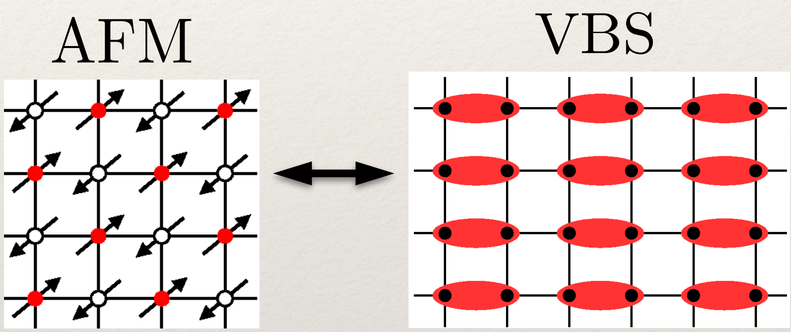
Editors' Suggestion

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)

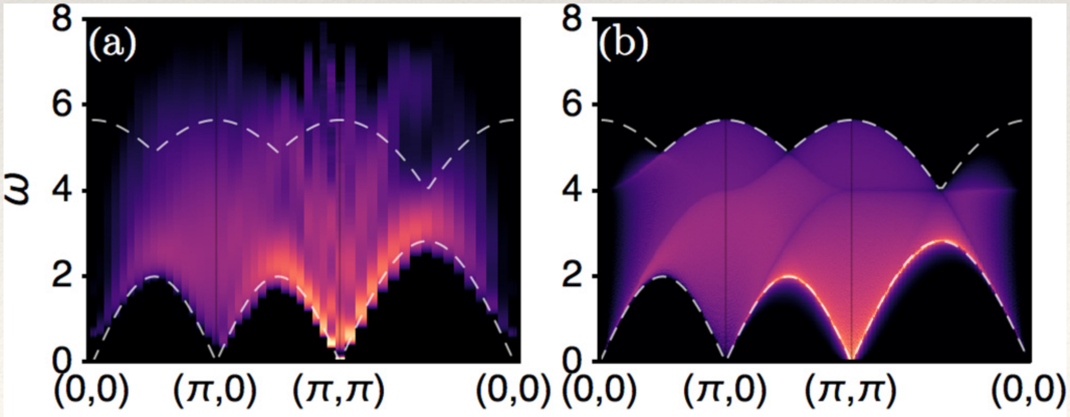


Close to critical point:
Good agreement with mean-field fermionic parton theory (π-flux)

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

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

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



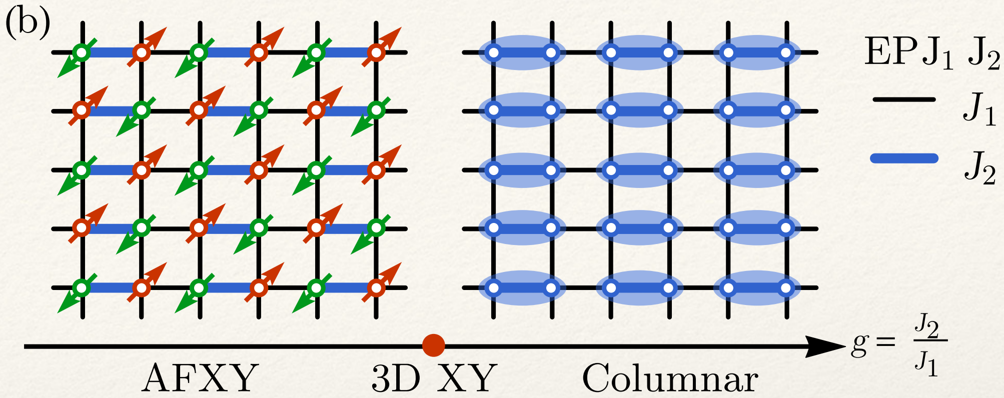
Deconfinment manifest on large length scales close to the phase transition

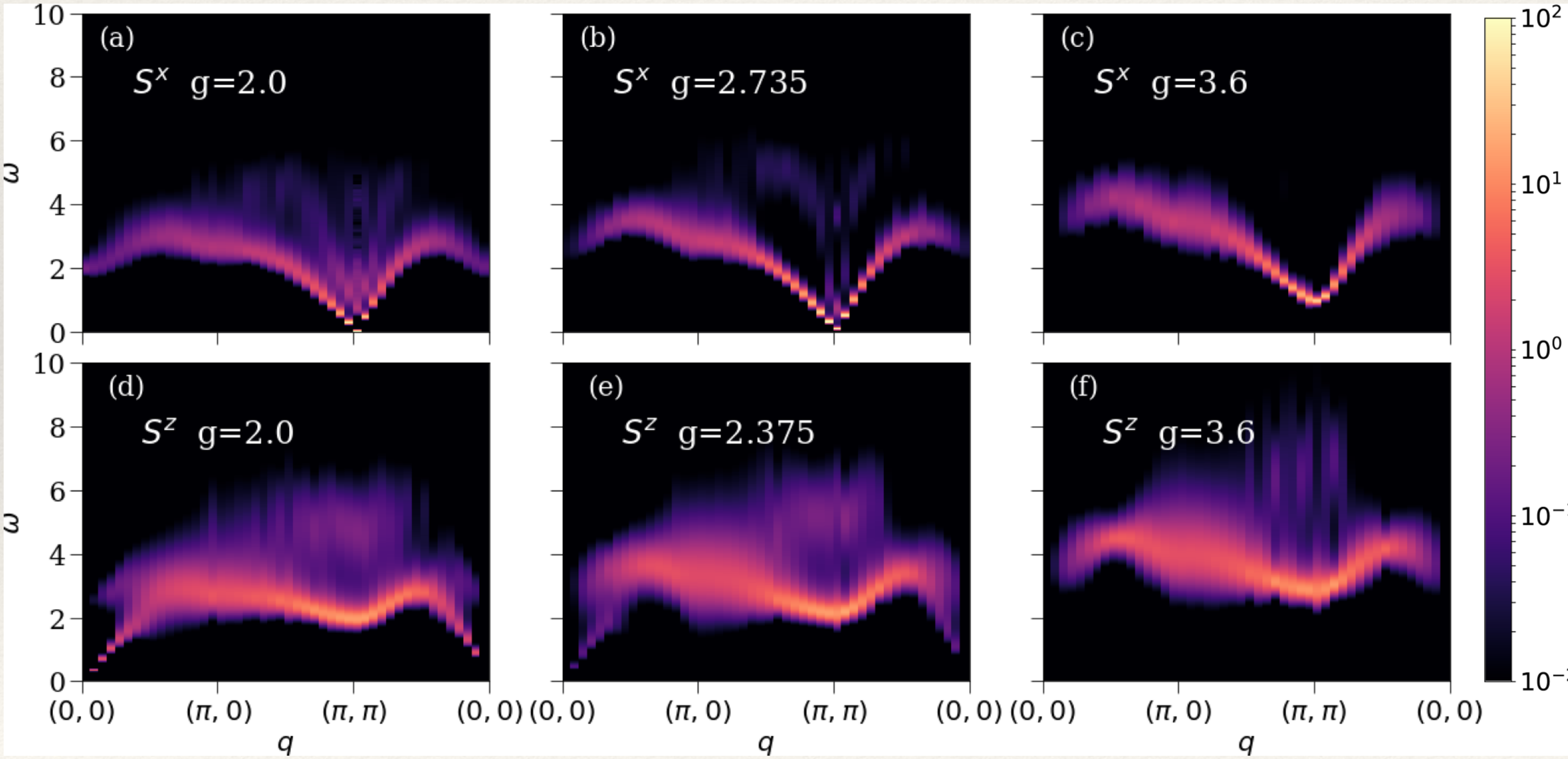
Conventional dynamics

Planar ("easy plane") columnar dimerized model

$$H_{\mathrm{J_1J_2}} = J_1 \sum_{\langle i,j\rangle'} D_{ij} + J_2 \sum_{\langle i,j\rangle''} D_{ij}$$

$$D_{ij} = S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z$$





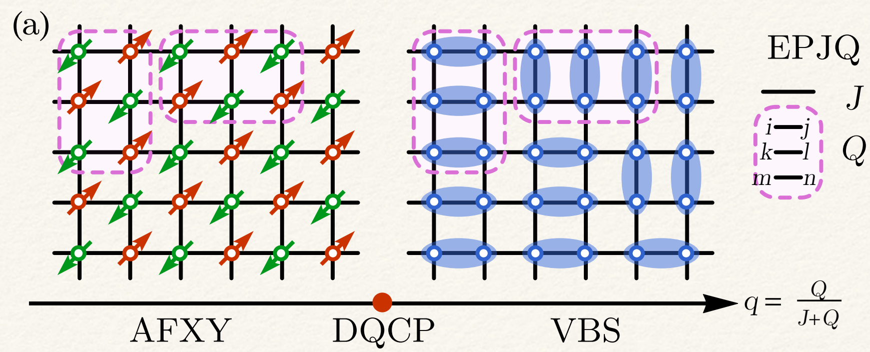
Gapless modes at (0,0) and (π,π)

