2D: 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

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 δ transition graph (33, 34) δ

scaling law controlled by n/n', which we confirm numerically below, is an unexpected feature of \mathcal{L}_max

• Unusual scaling properties [Shao, Guo, Sandvik (Science 2016)] 4

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

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

The 1D J-Q model has critical-dimerized transition of exactly the same kind as in the J₁-J₂ Heisenberg chain indicate diagonal and off-diagonal bond operators, respectively. The J-vertices are identical to those in the *l* as in the J₁-J₂ Heisenberg c = *J*1-*J*2 Heisenberg

2D J-Q models with first-order and (apparently) continuous out include all combinations of diagonal and off diagonal factors. Allowed loops pass only through one of transitions (deconfined quantum criticality) can be constructed **S***i* · **S** 0, (*m S* $i \in \mathbb{Z}$ *Sij* $\sqrt{2}$ *Smn*

Sij

bonds in a correlated fashion, using products of several

up to a constant, equal to a singlet projector operator:

completely destroying the antiferromagnetic order.

 $T_{\rm eff}$ is defined as a behavior lattice can be written as α

The pair-singlet, Eq. (19), is an eigenstate of this operator with eigenvalue 1, whereas a

different bonds. This favors a higher density of short valence bonds, thereby reducing or

Heisenberg models in Sec. 5.2.

Since the QMC sign problem prohibits large-scale studies of the *J*1-*J*² Heisenberg

FIGURE 88. In the J-Q3 model studied here, three singlet projectors are arranged in a staggered pattern.

Since the QMC sign problem prohibits large-scale studies of the *J*1-*J*² Heisenberg

Operator coding for J-Q models Slide by Ying Tang, Trieste School 2012

Linked vertex list and loop update:

- direct generaization of data structure and procedure for Heisenberg

C(*r*) = ⌅*S* ⌅ *ⁱ · S* \Box *ⁱ*+*r*⇧ ⇤ (1)*^r*e*r/*

Related 1D system: VBS state in J-Q chains

$$
\overbrace{0 \qquad \qquad \text{(Q/J)}_c \qquad \qquad \text{VBS}}
$$

Exactly the same physics (quantum phases and phase transition) as in J1-J2 Heisenberg chain

Evolution of VBS state during projector QMC $(J=0)$

Y. Tang and AWS, PRL (2011) r. Tang and Avv3, PRE (2011)
S. Sanyal, A. Banerjee, and K. Damle, PRB (2011)

VBS phase - always with fluctuations

Heisenberg chain with frustrated interactions

$$
H = \sum_{i=1}^{N} \left[J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2} \right]
$$

For the special point $J_2/J_1=0.5$, this model has an exact solution **Singlet-product states**

 $|\Psi_A\rangle = |(1,2)(3,4)(5,6)\cdots\rangle$ $|\Psi_B\rangle = |(1, N)(3, 2)(5, 4) \cdots\rangle$

It is not hard to show that these are eigenstates of H

$$
(a,b) = (\uparrow_a \downarrow_b - \downarrow_a \uparrow_b) / \sqrt{2}
$$

The system has this kind of order (with fluctuations, no exact solution) for all J2/J1>0.2411..... This is a **quantum phase transition** between

- a critical state
- a valence-bond-solid (VBS) state

The symmetry is not broken for finite N

• the ground state is a superposition of the two ordered states

 $|\Psi_0\rangle \sim |\Psi_A\rangle + |\Psi_B\rangle, \quad |\Psi_1\rangle \sim |\Psi_A\rangle - |\Psi_B\rangle$

J-Q chains: VBS with more fluctuations and critical state

$$
J/Q = 0.5
$$

\n
$$
J/Q = 0.5
$$

\n
$$
J/Q = (J/Q)_c \approx 6
$$

Extended valence-bond basis for S>0 states and this should, thus, be the most rapid way to approach

i lar S^z-S Consider $S^z = S$

- bond basis with two conditions.
In a pione of the pine of the pine was unpaired "un" enjoy. - for even N spins: N/2-S bonds, 2S unpaired "up" spins
- in replies in 20 sonds, 20 studies op opinon deconders. state $\left(1 + \frac{1}{2}\right)$ behave, $\frac{1}{2}\right)$ and $\left(1 - \frac{1}{2}\right)$. - for odd: (N-2S)/2 bonds, 2S unpaired spins
- transition graph has 2S open strings

$$
S = 0
$$
\n
$$
S = 1/2
$$
\n
$$
S = 1
$$
\n
$$
S
$$

 \bigcap \bigcup IS and matrix elements involve loops and strings Overlaps and matrix elements involve loops and strings

shown below and above the line of sites, respectively.

