Bootstrapping Nature: Non-perturbative Approaches to Critical Phenomena
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Anders Sandvik, Boston University

Multi-Critical Deconfined Quantum-Critical Point - numerics and experiments

SIMONS FOUNDATION

BOSTON UNIVERSITY

Outline

Brief introduction
- deconfined criticality, lattice models and field theory

The J-Q family of 2+1 dim quantum lattice models
- designer Hamiltonians for DQC and related phenomena

Critical and "pseudo critical" behavior
- continuous transitions vs weak first-order ones

Multi-criticality
- identification of second relevant operator

Shastry-Sutherland model and checker-board J-Q model
- emergent O(4) symmetry

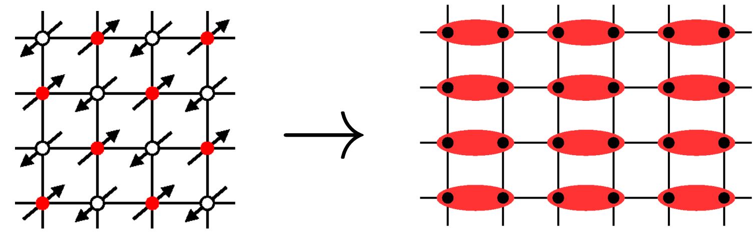
Unified phase diagram
- multi-critical DQCP as the tip of a gapless spin liquid

Experiments on $SrCu_2(BO_3)_2$
- case for proximate O(4) DQCP at high pressure and high magnetic field

Deconfined quantum criticality

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

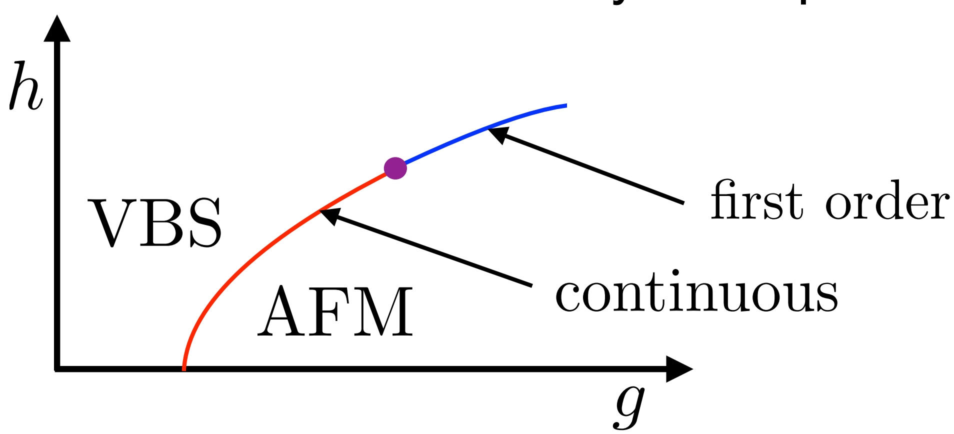
$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + g[\text{other symmetry preserving interactions}]$$

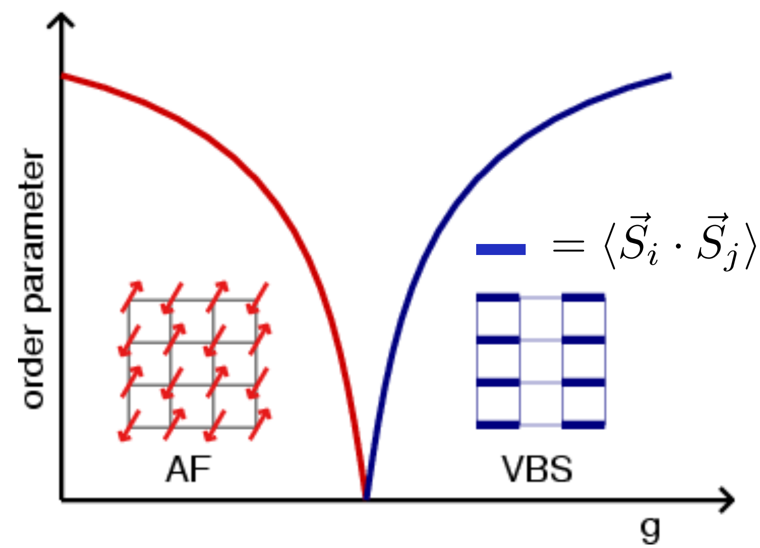


antiferromagnet for g=0
- breaks O(3) symmetry

valence-bond (or plaquette) solid for $g > g_c$
- breaks Z_4 (in other cases possibly Z_2) symmetry

Generic continuous transition at T=0
- would be violation of Landau rule
- first-order would normally be expected



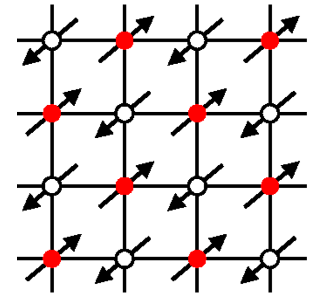


There can be a multi-critical end point of the generic critical line
- followed by 1st-order line

Field theory description; brief summary

Standard low-energy theory of quantum antiferromagnets

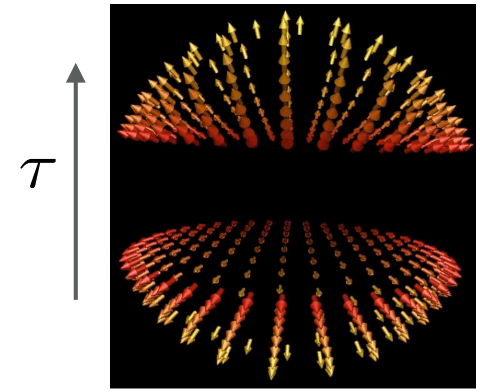
$$S = \int d^d r d\tau \tfrac{1}{2}[c^2(\partial_r\phi)^2 + (\partial_\tau\phi)^2 + m_0\phi^2 + u_o(\phi^4)]$$



Can describe Neel to featureless paramagnetic transition

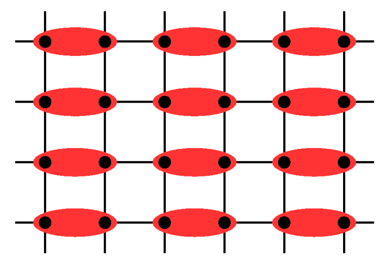
- VBS pattern or topological order cannot be captured

Graph:Senthil et al.



Topological defects (hedgehogs) in field configurations:

- suppressed in the Neel state
- proliferate in the quantum paramagnet



The VBS state corresponds to a certain **condensation of topological defects**

Neel vector described by spinors z; $\phi = z^*_\alpha \sigma_{\alpha\beta} z_\beta$ [Murthy & Sachdev 1991, Read & Sachdev 1991]

- coupled to U(1) gauge field where hedgehogs correspond to monopoles
- VBS on square lattice arises from condensation of quadrupled monopoles

Topological defects conjectured "dangerously irrelevant" at transition

- universality of defect suppressed O(3)
- topological defects relevant in VBS state only

Senthil, Vishwanath, Balents, Sachdev, Fisher (2004)

$$\mathcal{S}_z = \int d^2 r d\tau \left[|(\partial_\mu - iA_\mu)z_\alpha|^2 + s|z_\alpha|^2 + u(|z_\alpha|^2)^2 + \frac{1}{2e_0^2}(\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda)^2 \right]$$ non-compact (defect-free) CP^1 model

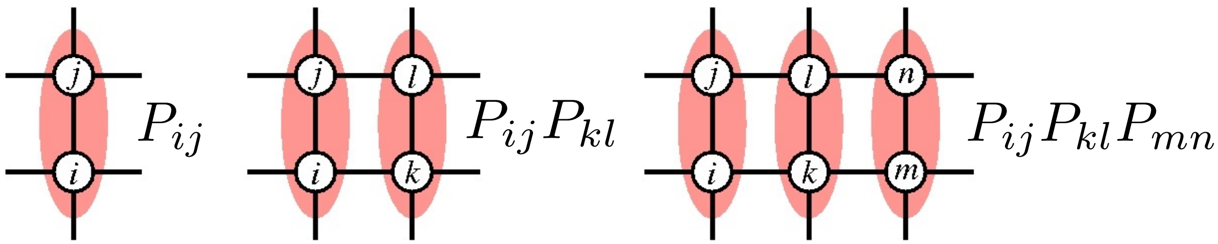
large-N calculations for SU(N) CP^{N-1} theory → continuous transition

SU(2): Designer Hamiltonian for DQC physics, J-Q model

The Heisenberg exchange = singlet-projector

$$P_{ij} = \frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j \qquad H_{\text{Heisenberg}} = -J \sum_{\langle ij \rangle} P_{ij}$$

- Extended models with products of singlet projectors

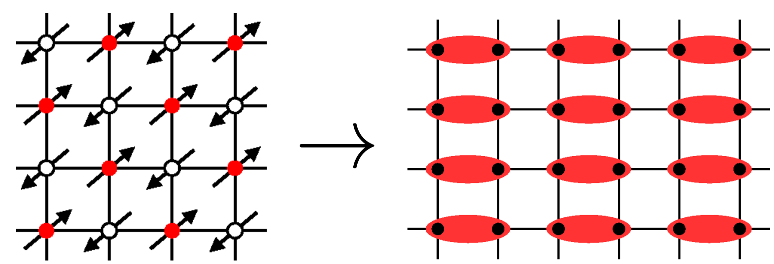


\+ all translations and rotations

- no frustration in the conventional sense (no QMC sign problem)
- correlated singlet projection still competes with antiferromagnetism

The J-Q model with two projectors (Sandvik 2007):

$$H_{JQ_2} = -J \sum_{\langle ij \rangle} P_{ij} - Q \sum_{\langle ijkl \rangle} P_{ij} P_{kl}$$

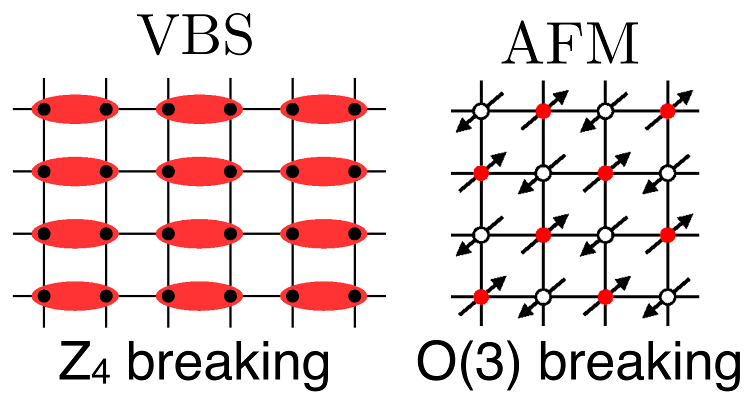


- Has **Néel-VBS transition of ground state**
- Sign-free in QMC simulations; large-scale simulations possible

Many variants, extensions of J-Q models

- test predictions from quantum field-theory, find new RG fixed points
- make contact with experiments on exotic quantum magnets

Phase transition in the J-Q_2 model



QMC simulations
- no approximations

Order parameters:

