Title: Quantum Spin Simulations (PHYS 7380) - Lecture 15

Date: Apr 23, 2010 11:00 AM

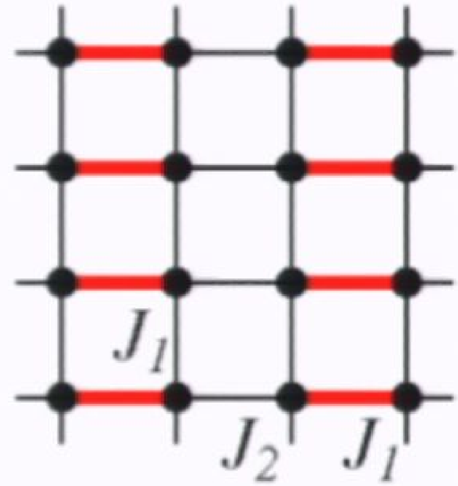
URL: http://pirsa.org/10040057

Abstract:

Analysis of the transition of dimerized (columnar) Heisenberg system

Two options of choosing the temperature in finite-lattice calculations

- get the ground state as $T \to 0$ limit
  - in practice **$T \ll \Delta$** (finite-size gap)
- use **$1/T = \beta = aL^z$** to analyze the transition
  - if z is known (or to test proposal)
  - the results should not depend on aspect ratio **a**



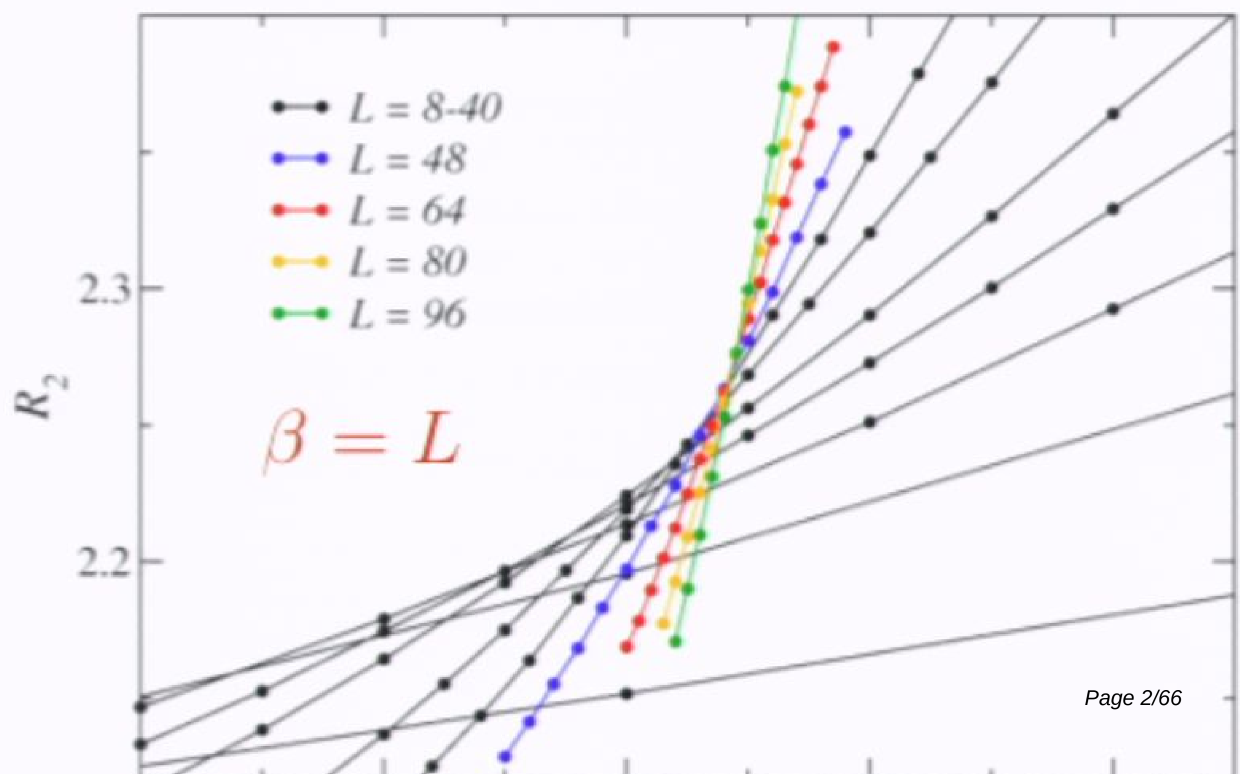
Use the Binder ratio

$$R_2 = \frac{\langle m_{sz}^4 \rangle}{\langle m_{sz}^2 \rangle^2}$$

to locate the critical coupling ratio g_c

Significant drifts in the crossing points, large lattices needed

$$g_c \approx 1.91$$



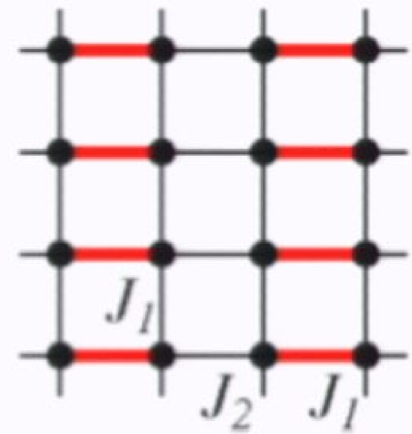
The spin stiffness at criticality

For a quantum-critical point with dynamic exponent z:

$$\rho_s \sim L^{-(d+z-2)}$$

d=2, z=1 → plot **$L\rho_s$** vs g for different L

- curves should cross (size independence) at g_c
- x- and y-stiffness different in this model



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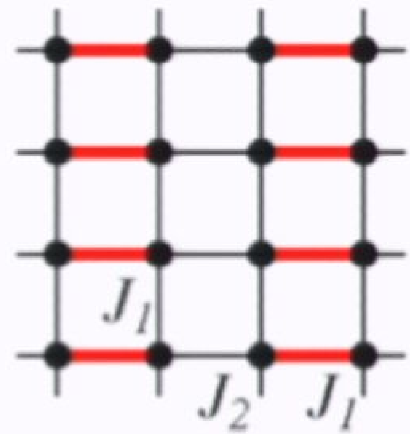
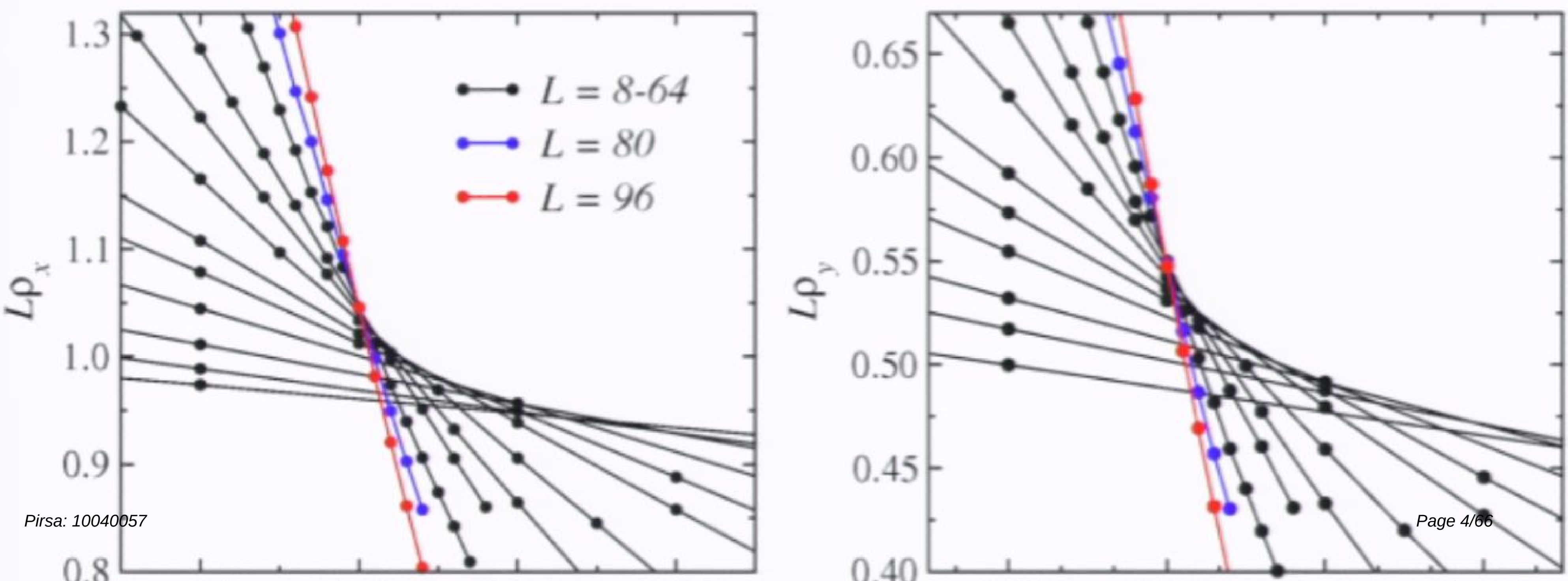


Finite-size scaling in agreement with z=1, $g_c \approx 1.9094$



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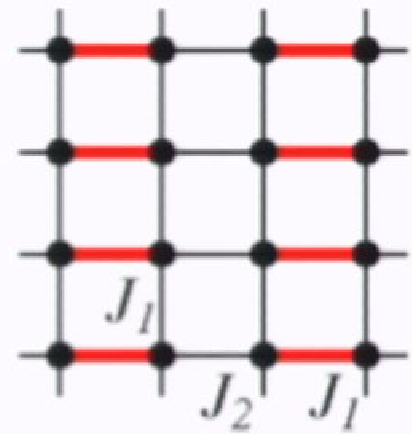

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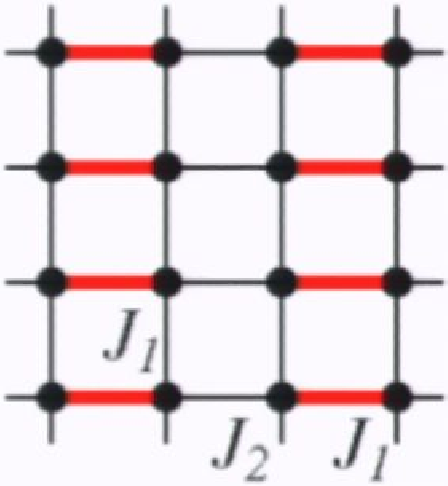

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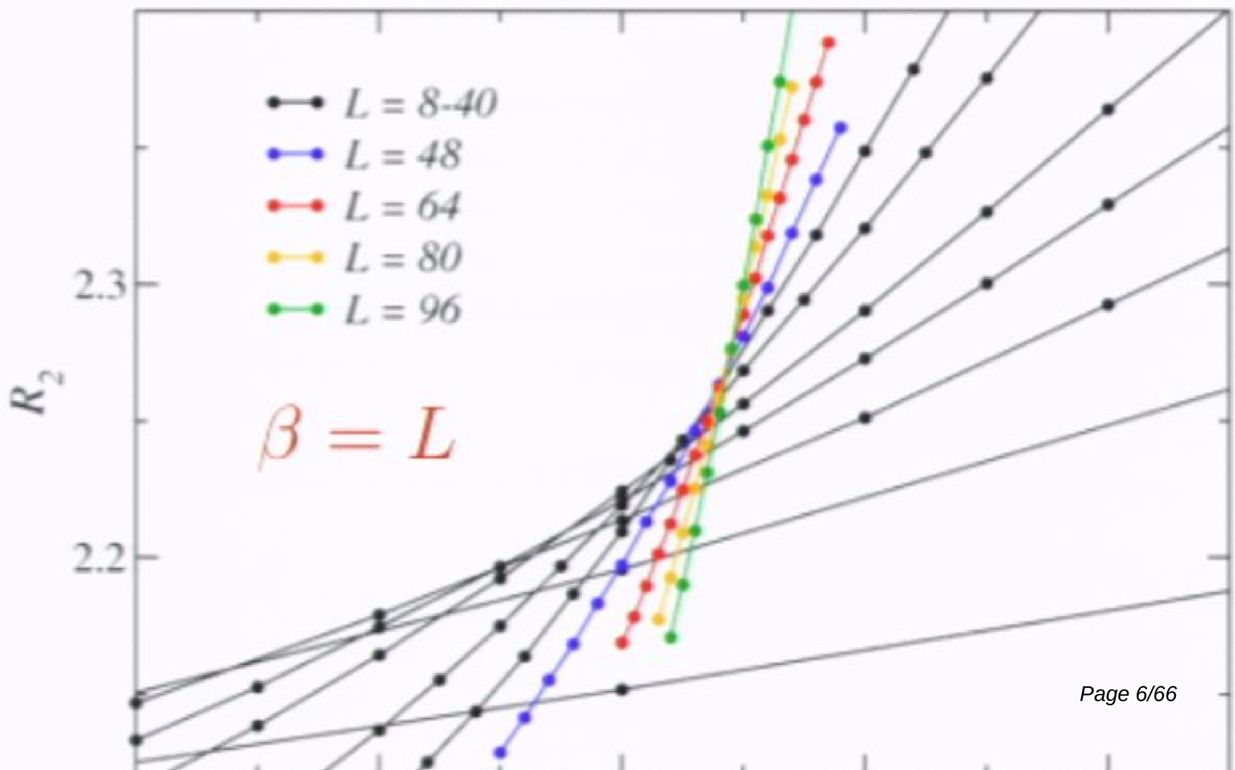

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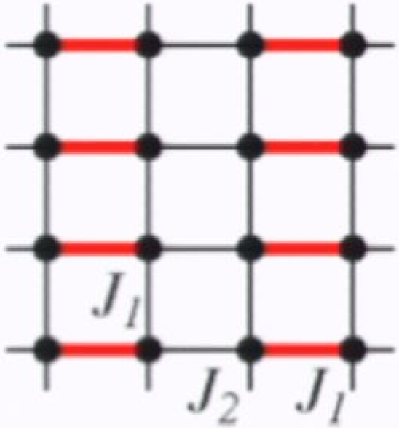