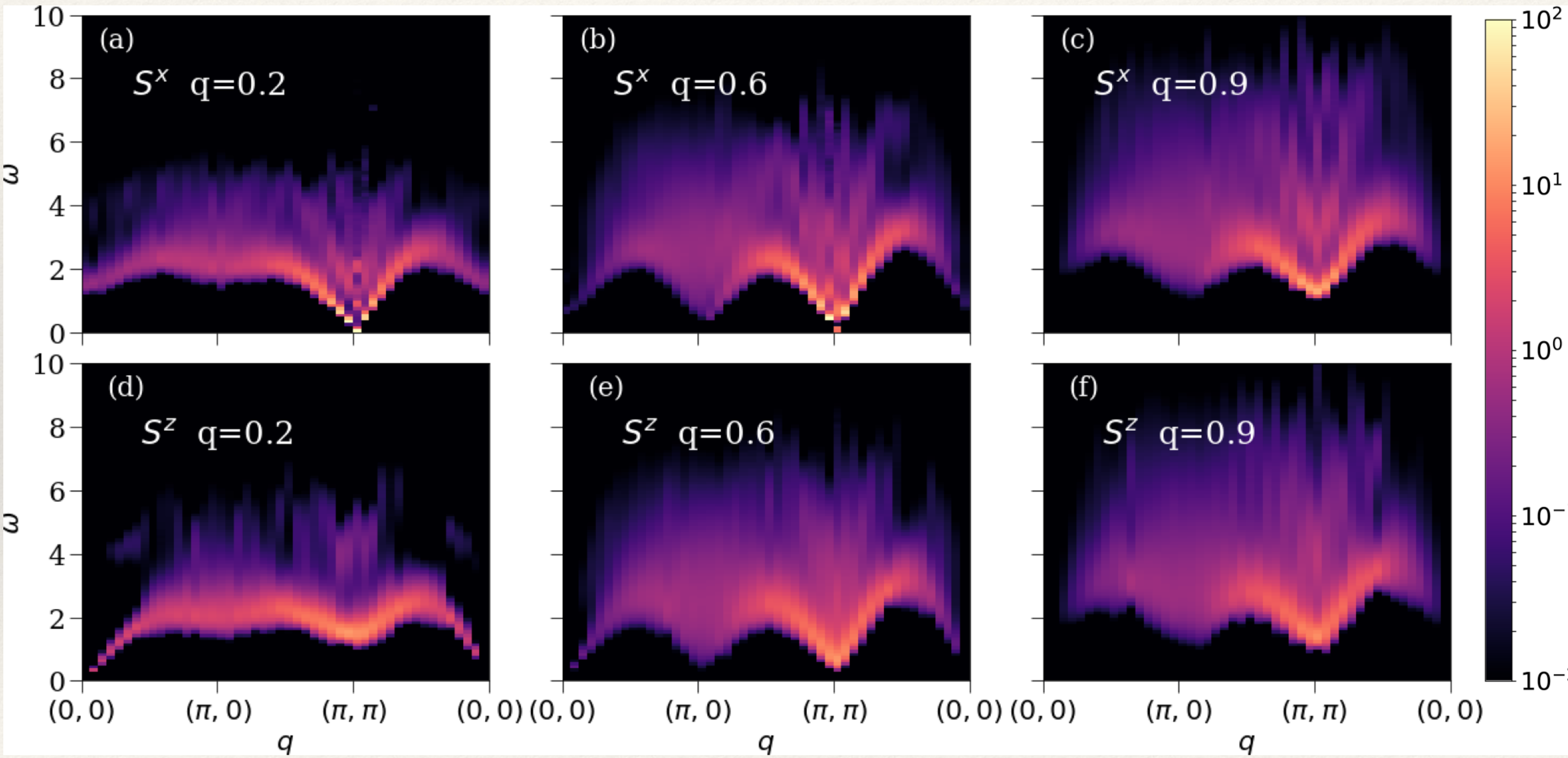
Dynamics at the DQCP

Planar ("easy plane") J-Q₃ model

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

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

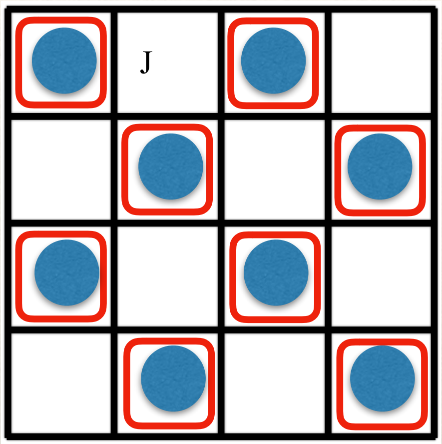


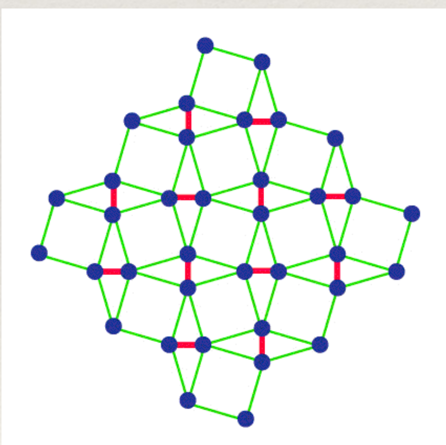


Additional gapless (π,0) mode; related to the VBS, critical dirac liquid

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?