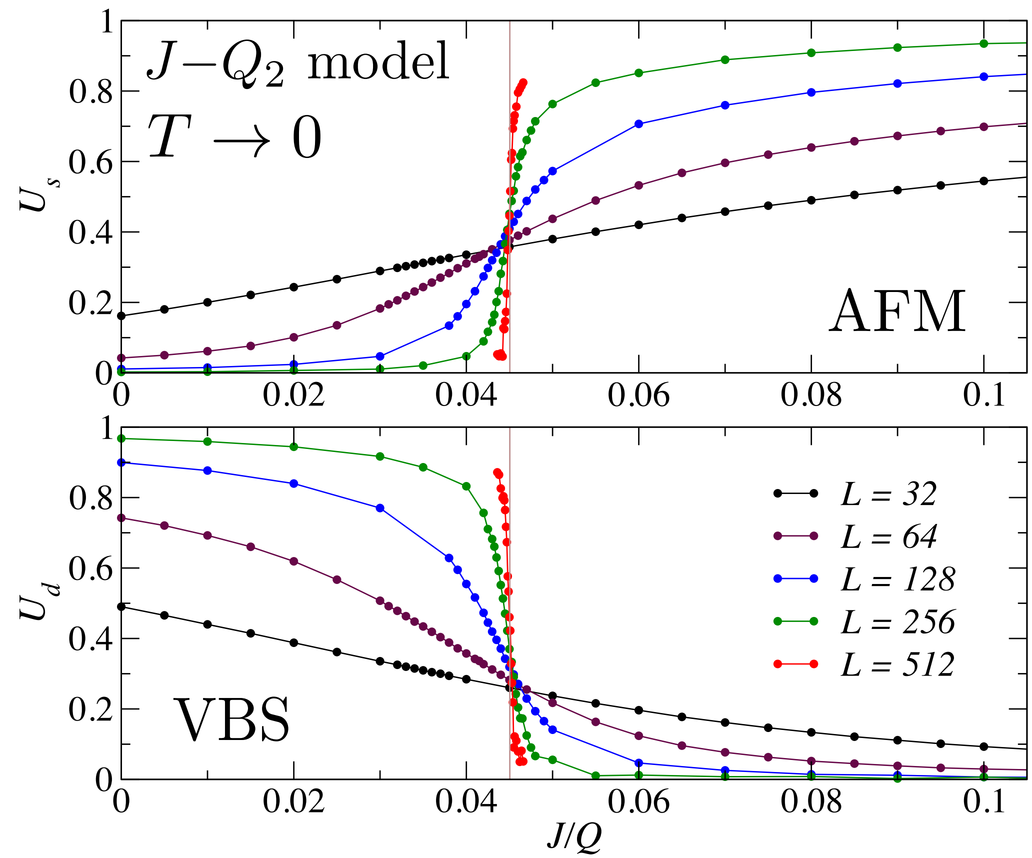
AFM: staggered magnetization

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

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 (finite-size scaling)
- consistent with simultaneous, continuous (or almost…) transition

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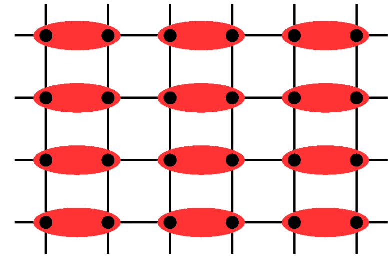
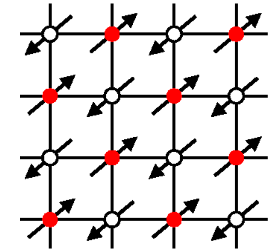
VBS

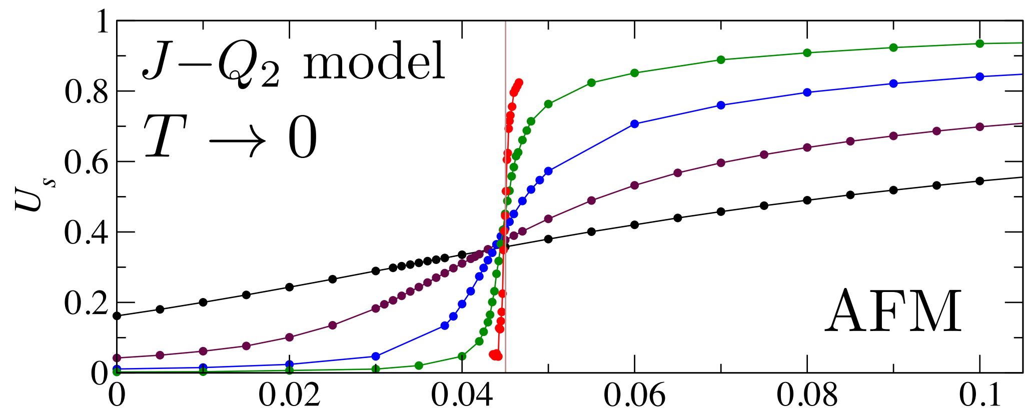


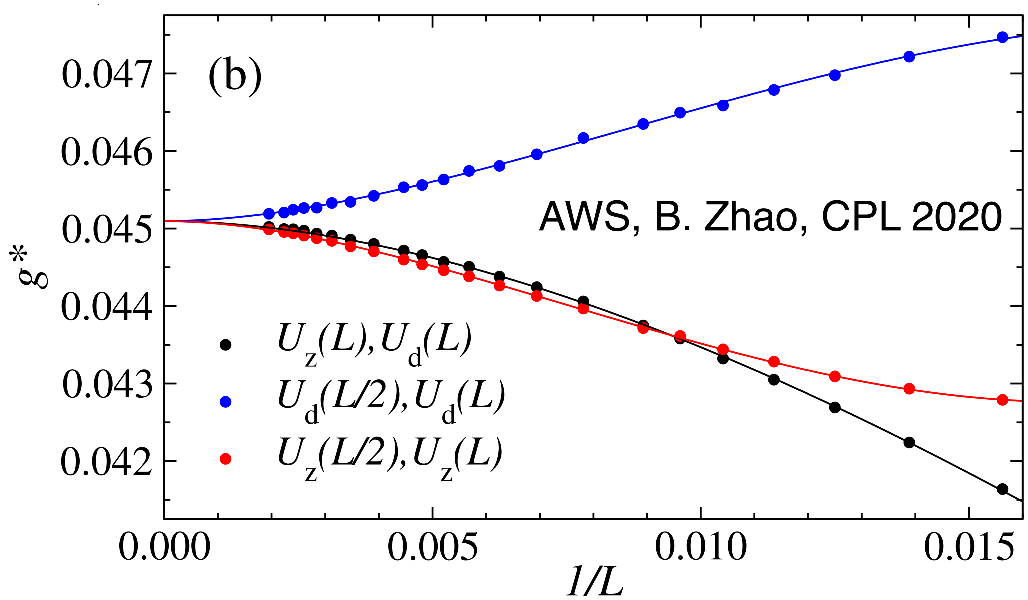
Z_4 breaking

AFM



O(3) breaking





Crossing-point analysis (finite-size scaling)
- consistent with simultaneous, continuous (or almost…) transition

Correlation-length exponent, J-Q_2

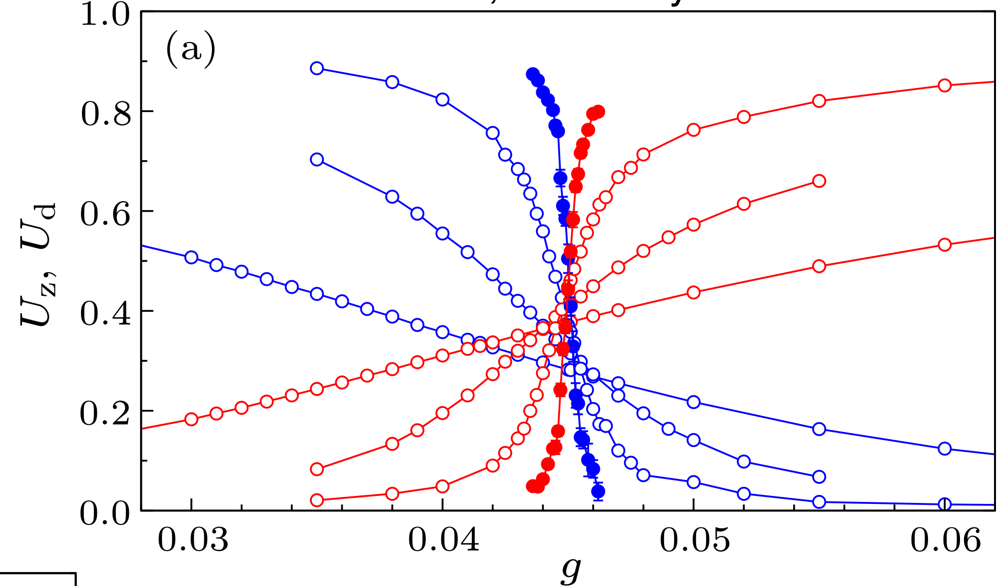
Binder cumulants give critical point

- slopes at g_c can be used to extract $1/\nu$

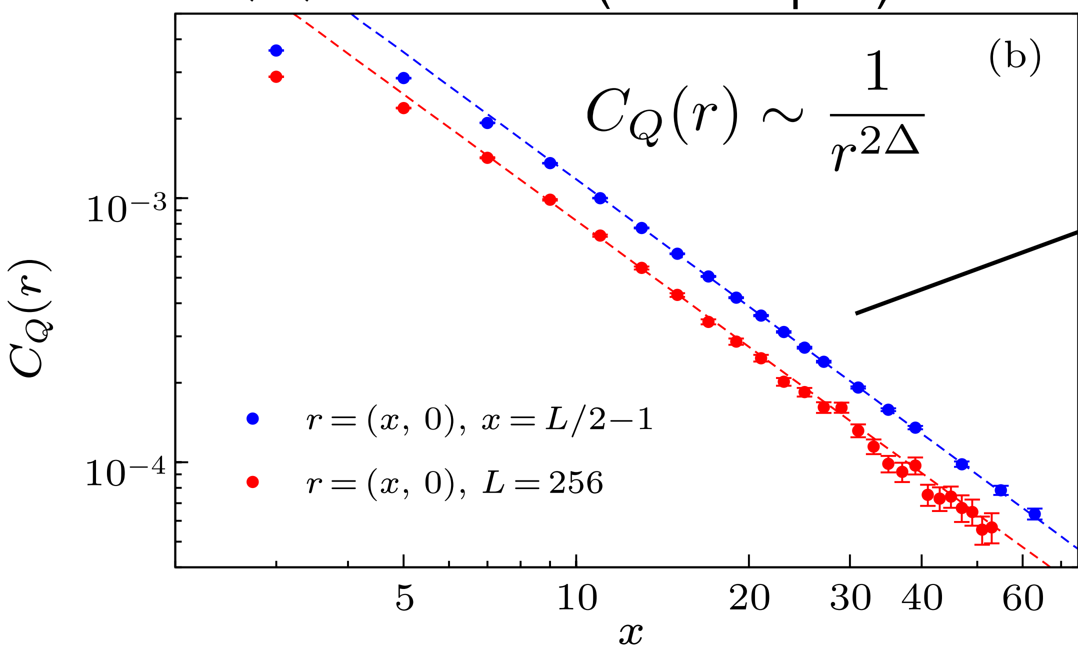
$$\frac{1}{\ln(2)} \ln\left(\frac{U'(2L)}{U'(L)}\right) \to \frac{1}{\nu} \quad = 3 - \Delta$$

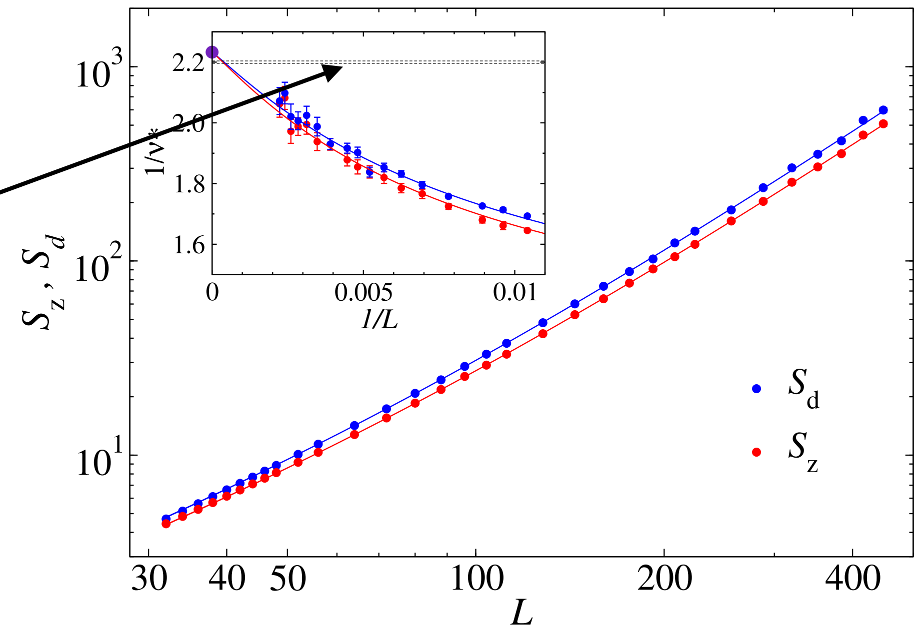
We can also calculate correlations of the relevant J and Q terms in H

Sandvik & Zhao, Chin. Phys. Lett. 2020



Q-Q correlations (uniform part)