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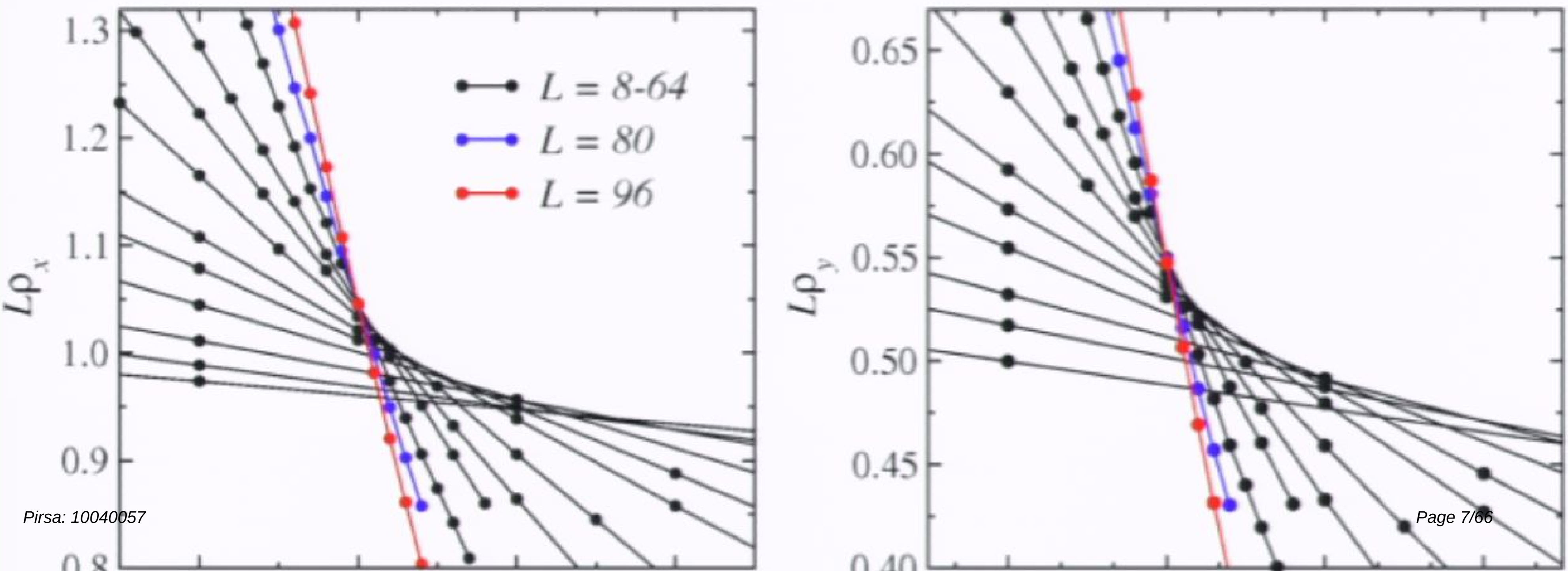
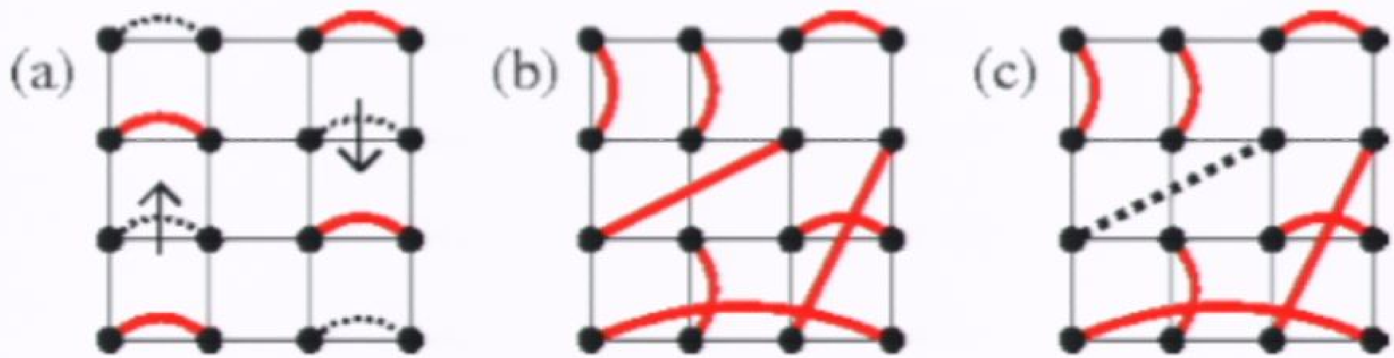


Valence-bond basis and resonating valence-bond states

As an alternative to single-spin ↑ and ↓ states, we can use singlets and triplet pairs



static dimers (complete basis)

arbitrary singlets (overcomplete in singlet subspace)

one triplet in the "singlet soup" (overcomplete in triplet subspace)

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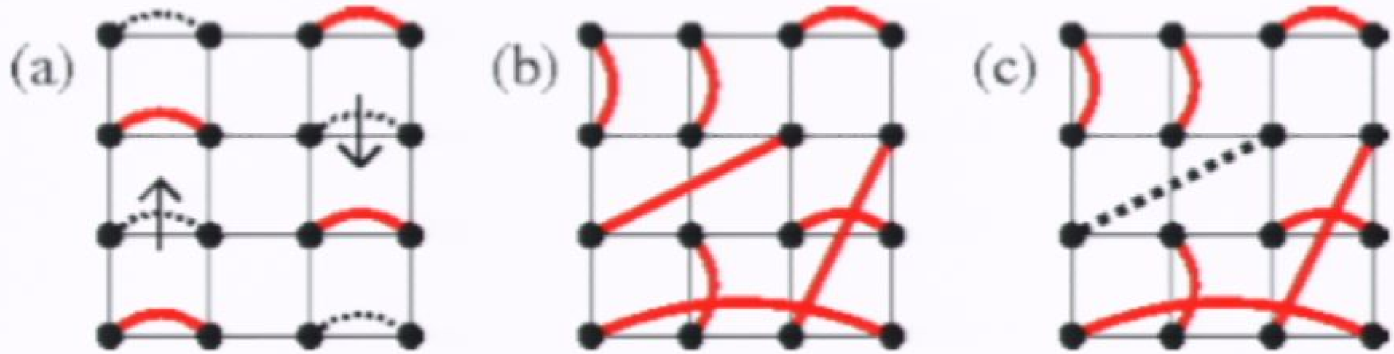

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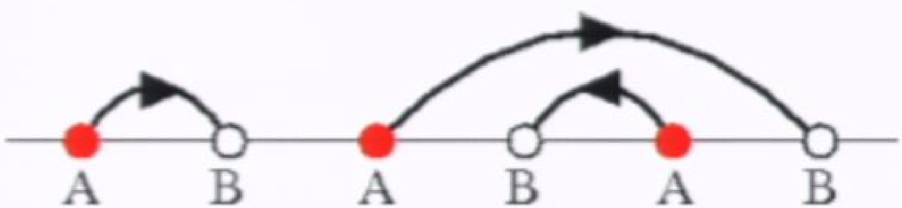

arrows indicate the order of the spins in the singlet definition

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

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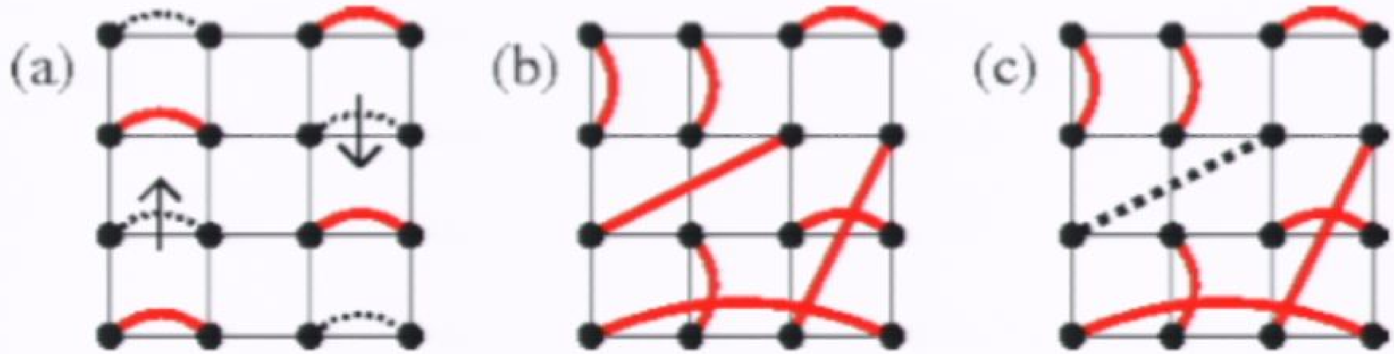

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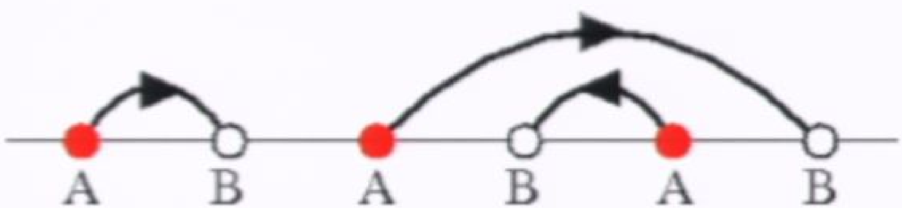

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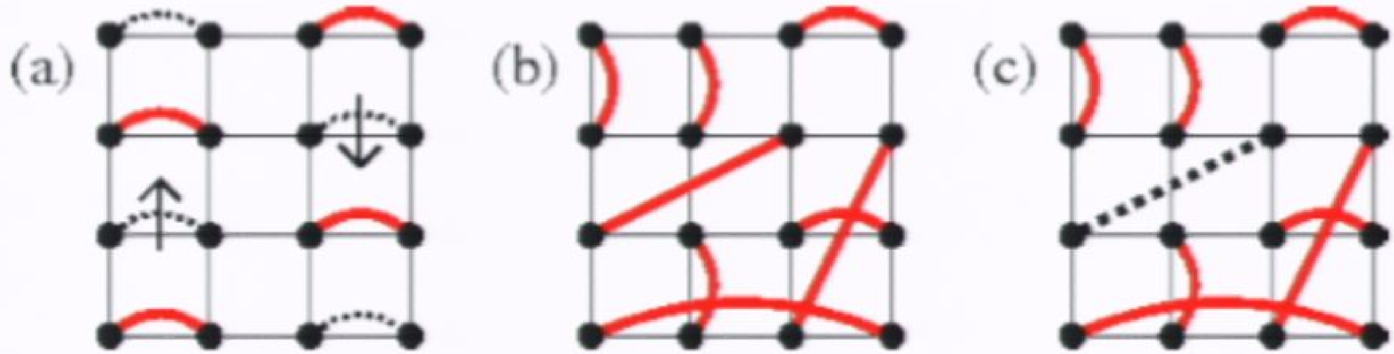

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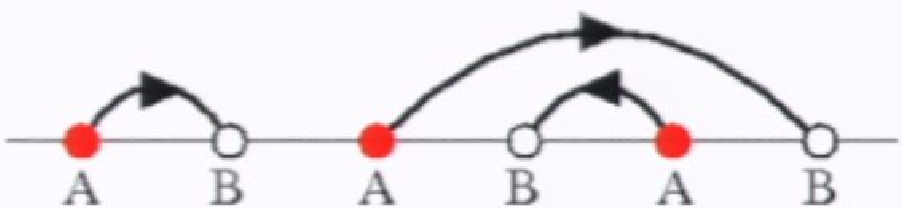

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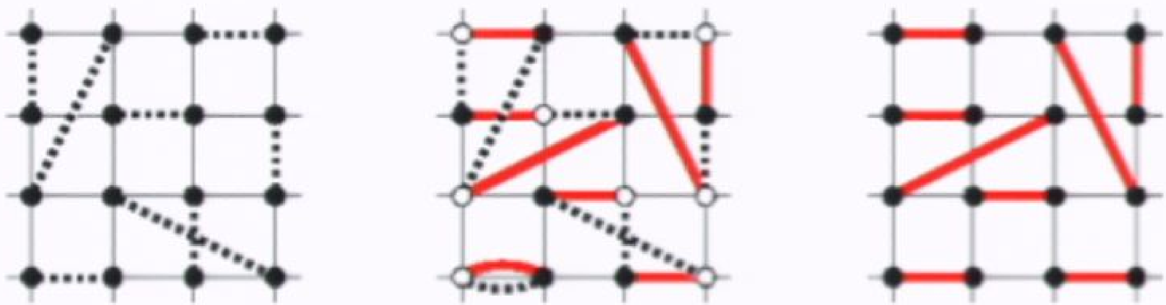
Calculating with valence-bond states

All valence-bond basis states are non-orthogonal

- the overlaps are obtained using transposition graphs (loops)



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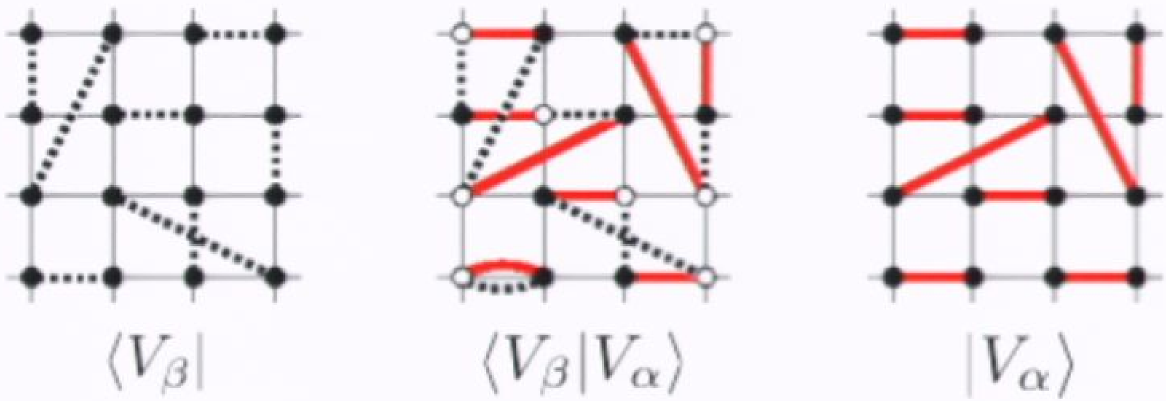

