Entanglement & Fidelity of quantum spin systems: a Valence-Bond approach

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Collaborations & References

- Fabien Alet (Toulouse)
- Matthieu Mambrini (Toulouse)
- Clément Sire (Toulouse)
- Fabricio Albuquerque (Toulouse)
- David Schwandt (Toulouse)
- Kevin Beach (Edmonton)
- Nicolas Laflorencie (Orsay)
- Ian McCulloch (Queensland)

- A few related references
  - Phys. Rev. Lett. **99**, 117204 (2007)
  - Phys. Rev. B **80**, 184401 (2009)
  - Phys. Rev. Lett. **103**, 170501 (2009)
  - arXiv:0912xxx

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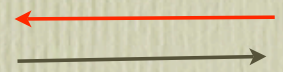
General context

- Recently, successful exchanges between

Quantum Information Theory  Condensed Matter

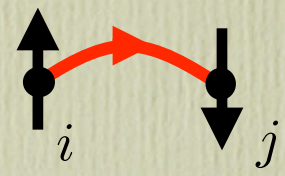
  - New concepts, tools and observables (entanglement, fidelity ...)
  - Automatic detection of quantum criticality
  - Design of efficient new algorithms (DMRG, MPS/TPS ...)

- This talk: Use standard condensed-matter toolbox on quantum information quantities

- Main tool : Valence bonds & Valence bond basis

Brief introduction to Valence Bonds

- Valence Bonds (VB) = singlets made out of two quantum spins 1/2



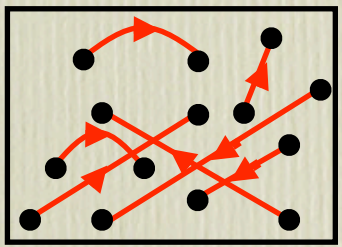
$$(i,j) = \frac{1}{\sqrt{2}}(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)$$

  - Origin: Quantum chemistry, first days of quantum mechanics
  - VB is a maximally entangled object

1st part : Entanglement Entropy

- Consider collection of (even) N spins
  - (Most) antiferromagnetic systems admit Total Singlet($S = 0$) ground-state
  - VBs form a basis of the singlet sector
- VB basis = all possible pairings of spins in VBs

$$|\varphi\rangle = 2^{-N/4} \prod_{(i,j)\in c} (|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)$$



Properties of VB basis

- Basis : Any singlet can be written as a linear combination of VB states

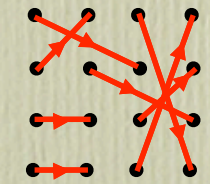
$$|\psi\rangle = \sum_i a_i |\varphi_i\rangle$$

VB QMC (Sandvik)

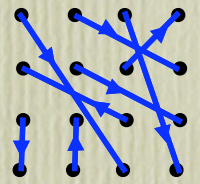
- Massively overcomplete $\mathcal{N}_{\rm VB}(N) \propto N^N \gg \mathcal{N}_{S=0}(N) \propto 2^N$
  - Linear relation between VB states
  - Non-orthogonality $\langle\varphi_1|\varphi_2\rangle \neq 0$

2nd part : Fidelity

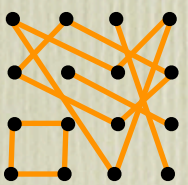
Overlap rules



$|\varphi_1\rangle$



$|\varphi_2\rangle$



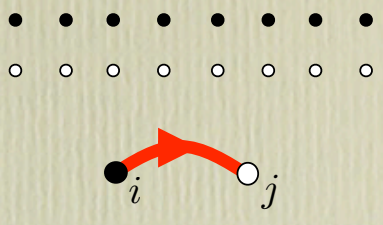
$\langle\varphi_1|\varphi_2\rangle = \pm 2^{N_l - N/2}$

Number of loops $N_l = 5$

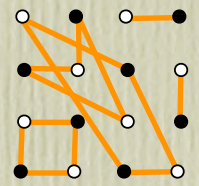
- Similar loop rules for observables $\dfrac{\langle\varphi_1|\mathcal{O}|\varphi_2\rangle}{\langle\varphi_1|\varphi_2\rangle}$

Properties of VB Basis

- Bipartite Valence Bond basis
  - Divide spins into 2 *arbitrary* sets
  - VBs go only from one set to the other
  - Still an overcomplete basis
  - Overlap rule



$$\mathcal{N}_{\mathrm{BVB}}(N) = (N/2)! \gg \mathcal{N}_{S=0}$$



$$\langle \varphi_1 | \varphi_2 \rangle = 2^{N_l - N/2}$$

- VB basis and numerics
  - Overcompleteness and non-orthogonality usually bring difficulties
  - Recent progress in stochastic sampling (Quantum Monte Carlo) in the VB basis

$$|\psi\rangle = \sum_i a_i |\varphi_i\rangle$$

Sandvik (2005)

Sandvik, Evertz (2008)

  - QMC samples the wave-function according to a_i
  - Need a_i positive and real to avoid sign problem

VB loop algorithm

- Heisenberg model

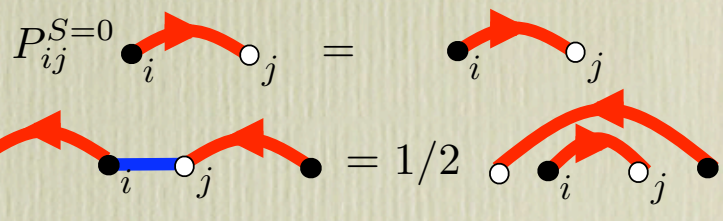
Sandvik, Evertz

Beach

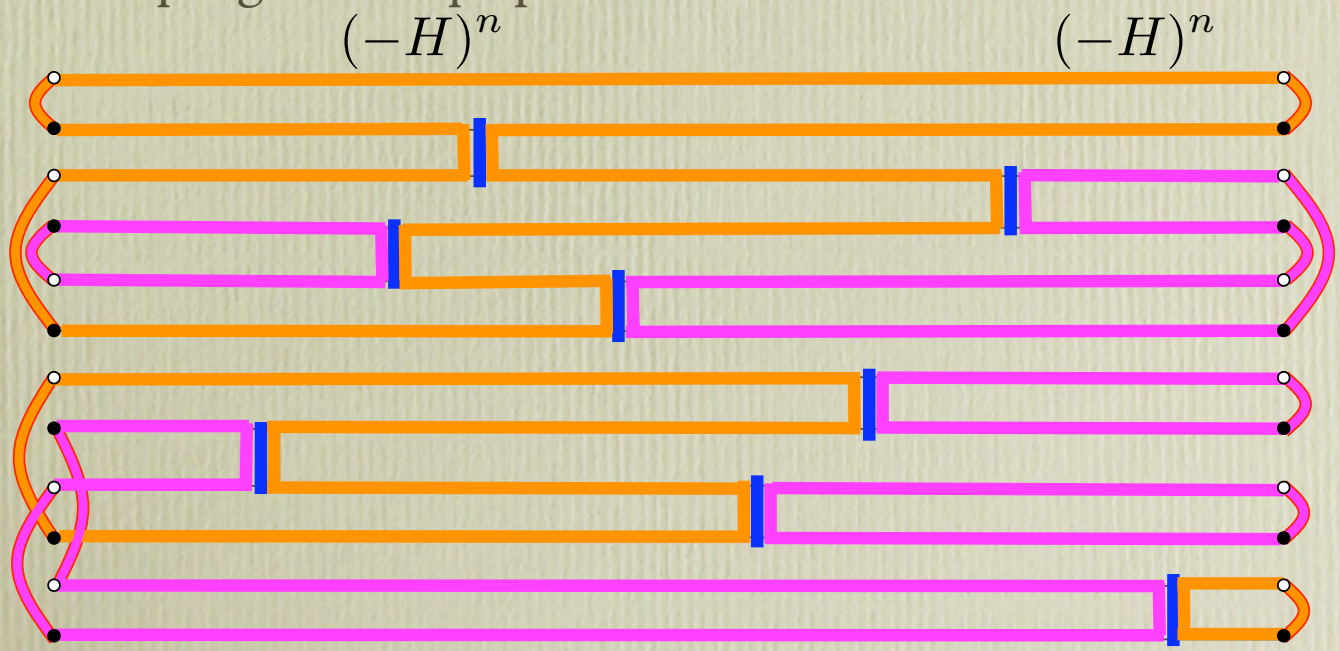
$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{\langle i,j \rangle} (P_{ij}^{S=0} - 1/4)$$

- Projection Quantum Monte Carlo $\lim_{n \to \infty} (-H)^n |\psi_T\rangle \sim |\psi_0\rangle$

- Simple update rules in bipartite VB basis



- Efficient sampling with loop updates



VB loop algorithm

- Heisenberg model

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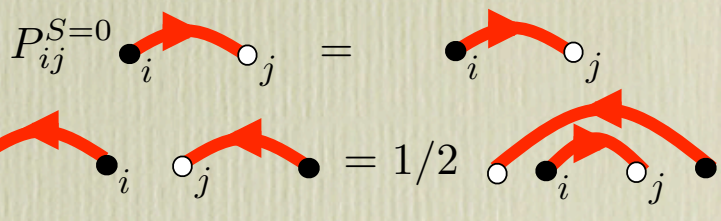


- Efficient sampling with loop updates

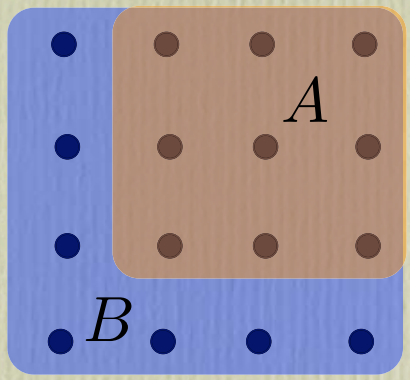
- VB states generated according to a_i of the ground-state of H on large systems

- Works only for non-frustrated lattices and SU(2) models

Part I :
Valence Bond Entanglement Entropy

Entanglement Entropy

- von Neumann Entanglement Entropy:

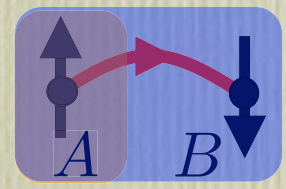


$$\rho_A = \mathrm{Tr}_B |\Psi\rangle\langle\Psi|$$

$$S = -\mathrm{Tr}(\rho_A \ln \rho_A)$$

  - How many degrees of freedom in A are determined by B ?