- $-v \epsilon$ A imple generalizations of the $S = 0$ case - very simple generalizations of the S=0 case
- $|$ O - loops have 2 states, strings have 1 state

Spinons in 1D: a single spinon in odd-N J-Q3 model

- one spin (spinon) doesn't belong to any bond
- bra and ket spinons at different locations; non-orthogonality

The distance between the bra and ket spins can be used to define the size of a spinon

- the spinon is not just the unpaired spin

Two spinons in 1D VBS are deconfined (no confining potential) - 2 separated (deconfined) sets of bra/ket spinons

Phase transition in the 2D J-Q model AFM VBS

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:

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

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

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

[Shao, Guo, Sandvik (Science 2016)] Phenomenological two-length scaling

Behaviors of crossing points \rightarrow exponents

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 0.07 From Binder ratio

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

- **Crossing of R₁(g,L), R₁(g,rL)**, g=J/Q, g*(L), analyze size dependence (using r=2)

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

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

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

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

- Small correction exponent; $\omega \approx 0.5$ $-v = 0.45 + (-0.01)$

the Binder ratio (right). The monotonic quantities are fitted with simple power law corrections,

Improved results to the *O*(3) value of ⌫.

LT. The lines have slope 2² = 3*.*188, corresponding

We define the coupling ratio *g* ⌘ *J/Q* and use the SSE

method to compute the *z* component of the staggered

[Sandvik & Zhao, Chin. Phys. Lett. 2020]

 $\overline{\mathbf{v}}$ rather modest distances, but the results still show a Binder cumulants give critical point $-$ slopes used to define 1/ ν

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

We can also calculate correlations of the relevant J and Q terms in H $\overline{0}$ r= (x, x) We can also calculate correlativ 119 can alco calculate correlation **b** and the sets exhibit the same determined the same determined the same decay.

Fig. 3. Correlation function, Eq. (9), of the *Q* terms in $\frac{1}{\sqrt{2}}$ is equaller exponential power-law term with smaller exponential power-law term with smaller exponential power-Mutual consistency between two ways of calculating $1/\nu$ for system sizes *L* = 64, 128, 256, and 512. The slopes

the critical *J*–*Q* model (*g* = 0*.*0451). In (a) results at

increase with *L* and the *L* = 512 data are shown with

nent, and exclude small systems until good fits are

 S_d

 S_{Z}

The VBS order parameter

N

i=1

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

coordinates on the square lattice. In this case as well Two possible types of order patterns
distinguished by histograms distinguished by histograms

Analogy with classical 3D clock model and the state of the state

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

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

Standard order parameter (m_x, m_y)

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

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

4, 32. The temperature *T=J* ! 2*:*17 for *Z*⁴ and 1.15 for *Z*8, both

FIG. 1 (color online). *P*%*mx; my*& at *h=J* ! 1 for *q* ! 4, 8, *L* ! Lou, Balents, Sandvik, PRL 2007

L L α *L* α *****L* α *L* α sponding to *!* " *"=*4 in *P*%*r; !*&. Arrows are color-coded accord-"angular order parameter":

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

 $q=6$

 $\varphi_{\rm q}$ > 0 only if q-fold anisotropy close to *Tc* we would expect the distribution to approach Finite-size scaling of φ_{q} can be *l* to extract length scale $\mathcal{E} > \mathcal{E}$ used to extract length scale $\xi > \xi$ and associated scaling dimension y_q [Lecture by Hui Shao] large number of configurations. We calculate the order

parameters h*m*i and h*mq*i, defined in Eqs. (3) and (4), and

Emergent U(1) symmetry of columnar VBS order

Realize stronger VBS order with J-Q3 model

Lou, Sandvik, Kawashima, PRB (2009), t_{total} discussed here could be even better suited for t_{total} . $tan m, + + + +$ **Sandvik, PRB (2012) Example 1. In the terms of the terms of the terms of the terms of the** *J***-***Q* **model used in the** this work. The circles are sites on the square lattice, labeled

$Strona$ columnar VDC when $I/O_{c}=O$ Strong columnar VBS when J/Q₃=0 contribution and the sites are the sites of the sites are the sites of the site

the honeycomb lattice.105–107 For the Hubbard model, 2D $J-Q_2$ model with $J/Q_2=0$ bars in the *Q* terms indicating products.