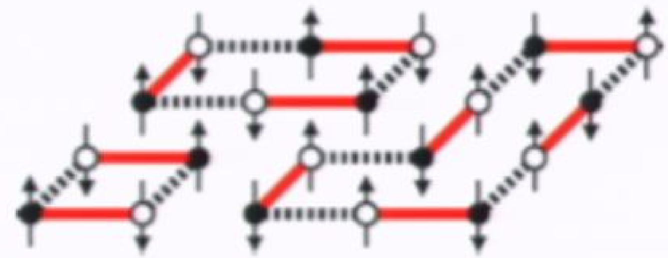

Each loop has two compatible spin states → $\langle V_\beta|V_\alpha\rangle = 2^{N_{\rm loop}-N/2}$

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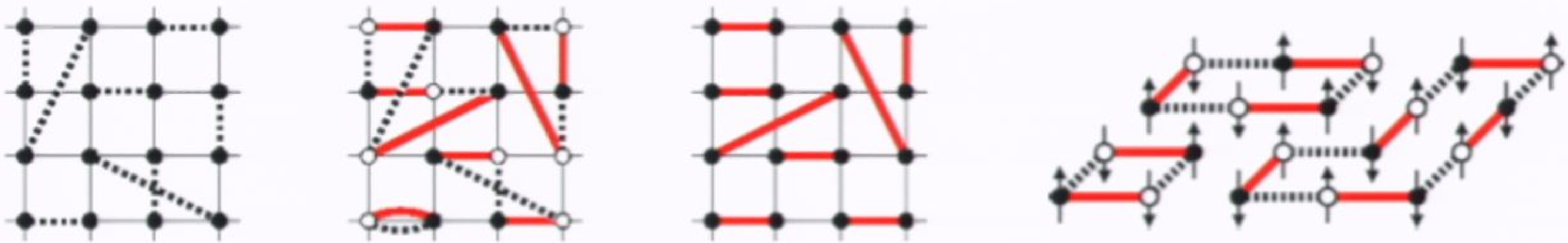

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Many matrix elements can also be expressed using the loops, e.g.,

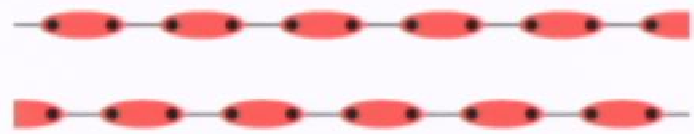
$$\frac{\langle V_\beta|\mathbf{S}_i\cdot\mathbf{S}_j|V_\alpha\rangle}{\langle V_\beta|V_\alpha\rangle} = \begin{cases} 0, & \text{for } \lambda_i \neq \lambda_j \\ \frac{3}{4}\phi_{ij}, & \text{for } \lambda_i = \lambda_j \end{cases}$$

λ_i is the loop index (each loop has a label), staggered phase factor

$$\phi_{ij} = \begin{cases} -1, & \text{for } i,j \text{ on different sublattices} \\ +1, & \text{for } i,j \text{ on the same sublattice} \end{cases}$$

Solution of the frustrated chain at the Majumdar-Ghosh point

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



We will show that these are eigenstates when $J_2/J_1=1/2$

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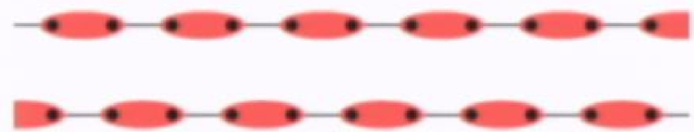

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Write H in terms of singlet projectors

$$H = -\sum_{i=1}^{N} (C_{i,i+1} + g C_{i,i+2}) + N\frac{1+g}{4}, \qquad C_{ij} = -(\mathbf{S}_i \cdot \mathbf{S}_j - -)$$

Useful valence-bond results
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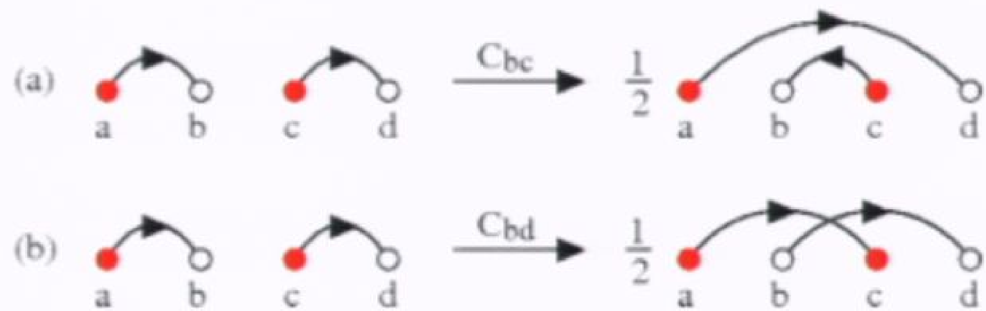

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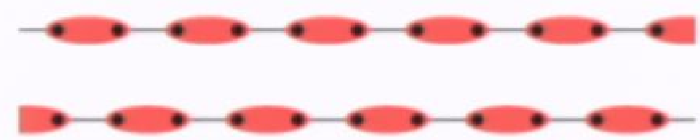

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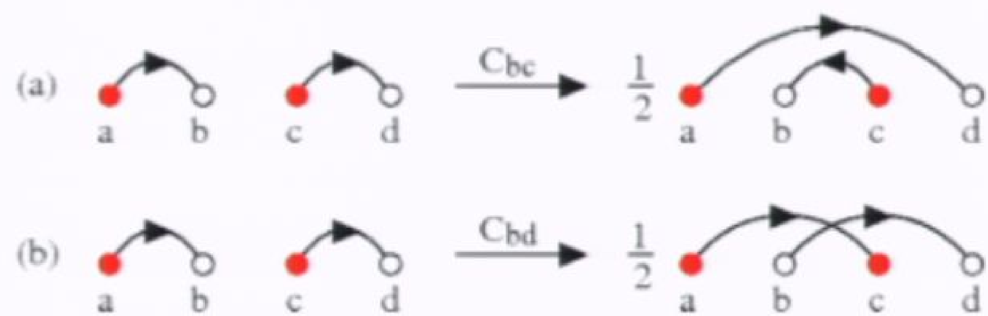

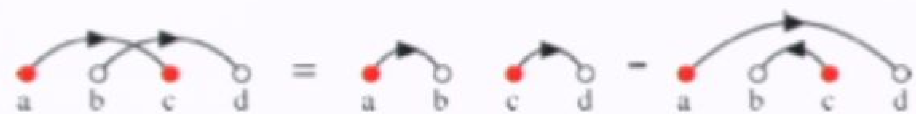

Act with one "segment" of the terms
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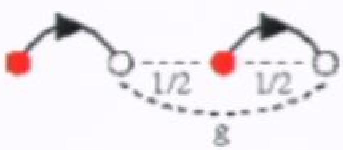

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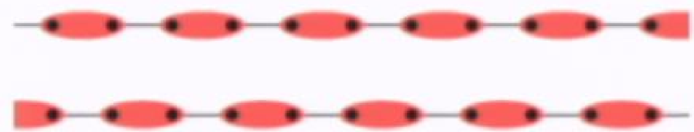

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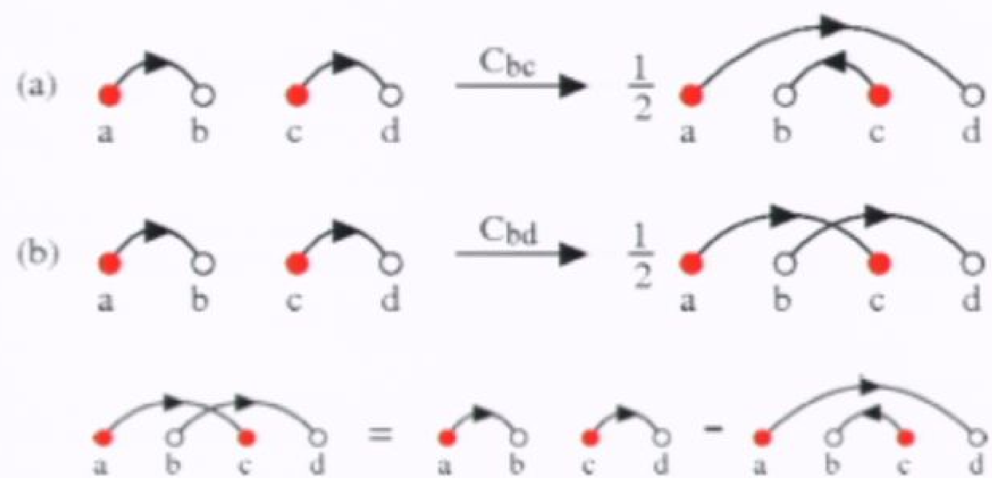

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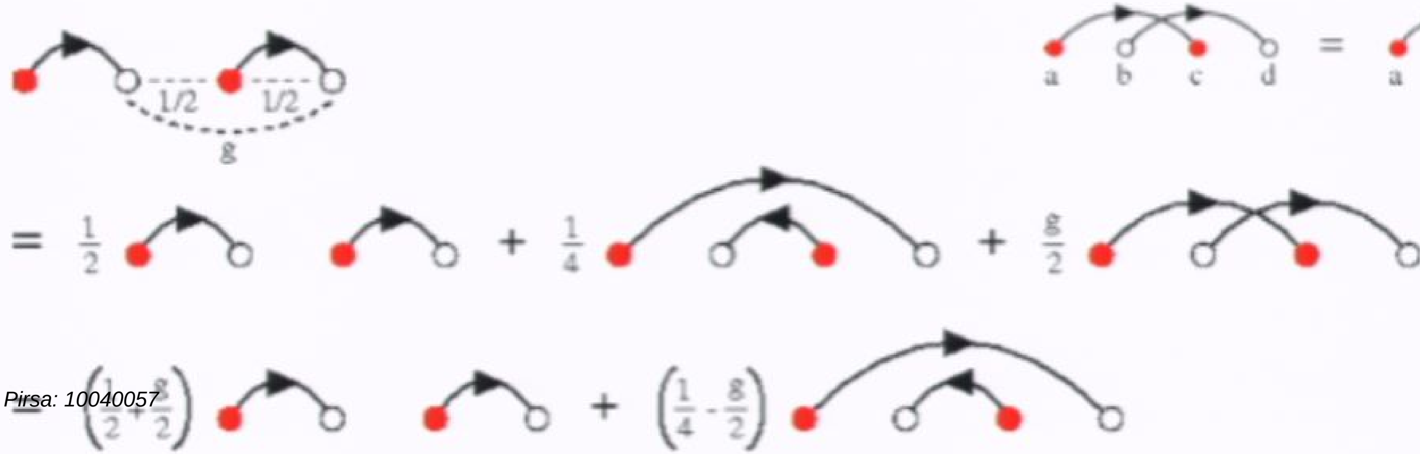

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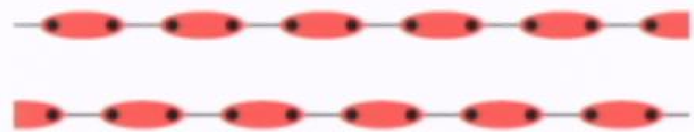

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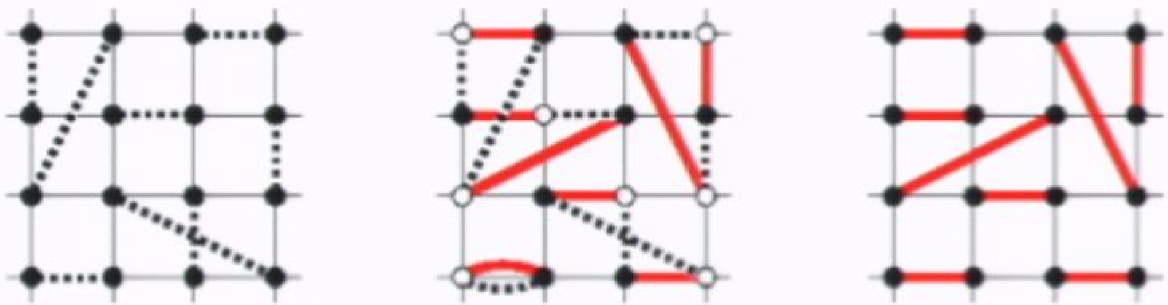

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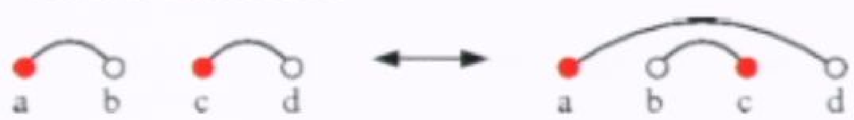