  - Example : A singlet



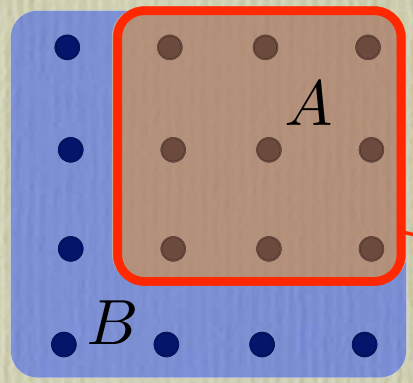
$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)$$

$$S = \ln 2$$

    - A singlet is a maximally entangled quantum state

Dimensional scaling and area law

- For pure states



$$S_A = -\mathrm{Tr}(\rho_A \ln \rho_A)$$
$$= -\mathrm{Tr}(\rho_B \ln \rho_B) = S_B$$

$$S \propto L^{d-1}$$

Area Law

- At criticality, log corrections may appear
  - In 1d, predictions from conformal field theory

Holzhey *et al.* Vidal *et al.*

Calabrese & Cardy

Critical systems $S \propto \frac{c}{3} \ln(L)$ (PBC)

Gapped systems $S \propto \ln(\xi)$

Can detect criticality

  - See also subleading corrections for topological systems
  - In higher dimensions, very few results
  - Analytics are hard, No good numerical method either

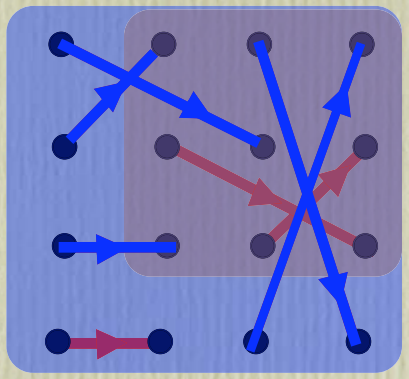
Kitaev & Preskill
Levin & Wen

Valence Bond Entanglement Entropy

- Consider a single VB state

PRL **99**, 117204 (2007)

Chhajlany *et al.*



$$S^{\mathrm{VB}} = \#\ \text{crossing VBs} \times \ln(2)$$

- If $|\Psi\rangle$ is a VB state, $S^{\mathrm{VB}} = S$
- If $|\Psi\rangle$ is a linear combination of VB states $|\Psi\rangle = \sum_i a_i |\varphi_i\rangle$

$$S^{\mathrm{VB}}(|\Psi\rangle) = \frac{\sum_i a_i S^{\mathrm{VB}}(|\varphi_i\rangle)}{\sum_i a_i}$$

Valence Bond Entanglement Entropy

- Well-defined, share good properties of an entropy
- Geometrical interpretation of entanglement
- Can be computed with VB Monte Carlo in any dimension
- What about scaling ?

