the case for deconfined quantum criticality in the

The J-K and J-Q models:

a comparative quantum Monte Carlo study

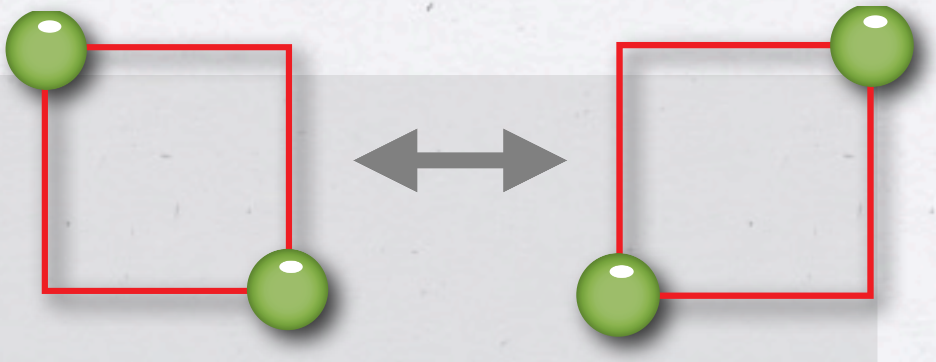
R. Melko, University of Waterloo

A. Sandvik, Boston University

R. Kaul, Harvard University

KITP, Nov 8, 2007

multi-particle ring-exchange



avenue to realize exotic quantum phases, phase transitions

- easy-plane models

QUANTUM MAGNETS, COLD ATOMS IN OPTICAL LATTICES:

Paramekanti, Balents, Fisher, Girvin
YB Kim, Isakov, Lauchli, Hermele, Buchler...
...many more

- exciton Bose liquid
- spin liquids
- cold atom simulators for lattice gauge theories

$$\mathcal{H}_{\text{ring}} = -J_{\text{ring}} \sum_{\bowtie} (S_1^+ S_2^- S_3^+ S_4^- + \text{h.c.}),$$

$$H_{\text{RE}} = K \sum_{\square} (b_1^\dagger b_2 b_3^\dagger b_4 + b_1 b_2^\dagger b_3 b_4^\dagger - n_1 n_3 - n_2 n_4)$$

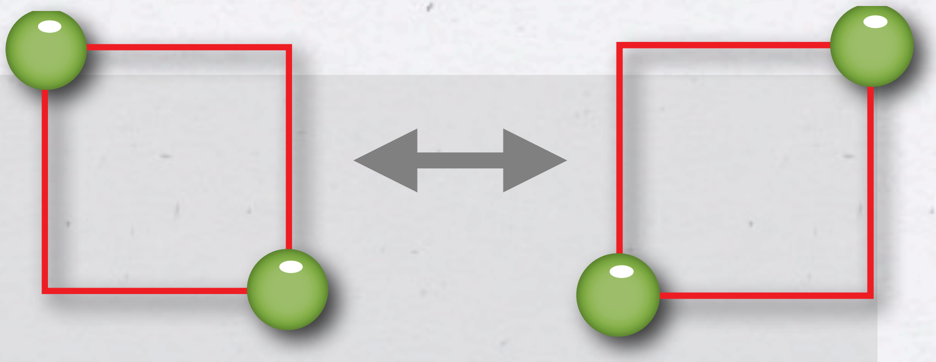
- SU(2) spin models

CUPRATES: low-energy effective theories of Hubbard model

destabilize “conventional” order WITHOUT the sign problem

solve with exact (unbiased) numerics

multi-particle ring-exchange



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outline

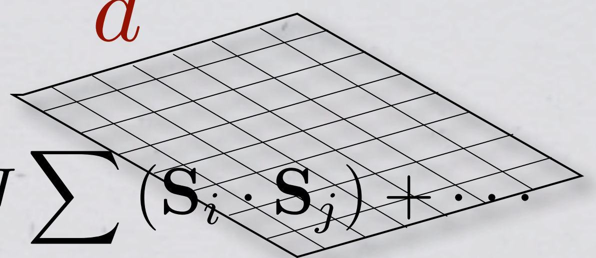
* Quantum Monte Carlo: SSE and the sign problem
* The J-K model, deconfined quantum criticality, and scaling
* The J-Q model: scaling in the quantum critical fan
* Emergent U(1) symmetries in the valence-bond-solid phases

Quantum Monte Carlo

$$Z = \mathrm{Tr}\{\mathrm{e}^{-\beta H}\}$$

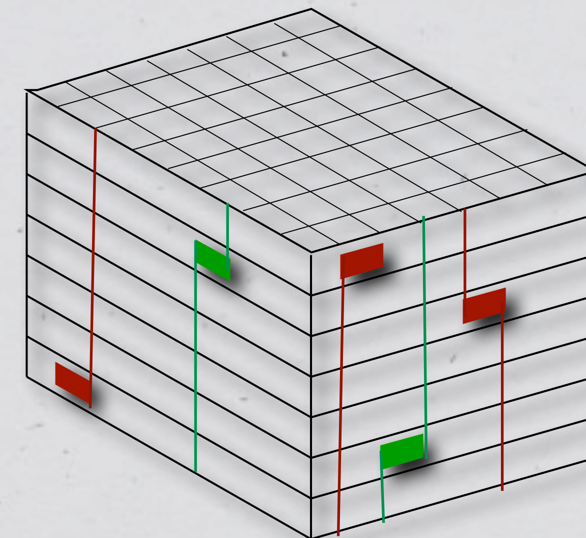
map to higher dimensional classical system

d



$$H = -J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j) + \cdots$$

$d+1$



weighted sampling of Hamiltonian operators
(particle trajectories/worldlines)

pros:

-numerically exact (unbiased)
-large system sizes
-no Trotter error

cons:

-fermionic sign problem
-ergodicity/freezing problems

Stochastic Series Expansion QMC

sandvik, PRA 25, 3667
sandivk and kurijarvi, PRB 43, 5950
RGM and sandvik, PRE 72, 026702

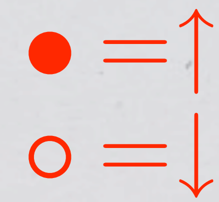
power series expansion of the partition function:

$$Z = \mathrm{Tr}\{\mathrm{e}^{-\beta H}\} = \sum_{\alpha} \langle \alpha \,|\mathrm{e}^{-\beta H}|\, \alpha \rangle$$

$$= \sum_{\alpha} \left\langle \alpha \left| \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} H^n \right| \alpha \right\rangle$$

$$= \sum_{\{\alpha_i\}} \sum_{n=0}^{\infty} \frac{(-1)^n \beta^n}{n!} \prod_{i=0}^{n} \langle \alpha_i \,|H|\, \alpha_{i+1} \rangle$$