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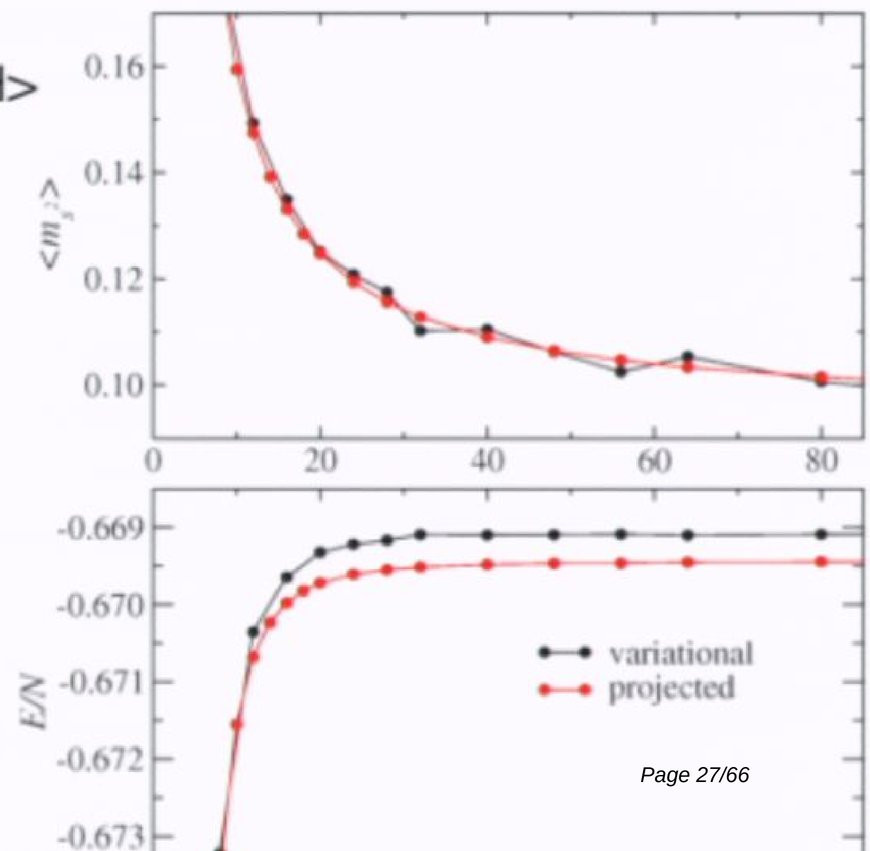

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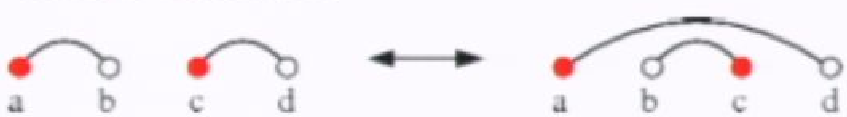
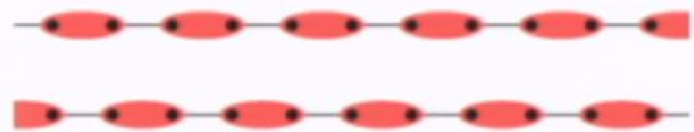


2D Heisenberg results

- $h(r) = 1/r^3$

Solution of the frustrated chain at the Majumdar-Ghosh point

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



We will show that these are eigenstates when $J_2/J_1=1/2$

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

Amplitude-product states

Good variational ground state for bipartite models can be constructed

$$|\Psi_s\rangle = \sum_\alpha f_\alpha |(a_1^\alpha, b_1^\alpha)\cdots(a_{N/2}^\alpha, b_{N/2}^\alpha)\rangle = \sum_\alpha f_\alpha |V_\alpha\rangle$$

Let the wave-function coefficients be products of “amplitudes” (real positive numbers)

$$f_\alpha = \prod_{\mathbf{r}} h(\mathbf{r})^{n_\alpha(\mathbf{r})},$$

Liang, Doucot, Anderson (PRL, 1990)

r is the bond length (n(r) = number of length **r** bonds)

The **amplitudes h(r) are adjustable parameters**

- use some optimization method to minimize E=<H>

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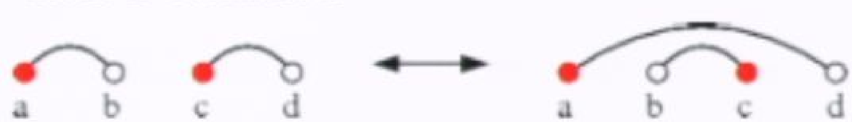
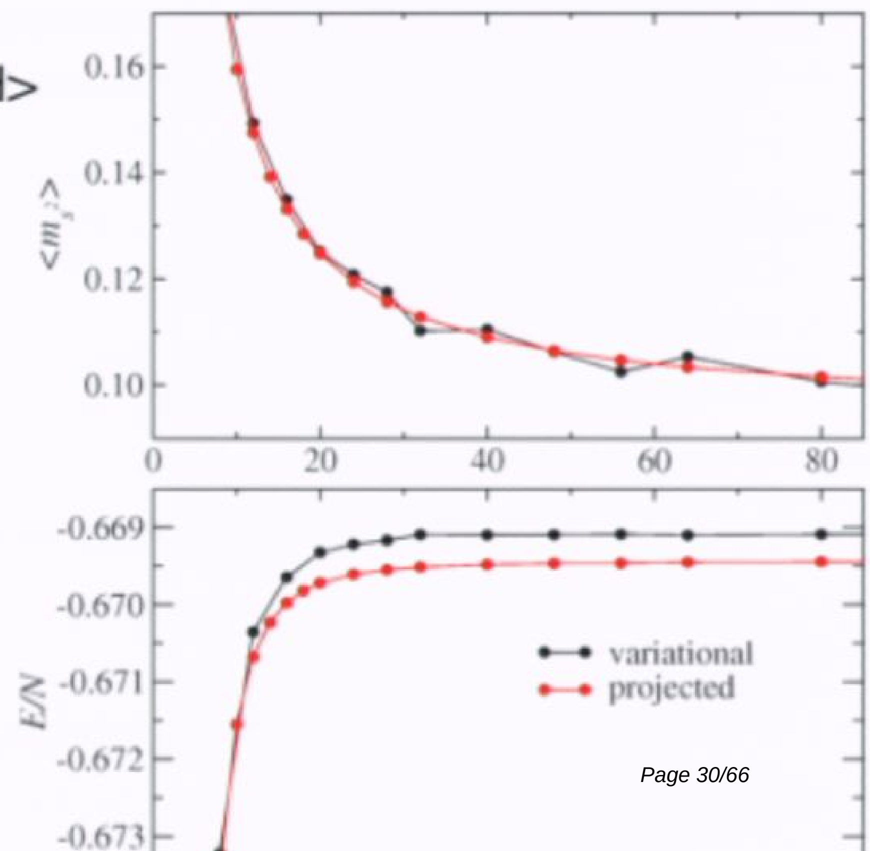
Variational QMC method

Given h(r), one can study the state using Monte Carlo sampling of bonds

- elementary two-bond moves
  - Metroplois accept/reject
- loop updates when spins are included
  - more efficient





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Projector Monte Carlo in the valence-bond basis

Liang, 1991; AWS, Phys. Rev. Lett 95, 207203 (2005)

(-H)^n projects out the ground state from an arbitrary state

$$(-H)^n|\Psi\rangle = (-H)^n \sum_i c_i|i\rangle \to c_0(-E_0)^n|0\rangle$$

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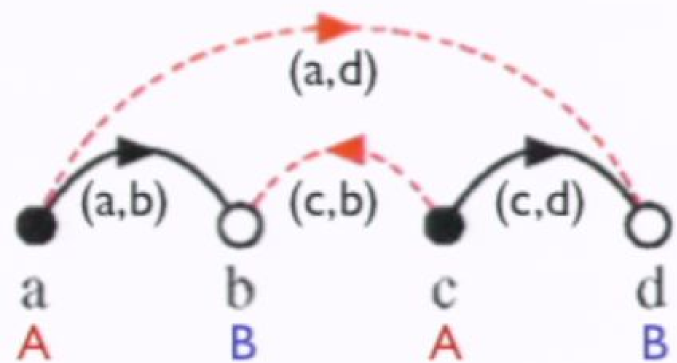
S=1/2 Heisenberg model

$$H = \sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j = -\sum_{\langle i,j\rangle} H_{ij}, \quad H_{ij} = (\tfrac{1}{4} - \vec{S}_i \cdot \vec{S}_j)$$

Project with string of bond operators

$$\sum_{\{H_{ij}\}} \prod_{p=1}^{n} H_{i(p)j(p)}|\Psi\rangle \rightarrow r|0\rangle$$ (r irrelevant)



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

Action of bond operators

$$H_{ab}|...(a,b)...(c,d)...\rangle = |...(a,b)...(c,d)...\rangle$$

$$H_{bc}|...(a,b)...(c,d)...\rangle = \frac{1}{2}|...(c,b)...(a,d)...\rangle$$

Simple reconfiguration of bonds (or no change; diagonal)

Expectation values: $\langle A \rangle = \langle 0|A|0 \rangle$

Strings of singlet projectors

$$P_k = \prod_{p=1}^{n} H_{i_k(p) j_k(p)}, \quad k = 1, \ldots, N_b^n \quad (N_b \ = \ \text{number of interaction bonds})$$

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$$\sum_k P_k|V_r\rangle = \sum_k W_{kr}|V_r(k)\rangle \rightarrow (-E_0)^n c_0|0\rangle$$

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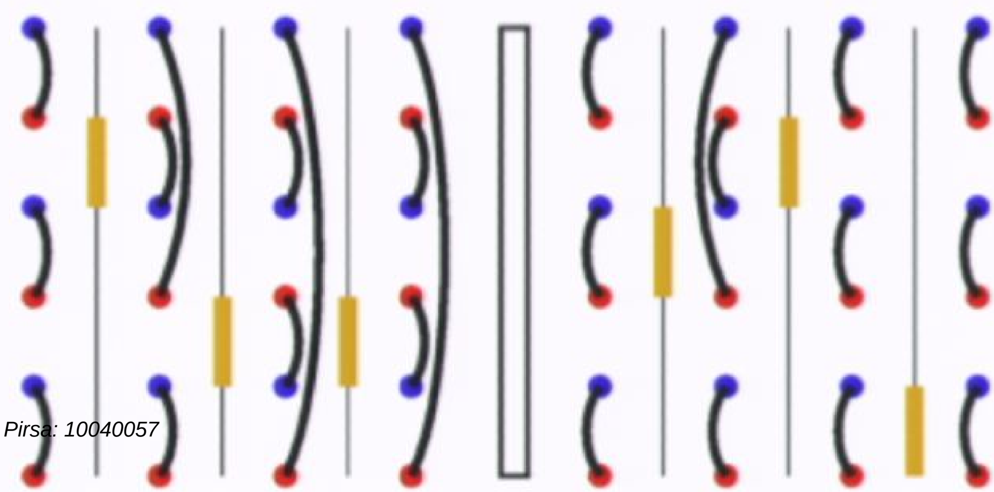
6-spin chain example:



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Monte Carlo sampling

More efficient ground state QMC algorithm → larger lattices

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AWS and H. G. Evertz, ArXiv:0807.0682

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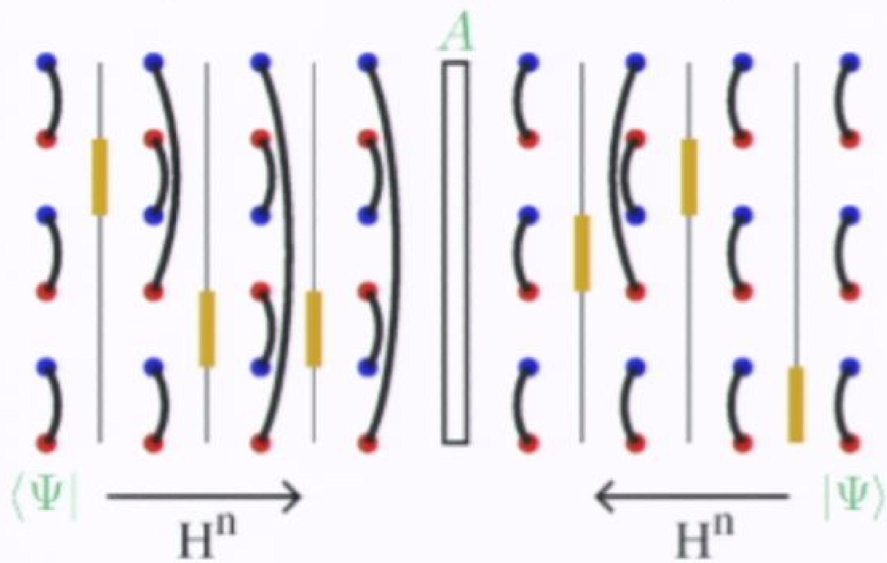

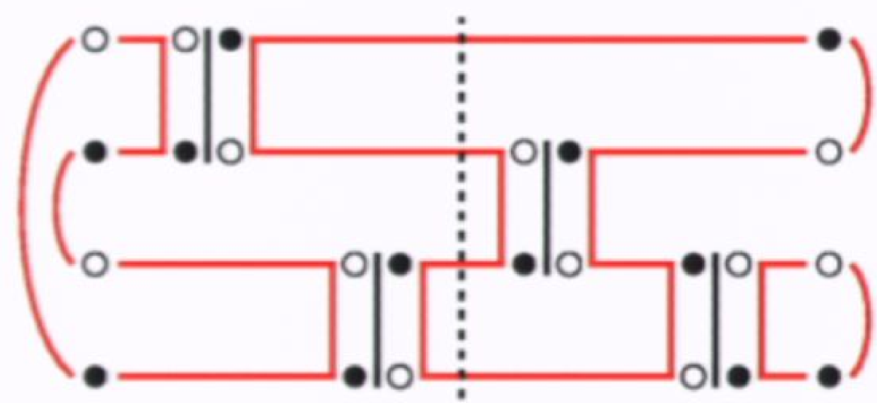

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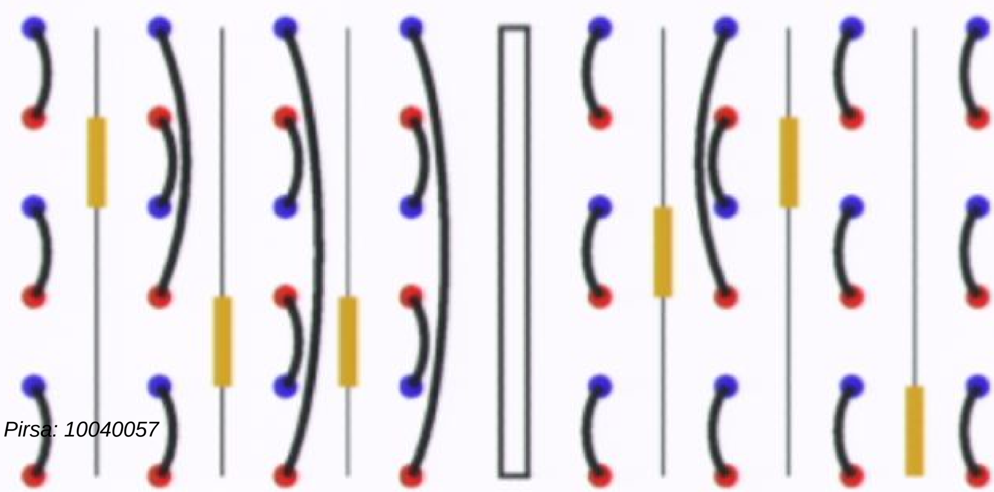