First results on Heisenberg spin chains

Periodic chain

CFT prediction

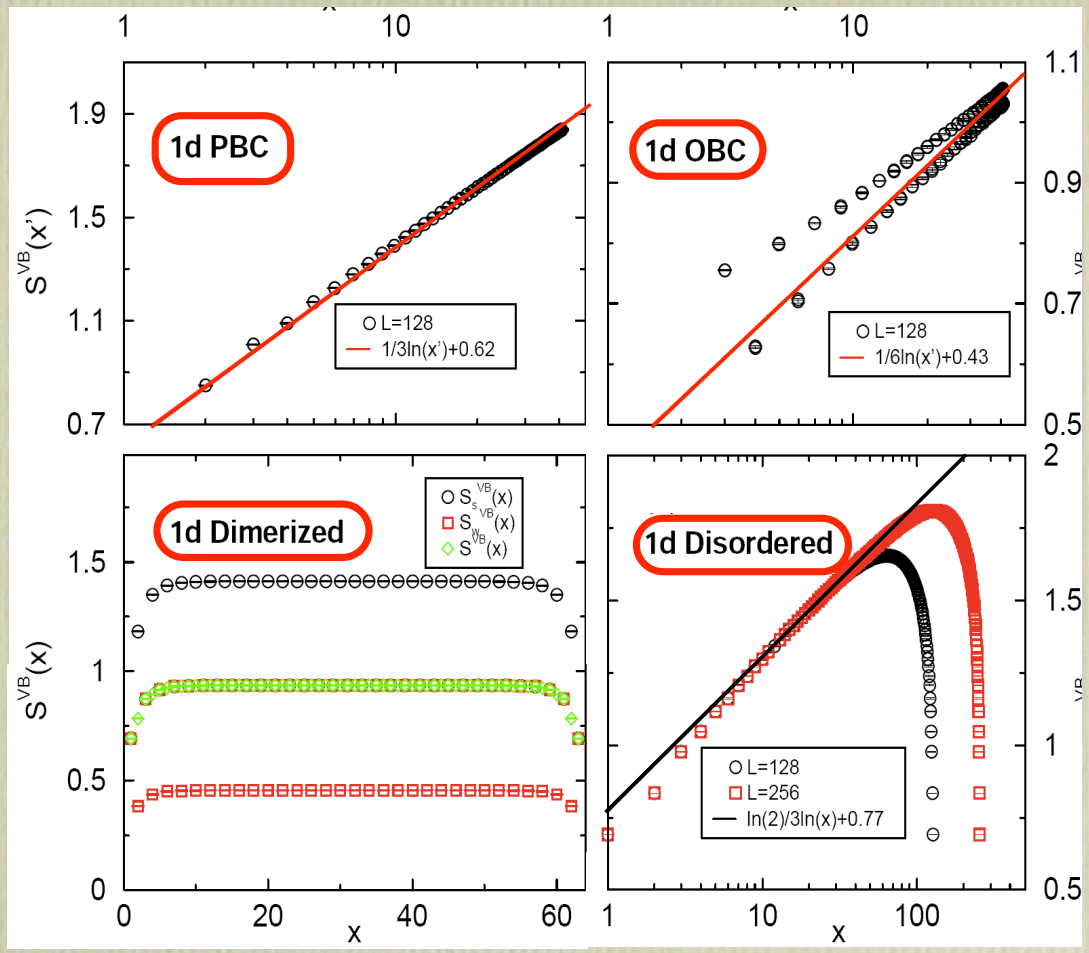
c=1

$$S \propto \frac{1}{3}\ln(x)$$

Dimerized chain

Gapped system

$$S \to C$$



Open chain

CFT prediction

$$S \propto \frac{1}{6}\ln(x)$$

Random chain

RSRG prediction

$$S \propto \frac{\ln 2}{3}\ln(x)$$

Refael & Moore

- S^{VB} appears to behave exactly like von Neumann entropy in 1d

Two-dimensional Heisenberg systems

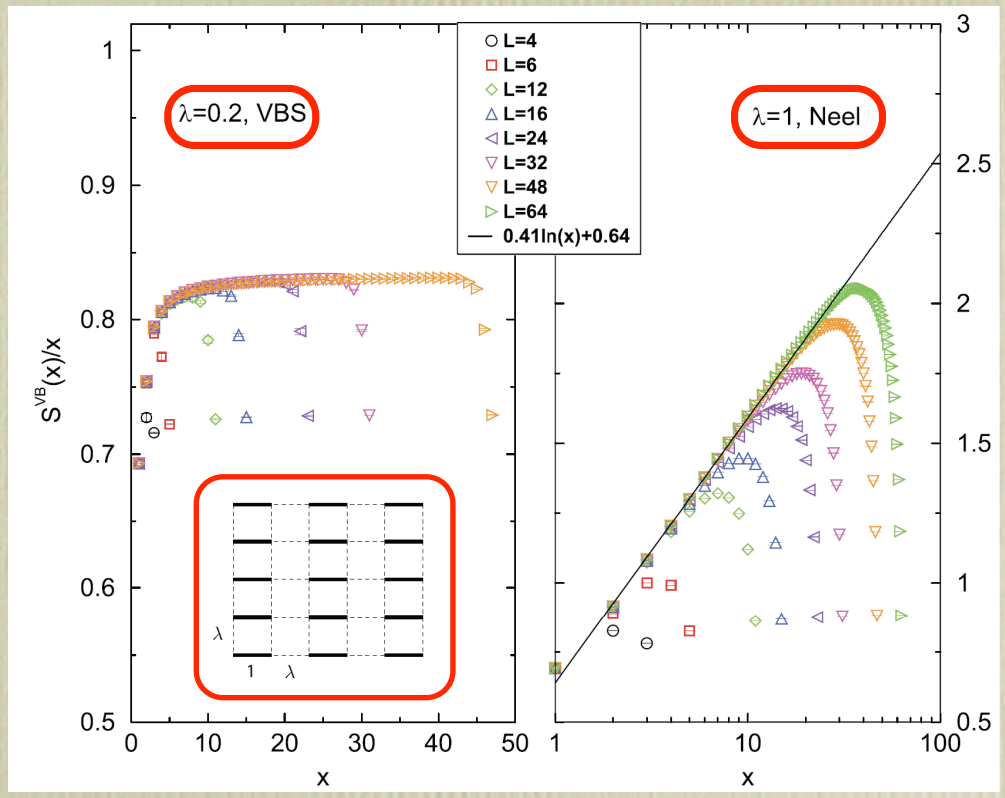
- Dimerized 2d model

Valence Bond Solid

Gapped system

$S^{\mathrm{VB}} \propto x$

Area Law



Néel

Gapless state

$S^{\mathrm{VB}} \propto x \ln x$

Log corrections

- Log corrections when Goldstone modes ?

Results in 1d, second take

- Exact asymptotics of S^{VB} for 1d Heisenberg chain (loop representation)

$$S^{\mathrm{VB}} \propto K \ln x \quad \text{with} \quad K = \frac{4 \ln 2}{\pi^2} \neq \frac{1}{3}$$

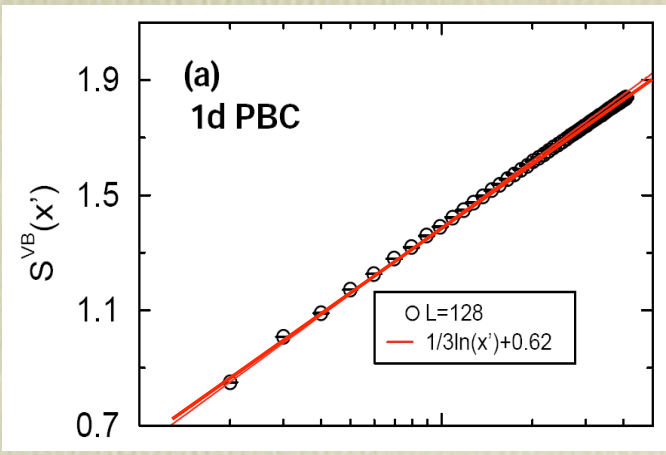
Jacobsen & Saleur

  - Best fit of numerical data

$$0.281 \sim \frac{4 \ln 2}{\pi^2} < K_{\mathrm{fit}} < \frac{1}{3} \sim 0.333$$

$$\sim 0.310$$

Log corrections at Heisenberg point?



- Results on N-leg ladders

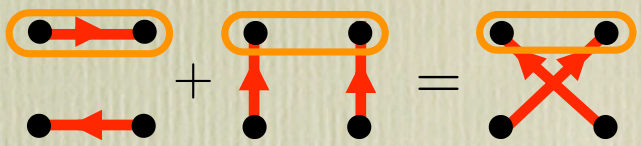
Kallin *et al*, PRL (2009)

$$S \propto N \quad \text{while} \quad S^{\mathrm{VB}} \propto N \ln N$$

  - Area law for von Neumann, log corrections for Valence Bond

Counting VBs

- Is it legal to count VBs occupation numbers, given overcompleteness ?
  - YES, but only for bipartite VBs ! Mambrini
  - Counter-example for non-bipartite



- "Average" VB occupation number between sites i and j in $|\Psi\rangle$

$$n_{ij}^{\mathrm{VB}}(|\Psi\rangle) = -\frac{\langle \text{Néel}|\mathcal{P}_{ij}|\Psi\rangle}{\langle \text{Néel}|\Psi\rangle}$$

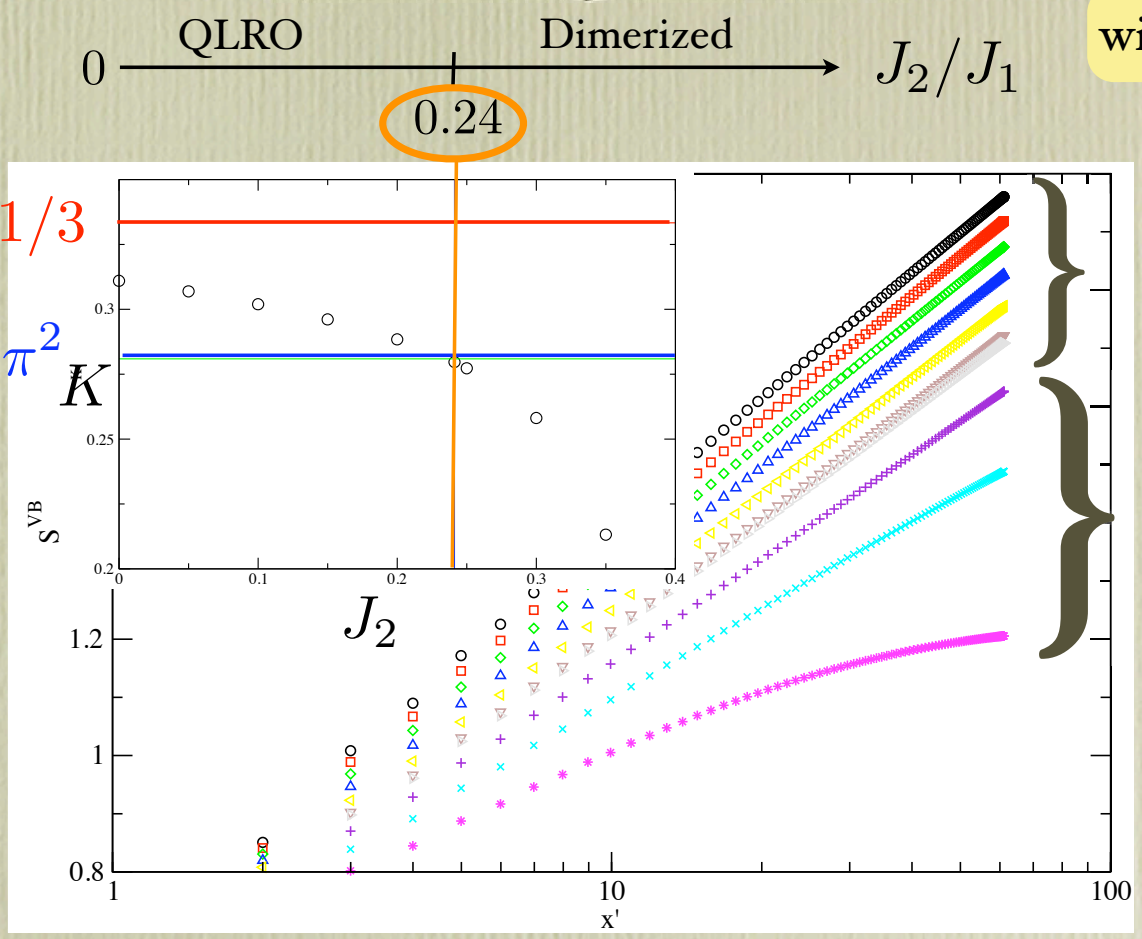
$\mathcal{P}_{ij}$ permutation operator

- Easy implementation in DMRG → frustrated systems

- Wave-functions must have a Marshall sign rule (Néel state)
  - Natural bipartition for VBs
  - No strong constraint, needed for QMC anyway

DMRG results on J1-J2 Heisenberg chain

with I. McCulloch



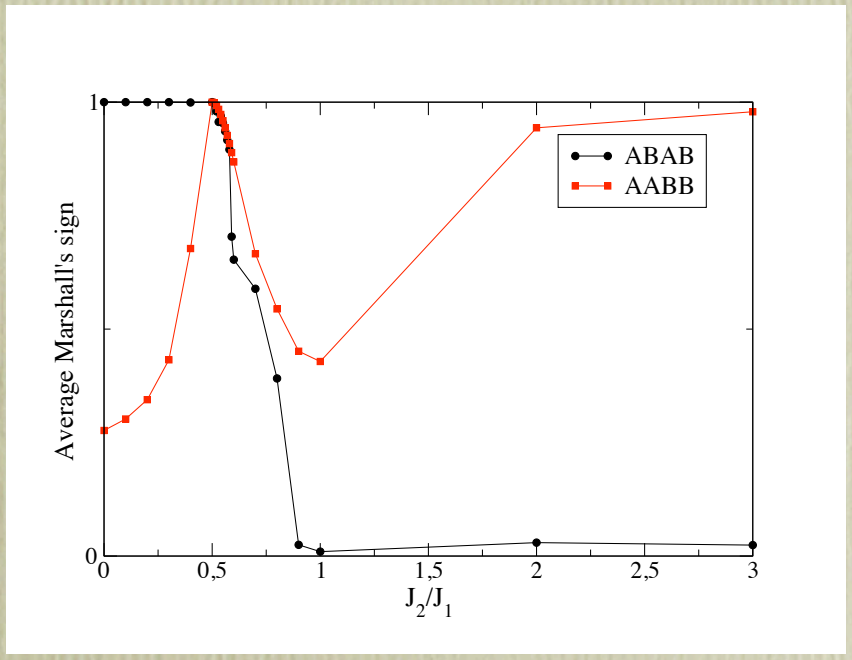
- Confirm
  - Jacobsen-Saleur result
  - No log corrections at critical point (marginally irrelevant operator)
  - S^{VB} detects criticality