- weak columnar VBS
- t system does not see the kind of problematic the k s scaling is very large angular fluctuations - very large angular fluctuations

on the basis of unbiased μ simulations would be a very simulations would be a very simulations would good test of the capabilities of the capabilities of the captures of these methods to capture α

 \blacksquare emergent \blacksquare (1) symmetry s_{in} - emergent U(1) symmetry

a VBS phase transition can be studied. The VBS should then be the one to which the "bare" honeycomb model is the most susceptible (which may in itself not be easy to determine in this case). **D. Bench-mark challenge** Finally, as a challenge to DMRG, tensor-product, and MERA techniques, it would be very interesting and useful to see these methods applied to *J* -*Q* models as well. Comparing $L = 64$ $L = 128$ tion and characterization and characterization of a 2D RS state with finite with finite with finite with finite with finite with finite with α dynamic exponent in a system without geometric frustratic Heisenberg a square-lattice Heisenberg a square-lattice Heisenberg and the square-lattice Heisenberg an romagnet with nearest-neighbor exchange *J* augmented with certain multi-spin interactions of strength *Q* (the *J*-*Q* model). The unadulterated translationally invariand $\mathbf{u} = \mathbf{u} + \mathbf{u}$ *H* = *J* \mathcal{L}

[−*D*max*,D*max], where *D*max = 3*/*8 (for a perfect columnar VBS).

a simpler one with one with only two singlet projectors \mathcal{A} ever, the critical coupling ratio *g^c* is then much larger, J-Q3 model $J_x=J_y, Q_x=Q_y$

 $\mathcal{L}_{\mathcal{L}}$ and $\mathcal{L}_{\mathcal{L}}$ and $\mathcal{L}_{\mathcal{L}}$ online) Angular distribution of the VBS order of the VBS order

n is an integer in the range [−*N/*2*,N/*2], with the extremal

0.154

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 **FINITE-SIZE SCALING AND BOUNDARY EFFECTS ...** PHYSICAL REVIEW B 87, 134407 (2012) **PHYSICAL REVIEW B 87, 134407 (2013) PHYSICAL REVIEW B 87, 134407 (2013) PHYSICAL REVIEW B 8**

Fugacity of topological defects ⁴ may work, but some interaction similar to the multispin *Q*

nontrivial ground states and quantum phase transitions. If the outcome is positive, it may be very useful to systematically systematically systematically systematically systematically $\mathcal{L}^{\mathcal{L}}$

ng Ratio v/v' plays important in finite-size scaling

parameter of the *Q*² model for system sizes *L* = 32, 64, and 128. To

P(*Dx* \overline{D} **Dx** \overline{D} \overline{D} **Example 24 (***C* \sim 25 (*C*) \sim 25 (*C*) squares corresponds to \sim **to the full space of the components of the components** *Dx**(Science 2016)* Shao, Guo, Sandvik

 MC RG flows for J- Q_3 model - work in progress *P*(*Dx ,Dy*) in the *Q*² model on periodic *L* × *L* lattices with *L* = 64 - WOTK III progress **corresponds** to both squares corresponds to both squares corresponds to both squares corresponds to \sim uration is associated with a pair of order parameters (*Dx ,Dy*), MC RG flows for J-Q $_3$ model $\hskip10mm$ $\overline{}$ **basis** matrix elements are of the form α

[−*D*max*,D*max], where *D*max = 3*/*8 (for a perfect columnar VBS).

values corresponding to both the bra and ket state (making up the transition graph) having the same perfect column \mathcal{A} and \mathcal{A} are perfect columnar patterns of \mathcal{A}

The simulations take a long time to rotate the VBS angle L=128: 10⁵ measurements require > 1 day of computation

building 100×10⁵ measurements 10⁵ measurements

Conventional first-order transition <u>CONVENTIONAL III ST-ORGER MANDITION</u> 8.2

Staircase J-Q3 model [Sen, Sandvik, PRB 2010]

c) d) **Binder cumulant of AFM order parameter**

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

EXAMPLE OF A FIRST-ORDER NÉEL TO VALENCE-… PHYSICAL REVIEW B **82**, 174428 !2010"

FIG. 6. !Color online" The probability density *P*!*Dx* ,*Dy*" shown

Negative Cumulant peak is a sign of phase coexistence: first-order transition gered, in the singlets preferential plants preferentially in the singlets preferential plants preferentially ture "*J*=*L*. Note that the minimum of the Binder cumulant is nega-**phase coexistence; first-order transition**

tive for *L*%8 and diverges to −# as *L*→# based on these sizes.

 $\frac{1}{\sqrt{2}}$

tity, either declines are considered as a construction of the construction of the