trace over standard basis

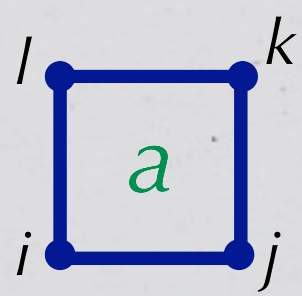


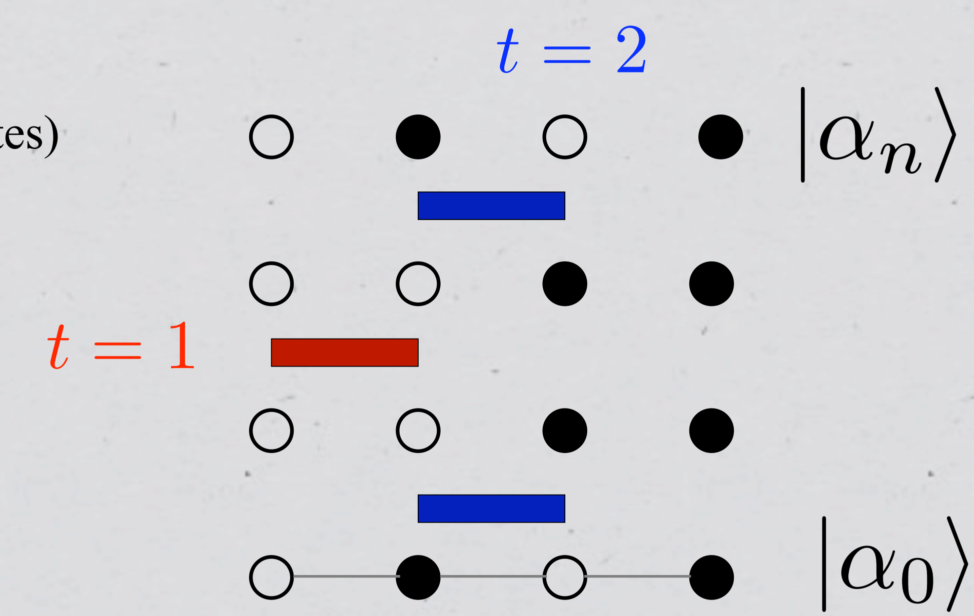
power series expansion

matrix elements = real numbers

decompose hamiltonian into basic "types" and "units" (bonds, plaquettes)

$$H = -\sum_{t} \sum_{a} H_{t,a}$$

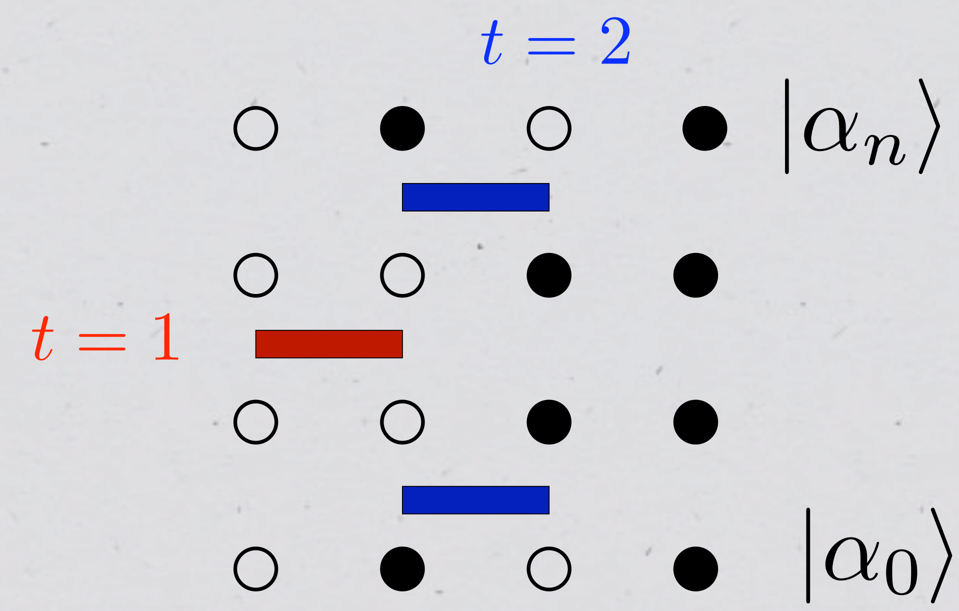




Stochastic Series Expansion QMC

$$Z = \sum_{\{\alpha_i\}} \sum_{n=0}^{\infty} \frac{(-1)^n \beta^n}{n!} \prod_{i=0}^{n} \langle \alpha_i | H | \alpha_{i+1} \rangle$$

$$H = -\sum_t \sum_a H_{t,a}$$



- construct weights from partition function

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \mathrm{Tr}\{\mathcal{O} \mathrm{e}^{-\beta H}\} \qquad \langle \mathcal{O} \rangle = \frac{\sum_{t=0}^{\infty} \mathcal{O}(x^t) W(x^t)}{\sum_{t=0}^{\infty} W(x^t)}$$

- Metropolis algorithm

$$r \leq \frac{W[x^{(t+1)}]}{W[x^t]}$$

$0 < r < 1$

need positive definite weights

Stochastic Series Expansion QMC

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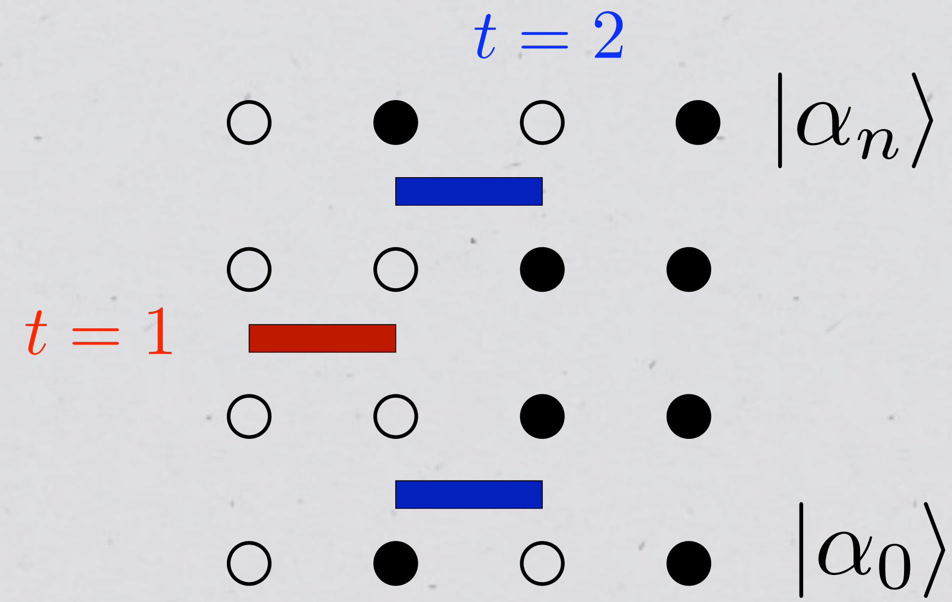


$$H = -\sum_t \sum_a H_{t,a}$$

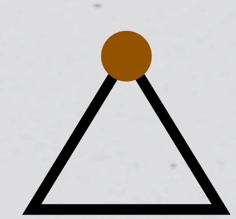
- weight of a given configuration

$$W_i \propto \langle \alpha_i | H_{t,a} | \alpha_{i+1} \rangle$$

- if $H_{t,a} < 0$

and an ODD number will satisfy the PBC of your simulation cell

(e.g. triangular lattice antiferromagnets)