Mutual consistency between two methods: $\nu = 0.455 \pm 0.002$

- at the very least, the model is extremely close to a critical point
- but violates CFT bound: $\nu > 0.51$ (if one relevant scalar; Nakayama, Ohtsuki, PRL 2016)

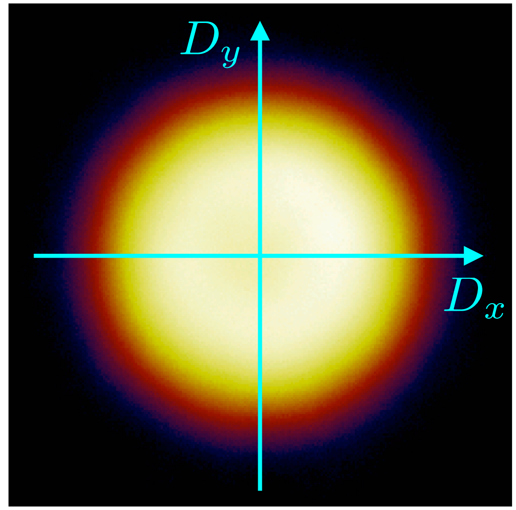
Emergent U(1) symmetry

VBS distribution $P(D_x,D_y)$

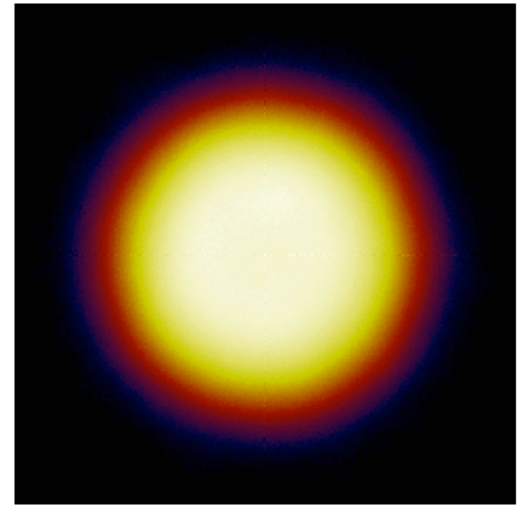
$$D_x = \frac{1}{N}\sum_{x,y}(-1)^x \mathbf{S}_{x,y}\cdot\mathbf{S}_{x+1,y}$$

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

L=64, J/Q_2 = 0.042



L=64 J/Q_2 = 0.043



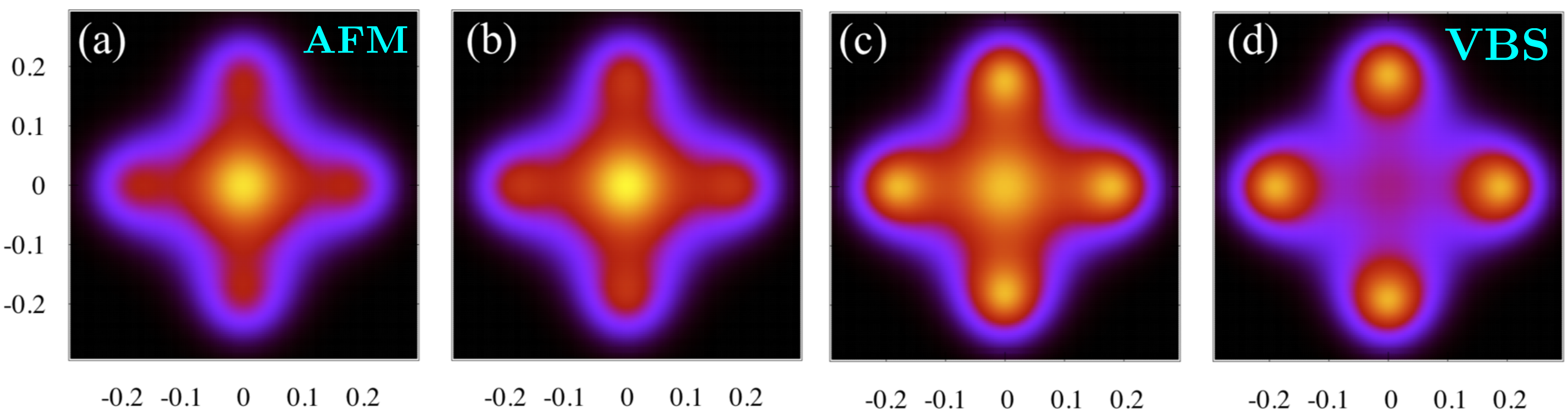
Emergent SO(5) symmetry has also been detected (3D loop model) (Nahum et al, PRL 2015)

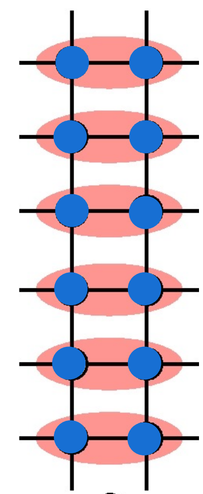
- emergent U(1) VBS combines with O(3) AFM

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

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

<u>J-Q_6 model (J. Takahashi, AWS, PRR 2020)</u>



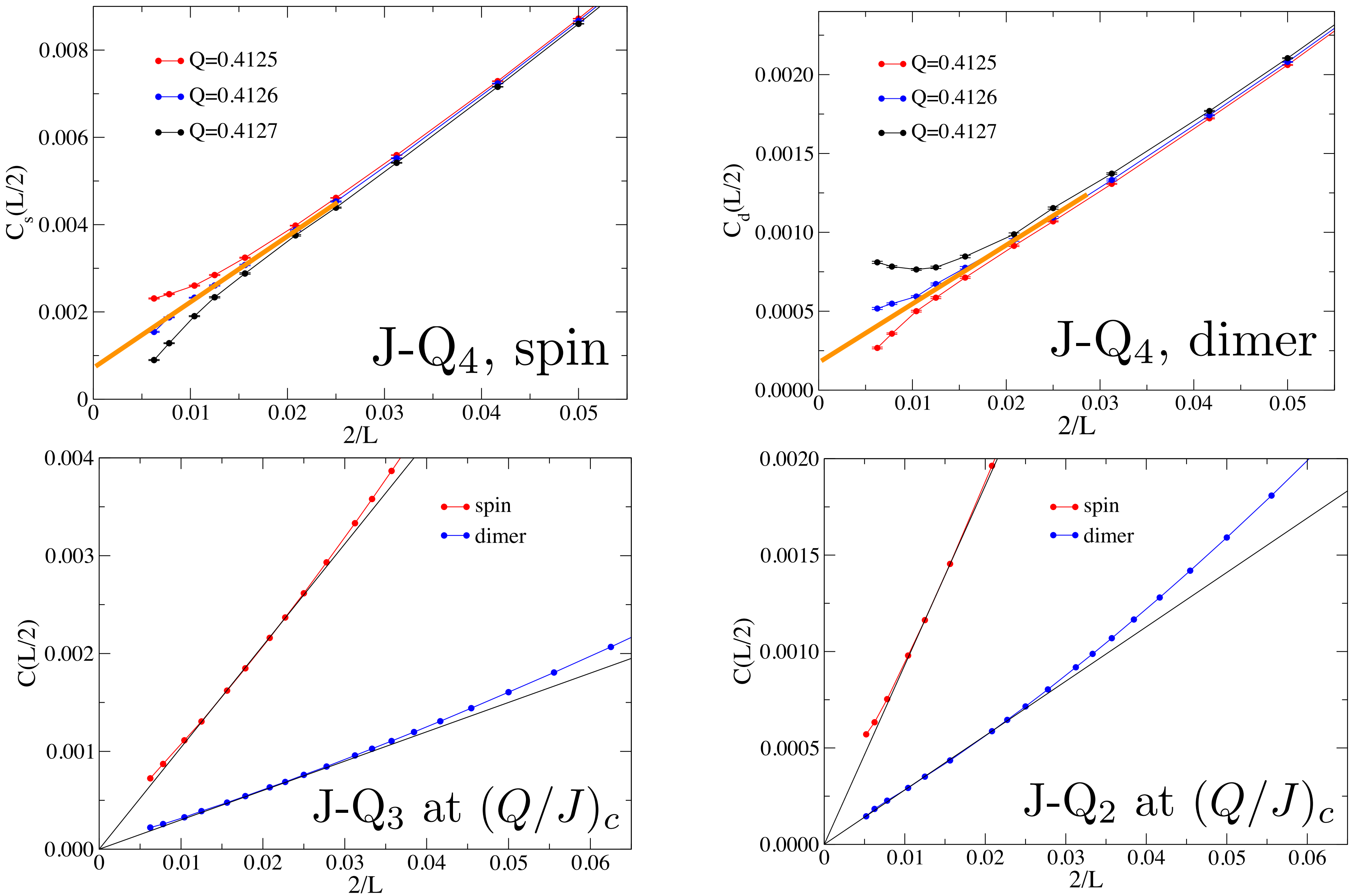


Coexistence between 4-fold degenerate columnar state and AFM

- J-Q_n model must have first-order transition above some n

Detection of coexistence; long-distance correlations

- a coexistence state should have long-ranged spin and dimer correlations



J-Q_3 and J-Q_4 have first-order transitions

(unpublished)

- very weak for J-Q_3; detectable only for L>200
- likely first-order also in J-Q_2, but not completely clear

Consistency of “quasi exponents” between models?

Are exponents extracted at a weak first-order transition really meaningful?

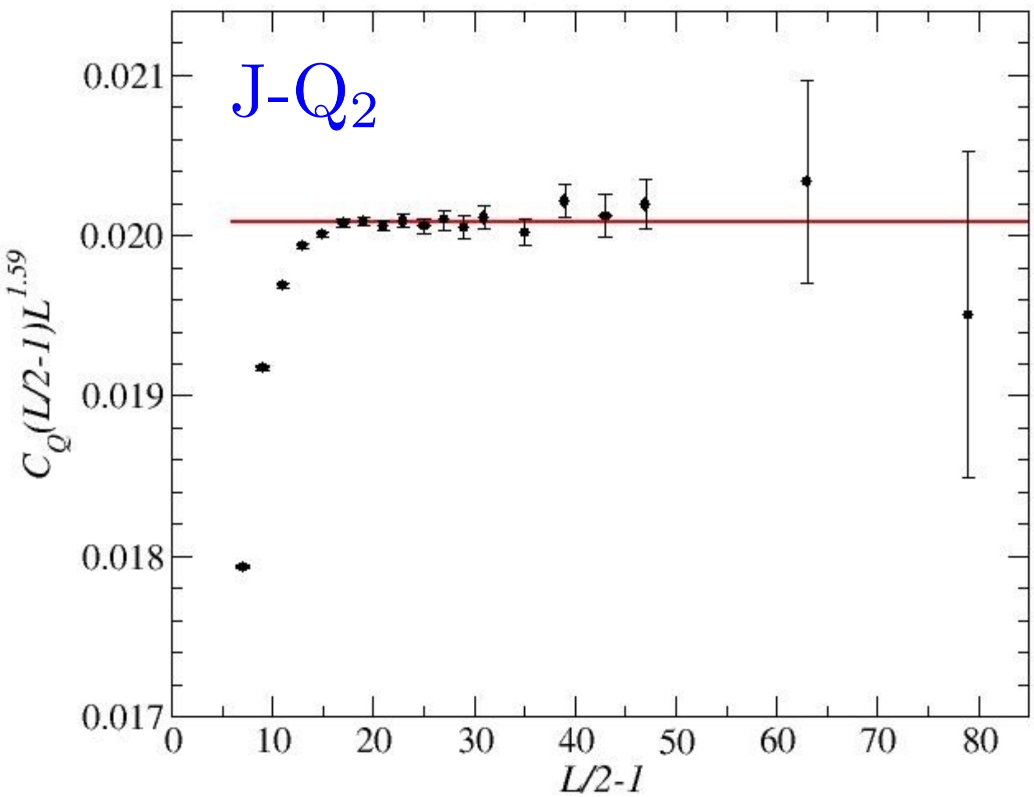
- critical exponents of some nearby critical point