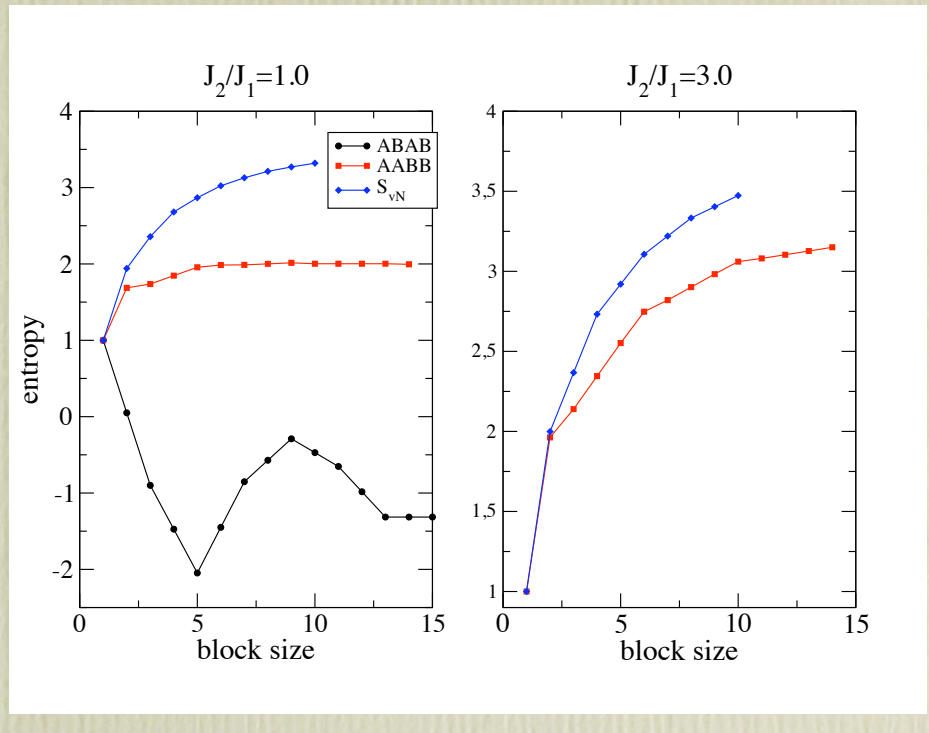
DMRG results on J1-J2 Heisenberg chain

- What happens for larger J2 ?
- Marshall's sign rule ?

with I. McCulloch

$$\langle s \rangle = \sum_i (-1)^{N_\uparrow^B} a_i |a_i|$$





- S^{VB} with a proper bipartition might still be a good quantity

Conclusions on VB entropy

- Valence Bond entanglement entropy
  - A valid entanglement quantifier for singlet states
  - Geometrical interpretation of entanglement
  - Equates von Neumann entropy for VB states
  - In general, different from von Neumann entropy, but ...
    - ✦ Captures criticality (1d), gapfullness / long-range order (2d)
    - ✦ Easy to compute numerically (QMC, DMRG)
    - ✦ Analytical understanding is possible

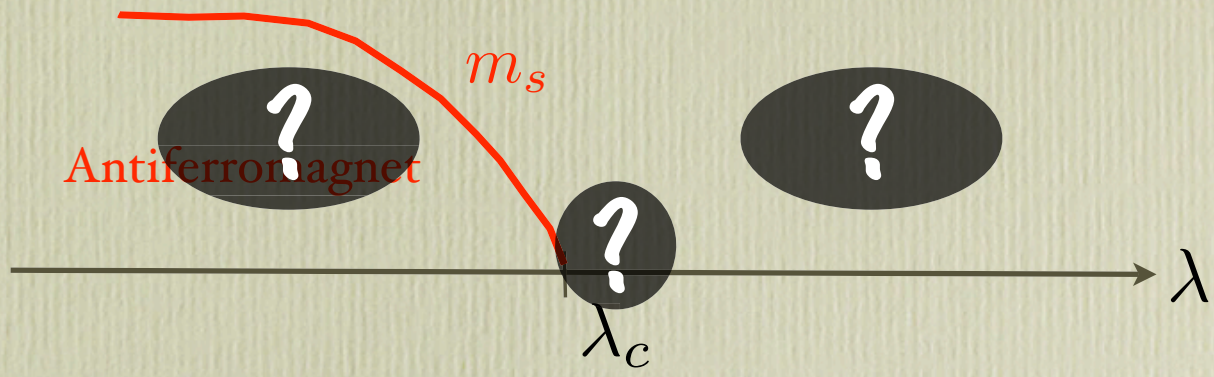
- Future directions (in progress)
  - Generalization for non-SU(2) systems ?
  - Precise relation to von Neumann's entropy ?
  - Connection with Marshall's sign rule

Part II :
Fidelity & quantum phase transitions

Fidelity and quantum phase transitions (I)

- What happens to the ground-state wavefunction across a quantum phase transition ?

$$H = H_0 + \lambda H_1$$



- How to locate the quantum critical point ?

▸ Standard approach: guess what is one phase (AF), measure order parameter (Ms), see where it vanishes

▸ Fidelity approach: search minima of $F(\lambda_1, \lambda_2) = |\langle \Psi(\lambda_1) | \Psi(\lambda_2) \rangle|$

Zanardi *et al.* Gu *et al.* Zhou *et al.* Gu, arXiv:0811.3127

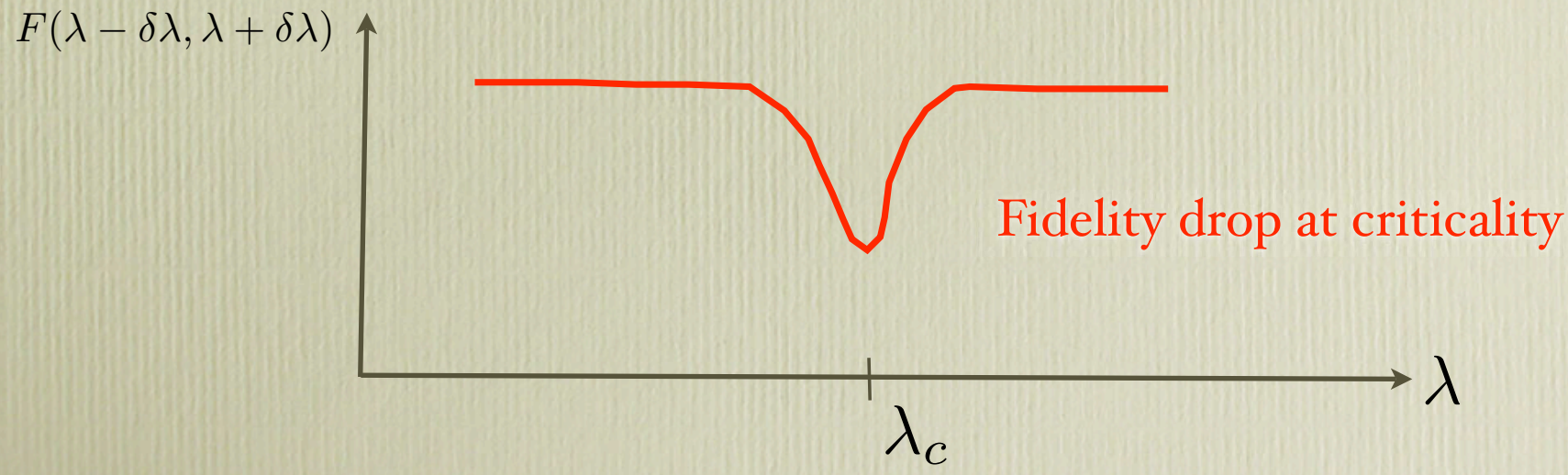
Fidelity and quantum phase transitions (II)

- Thermodynamic limit: $F(\lambda_1, \lambda_2) = 0 \quad \text{if} \quad \lambda_1 \neq \lambda_2$
- Finite system: $F(\lambda_1, \lambda_2) \sim O(1) \quad \text{if} \quad \lambda_1 \neq \lambda_2$
- Physically, we expect $F(\lambda_1, \lambda_2) \gg F(\lambda_1, \lambda_2)$

if λ_1 and λ_2 in the same phase

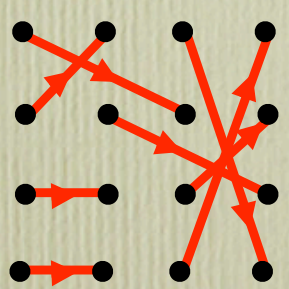
if not

- In practice, parametrize $\lambda_2 = \lambda_1 + \delta\lambda$

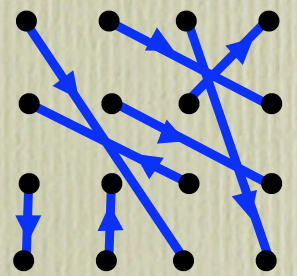


How to measure fidelity ?