a sign problem

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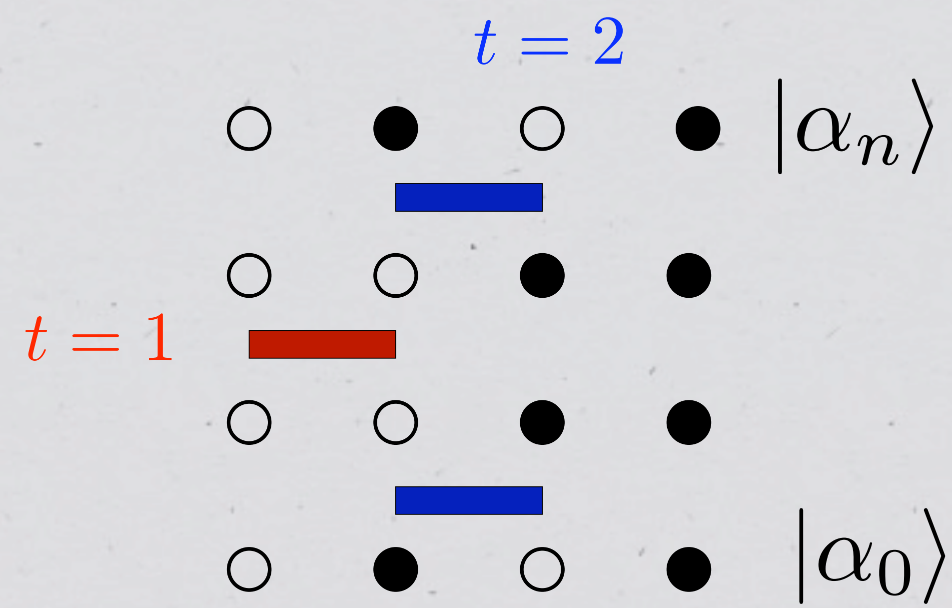

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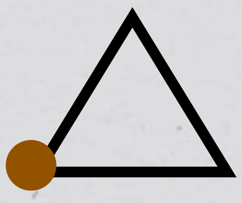

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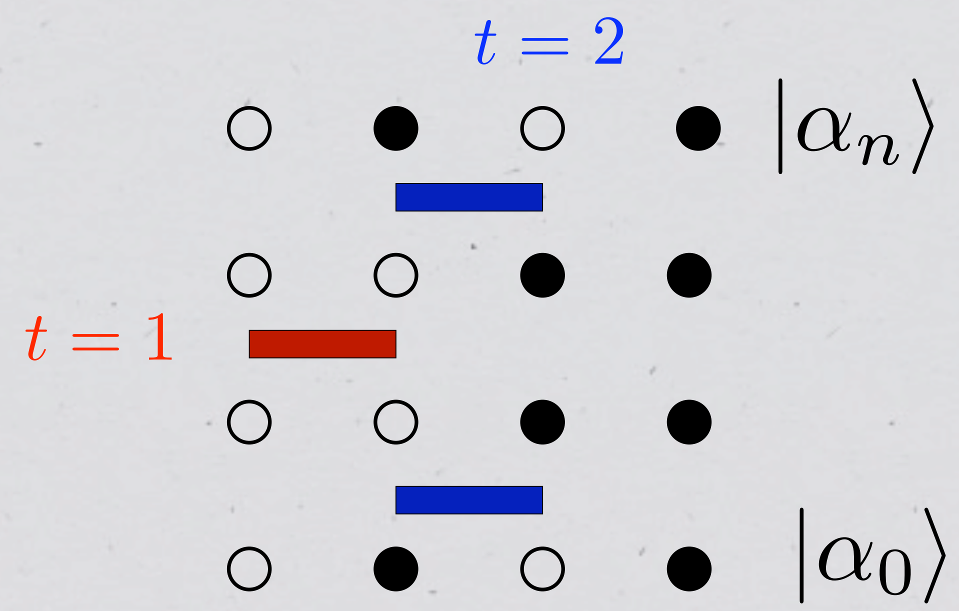

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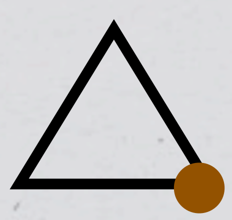
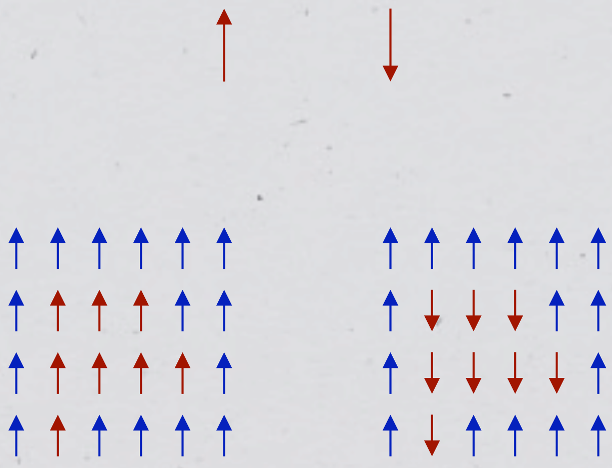


a sign problem

combat freezing (loss of ergodicity)

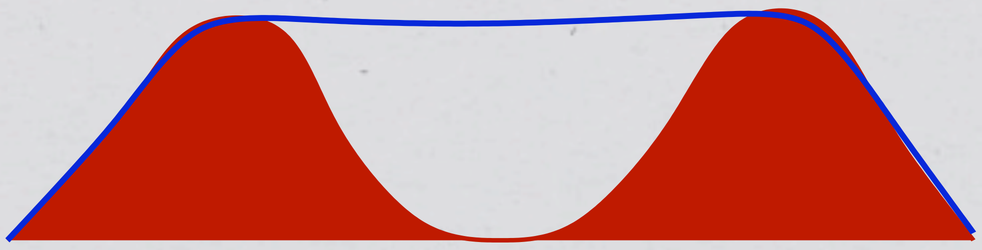
global updating procedures:

- operator (directed) loops
- multi-branch clusters



multilevel/optimized sampling

- annealing
- tempering (simulated or parallel)
- generalized ensembles



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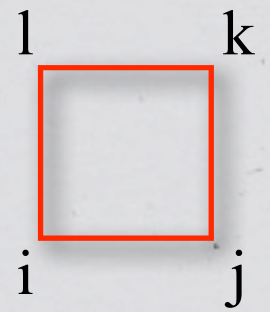
the J-K model

sandvik, daul, singh and scalapino, Phys. Rev. Lett. 89, 247201 (2002)



$$H = -J \sum_{\langle ij \rangle} B_{ij} - K \sum_{\langle ijkl \rangle} P_{ijkl}$$

spin 1/2 $\quad B_{ij} = S_i^+ S_j^- + S_i^- S_j^+ \quad P_{ijkl} = S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+$

hard-core bosons $\quad B_{ij} = b_i^\dagger b_j + b_i b_j^\dagger \quad P_{ijkl} = b_i^\dagger b_j b_k^\dagger b_l + b_i b_j^\dagger b_k b_l^\dagger$

six terms in the plaquette Hamiltonian decomposition

$$H = -\sum_t \sum_a H_{t,a}$$

$$\begin{aligned}
H_{1,a} &= C I_{ijkl}, \\
H_{2,a} &= (J/2) B_{ij} I_{kl}, \\
H_{3,a} &= (J/2) B_{jk} I_{il}, \\
H_{4,a} &= (J/2) B_{kl} I_{ij}, \\
H_{5,a} &= (J/2) B_{li} I_{jk}, \\
H_{6,a} &= K P_{ijkl},
\end{aligned}$$