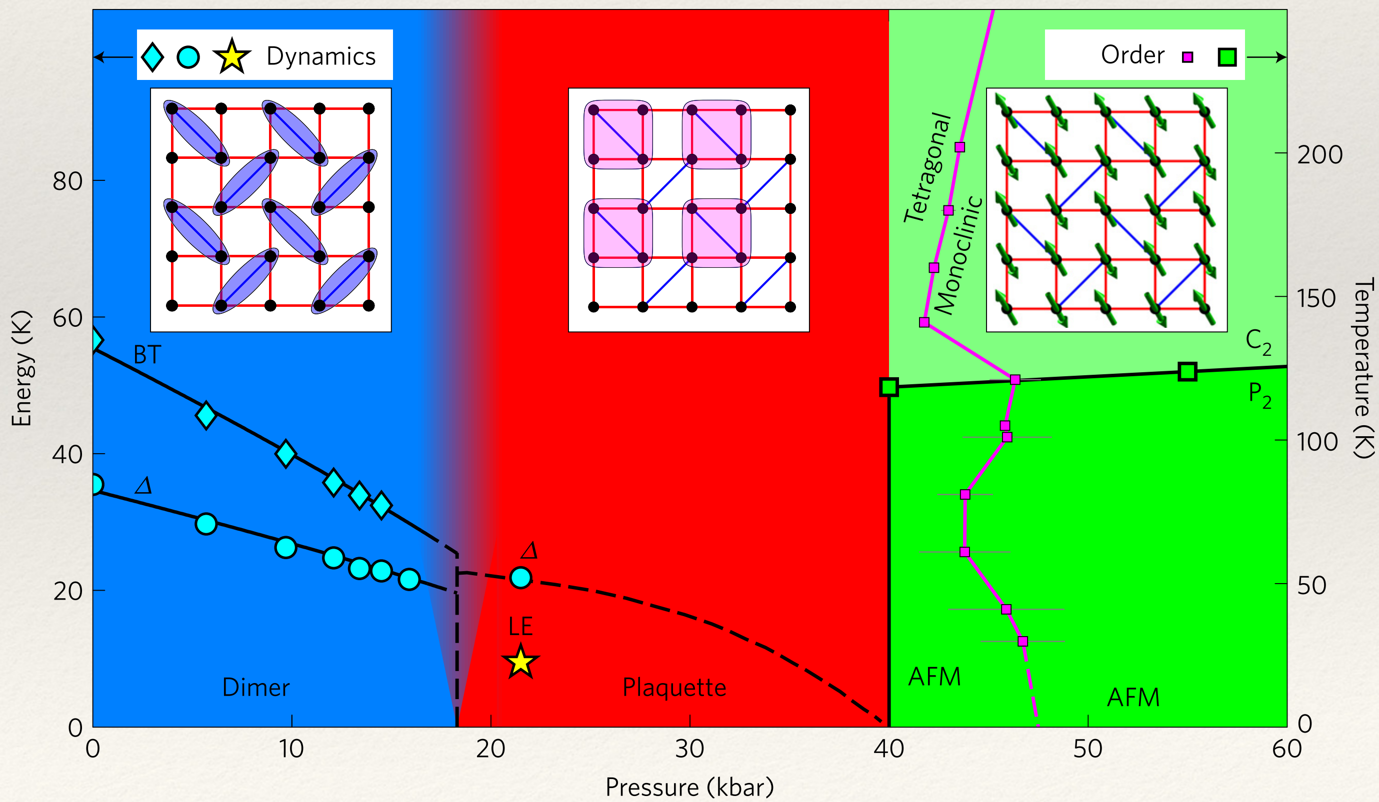
nature physics

LETTERS

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

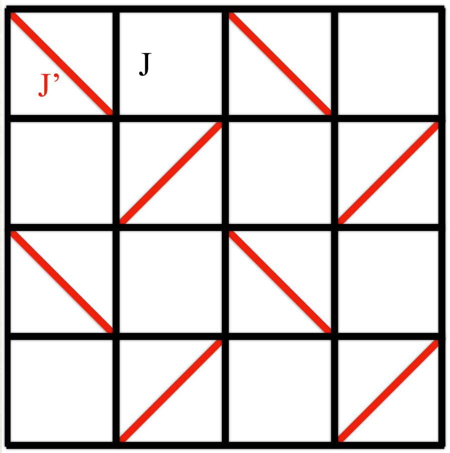
4-spin plaquette singlet state in the Shastry–Sutherland compound $SrCu_2(BO_3)_2$

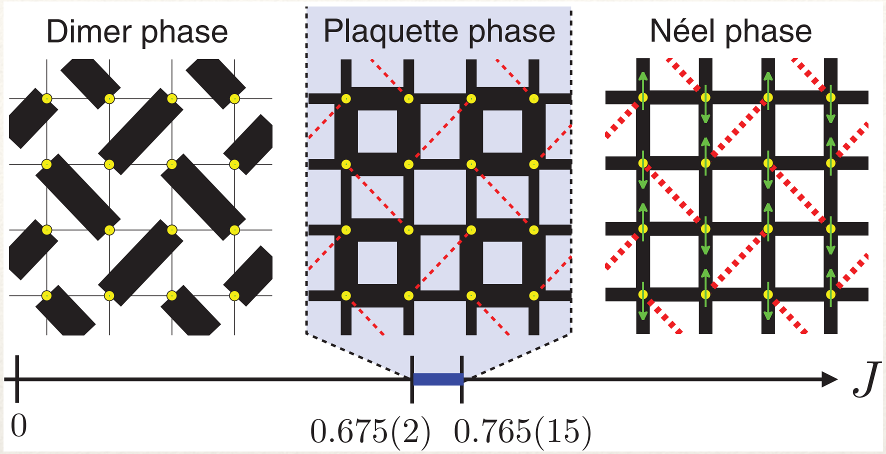
M. E. Zayed[1,2,3★], Ch. Rüegg[2,4,5], J. Larrea J.[1,6], A. M. Läuchli[7], C. Panagopoulos[8,9], S. S. Saxena[8], M. Ellerby[5], D. F. McMorrow[5], Th. Strässle[2], S. Klotz[10], G. Hamel[10], R. A. Sadykov[11,12], V. Pomjakushin[2], M. Boehm[13], M. Jiménez-Ruiz[13], A. Schneidewind[14], E. Pomjakushina[15],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



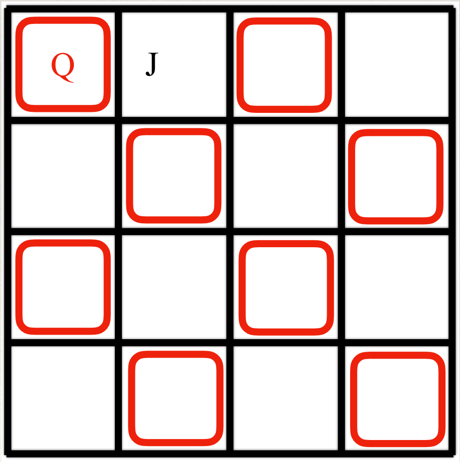


Corboz & Mila
PRB 2013

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

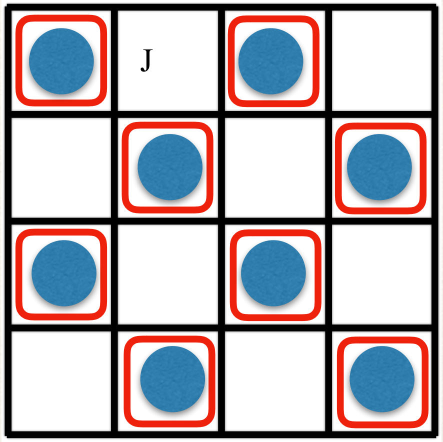
$$\mathcal{H} = -J \sum_{\langle ij \rangle} P_{ij} - Q \sum_{ijkl \in \square'} (P_{ij}P_{kl} + P_{ik}P_{jl})$$

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

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



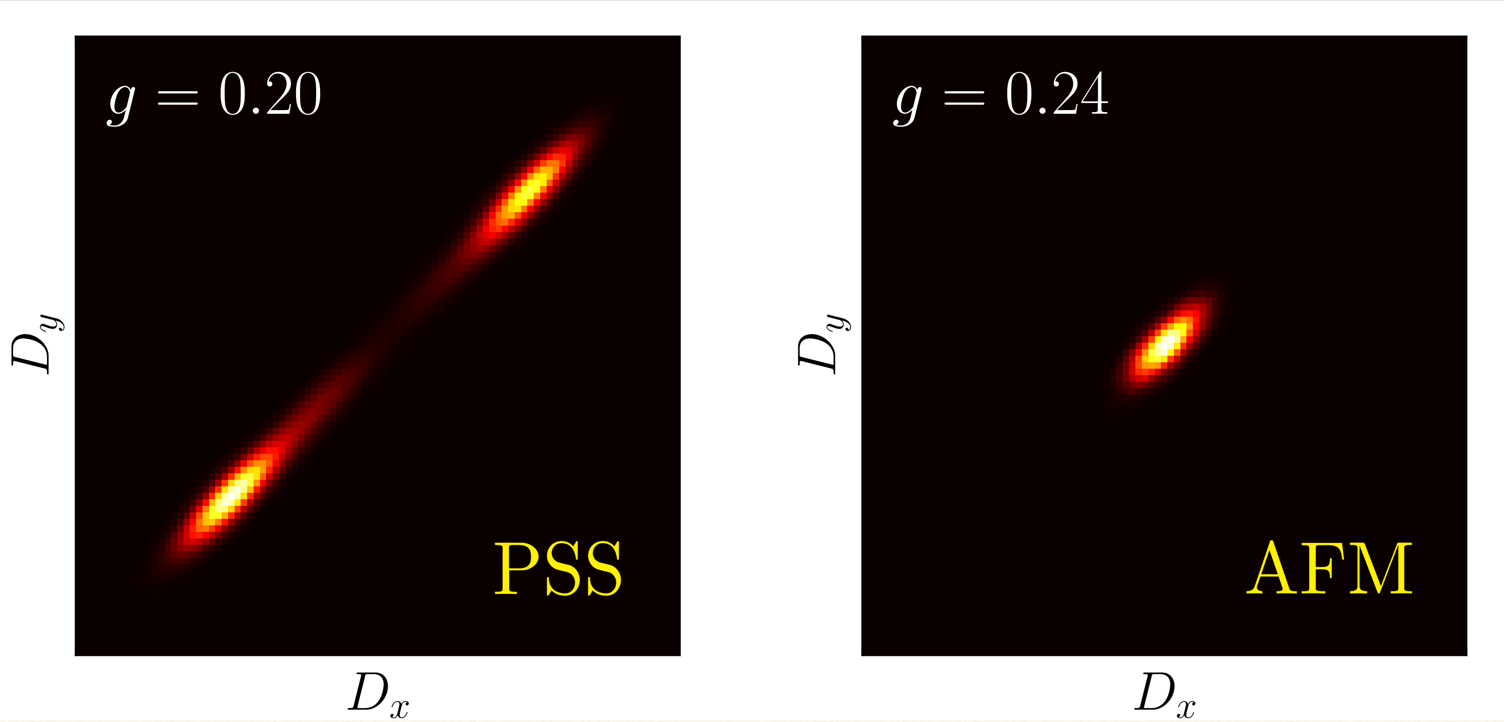
The lattice and interactions are compatible with