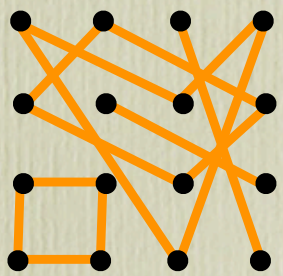
- Experiments : NO
- Theory:
  - Analytically : Only few examples
  - Numerics :
    - Variational methods: YES
    - Exact methods: YES, but limited to small systems
    - Stochastic methods: NO
- Way out : Use non-orthogonality of VB states



$|\varphi_i\rangle$



$|\varphi_j\rangle$



$$F = |\langle\varphi_i|\varphi_j\rangle| = 2^{\#\text{loops}-N/2} \neq 0$$

- Stochastic QMC evaluation of fidelity is possible!

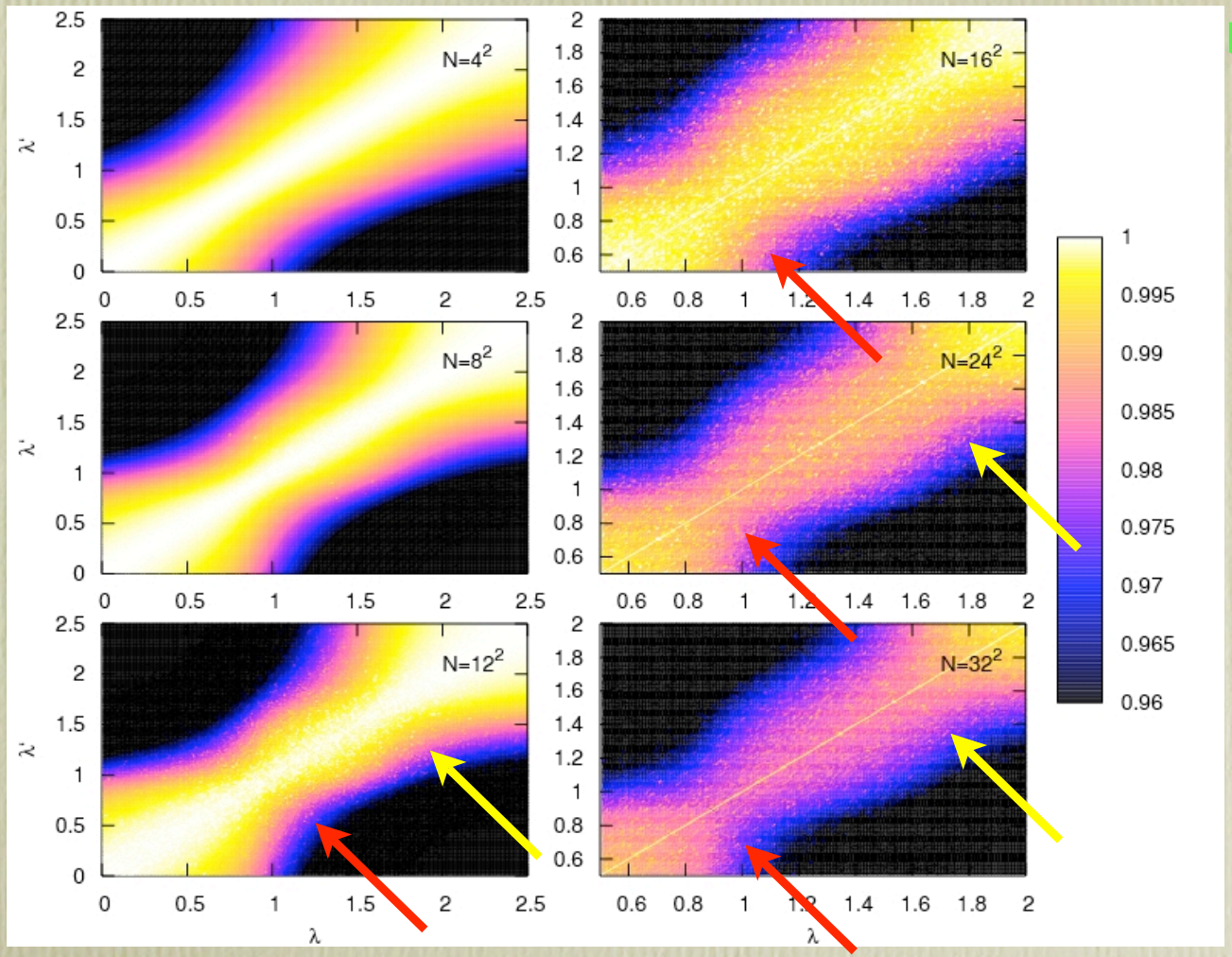
Schwandt, Alet, SC
PRL 103, 170501 (2009)

Results

- Guess where is the quantum phase transition ...

$$f = F^{1/N}$$

"Fidelity per site"



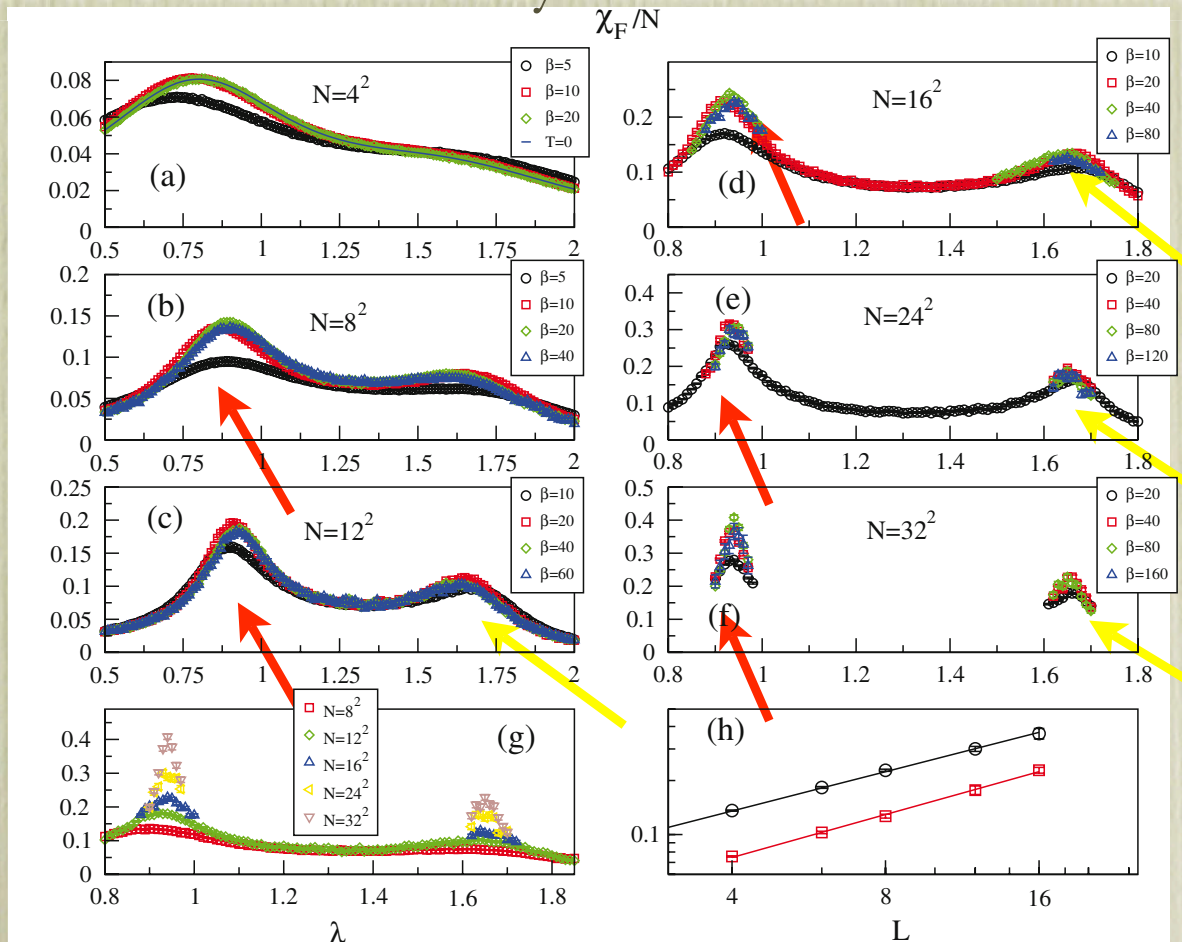
- Pinch points signal quantum critical points

Fidelity susceptibility

- Expand fidelity for $\delta\lambda \to 0$: $F(\lambda, \lambda+\delta\lambda) = 1 - \frac{(\delta\lambda)^2}{2}\chi_F + \dots$

Fidelity susceptibility $\chi_F = \int_0^\infty \tau \left[\langle H_1(0)H_1(\tau)\rangle - \langle H_1\rangle^2\right] d\tau$

- Can also be evaluated directly within Monte Carlo scheme



Two quantum critical points

$\lambda_c^1 \simeq 0.94$

$\lambda_c^2 \simeq 1.65$

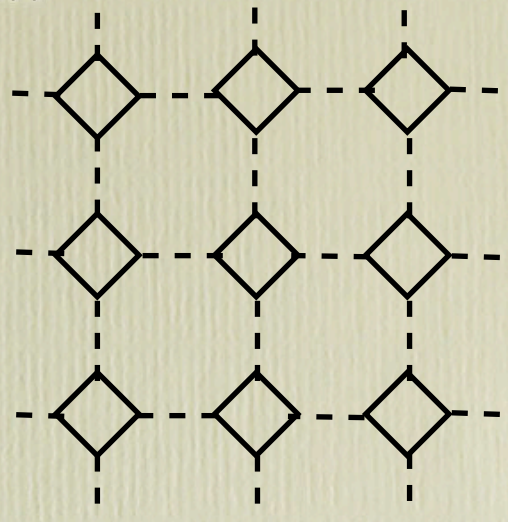
And the model was ...