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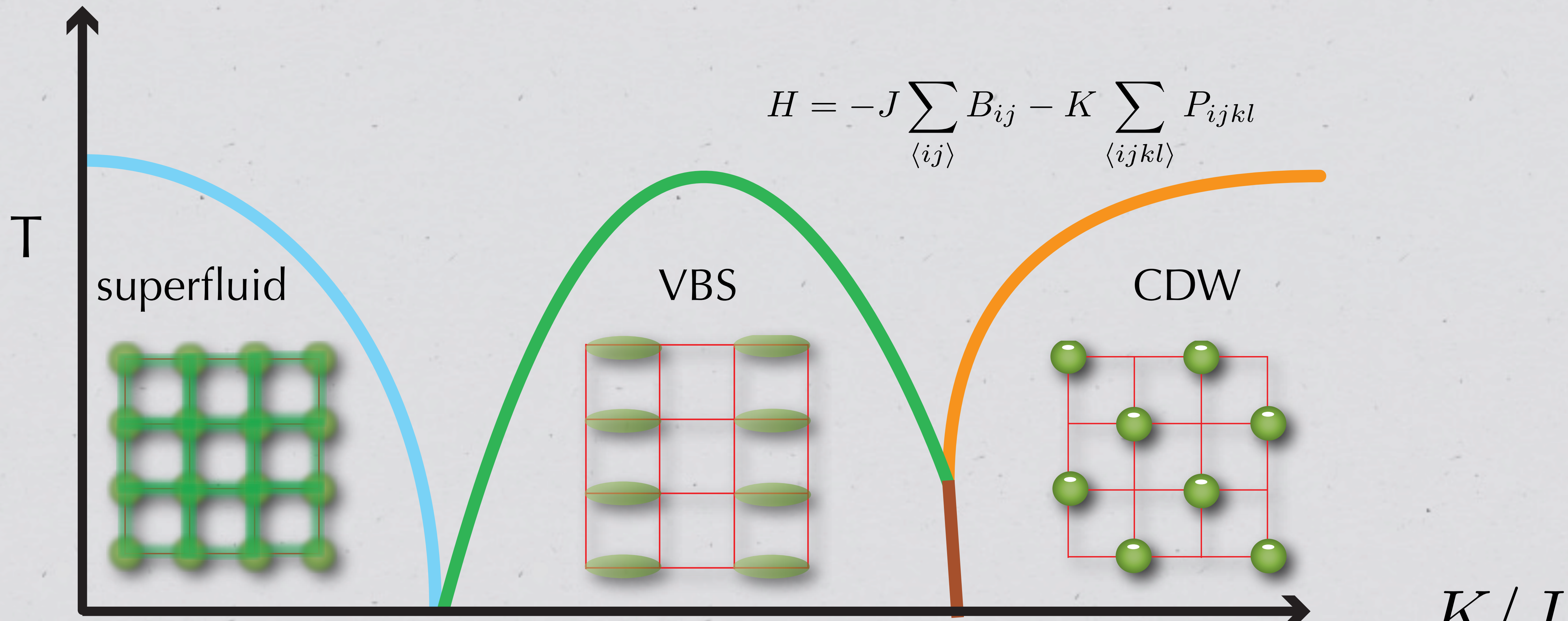


$$\rho_s = \frac{\partial^2 F}{\partial \phi^2} = \frac{\langle W^2 \rangle}{\beta}$$

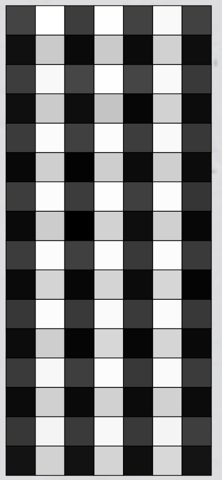
$$\langle m_P \rangle^2 = S_P(\pi, 0)/L^2$$

$$\langle m_S \rangle^2 = S_{S^z}(\pi, \pi)/L^2$$

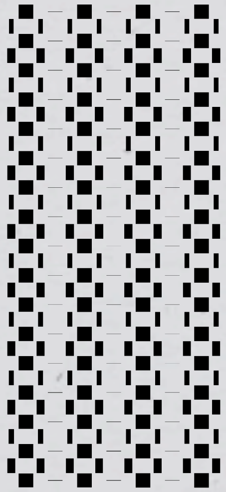
VBS: valence bond solid

$$S_p(q_x, q_y) = \frac{1}{N} \sum_{a,b} \mathrm{e}^{i(\mathbf{r}_a - \mathbf{r}_b)\cdot \mathbf{q}} \langle P_a P_b \rangle$$