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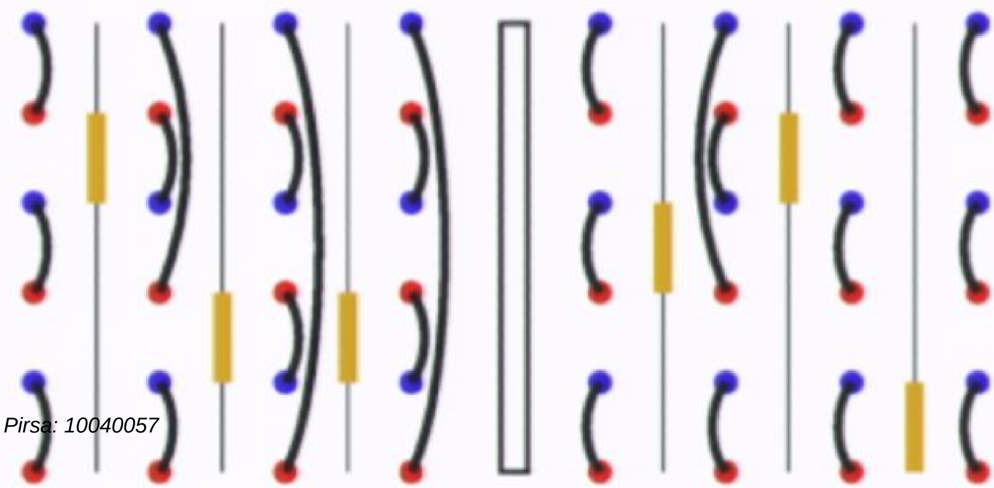

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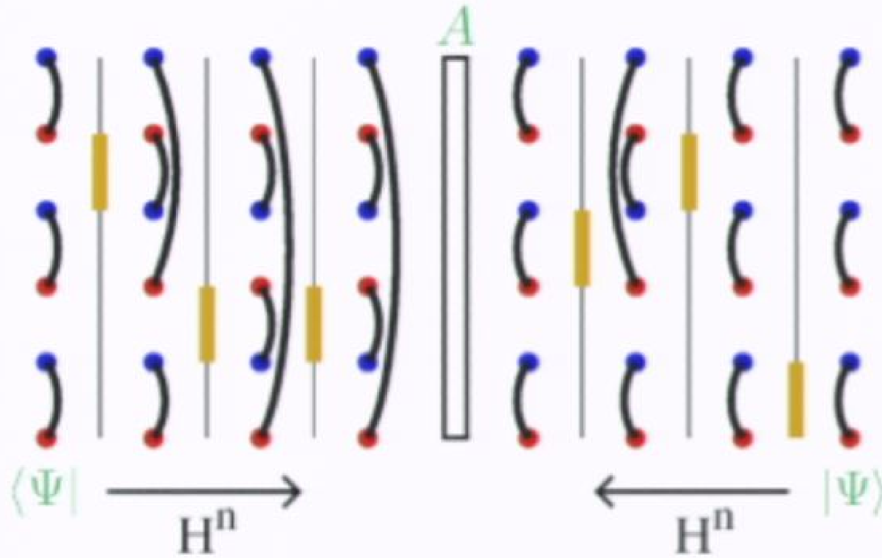

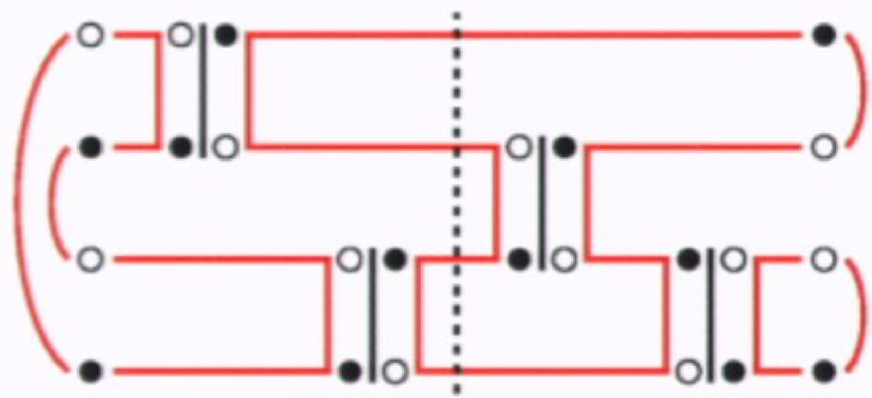

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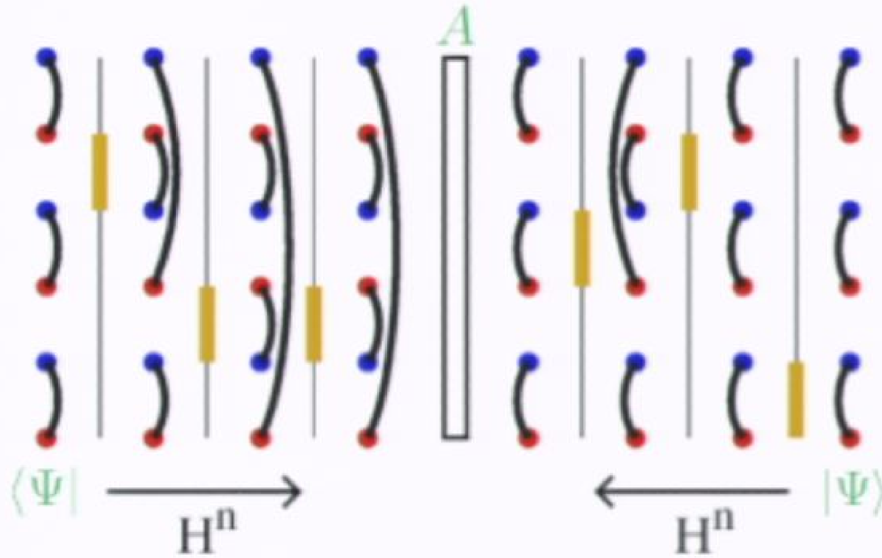

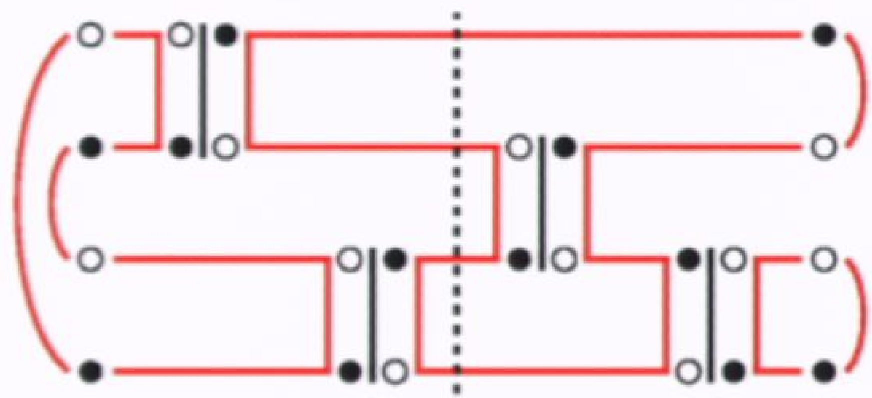

Loop updates similar to those in finite-T methods
(world-line and stochastic series expansion methods)

- good valence-bond trial wave functions can be used
- larger systems accessible

J-Q model: T=0 results obtained with valence-bond QMC

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

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Two different models: **J-Q₂ and J-Q₃**

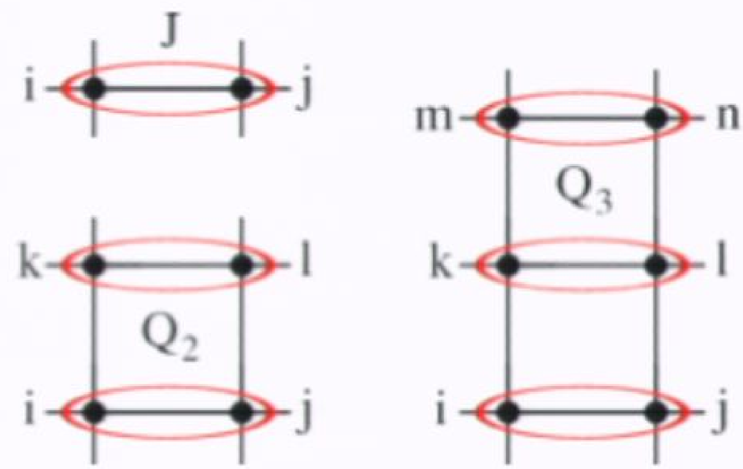
bond-singlet projector

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

$$H_1 = -J \sum_{\langle ij \rangle} C_{ij}$$

$$H_2 = -Q_2 \sum_{\langle ijkl \rangle} C_{kl} C_{ij}$$

$$H_3 = -Q_3 \sum_{\langle ijklmn \rangle} C_{mn} C_{kl} C_{ij}$$



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Two different models: **J-Q_2 and J-Q_3**

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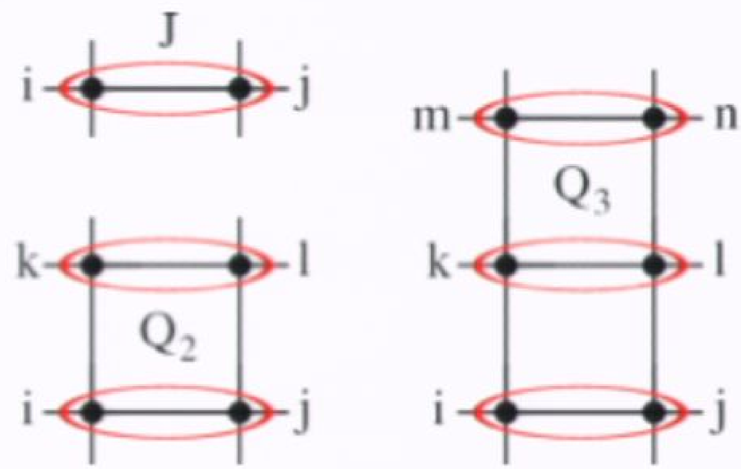
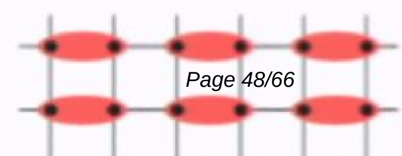


Studies of J-Q_2 model and J-Q_3 model on L×L lattices with L up to 64

Exponents η_s, η_d, and ν from the squared order parameters

$$D^2 = \langle D_x^2 + D_y^2 \rangle, \quad D_x = \frac{1}{N}\sum_{i=1}^{N} (-1)^{x_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}}, \quad D_y = \frac{1}{N}\sum_{i=1}^{N} (-1)^{y_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}}$$

$$M^2 = \langle \vec{M} \cdot \vec{M} \rangle \qquad \vec{M} = \frac{1}{N} \sum (-1)^{x_i + y_i} \vec{S}_i$$



Using coupling ratio

$$q = \frac{Q_p}{Q_p + J}, \qquad p = 2, 3$$

- AF order for q→0
- VBS order for q→1

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J-Q$_2$ model; q$_c$=0.961(1)

$$\eta_s = 0.35(2)$$
$$\eta_d = 0.20(2)$$
$$\nu = 0.67(1)$$

J-Q$_3$ model; q$_c$=0.600(3)

$$\eta_s = 0.33(2)$$
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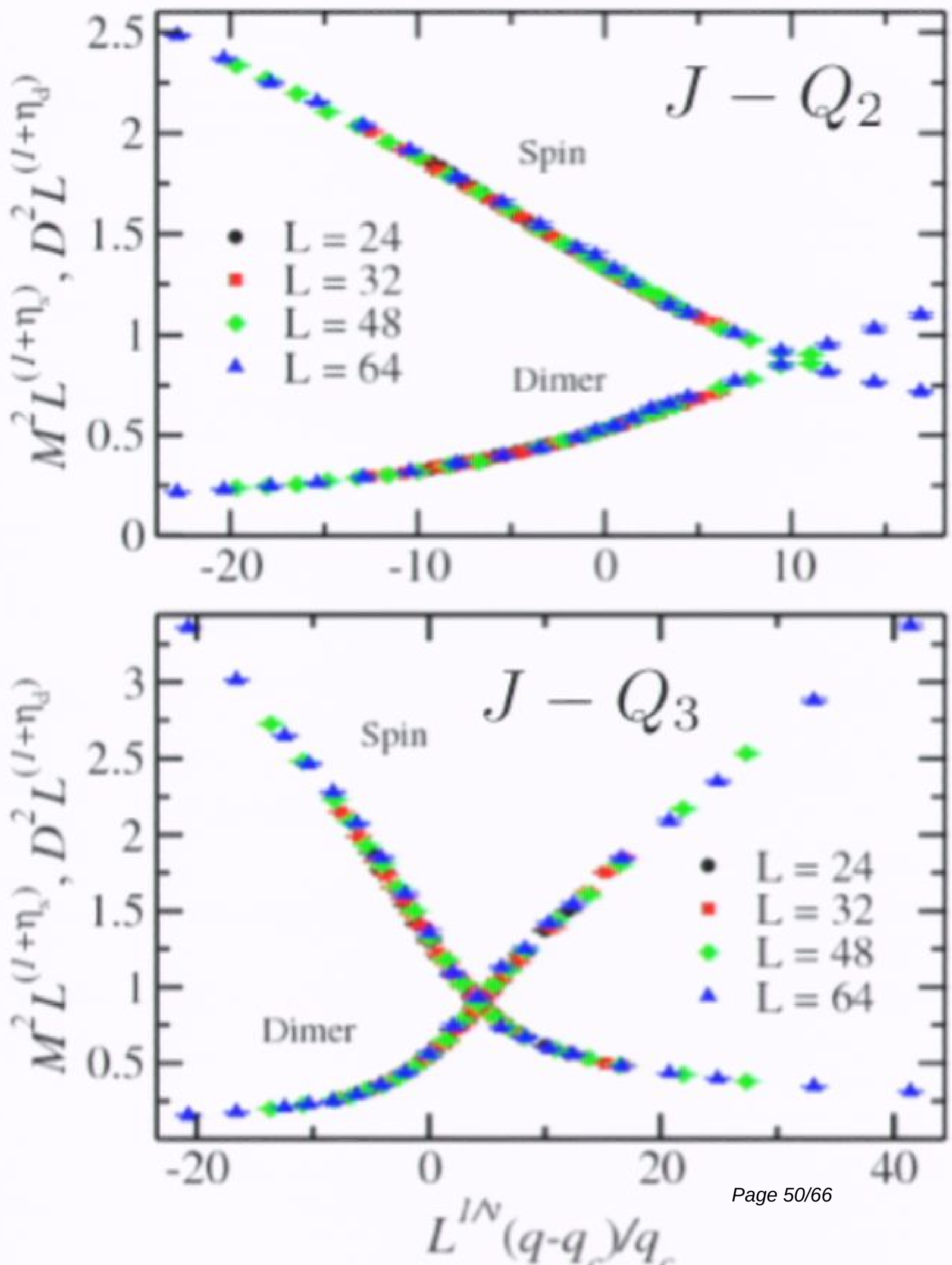
Finite-size scaling