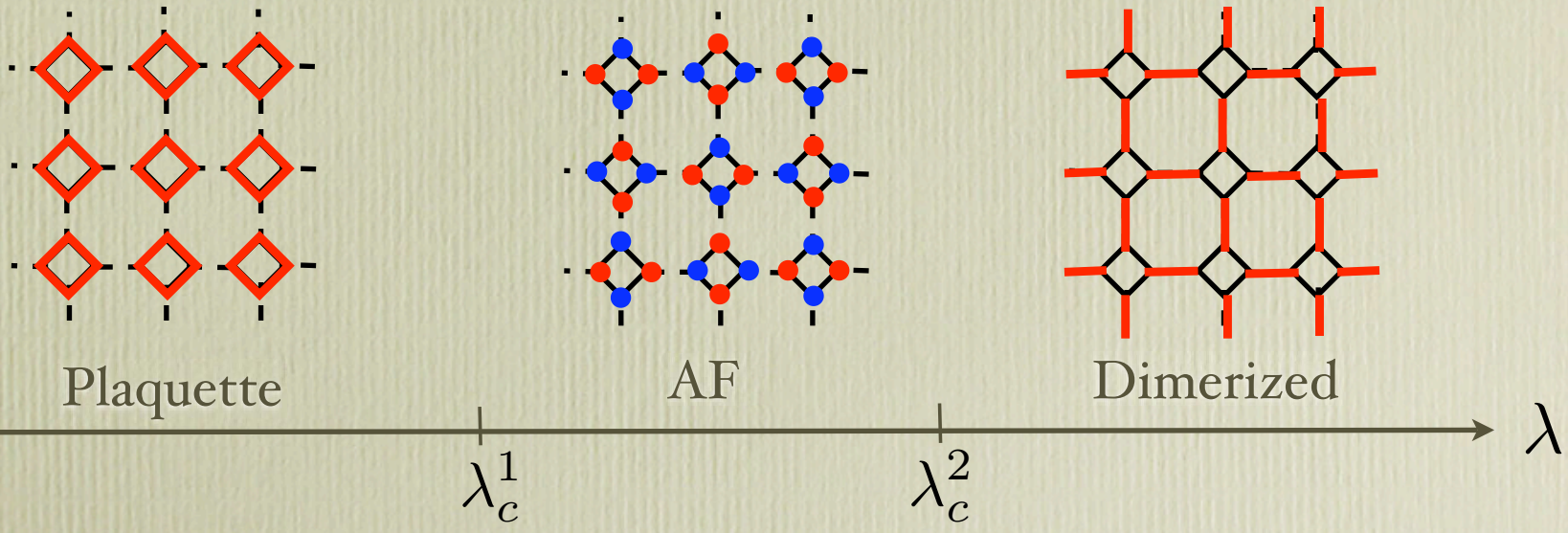
- S=1/2 Heisenberg model on the CaVO lattice

$$H = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

$J = 1$ —

$J = \lambda$ - - -





- Quantum critical points found by fidelity $\lambda_c^1 \simeq 0.94, \lambda_c^2 \simeq 1.65$ agree with works based on order parameters

Troyer *et al.*, Wenzel *et al.*

Scaling analysis

$$\delta\lambda \to 0 \qquad F(\lambda, \lambda+\delta\lambda) = 1 - \frac{(\delta\lambda)^2}{2}\chi_F + \dots$$

Susceptibility fidelity

$$\chi_F = \int_0^\infty \tau \left[\langle H_1(0) H_1(\tau)\rangle - \langle H_1\rangle^2\right] d\tau$$

$$L^{-d}\chi_F \sim |g - g_c|^{\nu(-2z+d+2\Delta_{H_1})}$$

L.C. Venuti and P. Zanardi, PRL (2007)

- By simply noticing that $\Delta_{H_1} = z - 1/\nu$ and $\xi \sim (g - g_c)^{-\nu}$

$$L^{-d}\chi_{\mathrm{F}} \sim L^{\frac{2}{\nu}-d}$$

D. Schwandt, F. Alet, SC

C. De Grandi, V. Gritsev, A. Polkovnikov

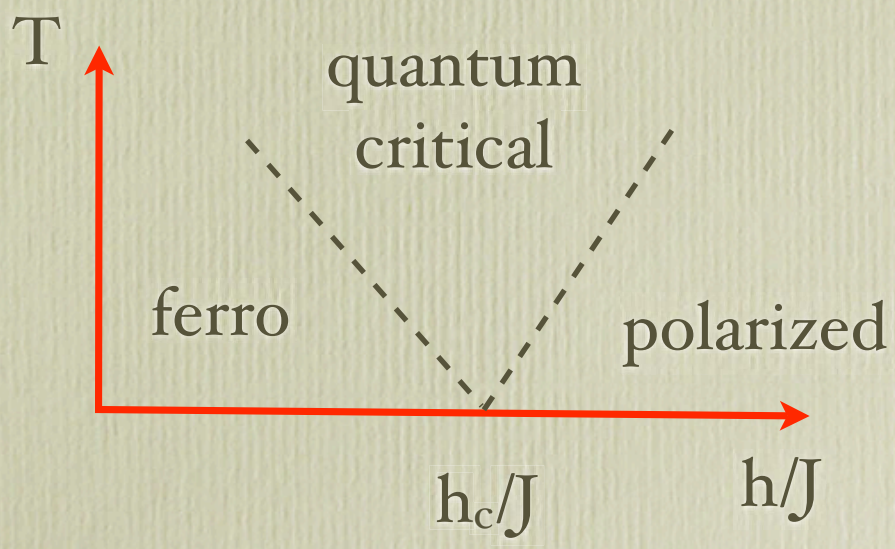
- to be compared to the more usual energy derivative

$$L^{-d}\chi_{\mathrm{E}} \sim L^{\frac{2}{\nu}-(d+z)}$$

Transverse Ising model

$$\mathcal{H}(h) = JH_J + hH_h = -J\sum_{\langle i,j\rangle}\sigma_i^x\sigma_j^x - h\sum_i \sigma_i^z$$

- Paradigm of Quantum Phase Transition (T=0)