- 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 $P(D_x,D_y)$



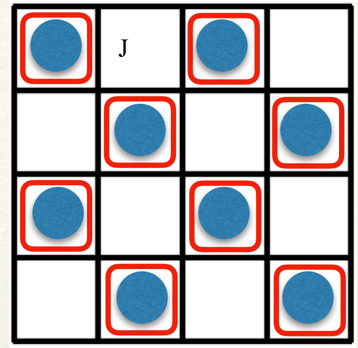
We find 2-fold PSS order for small g=J/Q

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:

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

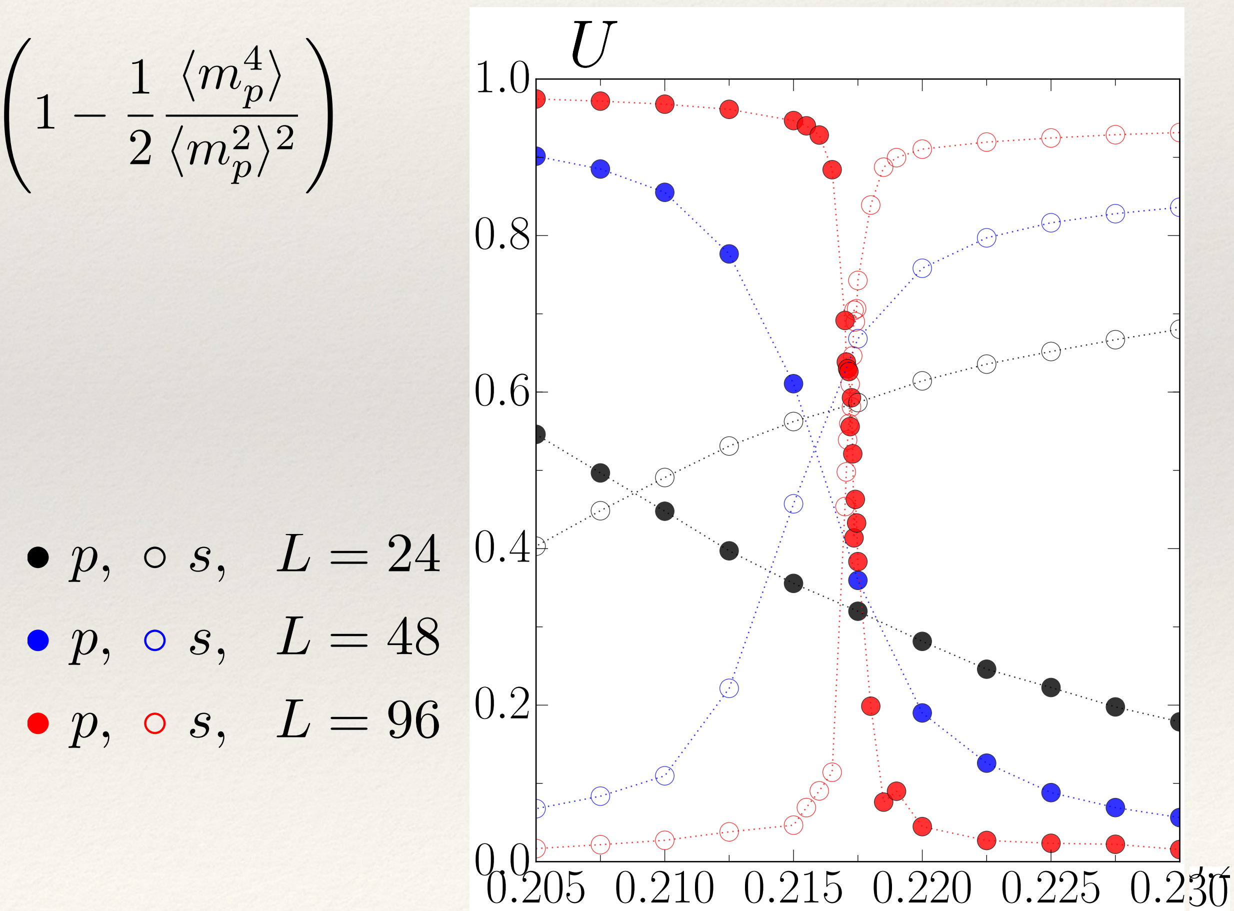
Expectation:

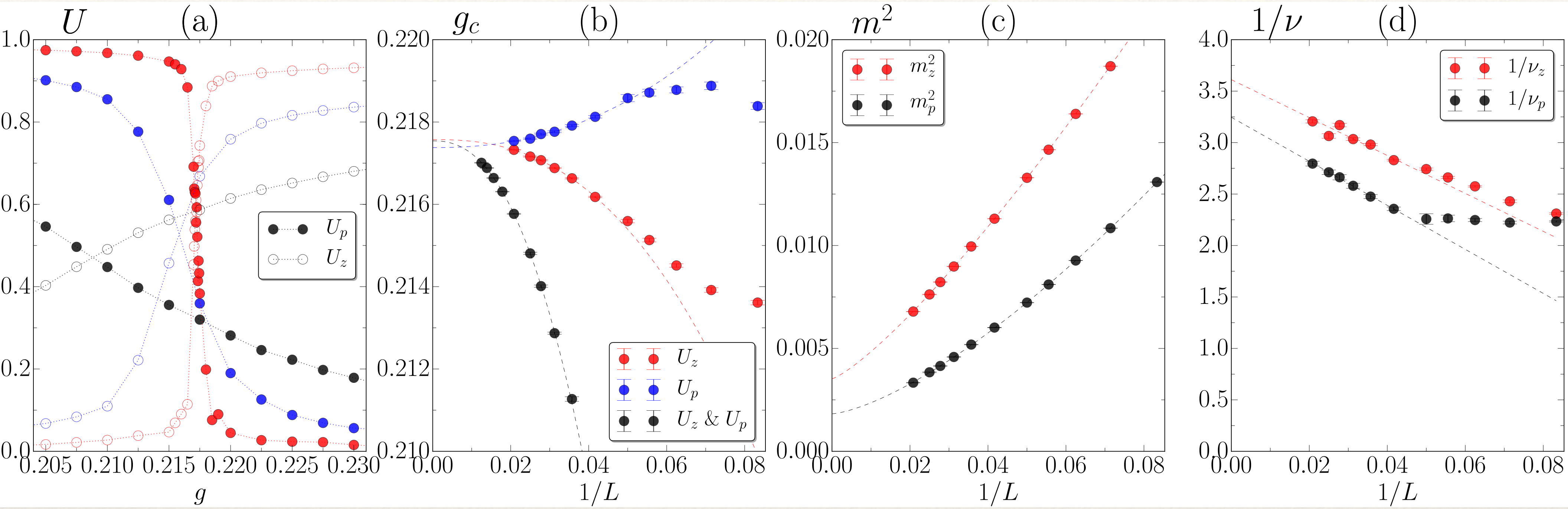
$U_s \rightarrow 1$, $U_p \rightarrow 0$ in AFM phase

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

Crossing points used
to analyze the transition

No negative peaks in U
- continuous transition?