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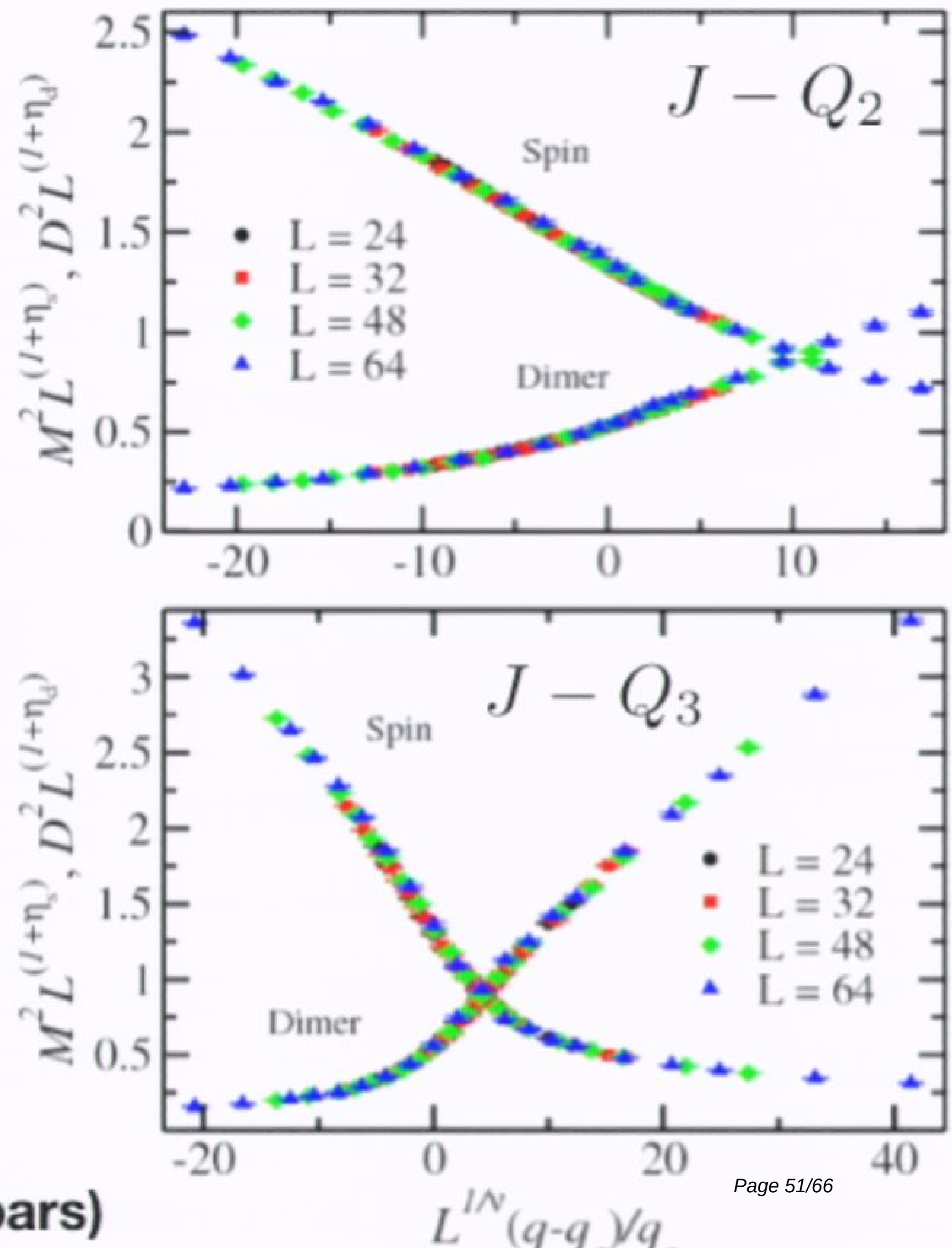
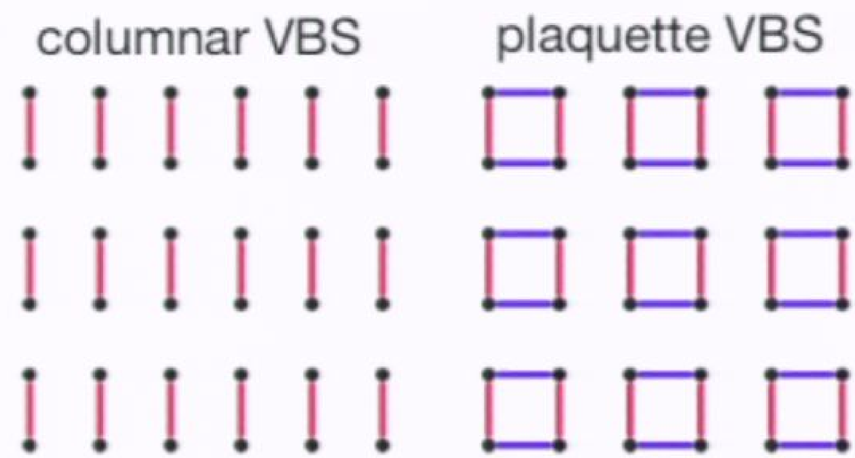


Exponents universal (within error bars)

Columnar or plaquette VBS?



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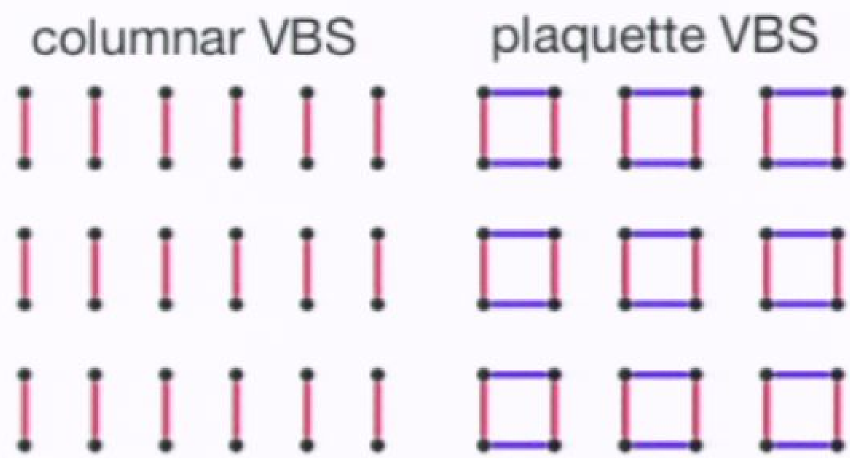

QMC sampled state in the valence-bond basis

$$|0\rangle = \sum_k c_k |V_k\rangle$$

Joint probability distribution **P(D_x,D_y)** of x and y columnar VBS order parameters

$$D_x = \frac{\langle V_k | \frac{1}{N} \sum_{i=1}^{N} (-1)^{x_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}} | V_p \rangle}{\langle V_k | V_p \rangle}$$

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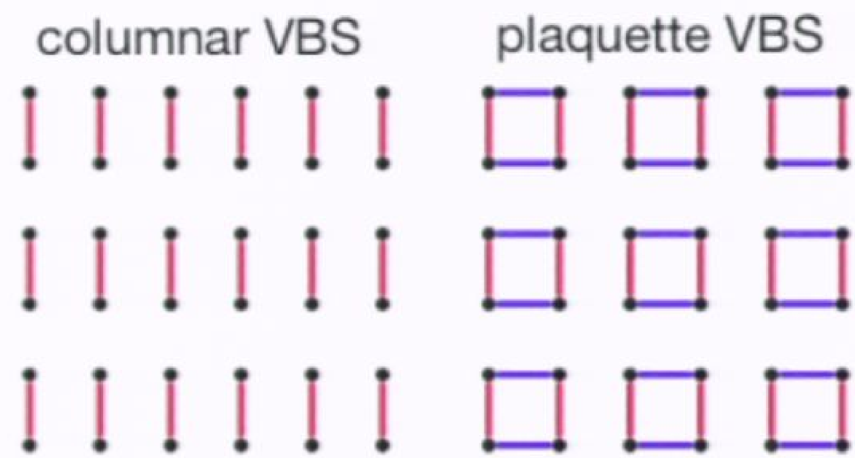

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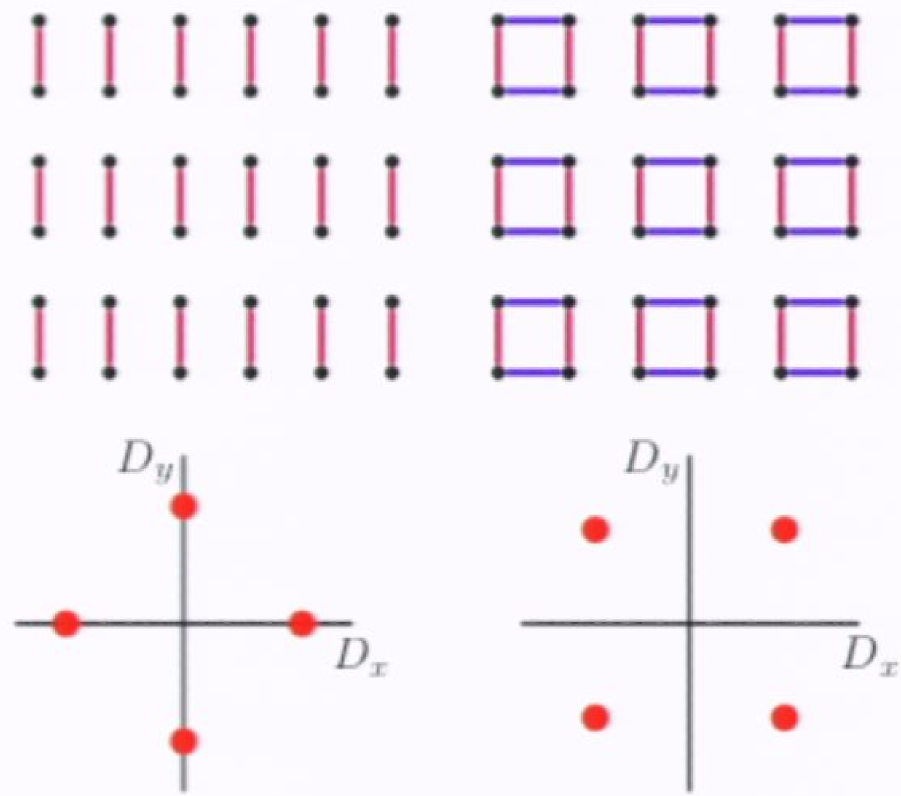