$\langle H_K \rangle$



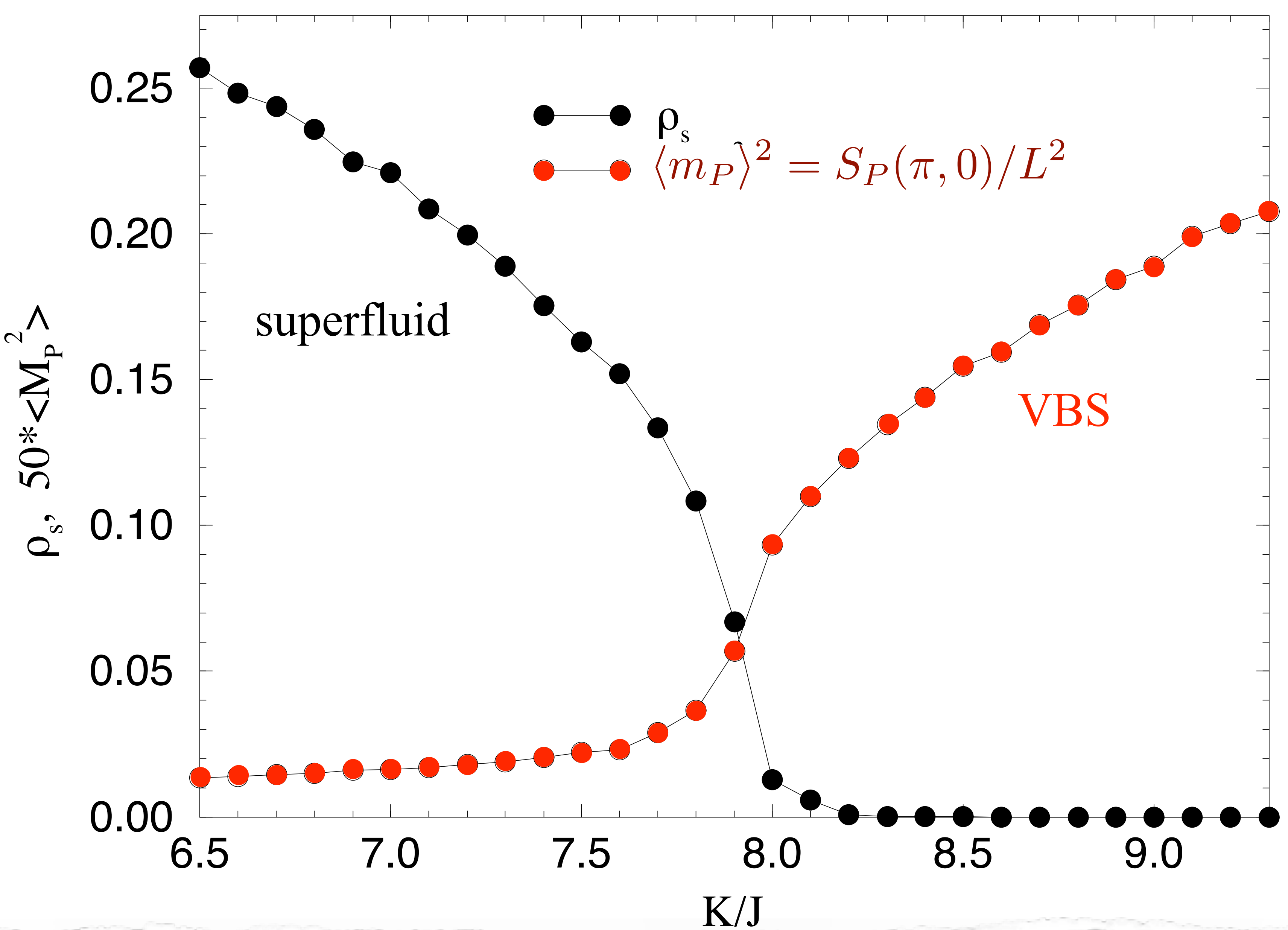
$\langle H_J \rangle$



superfluid-VBS quantum phase transition

$$H = -J\sum_{\langle ij\rangle} B_{ij} - K\sum_{\langle ijkl\rangle} P_{ijkl}$$

sandvik, daul, singh and scalapino, Phys. Rev. Lett. 89, 247201 (2002)



looks like a continuous (!) quantum phase transition

Does the J-K model have a deconfined quantum critical point?

senthil, vishwanath, balents, sachdev, fisher, science 303, 1490 (2004)

manifest as:

- continuous Néel (superfluid)-VBS quantum phase transition
- fractionalized excitations (spinons)
- emergent global U(1) symmetry

- dynamical scaling exponent $z = 1$
- anomalous dimension $\eta > 0.038$ ("large")

Scaling near the quantum phase transition

sandvik, RGM, cond-mat/0604451, Annals of Physics 321, 1651 (2006)

does the superfluid-VBS transition scale like a QCP?

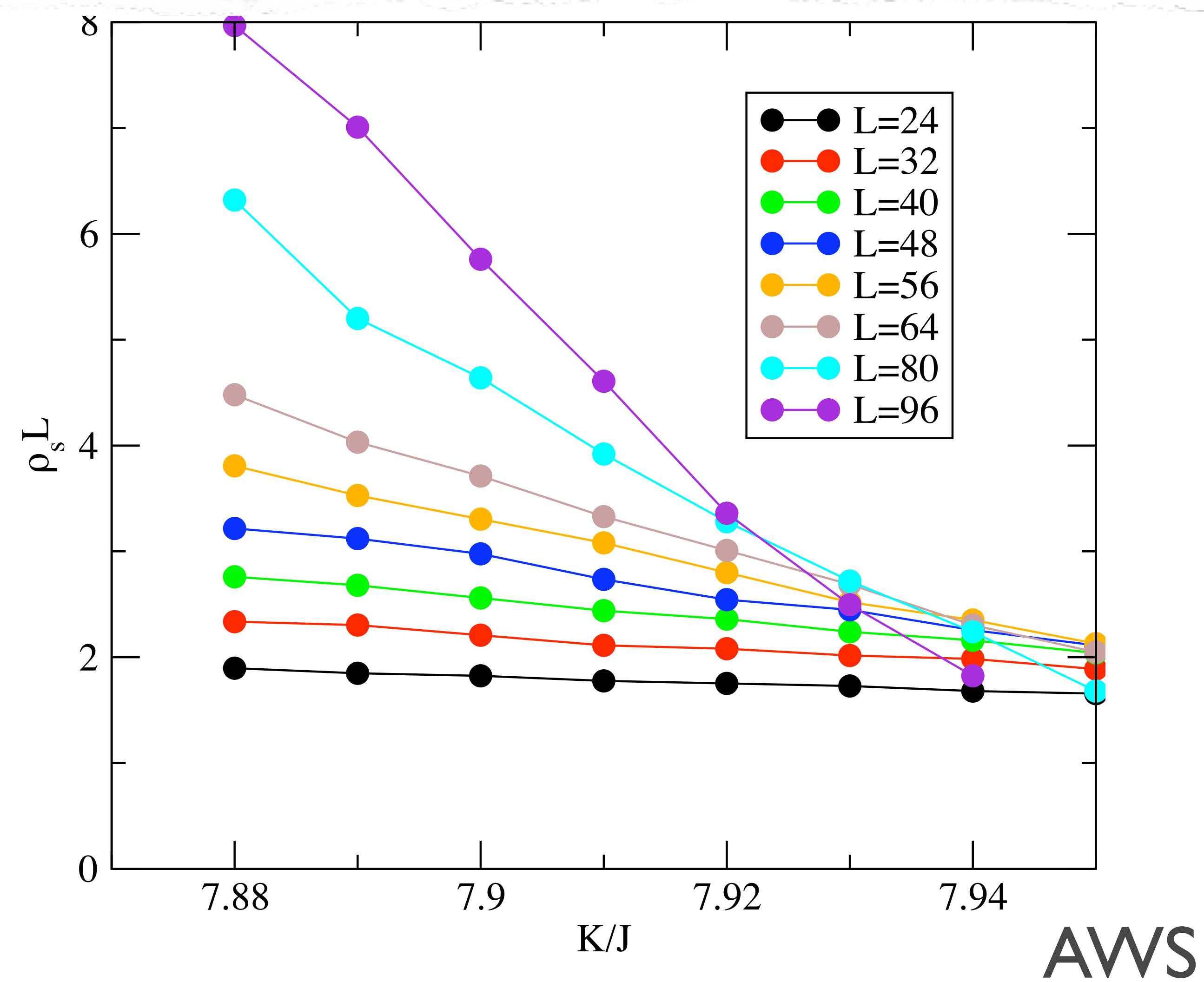
Spin stiffness/superfluid density:

dynamical scaling exponent z

DQCP: $z=1$

$$\xi \propto (g - g_c)^{-\nu}$$

$$\xi_\tau \propto (g - g_c)^{-\nu z}$$



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

Fisher *et al.*
PRB 40, 546 (1989)