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?

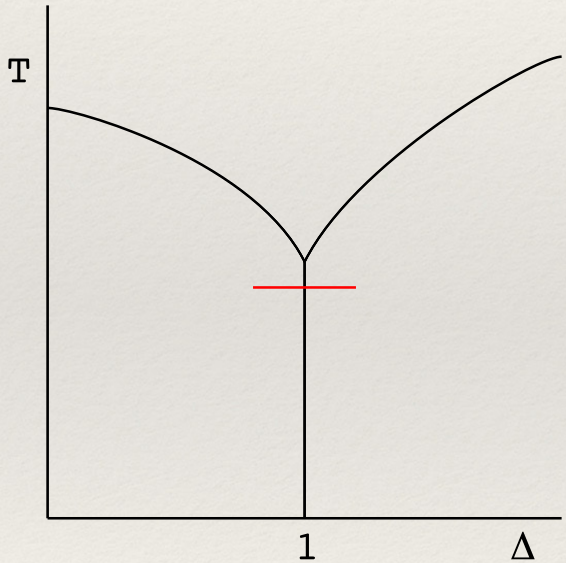
Yes: 3D O(N) models with N=3,4,5,… in their ordered states ($T < T_c$)

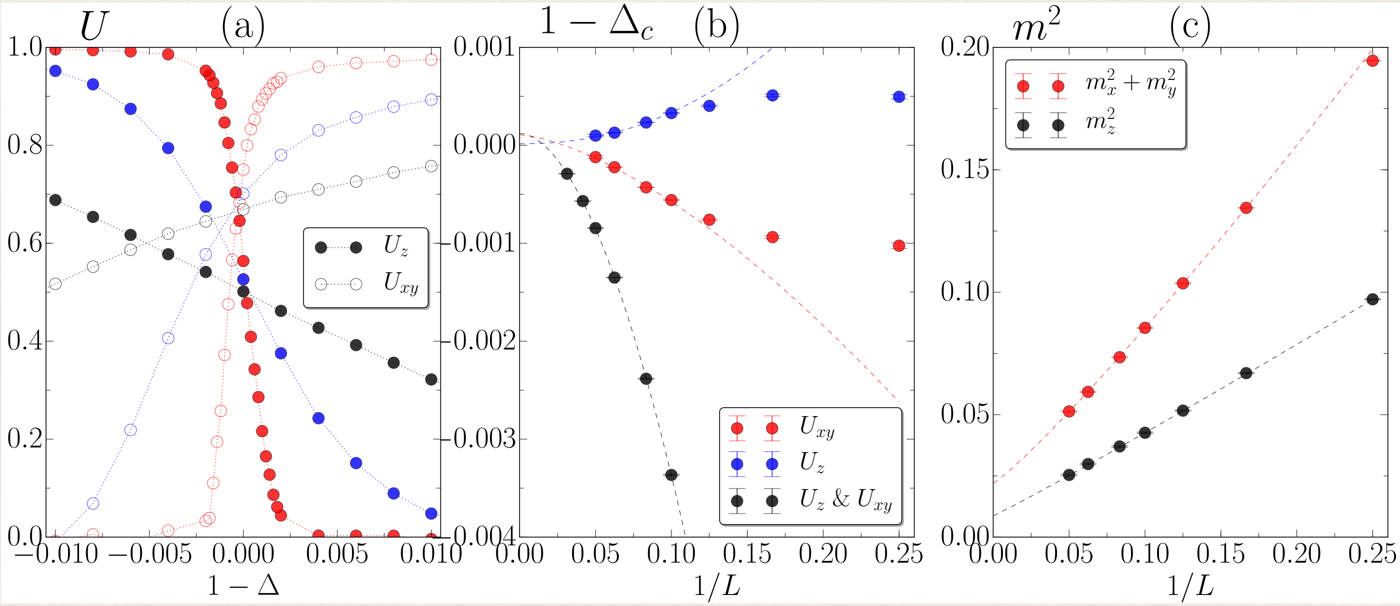
Example: **Classical 3D O(3) (Heisenberg) model** with tunable anisotropy

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

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





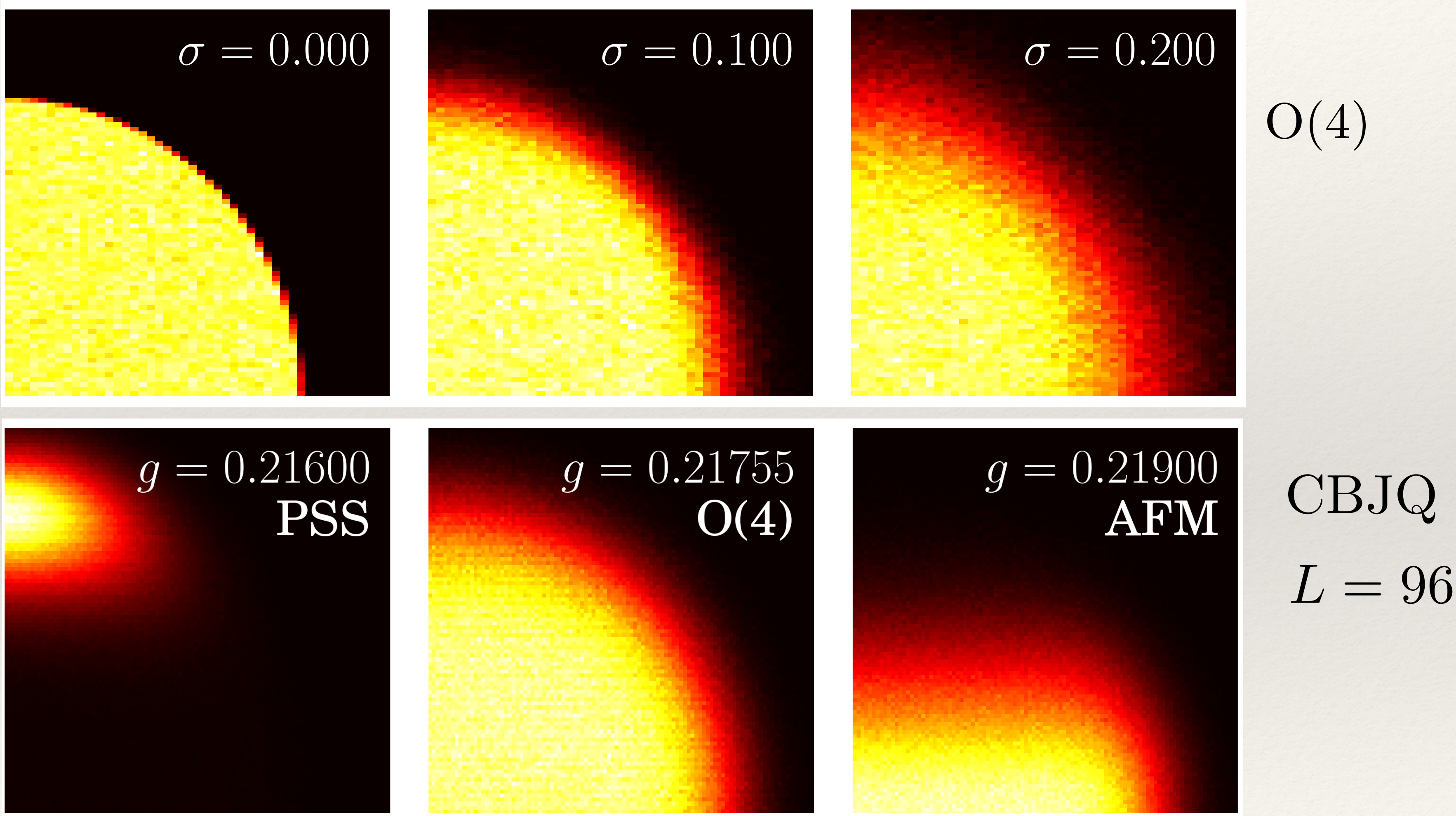
Very similar behaviors as CBJQ model!