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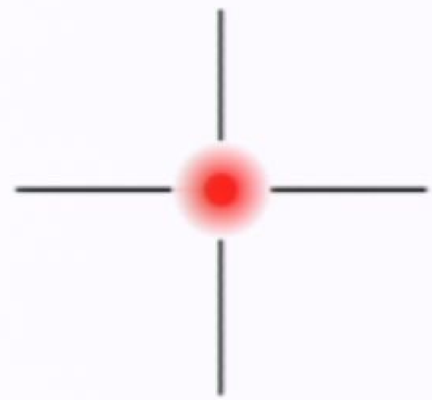
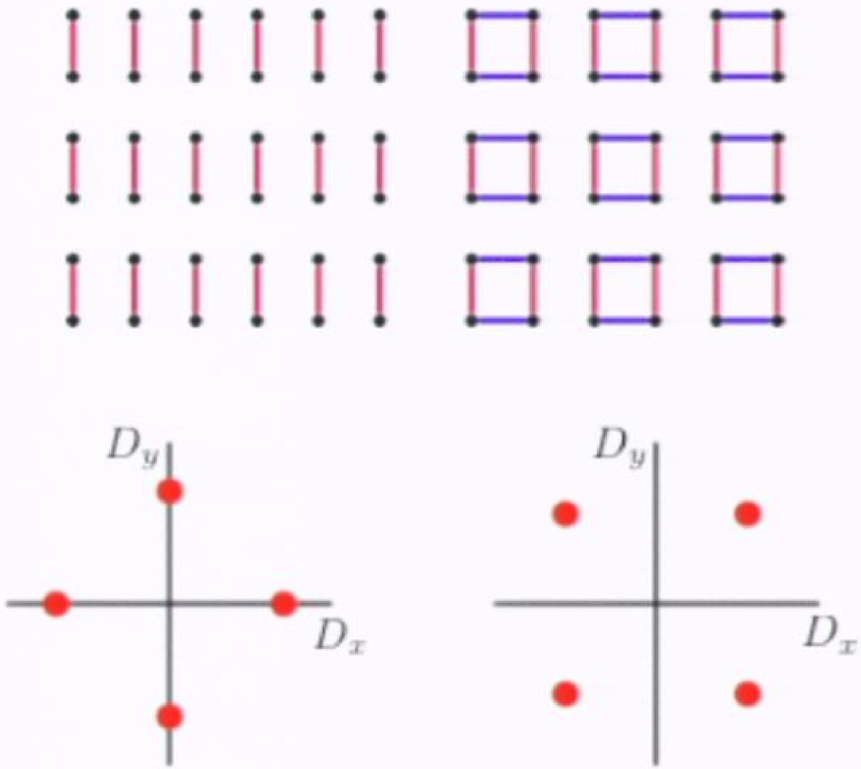
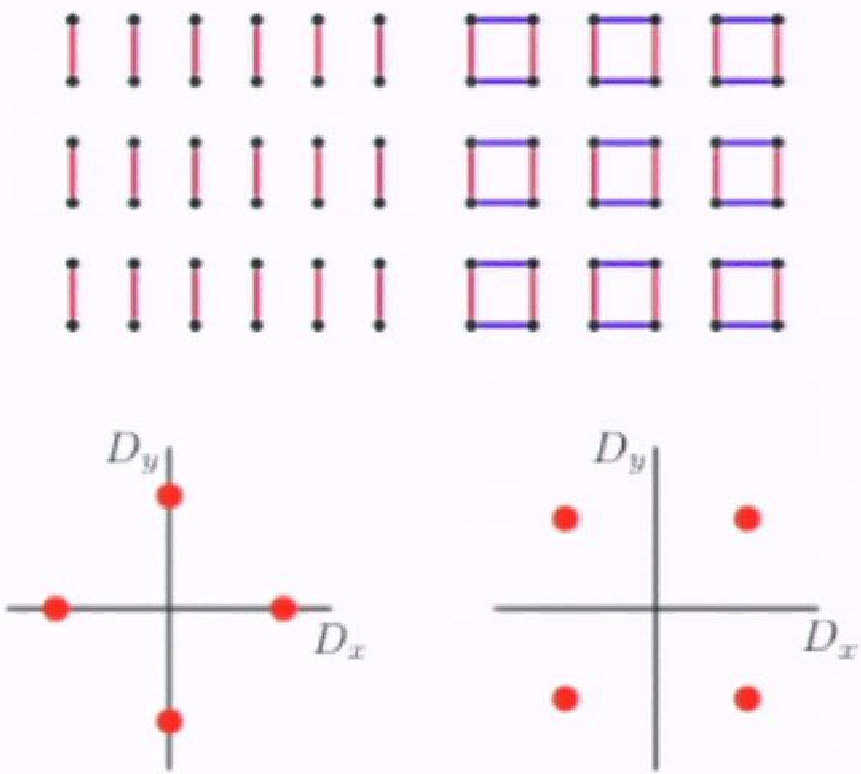
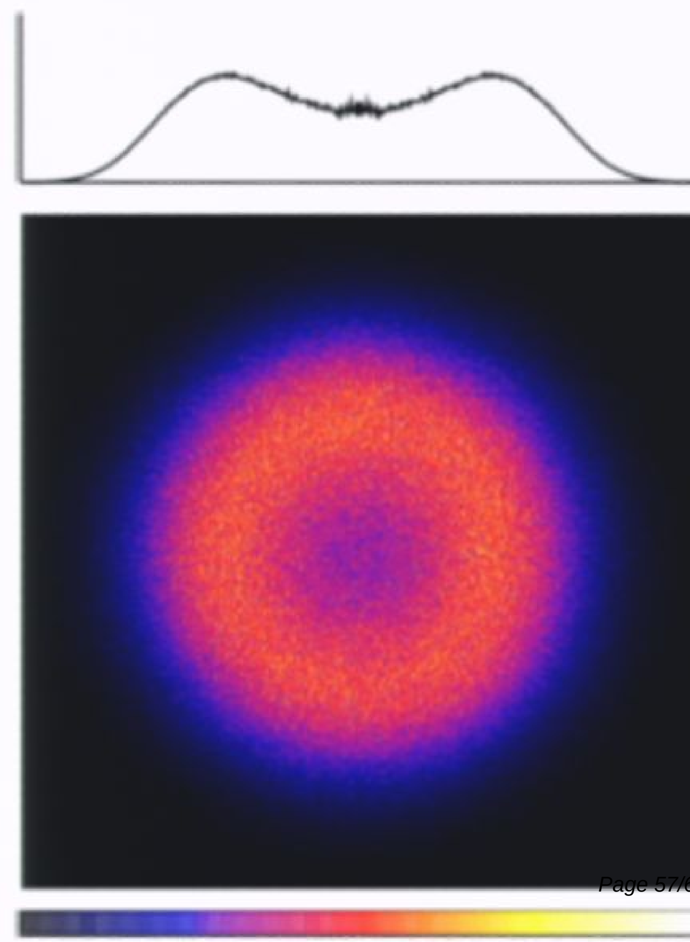


critical

4 peaks expected in VBS phase


D_y
D_x
D_y
D_x

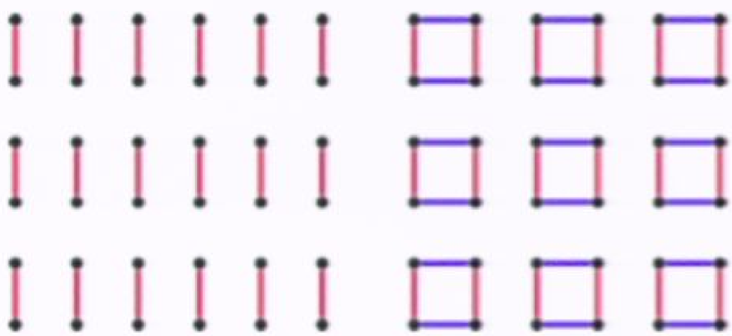


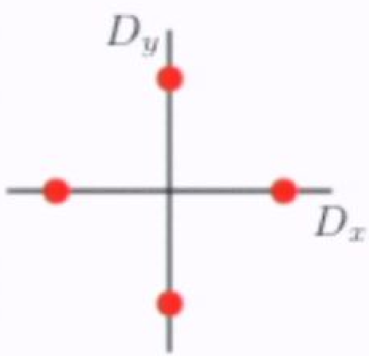


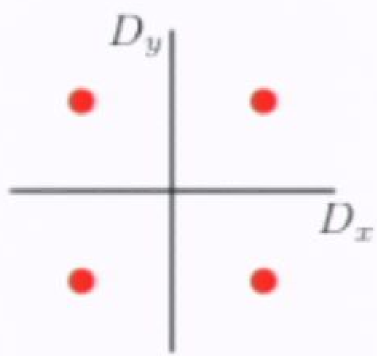
No sign of cross-over to Z_4 symmetric order parameter seen in the J-Q_2 model

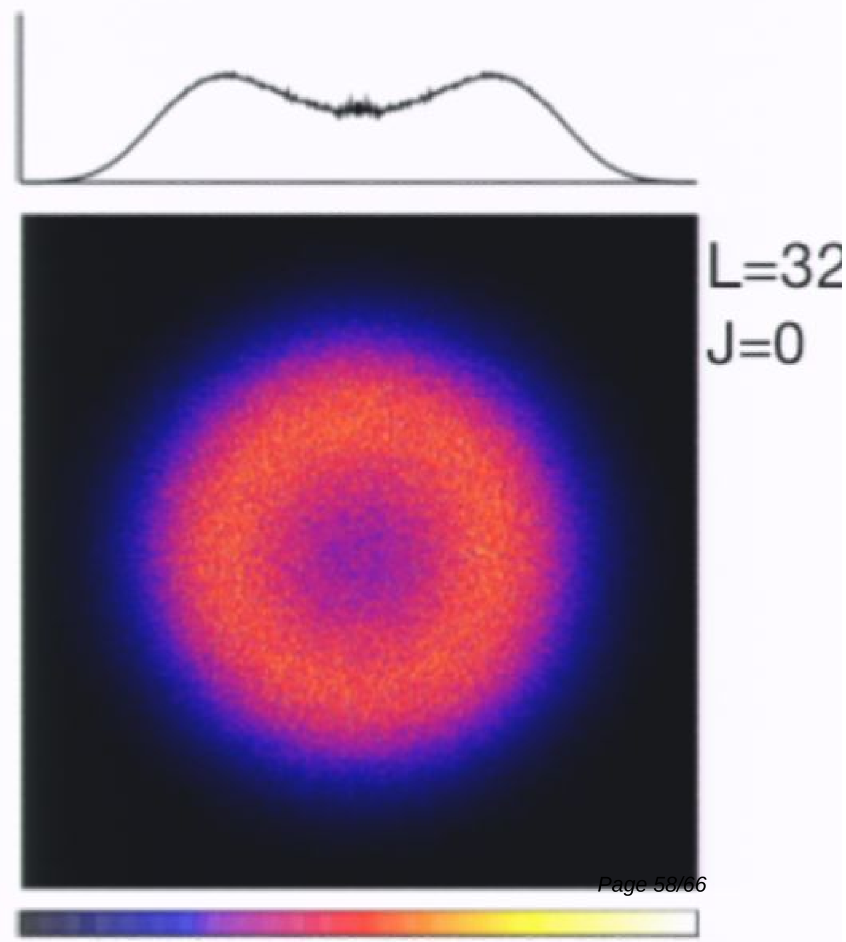
VBS fluctuations in the theory of deconfined quantum-critical points

- plaquette and columnar VBS "degenerate" at criticality
- Z_4 "lattice perturbation" irrelevant at critical point
  – and in the VBS phase for $L<\Lambda \sim \xi^a$, $a>1$ (spinon confinement length)
- **emergent U(1) symmetry**
- **ring-shaped distribution expected for L<Λ**









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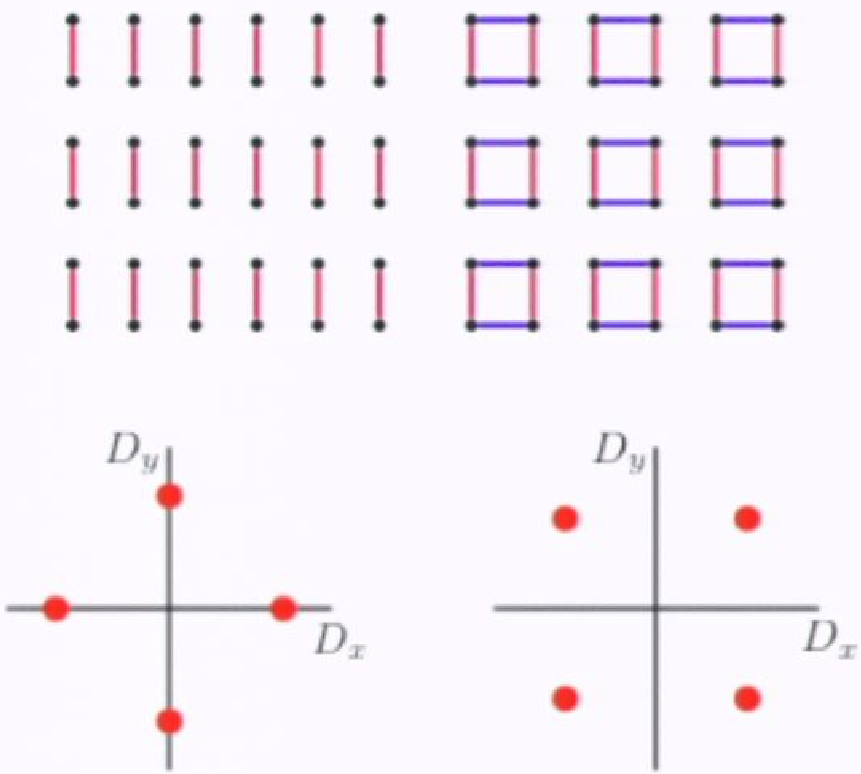
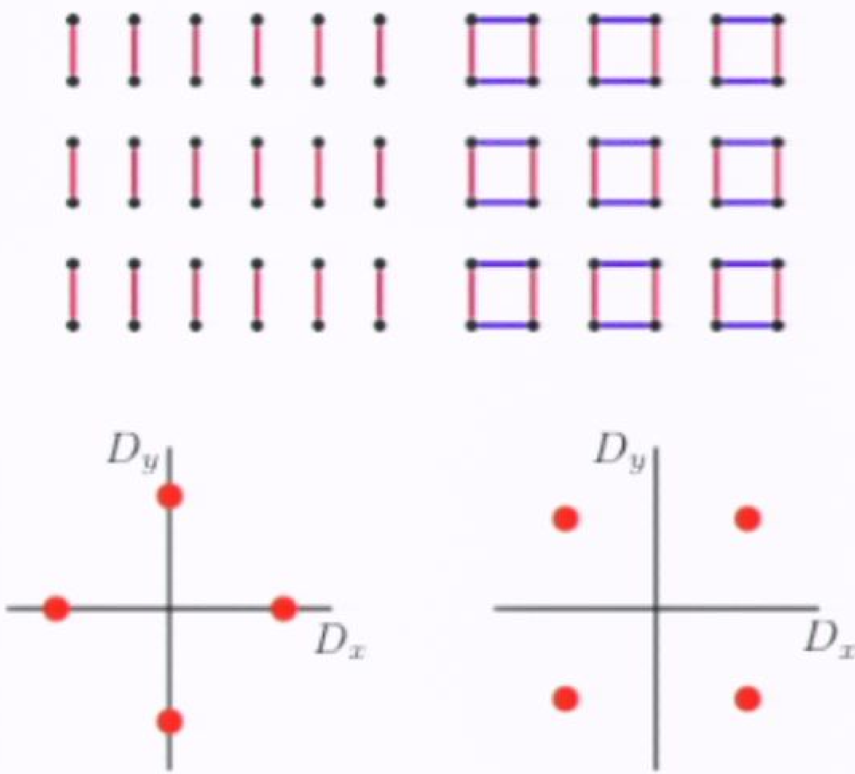
Order parameter histograms $P(D_x,D_y)$, J-Q_3 model