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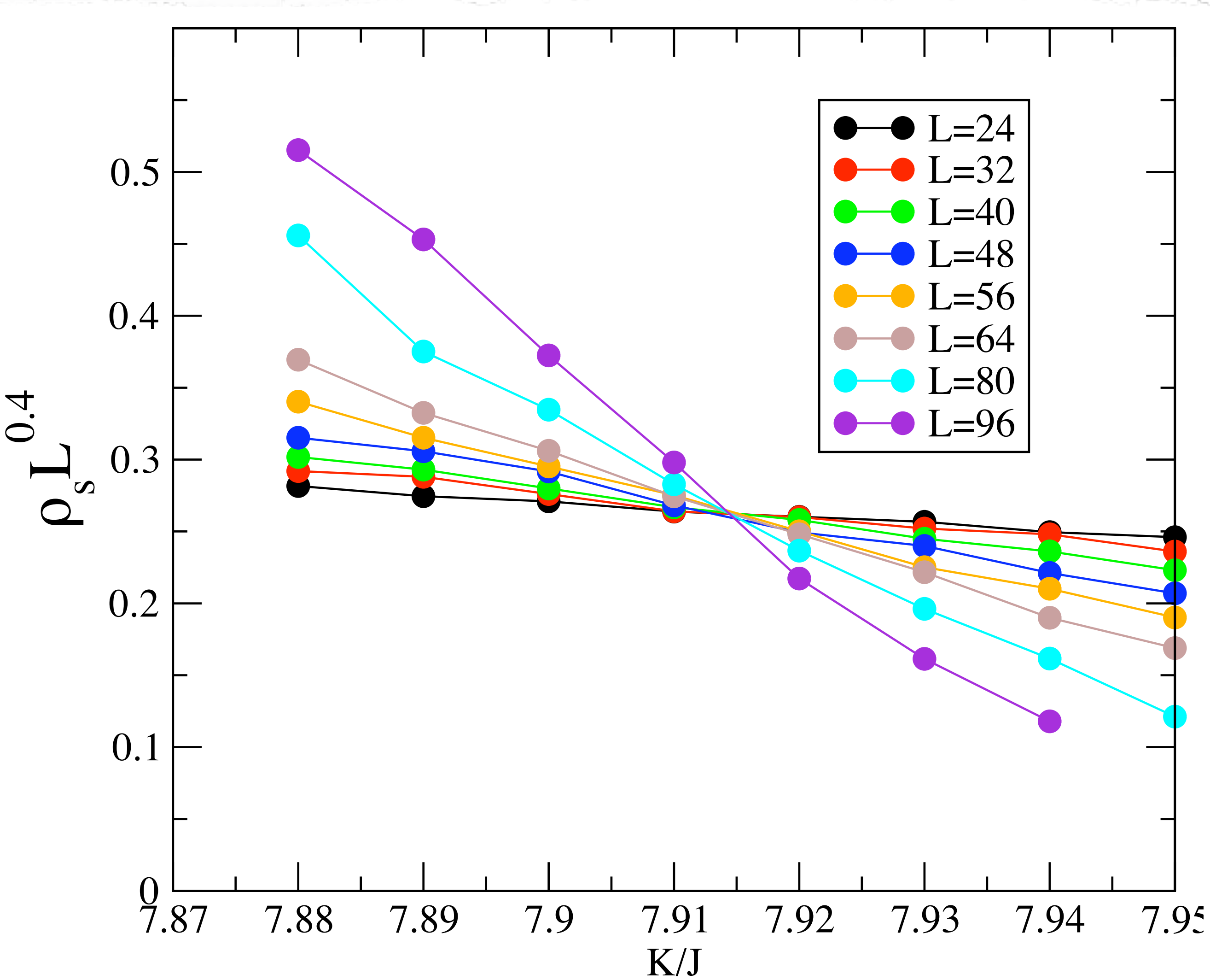


$$\rho_s \sim L^{-z}$$

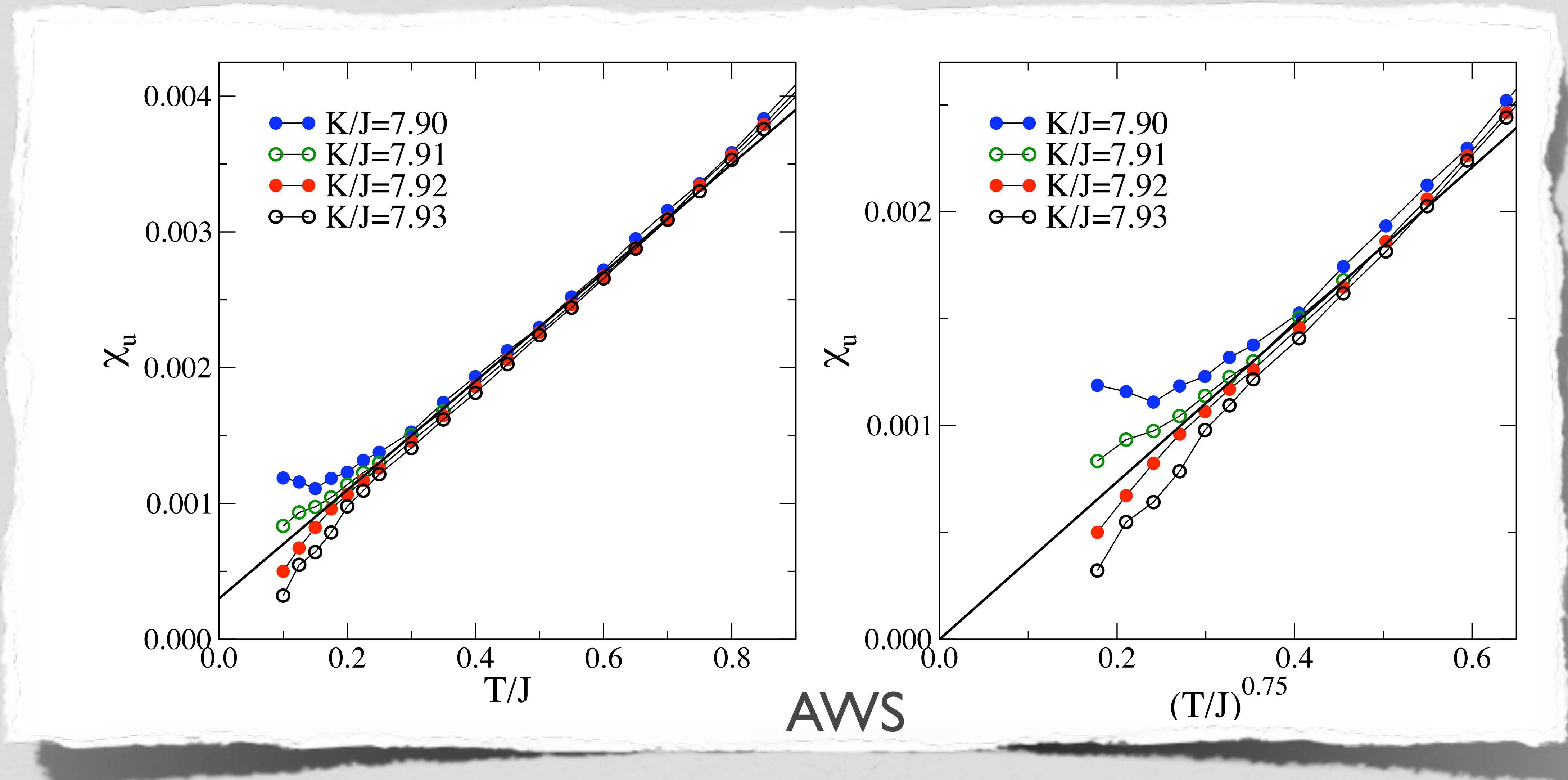
$$z = 0.4?$$

$$7.91 < (K/J)_c < 7.92$$

Uniform spin susceptibility: $\chi_u = \frac{\langle (\sum_i S_i^z)^2 \rangle}{TN}$

$\chi_u \propto T^{d/z-1}$ Chubukov *et al.* PRB 49, 11919 (1994)