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

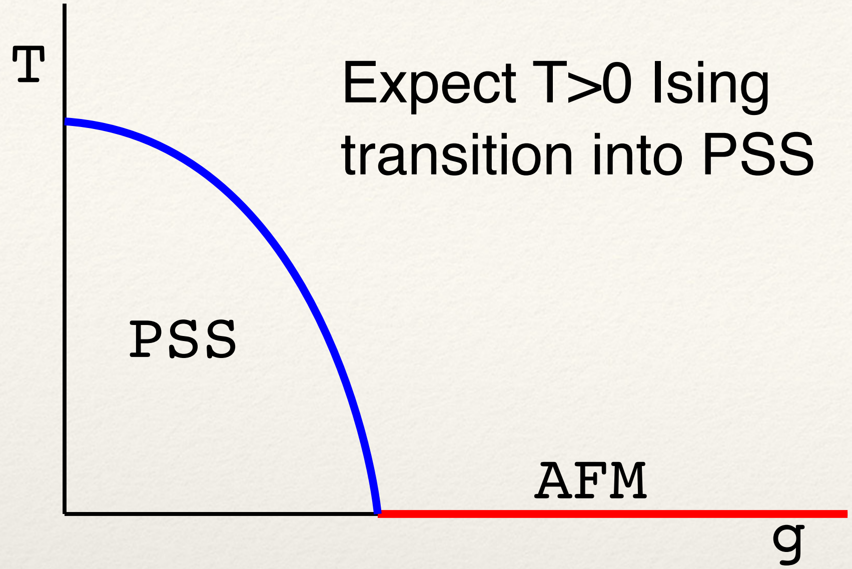
Detecting O(4) symmetry in the CBJQ model

- 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:

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

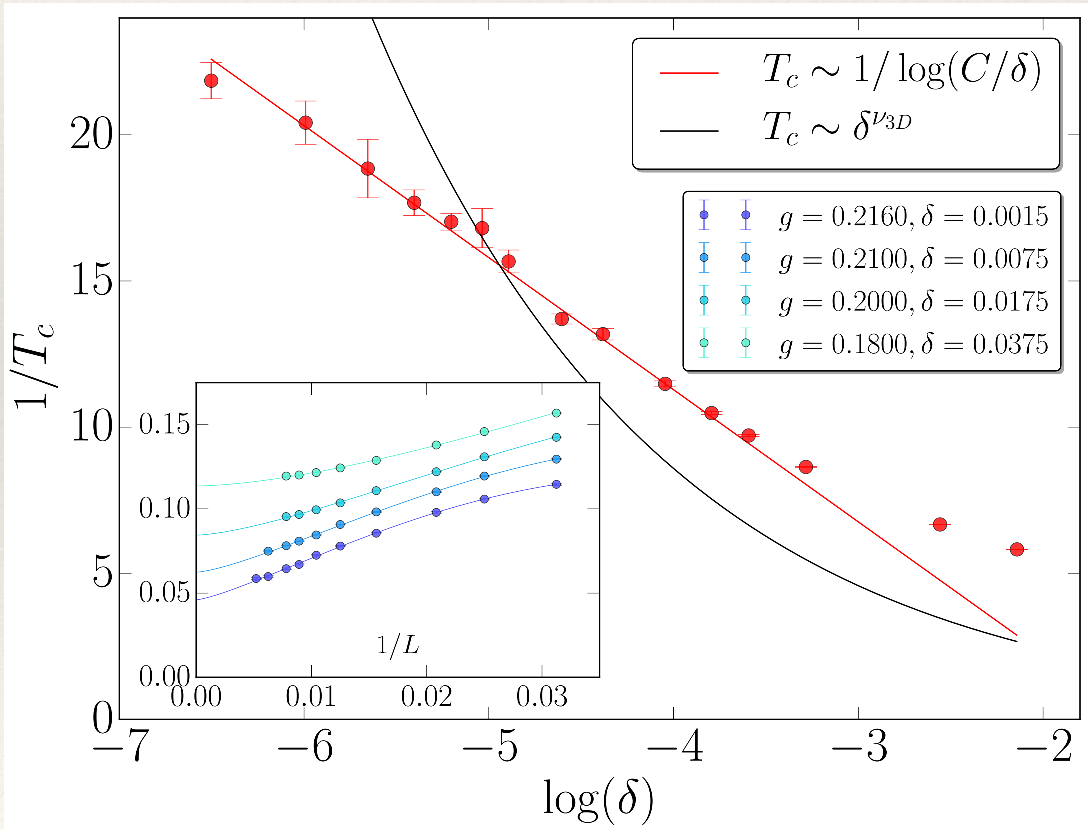
- cut off at low T_c if the transition is eventually first-order

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

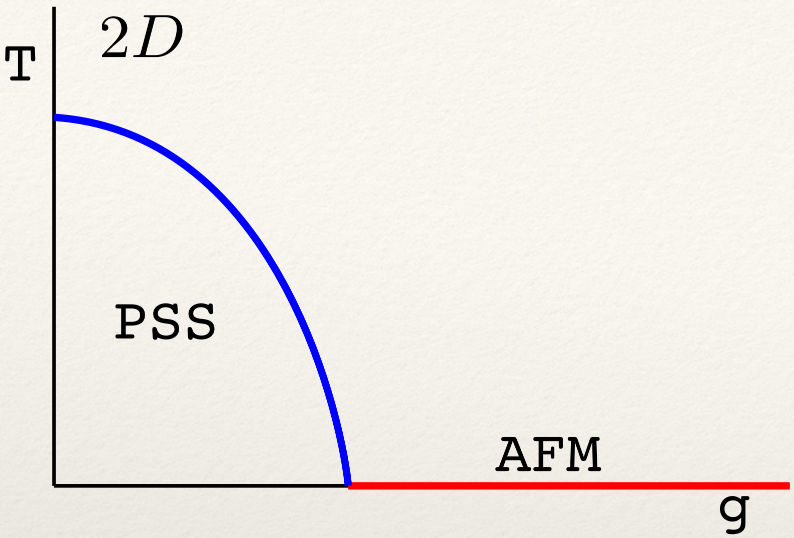
$$T_c \propto \frac{1}{\ln(C/|g - g_c|)}$$