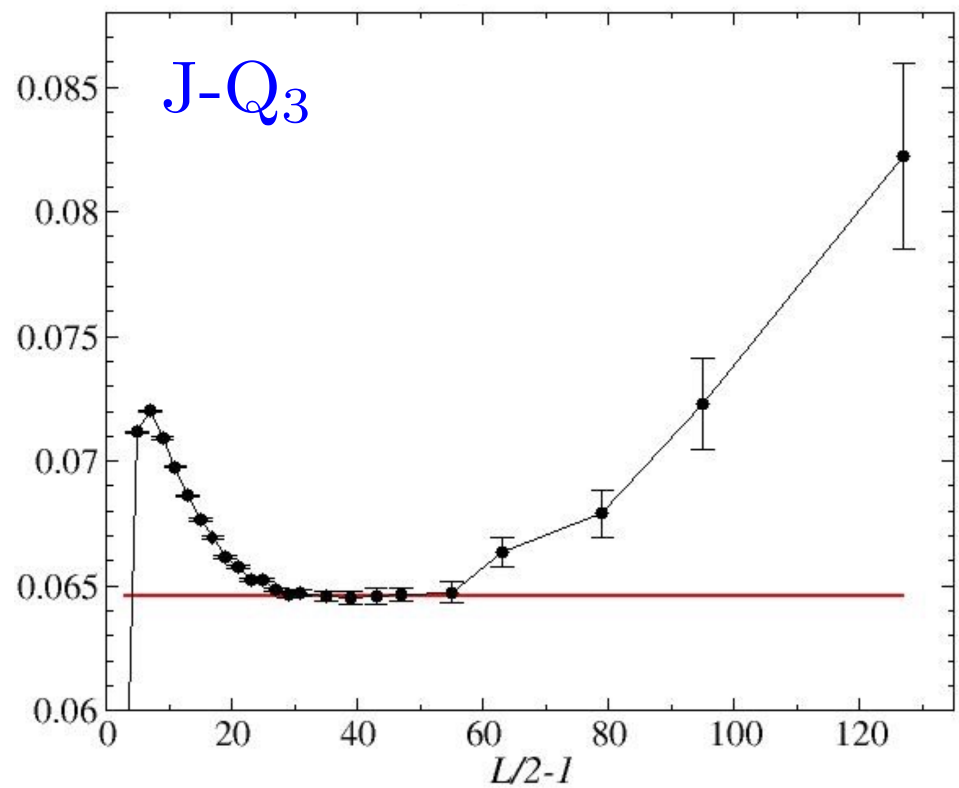
The J-Q_2 and J-Q_3 models are presumably close to the same DQCP

Q-Q correlations for both models

$$C_Q(r) \sim \frac{1}{r^{2\Delta}} \quad \rightarrow C_Q(r)r^{2\Delta} \rightarrow \text{constant}\ (L \rightarrow \infty) \qquad 2\Delta \approx 1.6$$

Showing for r=L/2 -1 versus L/2-1 (T=0 projector QMC, unpublished results)





J-Q_3 model exhibits same criticality as J-Q_2 before “running away” from DQCP

Dynamic signatures of deconfined quantum criticality

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

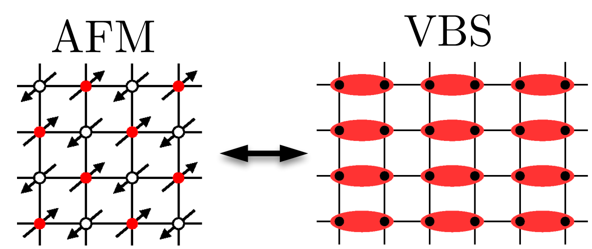
Editors' Suggestion

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: $H_{\mathrm{JQ}} = -J\sum_{\langle ij\rangle}(P_{ij} + \Delta S_i^z S_j^z) - Q\sum_{\langle ijklmn\rangle} P_{ij}P_{kl}P_{mn}$ $\qquad P_{ij} = \frac{1}{4} - \mathbf{S}_i\cdot\mathbf{S}_j$

Spin structure factor S(q,ω) at the transition point (weak 1st order transition)



QMC + analytic continuation

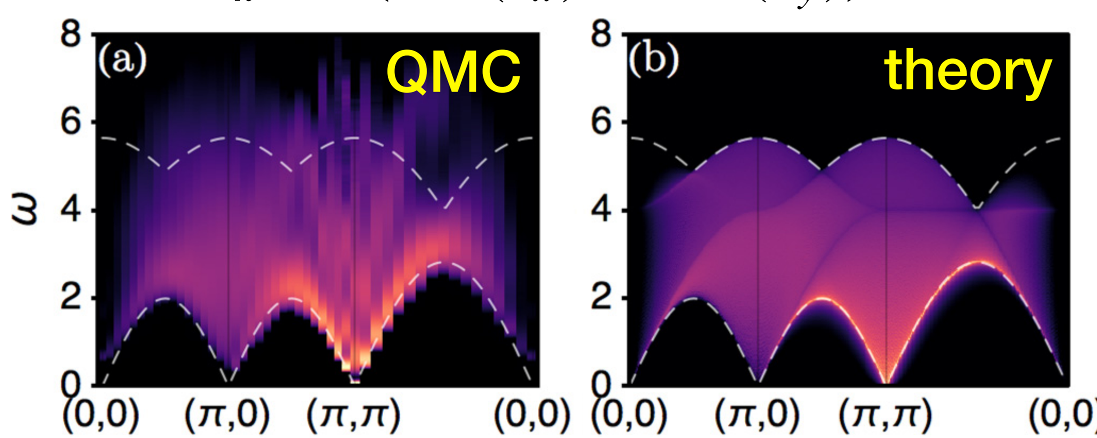
Good agreement with mean-field calculation of fermionic parton theory; N_f=4 compact QED_3

π-flux square-lattice model

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

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

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



Spinon deconfinment manifested on large length scales close to the phase transition

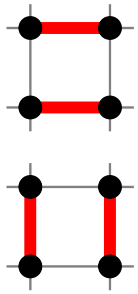
DQCP phenomenology applies even for weak first-order transitions

Multi-Critical DQCP Scenario

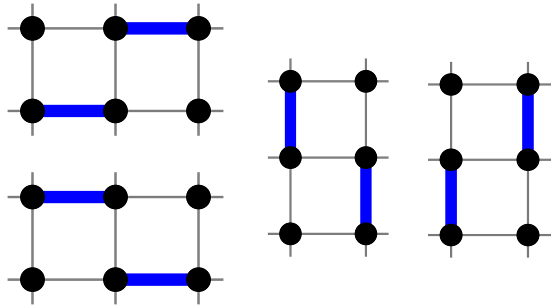
Zhao, Takahashi, Sandvik, PRL 2020

Identified a second symmetric relevant operator

Q



Z



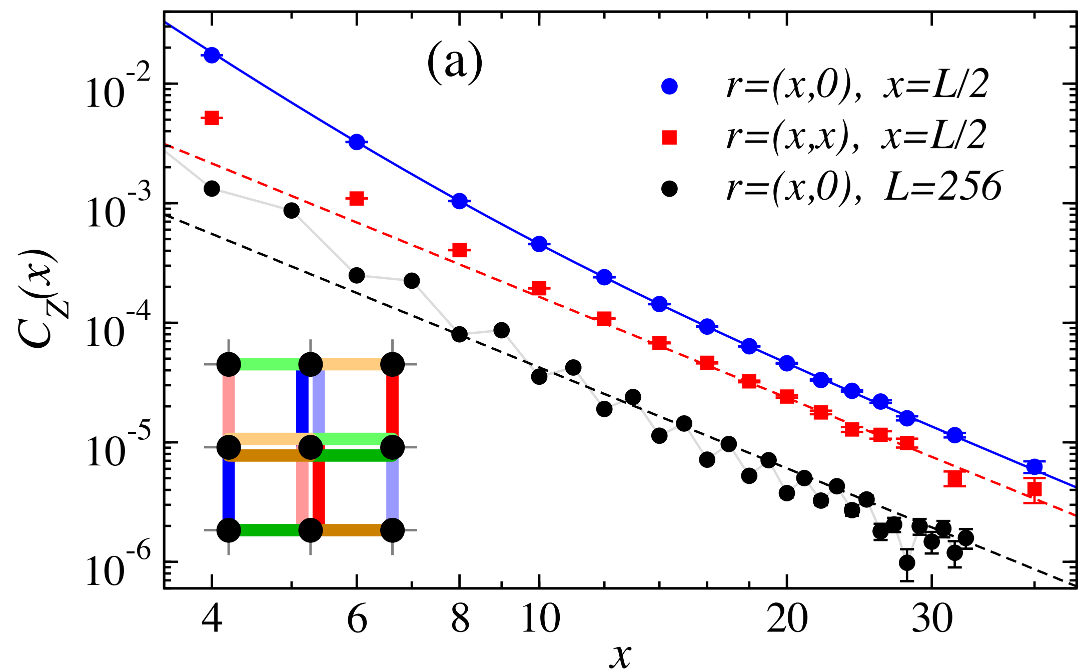
summed over all lattice positions

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

No change in symmetry

Compute scaling **dimension of the Z perturbation** in the (near) critical J-Q_2 model

- ZZ Correlations at δ=0 decay with a power corresponding to
  $\Delta_Z \approx 1.40$
  different from
  $\Delta_Q \approx 0.80$
- Bootstrap bound assumed a single relevant scalar
- Why is $C_Z(r)$ not contaminated by Δ_Q?



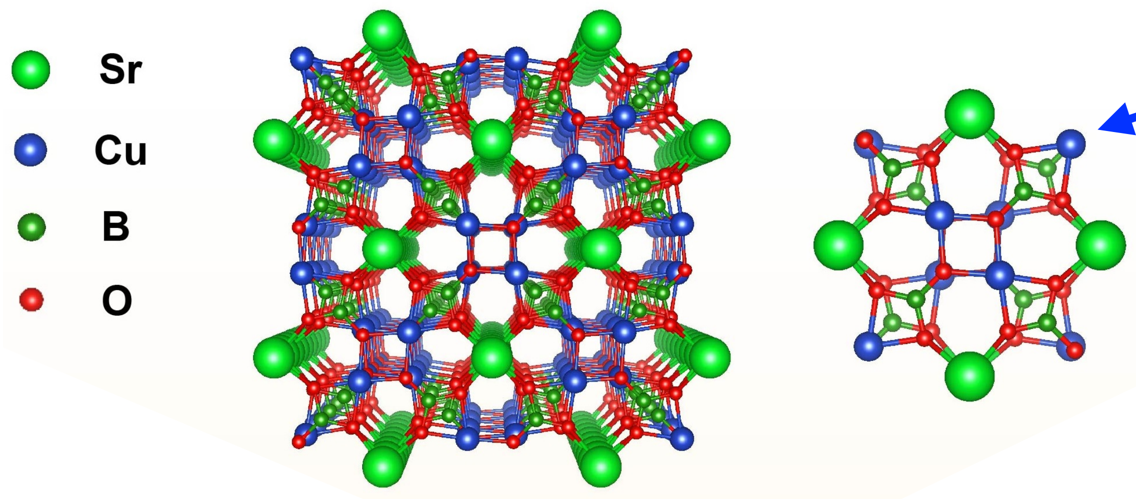
The Q term may be slightly contaminated by Δ_Z - reason for weak 1st-order?