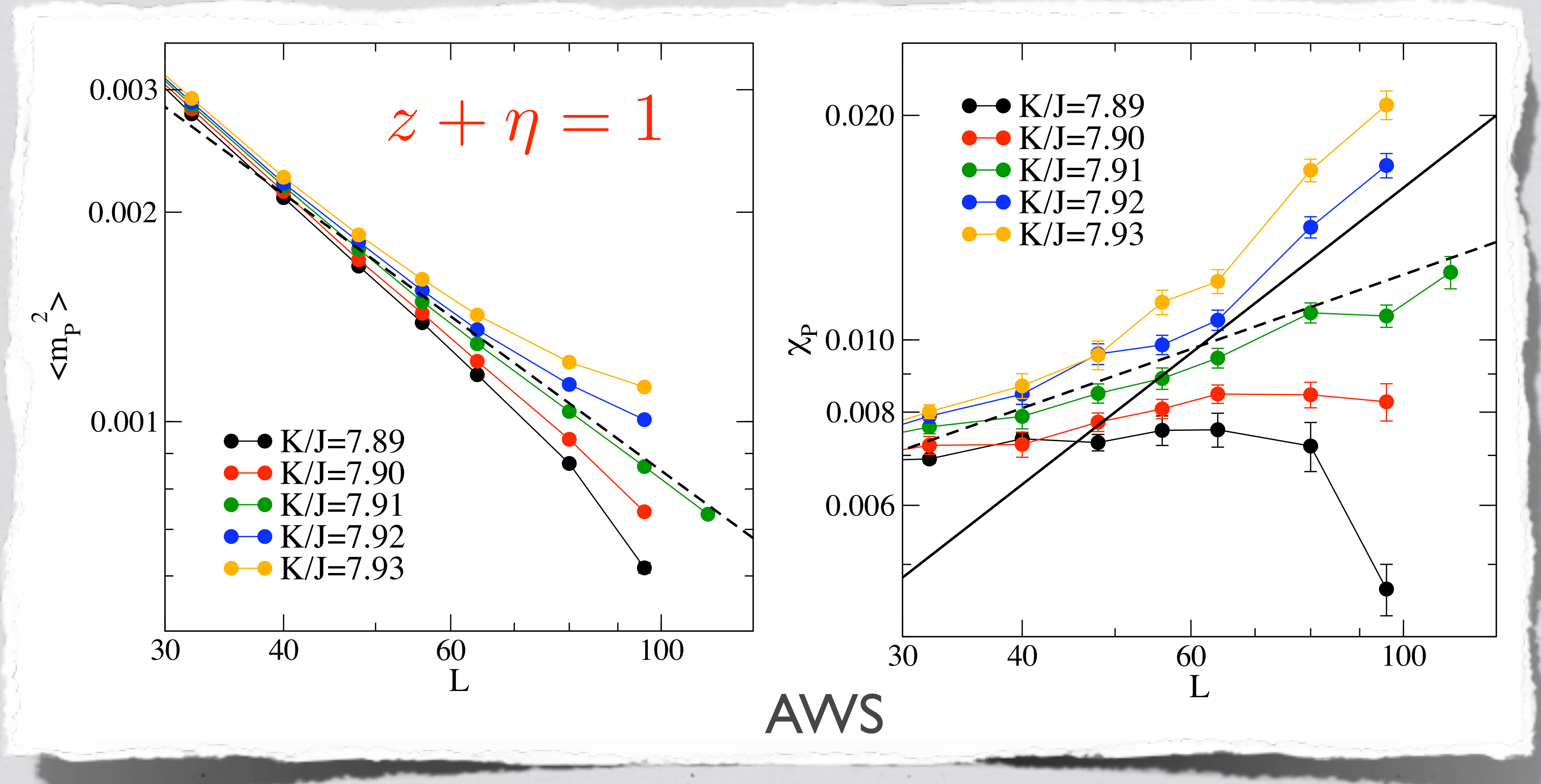
$L = 256$



$7.91 < (K/J)_c < 7.92$

VBS (plaquette) order parameter and susceptibility

$$\langle m_P^2 \rangle \sim L^{-(z+\eta)} \qquad \langle \chi_P \rangle \sim L^{-\eta}$$



$\eta = -1$

$\eta = -0.5$

discussion: J-K model scaling

* spin stiffness scaling $z<1$: evidence for development of a discontinuity ?
* anomalous dimension may be negative - seen in other "candidate" DQCPs in boson models (kagome lattice XXZ)

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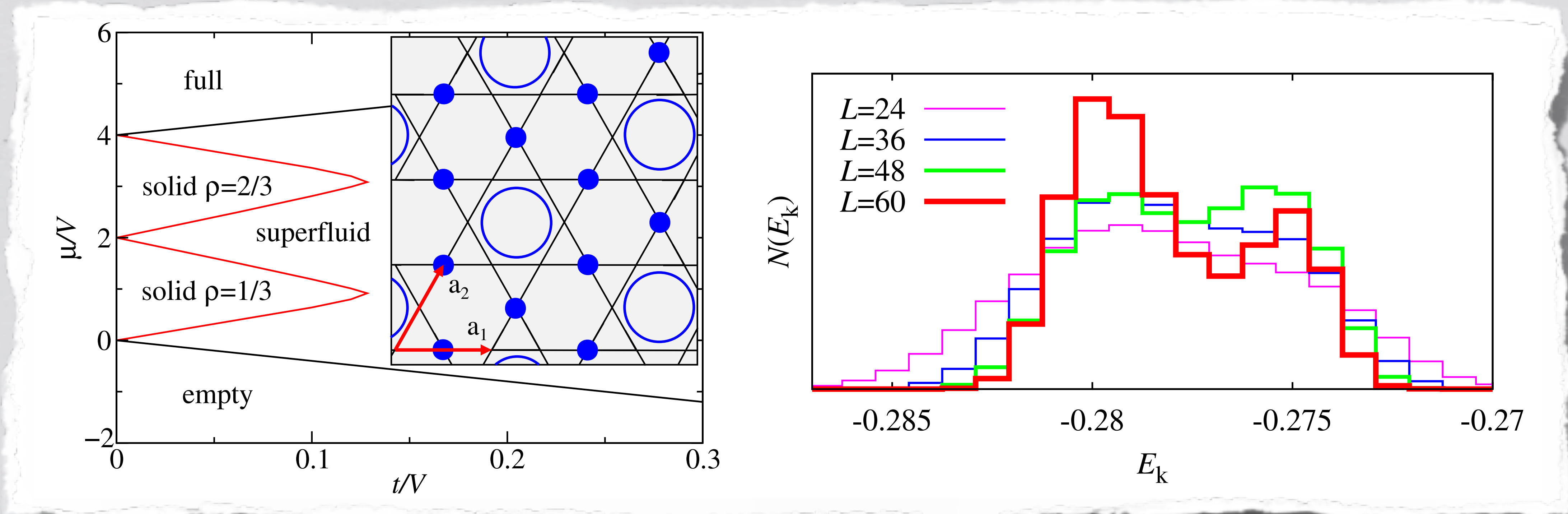

Isakov et al. Phys. Rev. Lett. 97, 147202 (2006)

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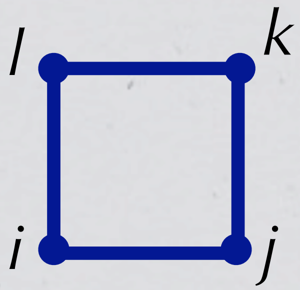
Sandvik's J-Q model

Sandvik, Phys. Rev. Lett. 98. 227202 (2007)