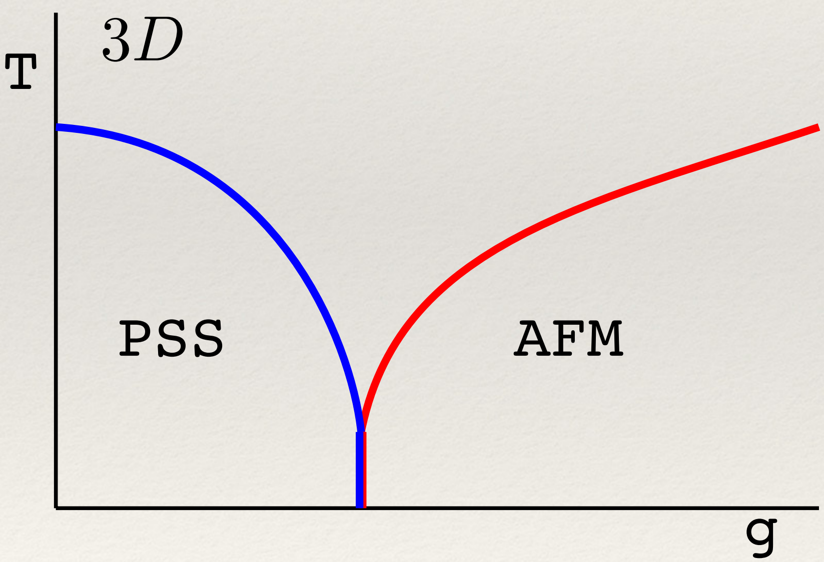
Results support the log form

manifestation of O(4) symmetry in physical observable



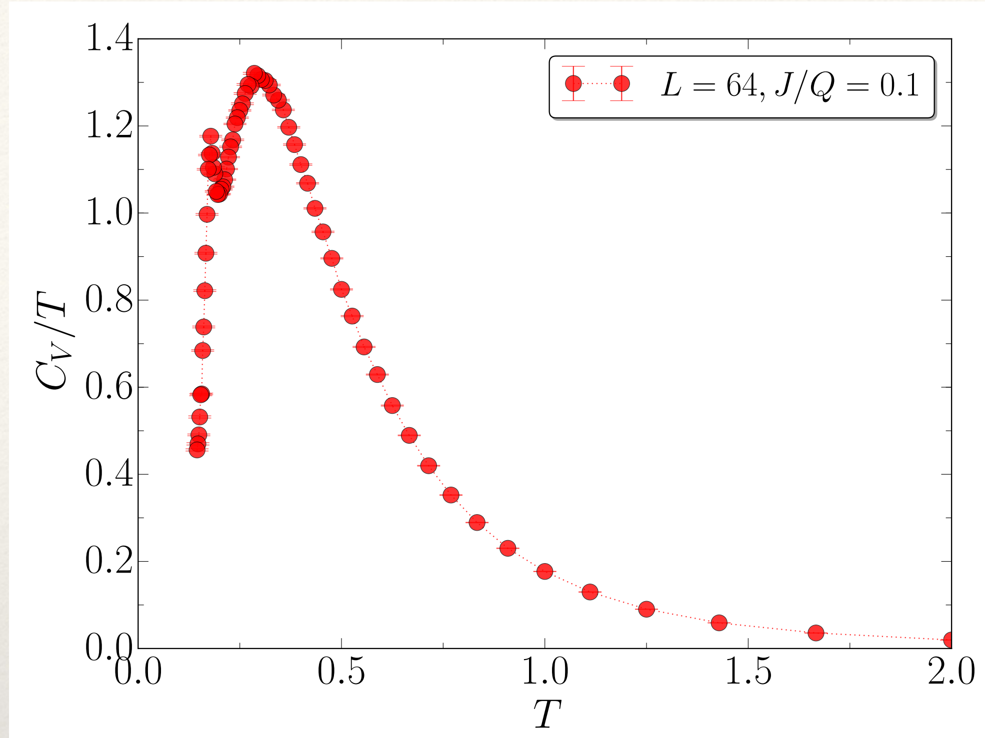
Specific heat, 3D T>0 phase diagram





Similar behavior in $SrCu_2(BO_3)_2$

- high-pressure, low-T experiments: J. Guo et al. (IOP), PRL 2020



Entropy change small at T>0 transition

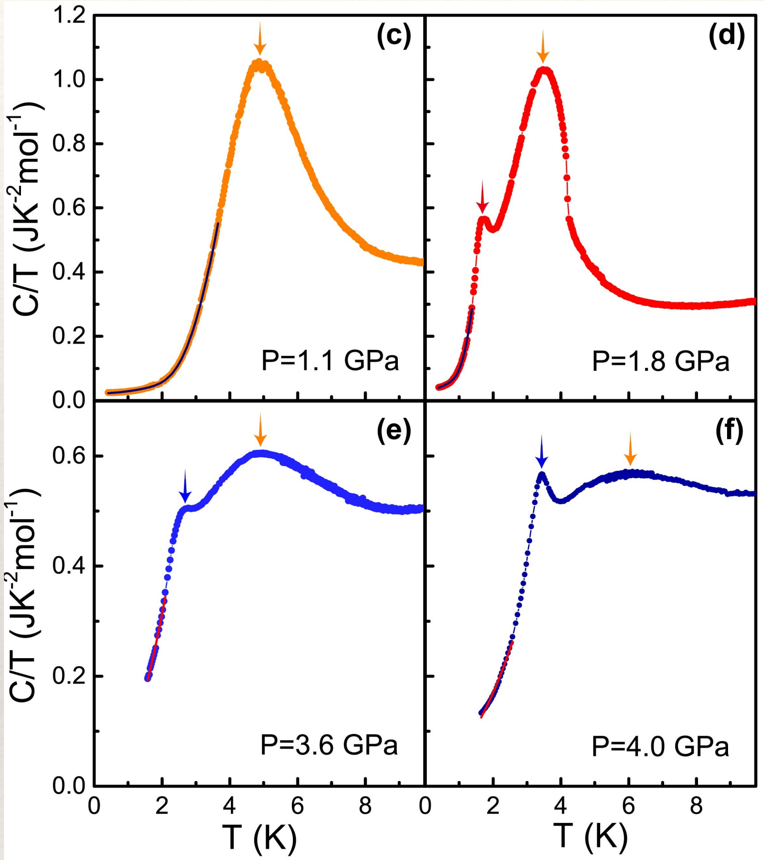
- a lot of entropy goes to freezing out higher states on the plaquettes

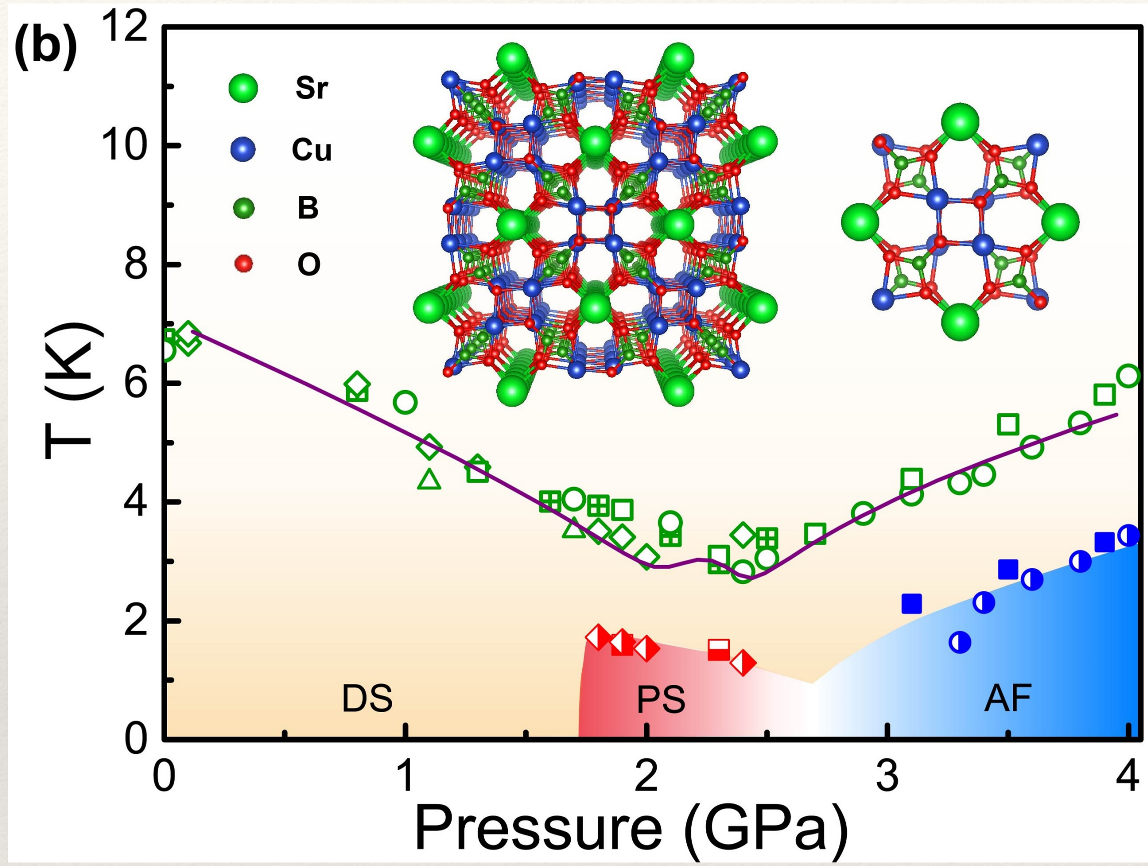
3D effects should cause first-order line

- could there be remnant O(4) above?
- G. Sun et al (in progress)