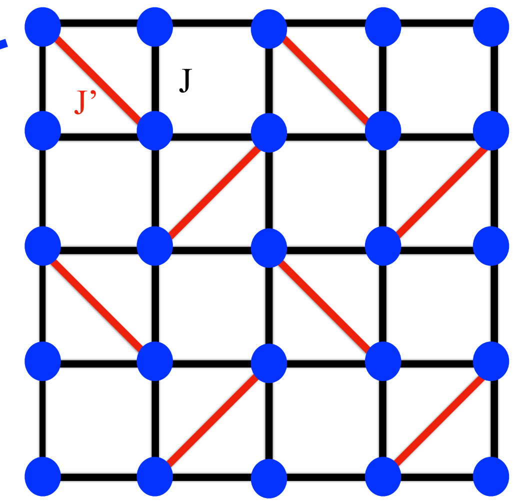
- agrees with theoretical analysis of Z interaction; Lu, You, Xu, PRB 2021
- in J-Q_n model, “contamination” increases with n (stronger first-order)

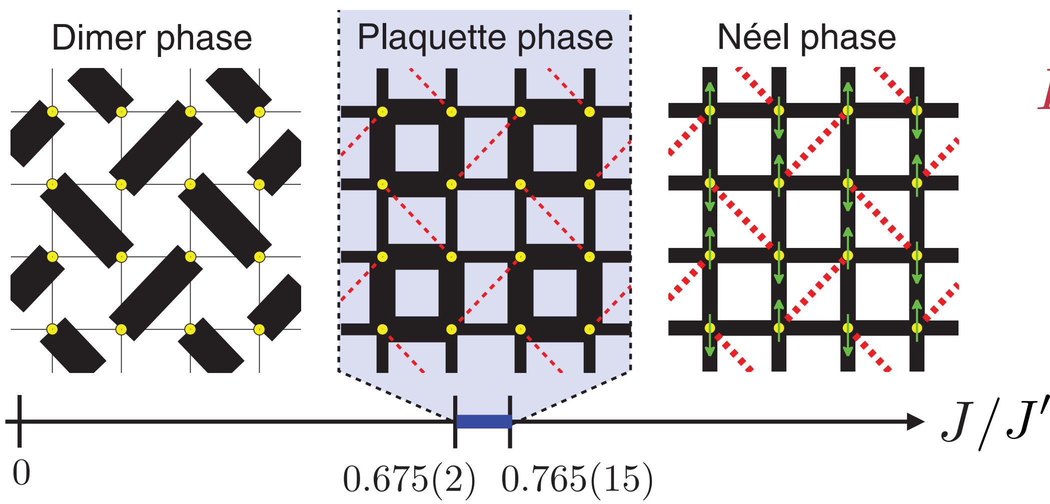
Multi-critical scenario goes beyond original DQC proposal

Plaquette-singlet (PS) state and the Shastry-Sutherland model

Realized in the quasi-2D quantum magnet $SrCu_2(BO_3)_2$







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

three ground state phases versus ratio g=J/J'

- g in $SrCu_2(BO_3)_2$ increases with applied (high) pressure

Corboz & Mila, PRB 2013 (tensors)
- T=0: weak first-order Neel to PS transition

Lee, You, Vishwanath, Sachdev PRX 2020 (DMRG)
- continuous DQCP transition with emergent O(4) symmetry

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

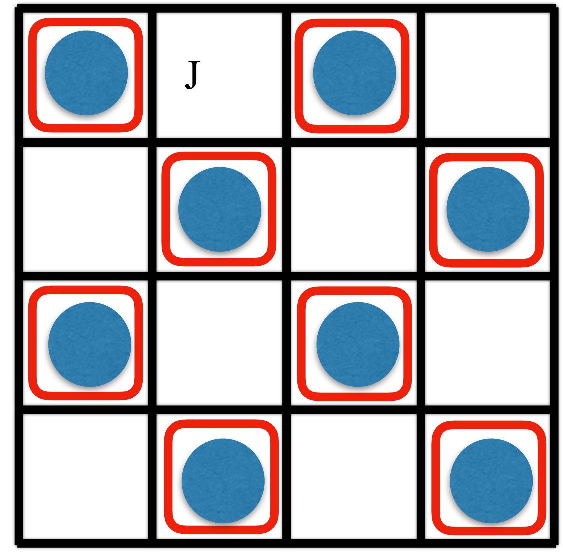
B. Zhao, P. Weinberg, AWS, Nature Physics 2019

Replace frustrated SS bonds by 4-spin Q terms

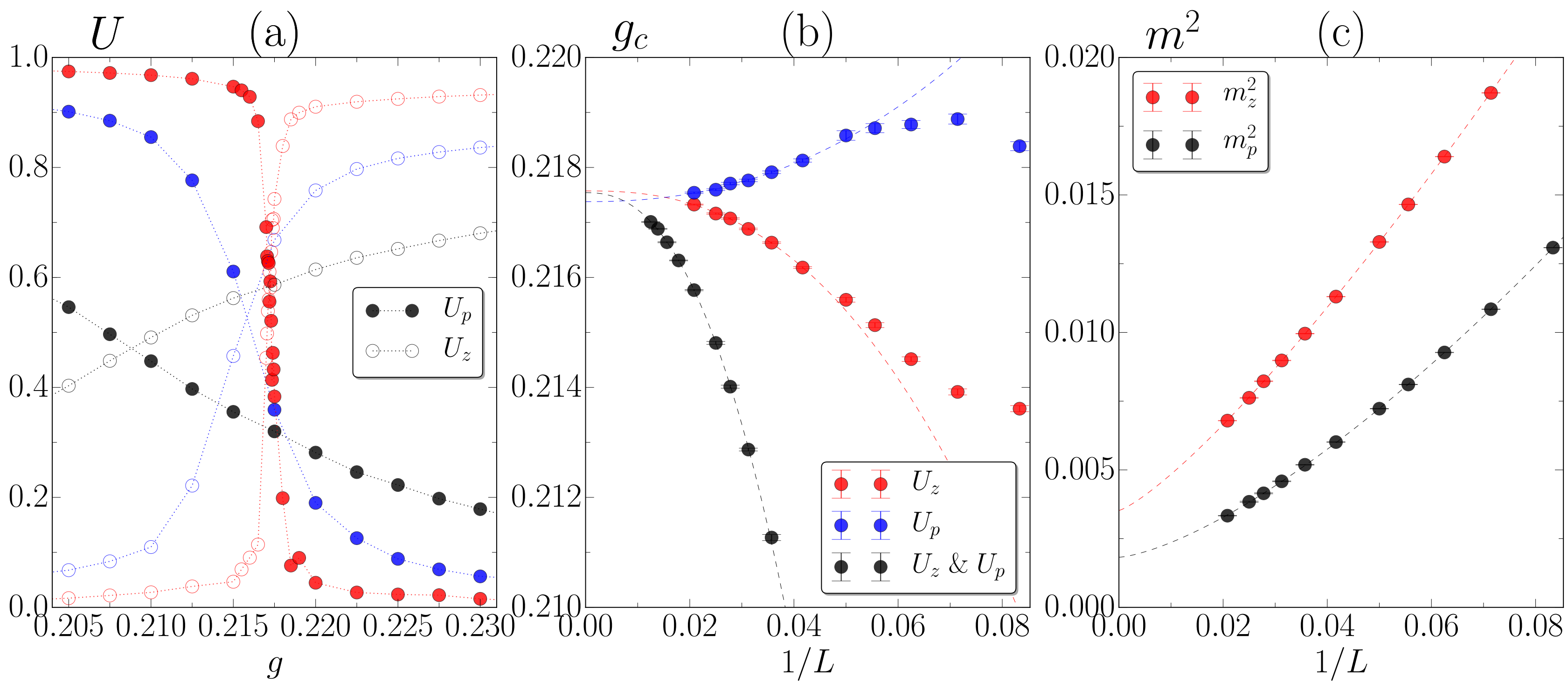
$$\mathcal{H} = -J \sum_{\langle ij \rangle} P_{ij} - Q \sum_{ijkl \in \square'} (P_{ij}P_{kl} + P_{ik}P_{jl})$$

Allows 2-fold degenerate PS state

- Z_2 symmetry breaking



QMC results vs 1/L, $g = J/Q$

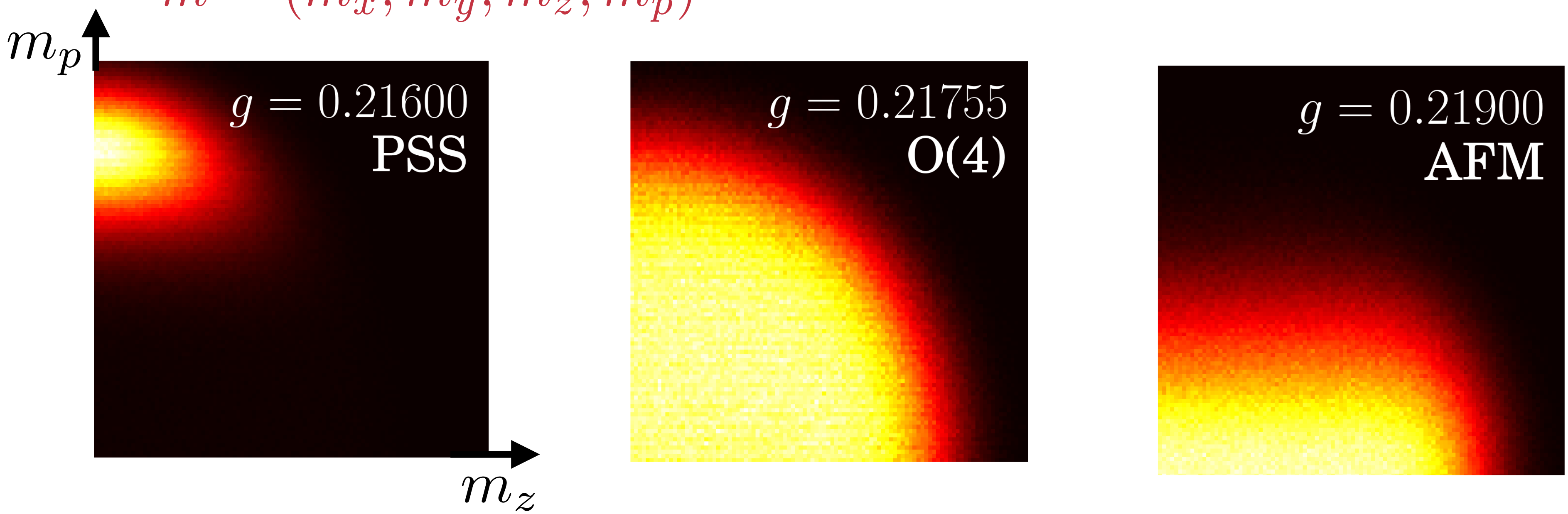


(a) AF-PS transition, (b) g_c = 0.2175(1), (c) coexisting orders

→ **clearly first-order transition**

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

$$\vec{m} = (m_x, m_y, m_z, m_p)$$



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

- fluctuating radius due to finite size

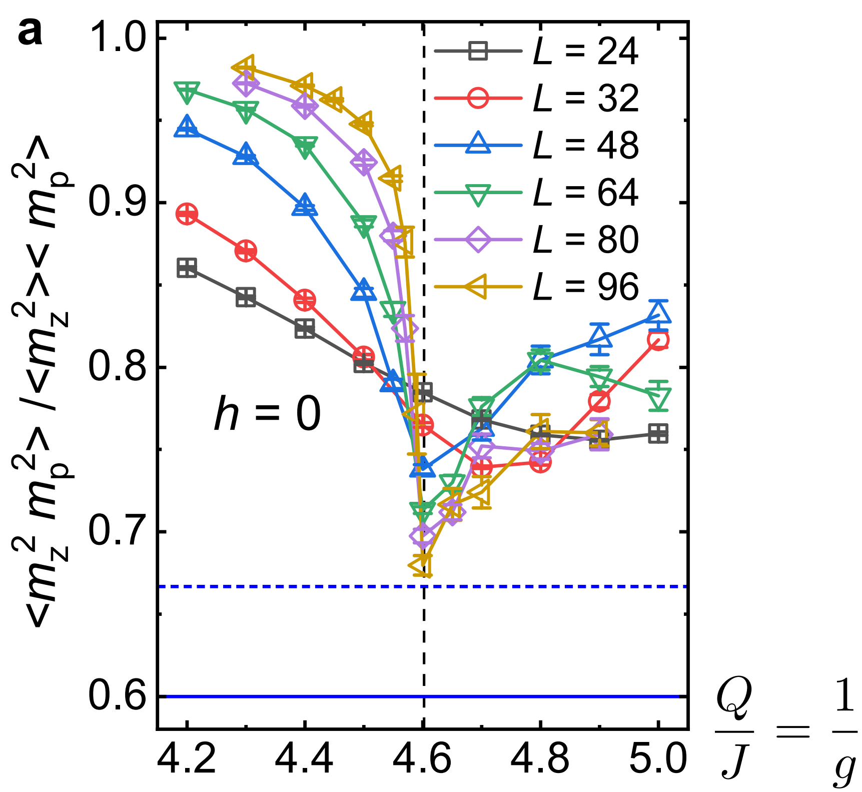
Further demonstration (arXiv:2204.08133)

- cross-correlations of the order params

$$C = \frac{\langle m_z^2 m_p^2 \rangle}{\langle m_z^2 \rangle \langle m_p^2 \rangle}$$