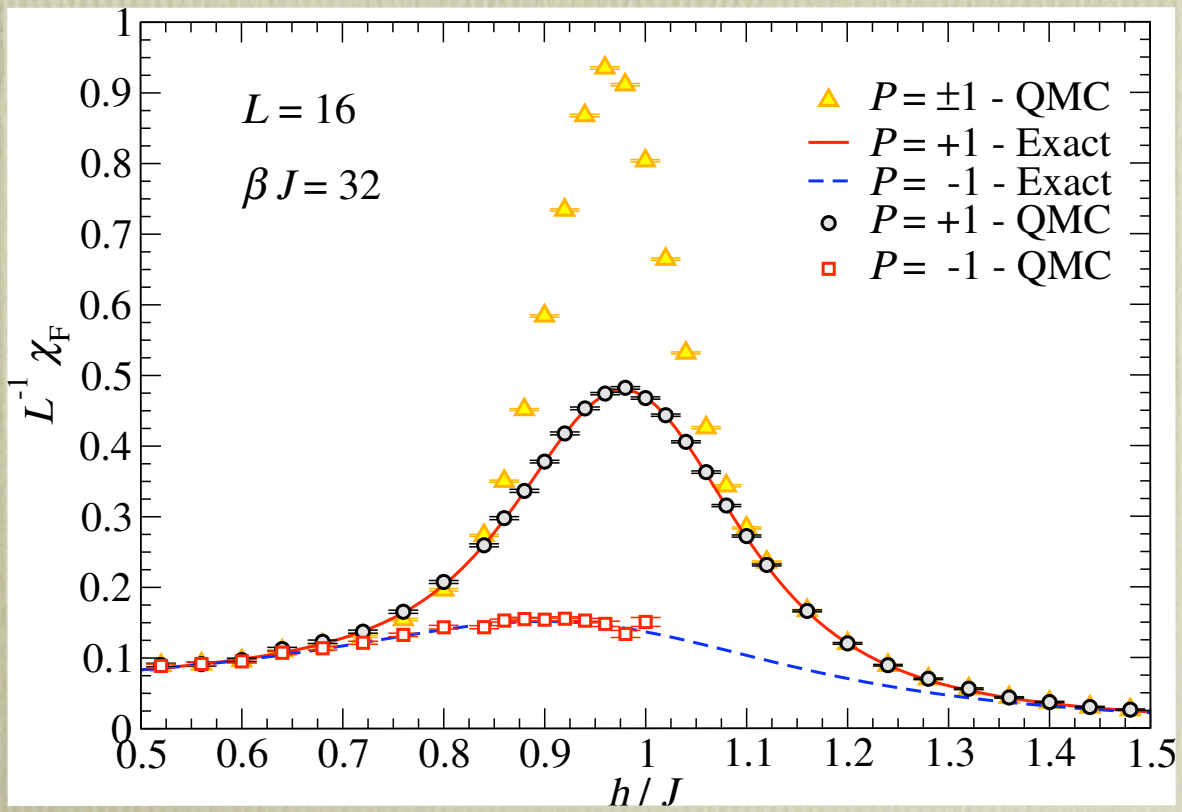


- Same universality class as finite-T Ising model in dimension (d+1), dynamical exponent z=1
- Can it be detected using fidelity estimators ?

Parity issues

- Transverse field Ising model has a conserved quantity: $\mathcal{P} = \prod_{i=1}^{N} \sigma_i^z$
- ground-state has P=+1.
- Lowest P=−1 excitation has *vanishing* gap
  - If P is not fixed, then needs exponentially small T !

$$[\mathcal{P}, \mathcal{H}] = 0$$



In 1d, exact solution h_c=J

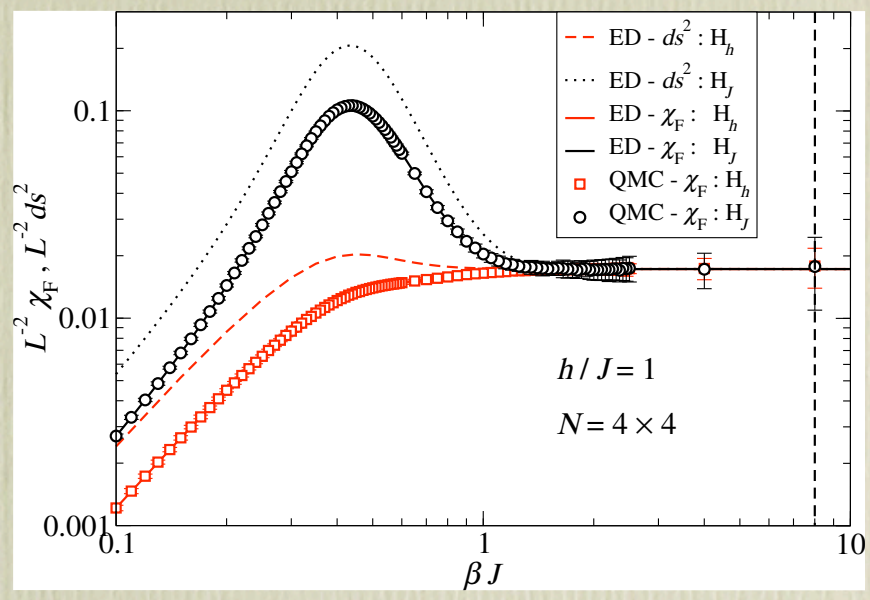
Finite temperature issues

- For mixed states, fidelity is defined as $F(\rho,\rho') = \mathrm{tr}\sqrt{\rho^{1/2}\rho'\rho^{1/2}}.$
  - ✓ so-called Bures' metric $ds(\rho,\rho') = \sqrt{2(1-F(\rho,\rho'))}$
  - ✓ Let us define a finite-T susceptibility as

$$\chi_F(g,\beta) = \int_0^{\beta/2} \tau \left(\langle H_1(\tau) H_1(0) \rangle - \langle H_1 \rangle^2 \right)$$

- ✓ Two measures are equivalent

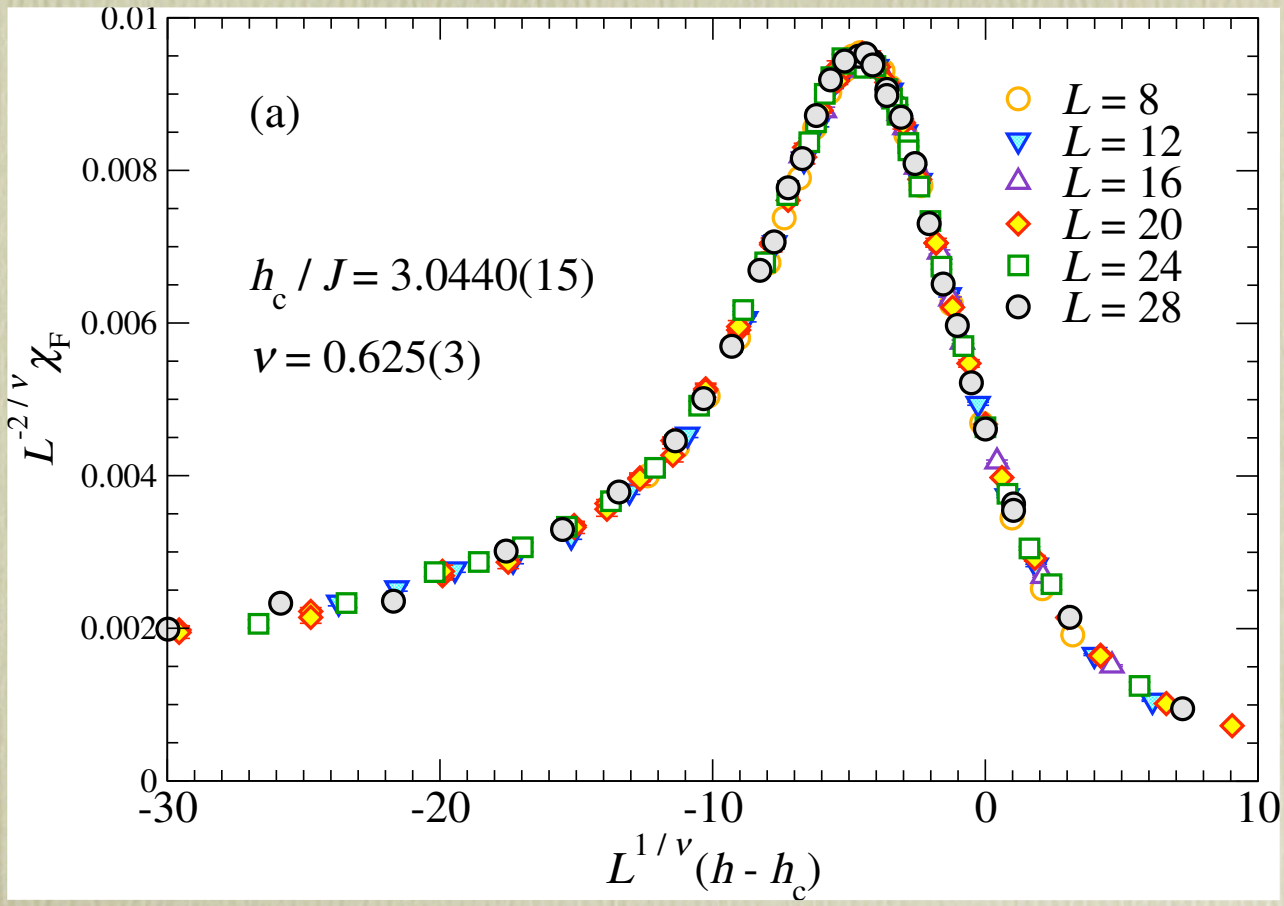
$$\frac{1}{2} ds^2(g,\beta) \leq \chi_{\mathrm{F}}(g,\beta) \leq ds^2(g,\beta)$$



F. Albuquerque et al.

Transverse Ising model (2d)

- Data collapse gives access to all exponents with great accuracy



F. Albuquerque, F. Alet, SC, and C. Sire

Conclusions on fidelity

- Fidelity approach of quantum phase transitions
  - Rooted in quantum information theory
  - Focus on changes of overlap of wave-functions
  - Can locate quantum phase transitions without prior information
  - Interesting alternative to order-parameter based methods

- Central quantities can be computed with stochastic simulations

$$F(\lambda_1, \lambda_2) = |\langle \Psi(\lambda_1) | \Psi(\lambda_2) \rangle| \qquad F(\lambda, \lambda + \delta\lambda) \simeq 1 - \frac{(\delta\lambda)^2}{2} \chi_F$$

Valence Bond method

Standard methods (SSE)

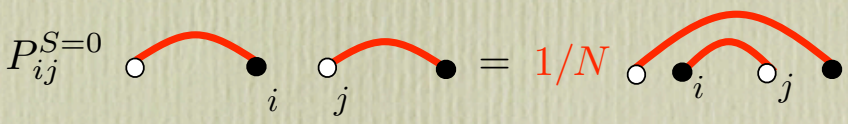
- Very first results ... PRL (2009); arXiv:0912 (in preparation)
- Much more to understand