Quantum phases of $SrCu_2(BO_3)_2$ from high-pressure thermodynamics PRL 2020

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 smaller than expected
- new AF phase

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

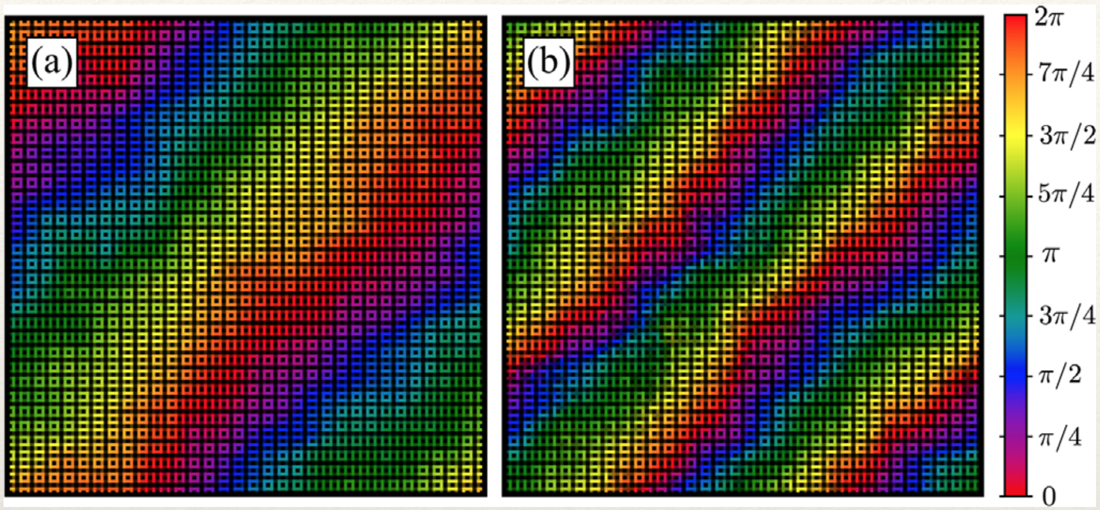
$$J'(P) = [75 - 8.3P/\mathrm{GPa}]\ \mathrm{K}$$

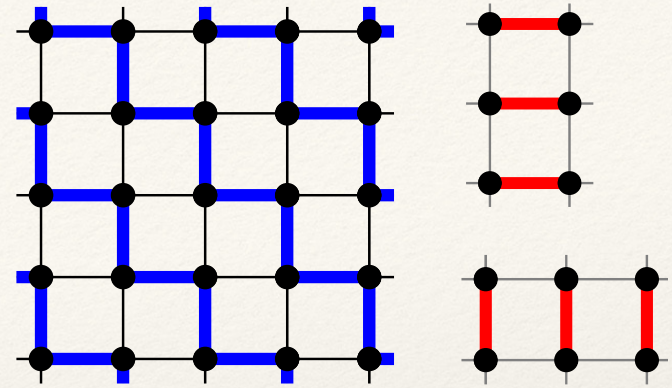
$$J(P) = [46.7 - 3.7P/\mathrm{GPa}]\ \mathrm{K}$$

Helical VBS in a deformed J-Q model

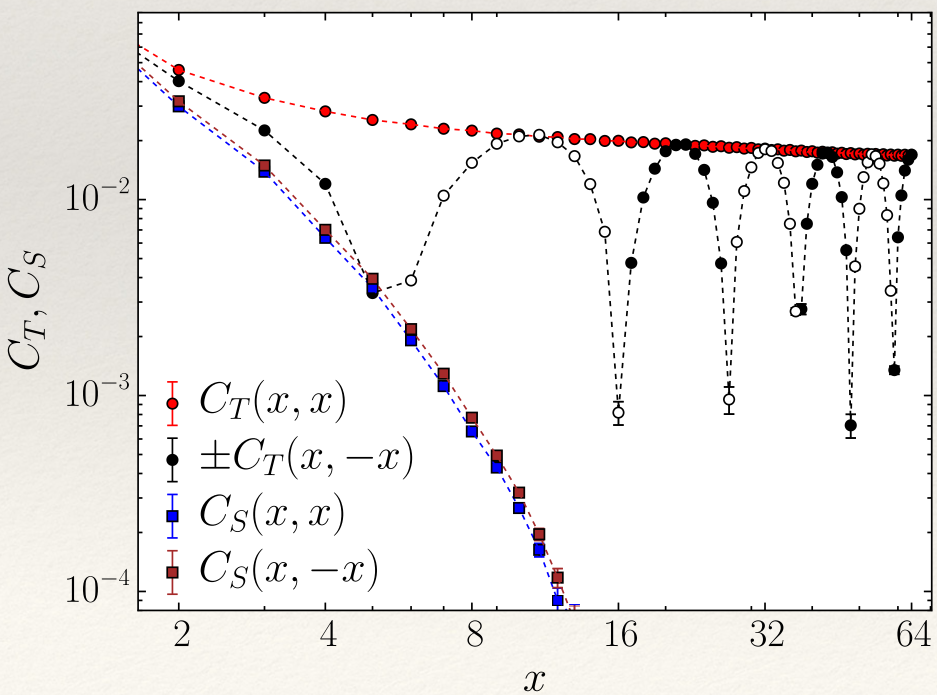
Zhao, Takahashi, Sandvik [PRL 2021]

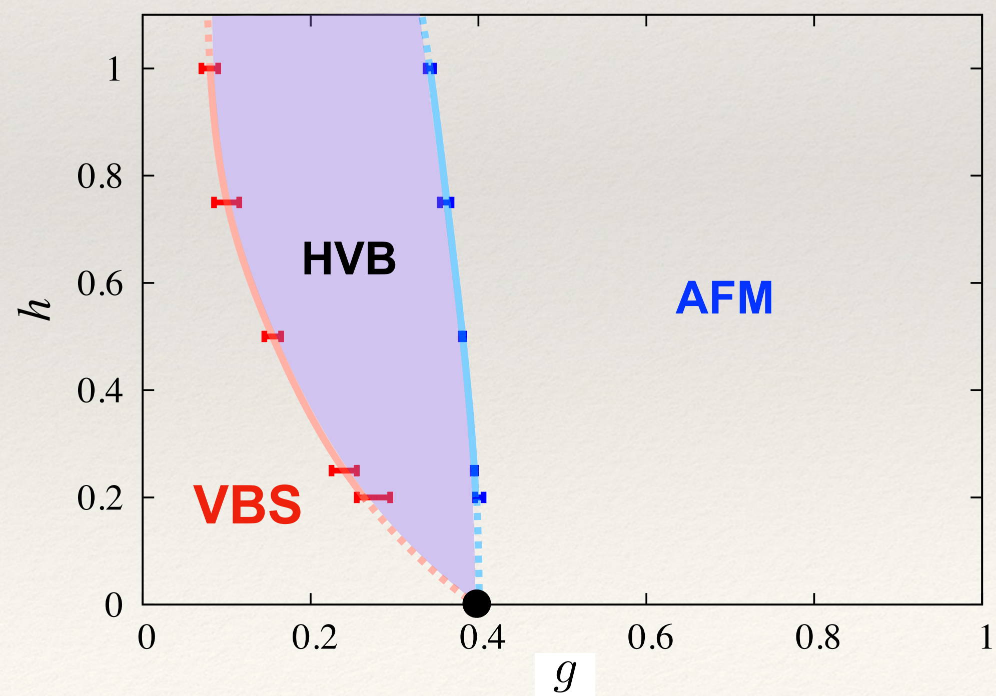
J-Q_3 model with staircase modulation of J terms
- induced a phase with winding (helical) VBS





$$J \to J(1 \pm h)$$





Quantum magnetism as a research field

Many different aspects/contexts

- materials
- artificial structures

Interesting theoretical questions

- how can we understand “exotic” quantum phases
- how can we do reliable quantitative calculations?
- connections to quantum field theory, particle physics

Experiments

- improving technologies allow better experiments

Technology

- future technologies; spintronics
- quantum computing/information

Education

- S=1/2 quantum spin contains a lot of basic quantum mech!
- quantum many-body physics with interacting spins