O(4) value is C=2/3

- approached vs L at the transition point

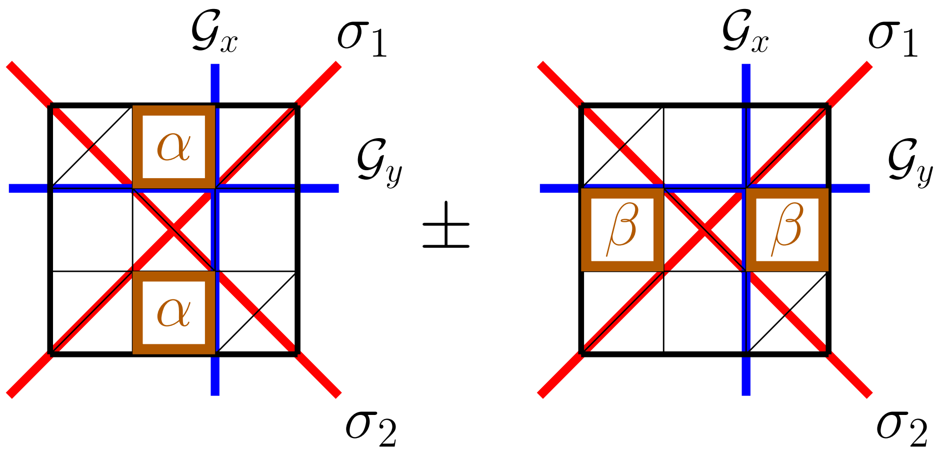


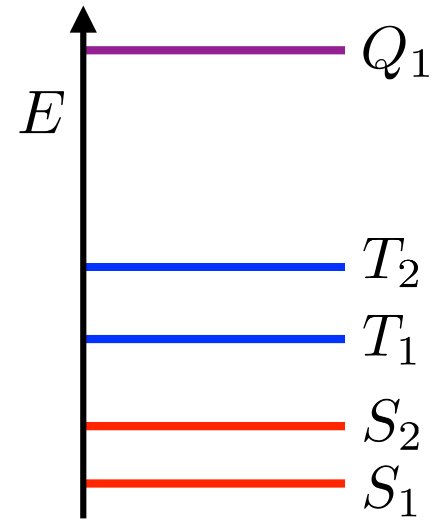
Revisiting the Shastry-Sutherland model

Wang, Zhang, Sandvik, CPL 2022 (arXiv:2205.02476)
Yang, Sandvik, Wang, PRB 2022

Level spectrum → locate quantum phase transitions

quasi-degenerate singlet ground state of the plaquette-singlet-solid (PSS)





Singlets S_1, S_2
Triplets T_1, T_2
Quintuplet Q

Gaps: $\Delta(S_2) = E(S_2) - E(S_1)$ $\quad \Delta(T_1) = E(T_1) - E(S_1)$

Composite gaps: $\delta_T = E(T_2) - E(S_2)$ $\quad \delta_Q = E(Q_1) - E(T_1)$

<u>Gap criteria for PSS and AFM ordered phases</u>

PSS: $\Delta(S_2) < \Delta(T_1)$ doubly-degenerate ground state, triplet gapped

AFM: $\Delta(Q_1) < \Delta(S_2), \quad \delta_T < \Delta(S_2)$

$E_S \propto S(S+1)/N$

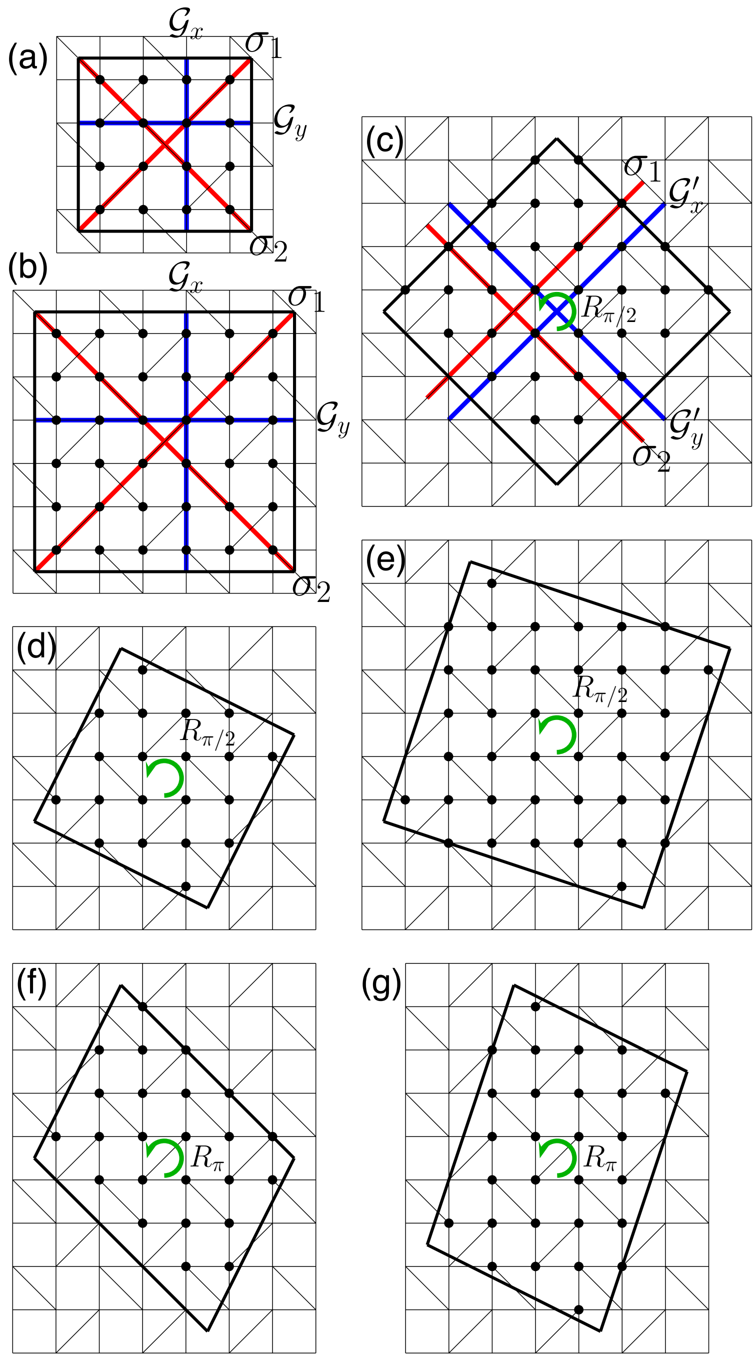
S_2 gapped; amplitude mode

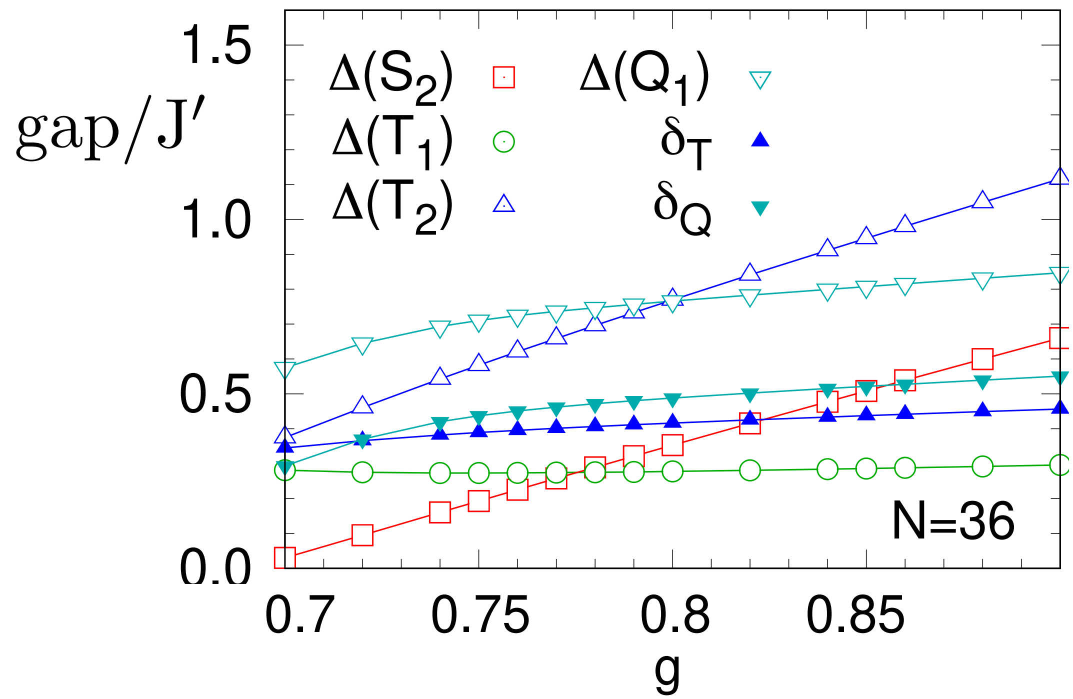
Gap crossings vs g to detect quantum phase transitions

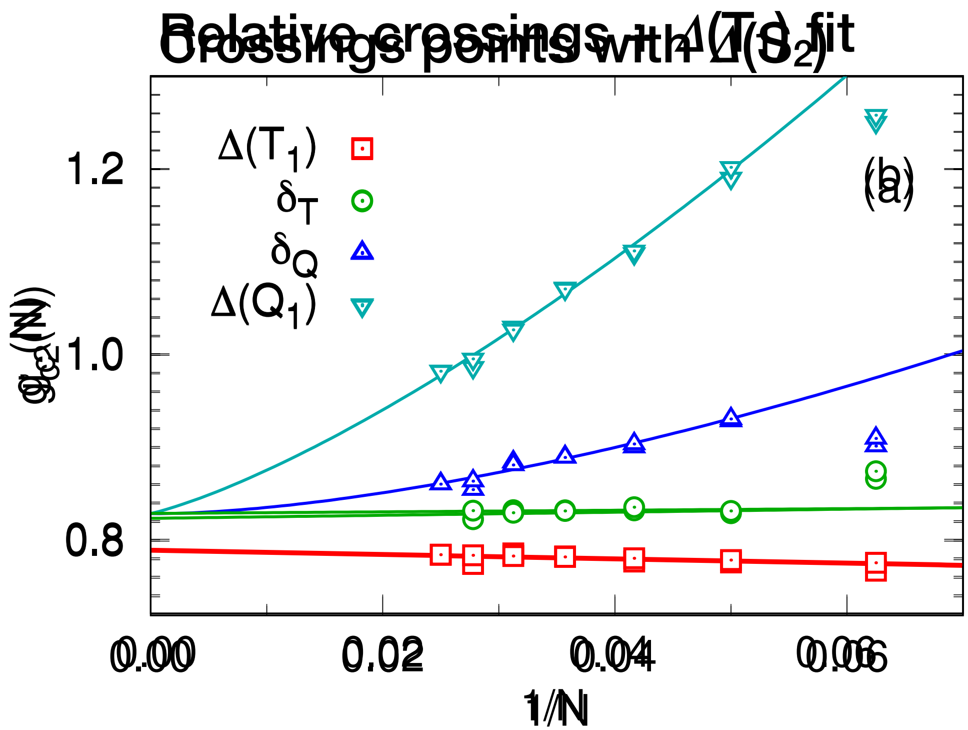
Lanczos calculations for periodic small clusers, N up to 36

DMRG for cylinders, up to N=12*24 (slightly different crossing arguments)

Clusters and symmetries





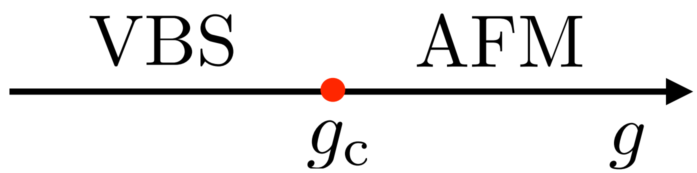


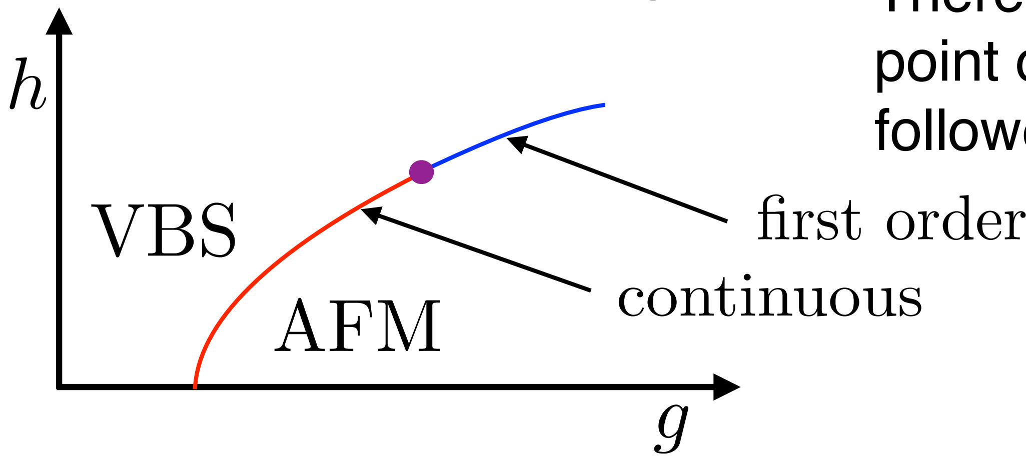
Gapless spin liquid phase for g ∊ (0.79,0.83)? DMRG gives compatible results.