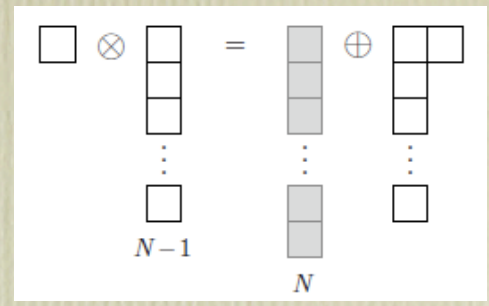
Part III :
Néel - VBS transition

Valence bonds for SU(N)

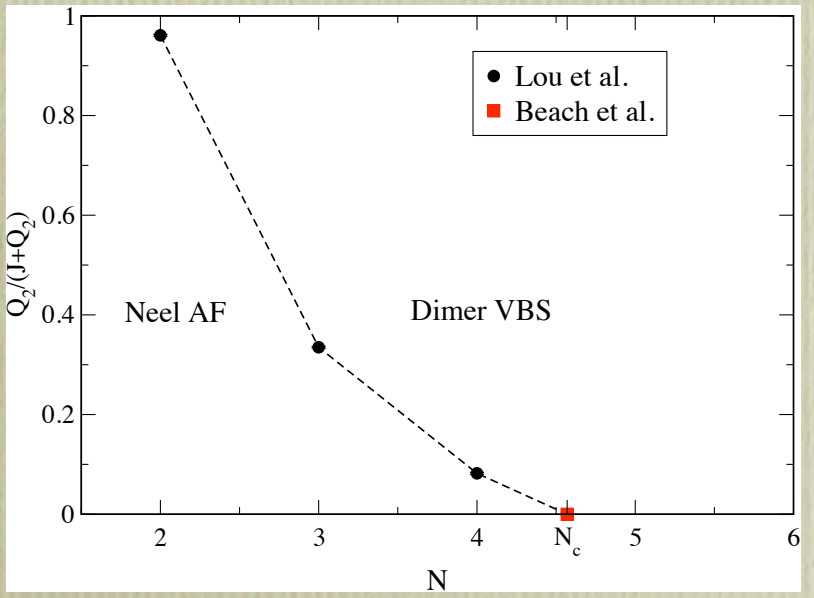
- Square lattice SU(N) model

$$P_{ij}^{S=0} = 1/N$$





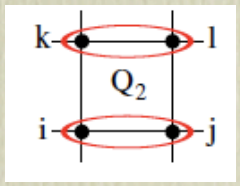
  - large N tend to favor small bonds ⟶ destroy Néel order



Study Heisenberg model for arbitrary N

  - Néel-VBS transition in 2d at N_c=4.57

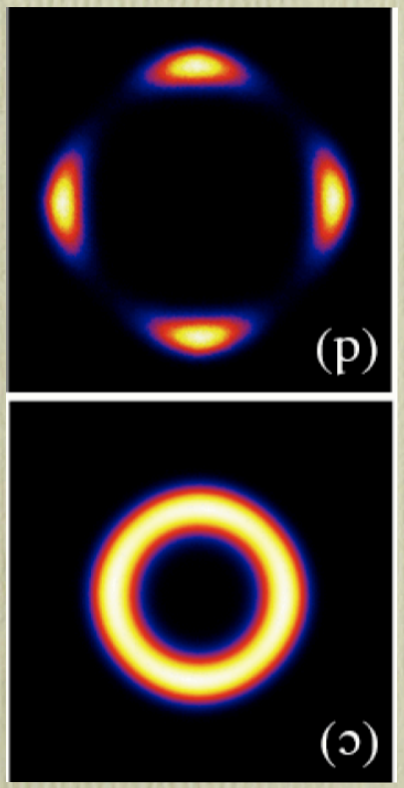
K. Beach, F. Alet, M. Mambrini, SC, PRB (2009)

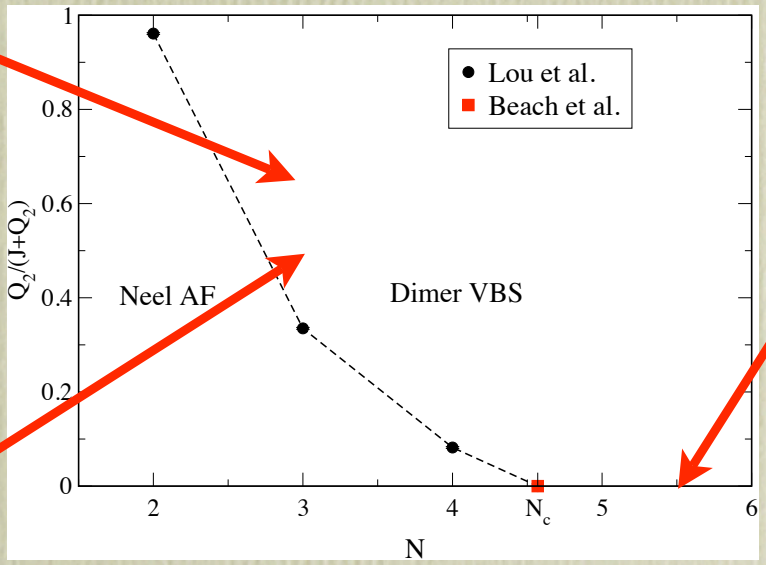
Add  term

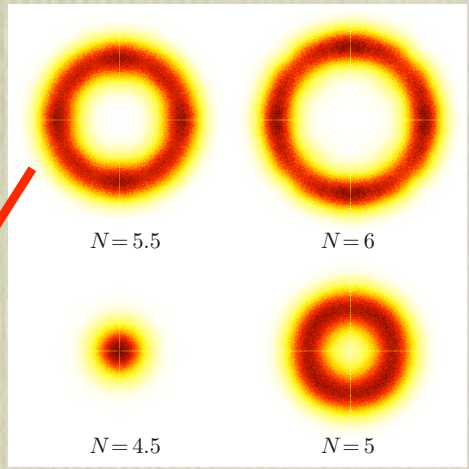
J. Lou, A. Sandvik, N. Kawashima, PRB (2009)

Nature of the VBS phase

- Dimer order points towards columnar order VBC







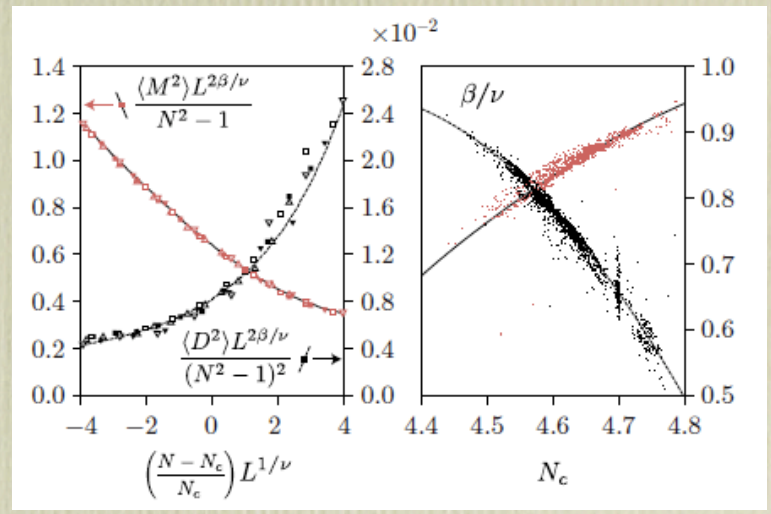
J. Lou et al., PRB (2009)

K. Beach, et al., PRB (2009)

Quantum phase transition

- Data collapse indicate *second* order phase transition

	SU(2)	SU(3)	SU(4)	SU(N_c)
η_s	0.35(2)	0.38(3)	0.42(5)	0.63(4)
η_d	0.20(2)	0.42(3)	0.64(5)	0.63(4)
ν	0.67(1)	0.65(3)	0.70(2)	0.8(1)



J. Lou et al., PRB (2009)

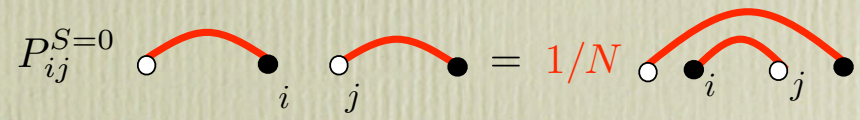
K. Beach, et al., PRB (2009)

Are these new universality classes ?

Is it related to deconfined quantum criticality (Senthil et al.) ?

Summary

- Valence Bond Basis, Fidelity & Entanglement :
  - Old-school Quantum Mechanics can help to sustain the quantum information approach to condensed-matter
  - Condensed-matter side: automatic detection of quantum criticality
  - New numerical methods are very efficient in the VB basis
  - New simple analytical results are also possible
- Other applications of valence bond



  - SU(N) models: Néel-VBS transition in 2d
  - $SU(2)_k$ anyonic spin chains

$$N = 2\cos(\frac{\pi}{k+2})$$

Trebst *et al.*