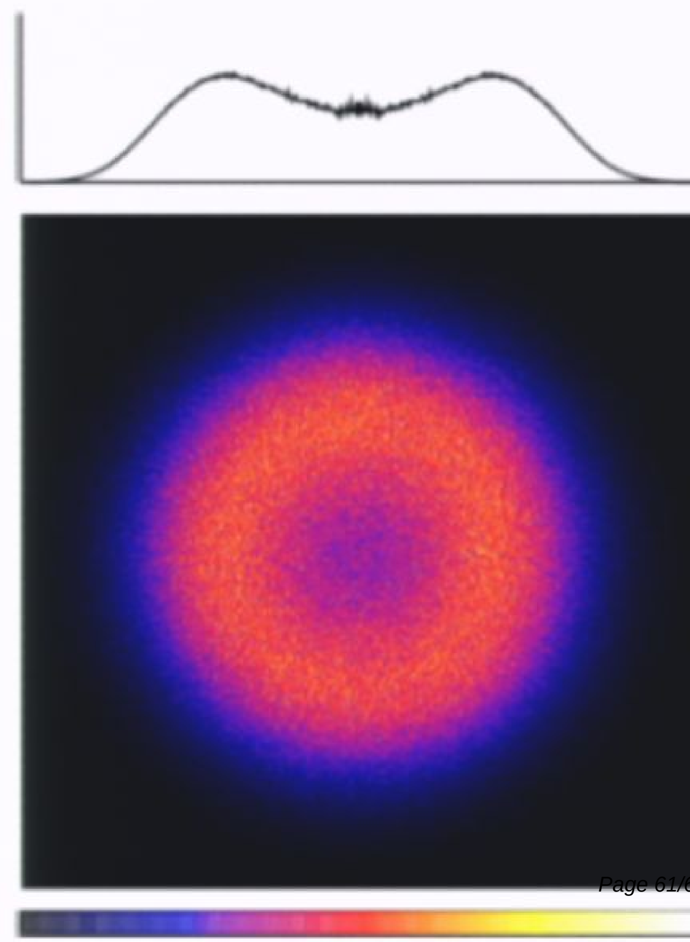
J. Lou, A.W. Sandvik, N. Kawashima, PRB (2009)

This model has a more robust VBS phase

- can the symmetry cross-over be detected?


D_y
D_x
D_y
D_x





No sign of cross-over to Z_4 symmetric order parameter seen in the J-Q_2 model

Order parameter histograms $P(D_x,D_y)$, J-Q_3 model

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

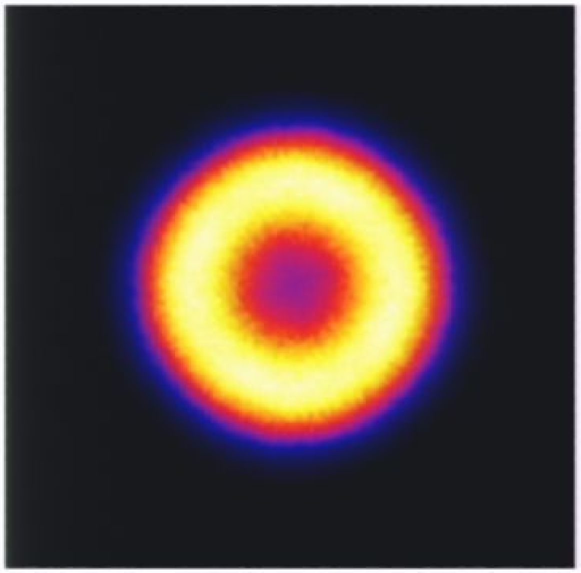
This model has a more robust VBS phase

- can the symmetry cross-over be detected?

$q = 0.635$

$(q_c \approx 0.60)$

$L = 32$



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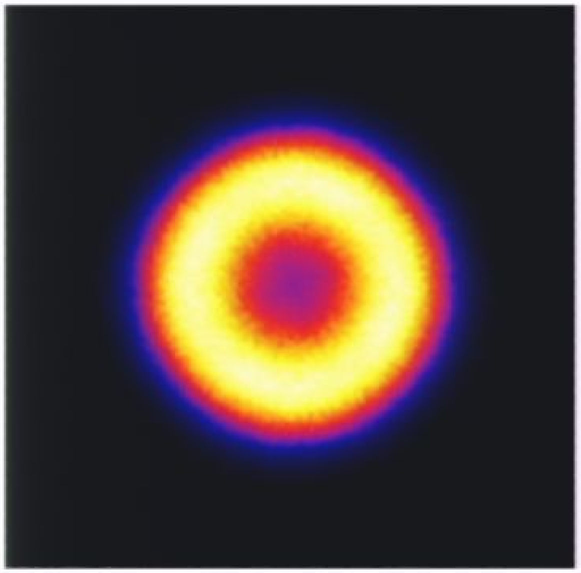

$q = 0.85$

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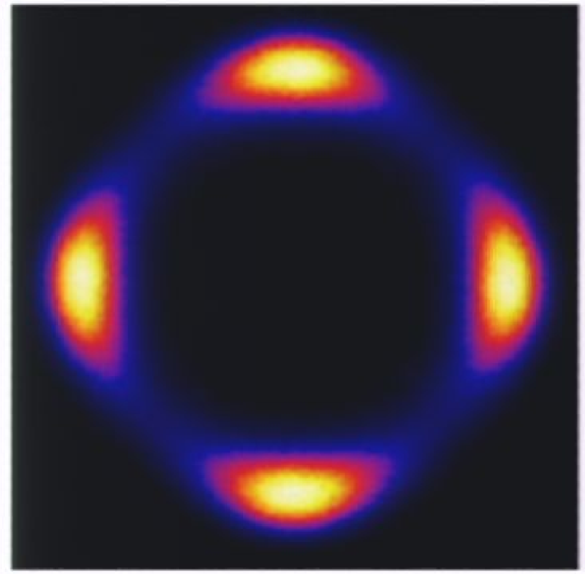

Order parameter histograms P(D_x,D_y), J-Q_3 model

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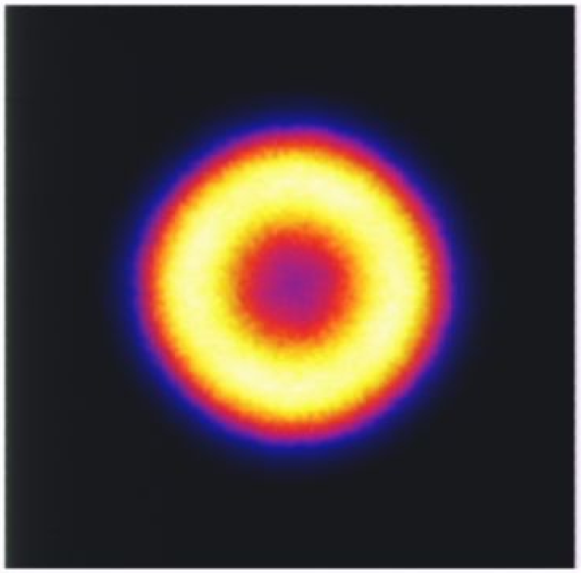

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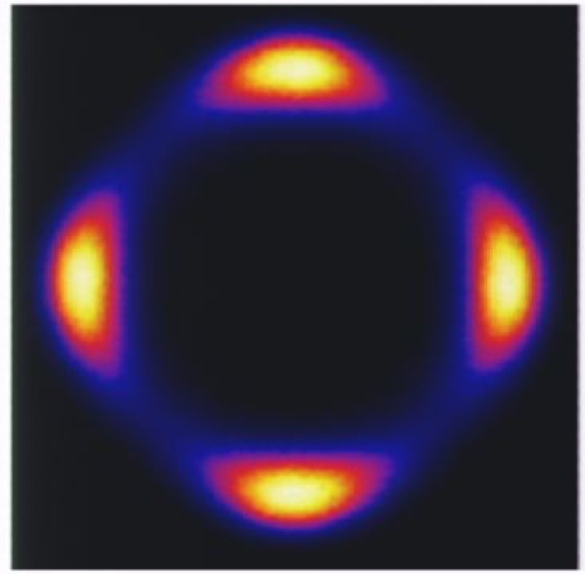
$L = 32$



VBS symmetry cross-over
- Z_4-sensitive order parameter

$$D_4 = \int r dr \int d\phi P(r,\phi) \cos(4\phi)$$

Finite-size scaling gives U(1)
(deconfinement) length-scale

Order parameter histograms $P(D_x,D_y)$, J-Q_3 model

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

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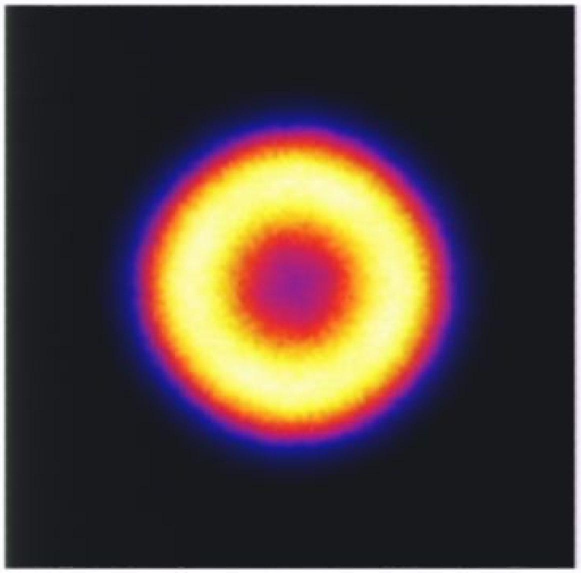
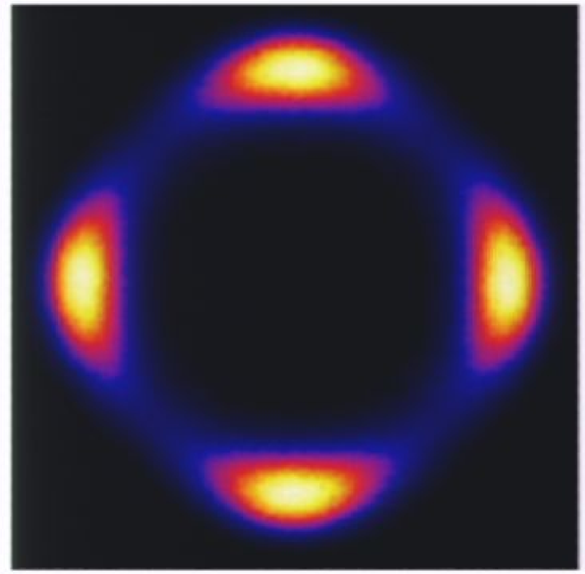


$q = 0.85$

$L = 32$



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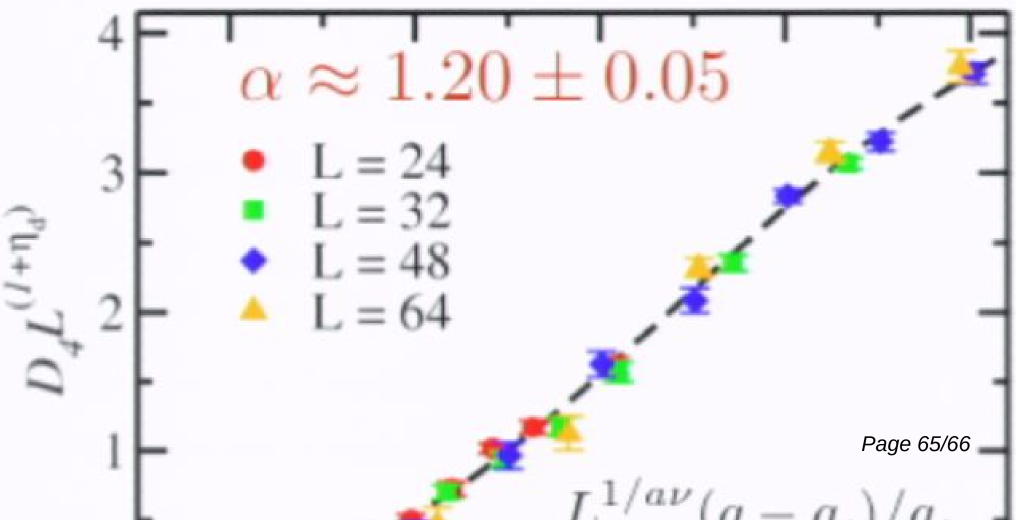


Order parameter histograms P(Dx,Dy), J-Q

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

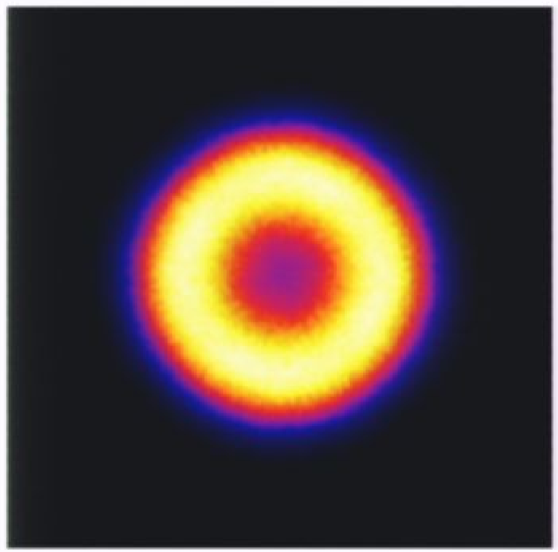
This model has a more robust VBS phase

- can the symmetry cross-over be detected?

$q = 0.635$

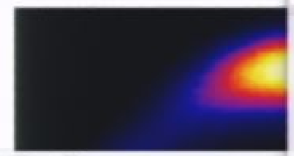
$(q_c \approx 0.60)$

$L = 32$



$q = 0.85$

$L = 3$



VBS symmetry cross-over

- Z_4-sensitive order parameter

$$D_4 = \int r dr \int d\phi P(r,\phi) \cos(4\phi)$$