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

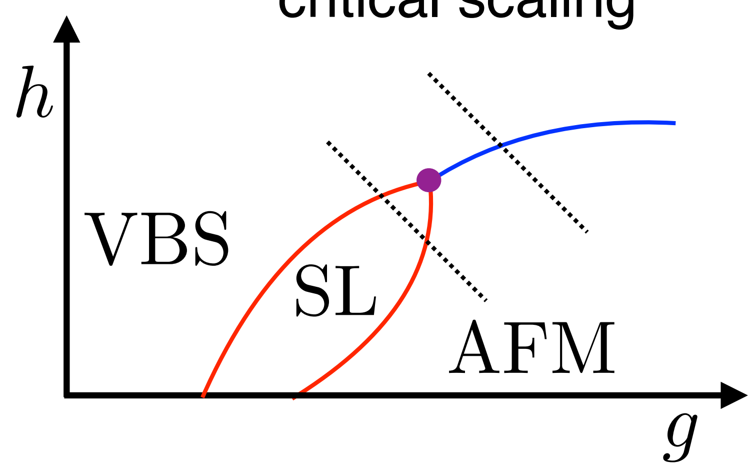
There can be a multi-critical end point of the generic critical line, followed by 1st-order line

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

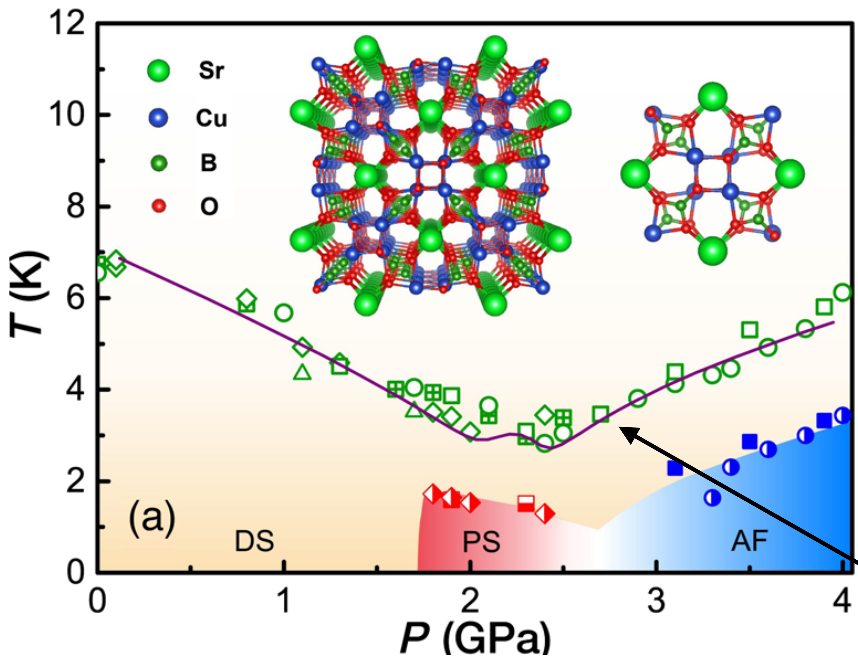


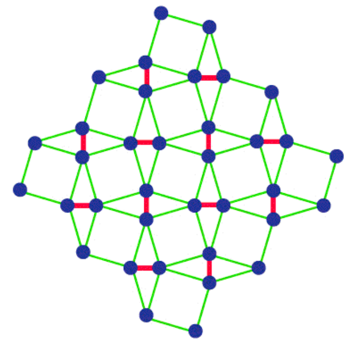
Experiments: Shastry-Sutherland material $SrCu_2(BO_3)_2$

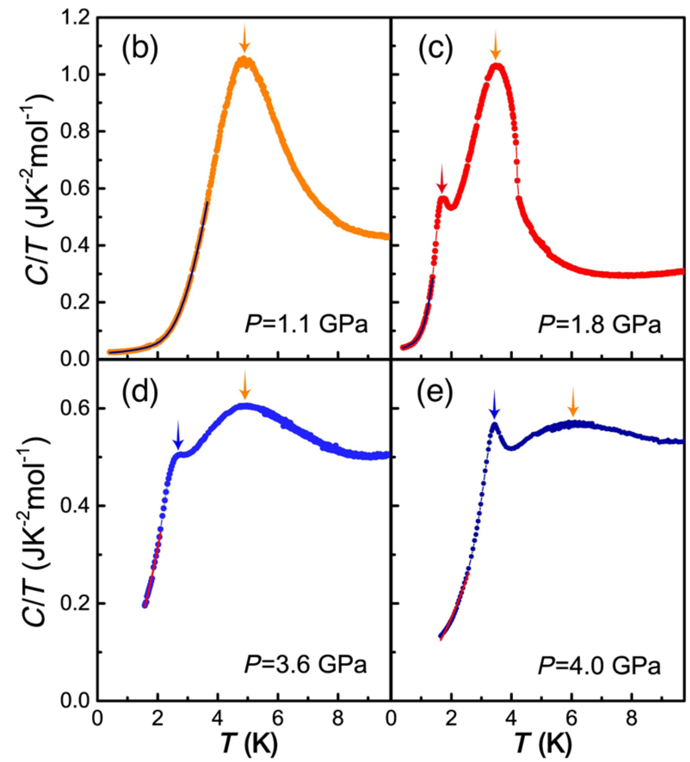
PHYSICAL REVIEW LETTERS **124**, 206602 (2020)

Quantum Phases of $SrCu_2(BO_3)_2$ from High-Pressure Thermodynamics

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







g=J/J' depends on the pressure

hump location compared with numerical result

First experimental phase diagram consistent with the SS model

Spin liquid phase between PS and AFM?

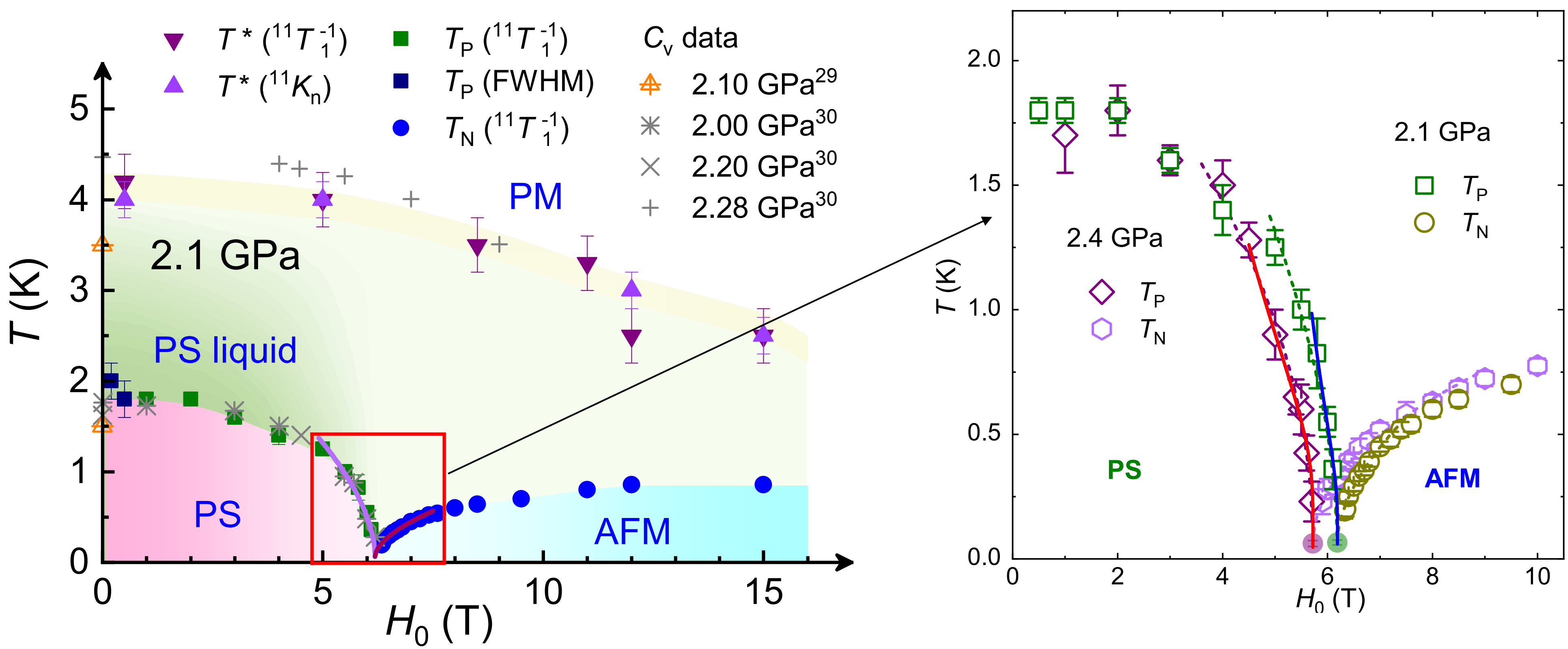
Experimental limitations for P > 2.6 GPa, T < 1.5 K

arXiv:2204.08133v1 [cond-mat.str-el] 18 Apr 2022

Proximate deconfined quantim-critical point in $SrCu_2(BO_2)_3$

Yi Cui,[1,*] Lu Liu,[2,*] Huihang Lin,[1,*] Kai-Hsin Wu,[3] Wenshan Hong,[2] Xuefei Liu,[1] Cong Li,[1]
Ze Hu,[1] Ning Xi,[1] Shiliang Li,[2,4,5] Rong Yu,[1,†] Anders W. Sandvik,[3,2,‡] and Weiqiang Yu[1,§]

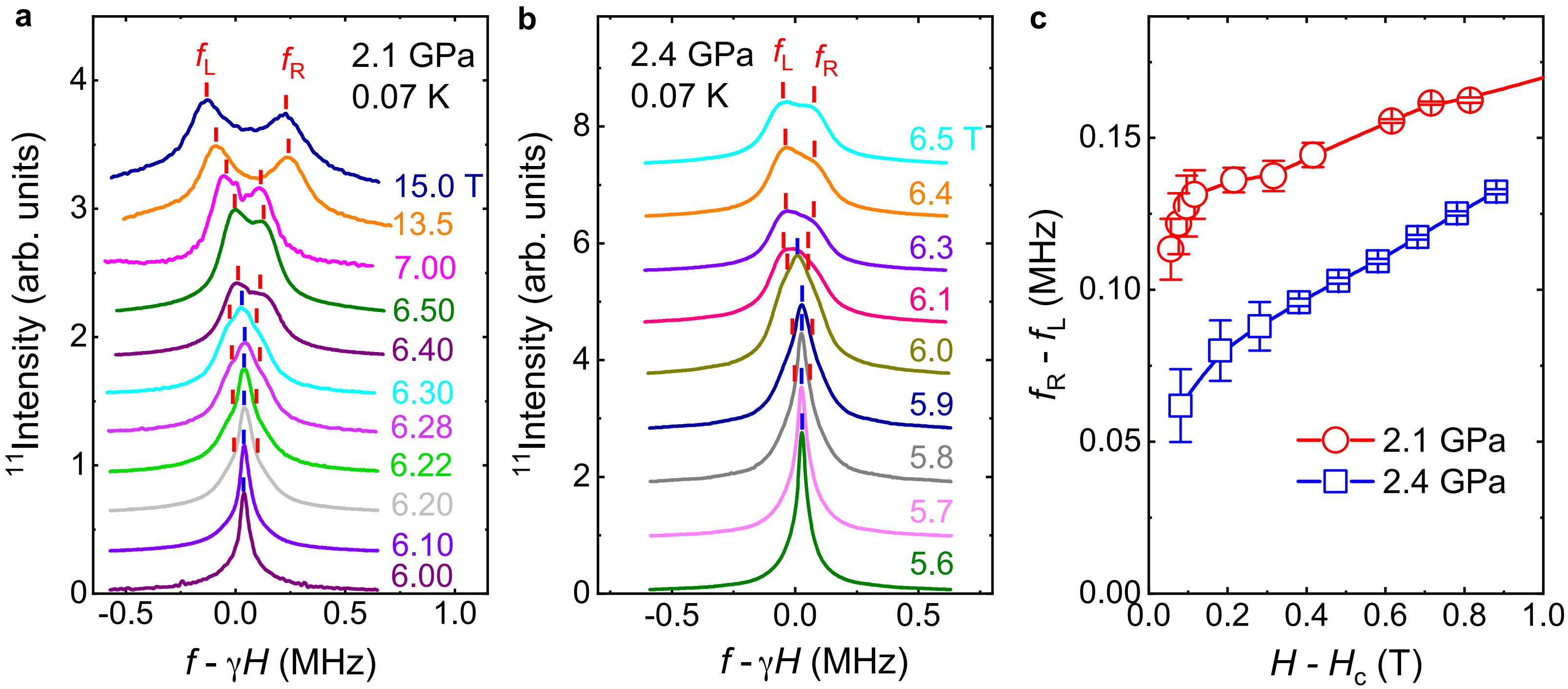
Suppression of PS phase by magnetic field, NMR (^{11}B) measurements



Common PS and AFM transition at T_c ~ 0.07 K, H_0 ~6 T

- Unusually low Tc for a first-order transition

AFM order parameter: NMR line splitting

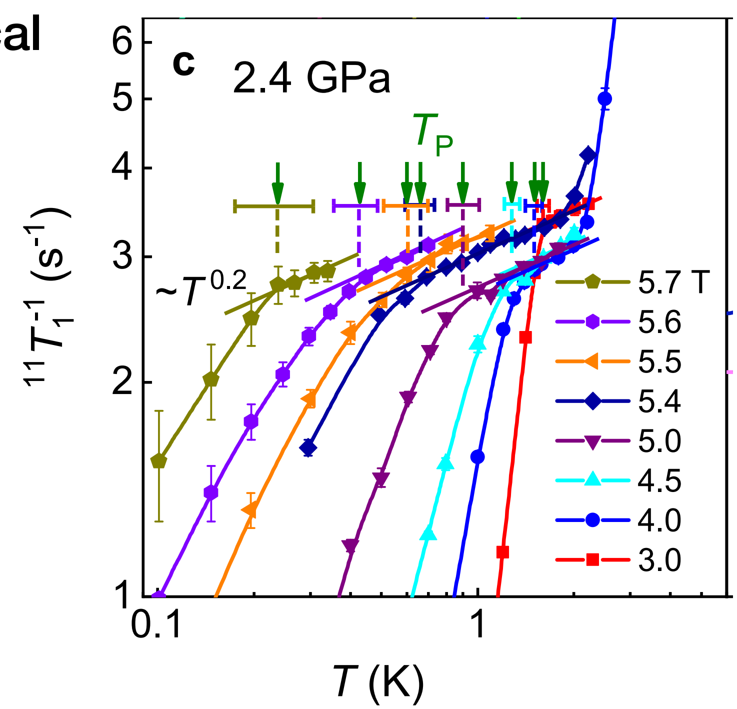


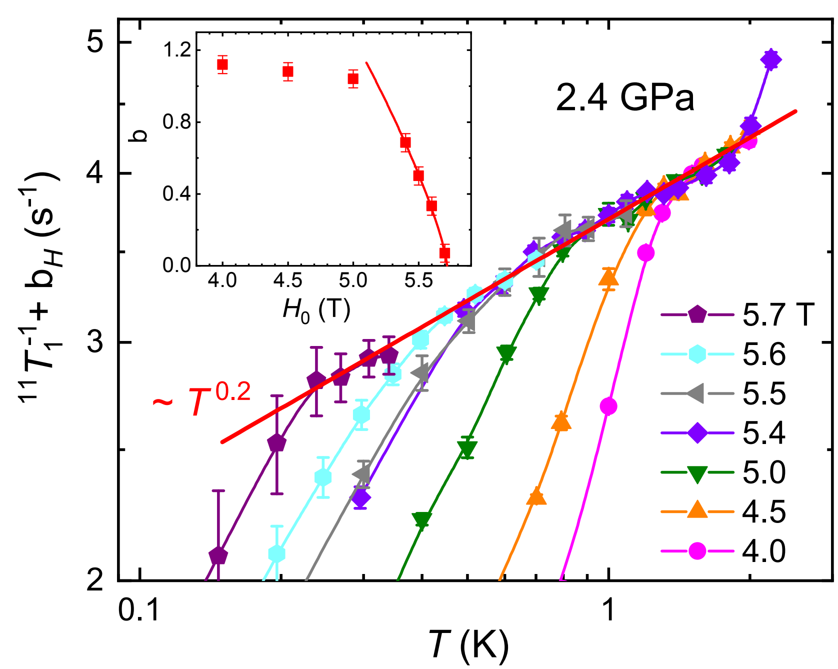
Phase coexistence at the low-T phase transition

Discontinuity at H_c is smaller at the higher pressure

Quantum-critical T>0 scaling of spin-lattice relaxation at 2.4 GPa

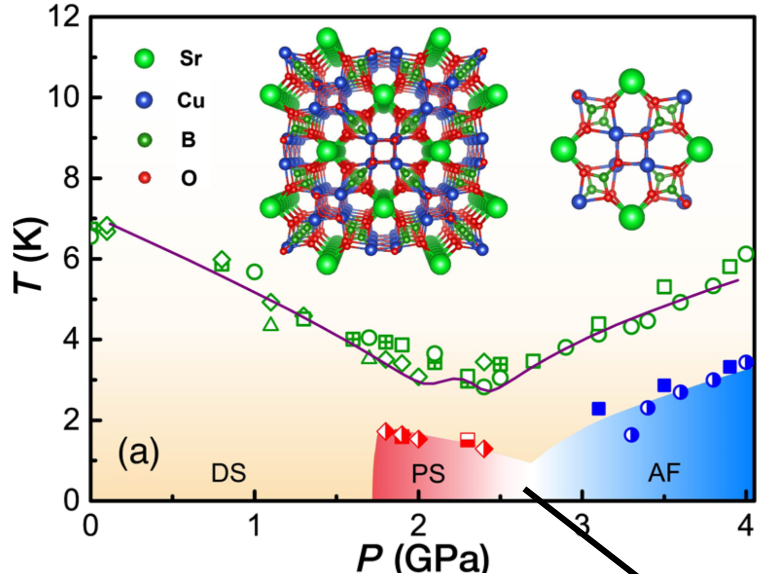
Exponent η ~ 0.20 intruguingly close to DQCP estimate

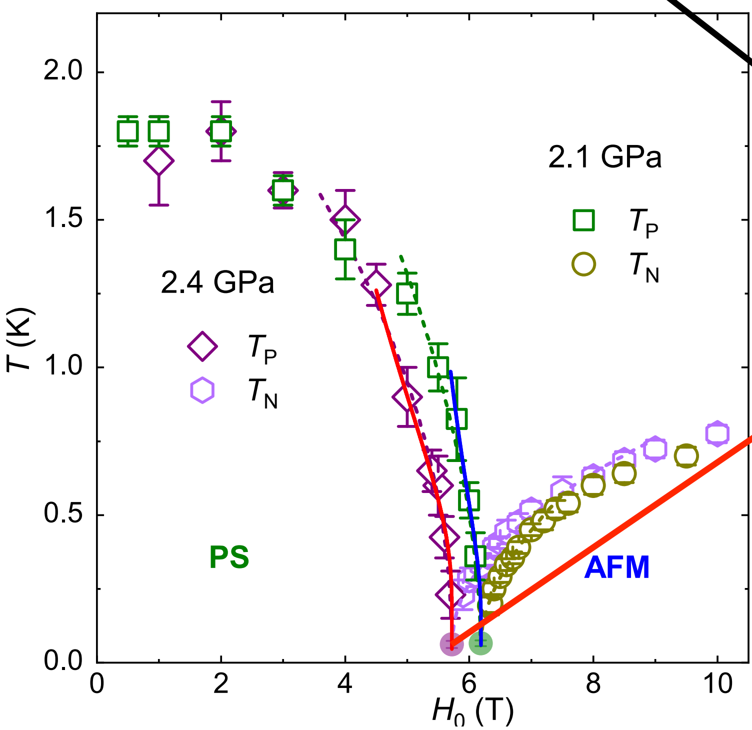


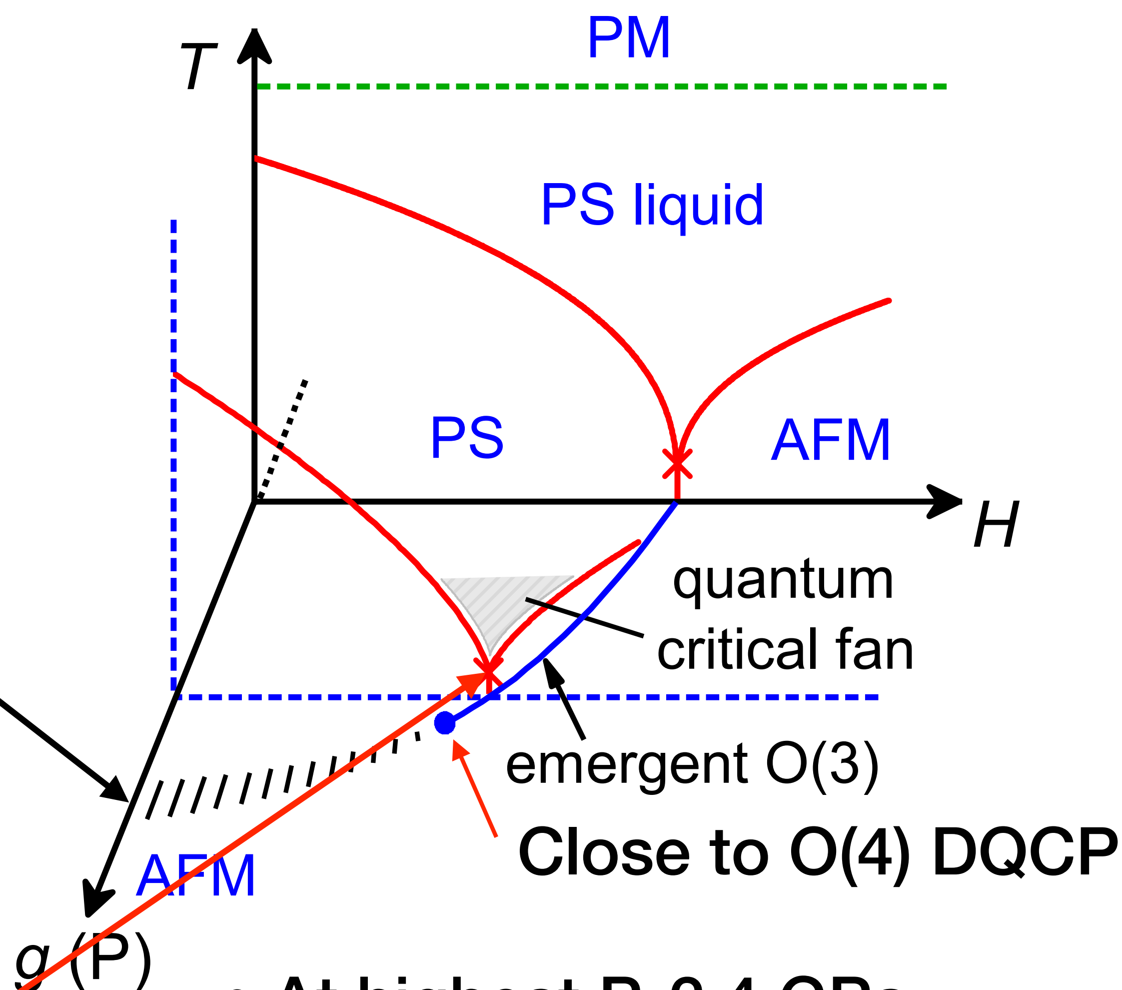


Theoretical scenario

Picture emerging from models and experiments







- At highest P, 2.4 GPa, influence of DQCP
- Only weak 3D effects
- Spin liquid around 2.8 GPa?