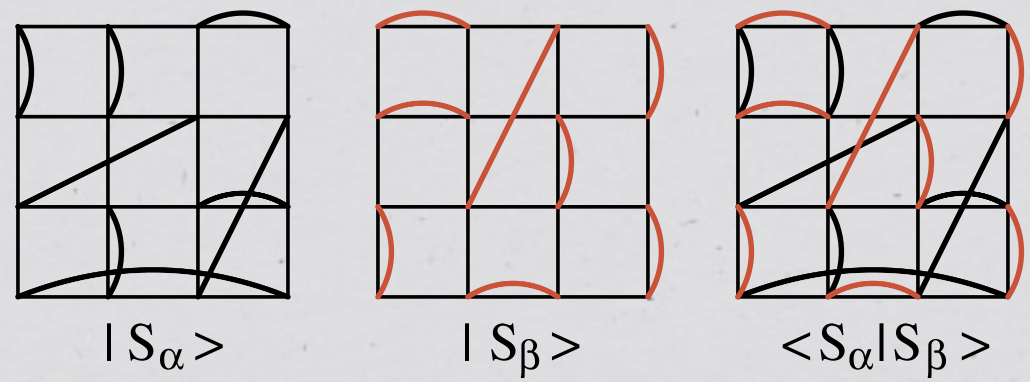


$$H = J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j - Q\sum_{\langle ijkl\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4})(\mathbf{S}_k\cdot\mathbf{S}_l-\tfrac{1}{4})$$

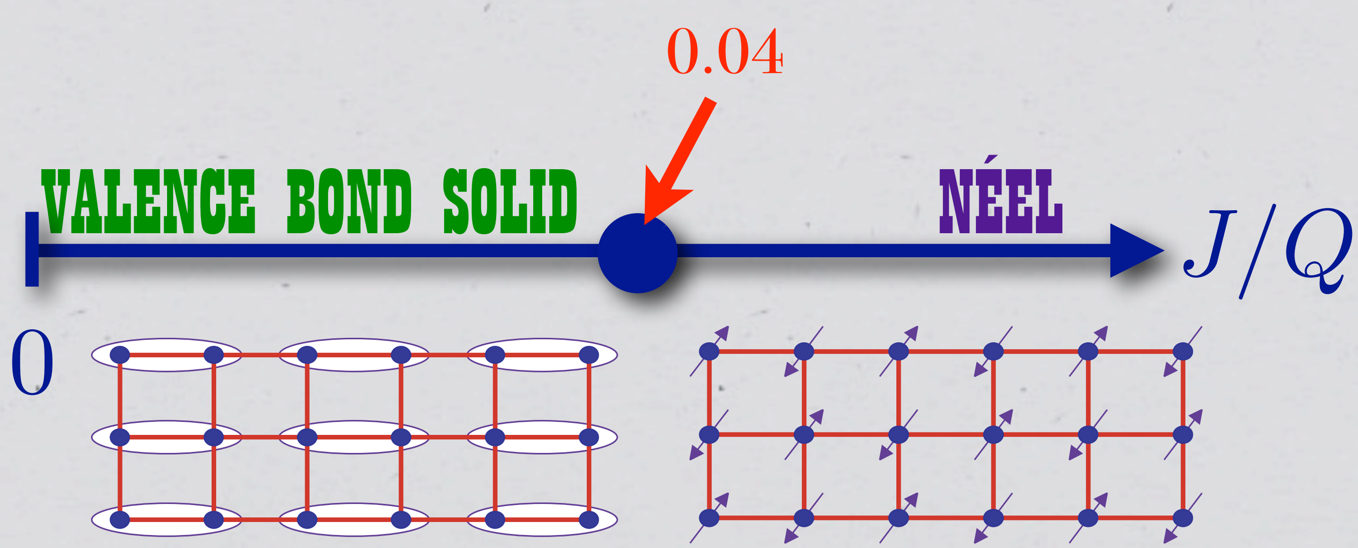
Valence Bond Basis

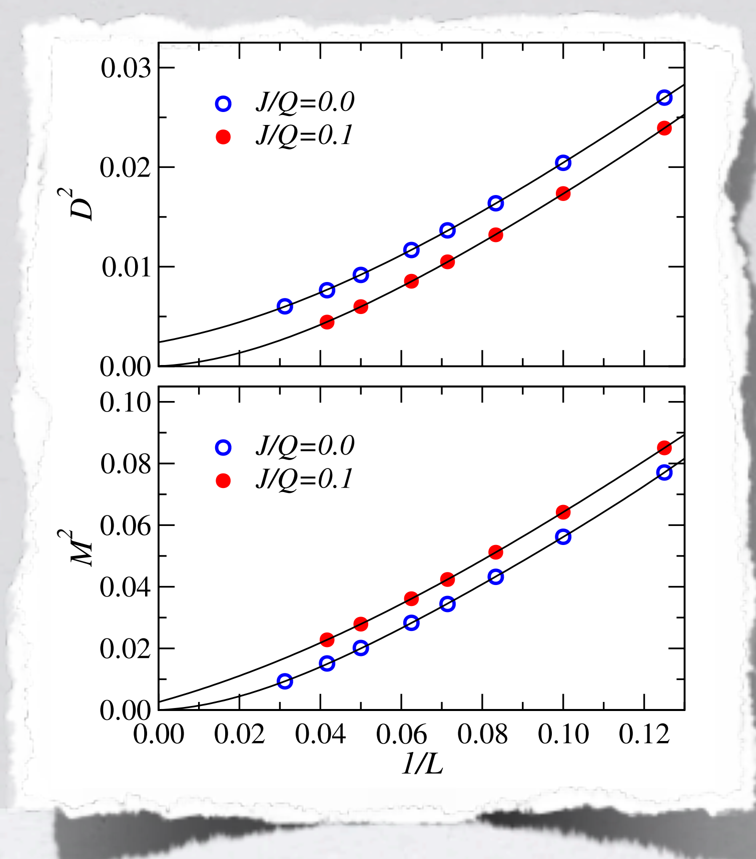
Sandvik

Phys. Rev. Lett. **95**, 207203 (2005)



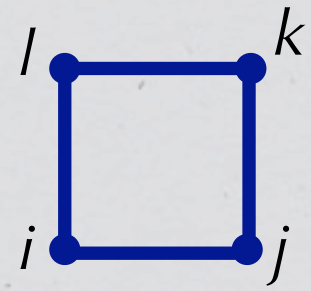
T=0 projector QMC up to L=32





Sandvik's J-Q model

RGM and Kaul, Phys. Rev. Lett. (2007)



$$H = J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j - Q\sum_{\langle ijkl\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j - \tfrac{1}{4})(\mathbf{S}_k\cdot\mathbf{S}_l - \tfrac{1}{4})$$

What about S^z basis suitable for finite-T QMC?

$$H = -\sum_t\sum_a H_{t,a}$$

$$H_{1,a} = -J(S_i^z S_j^z I_{k,l})$$

$$H_{2,a} = -J/2(S_i^+ S_j^- I_{k,l})$$

negative

$$H_{3,a} = Q(S_i^z S_j^z - 1/4)(S_k^z S_l^z - 1/4)$$

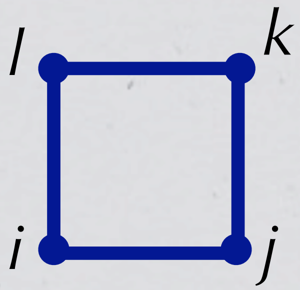
$$H_{4,a} = Q/2(S_i^z S_j^z - 1/4)(S_k^+ S_l^- + S_k^- S_l^+)$$

negative

$$H_{5,a} = Q/4(S_i^+ S_j^- + S_i^- S_j^+)(S_k^+ S_l^- + S_k^- S_l^+)$$

Sandvik's J-Q model

RGM and Kaul, Phys. Rev. Lett. (2007)



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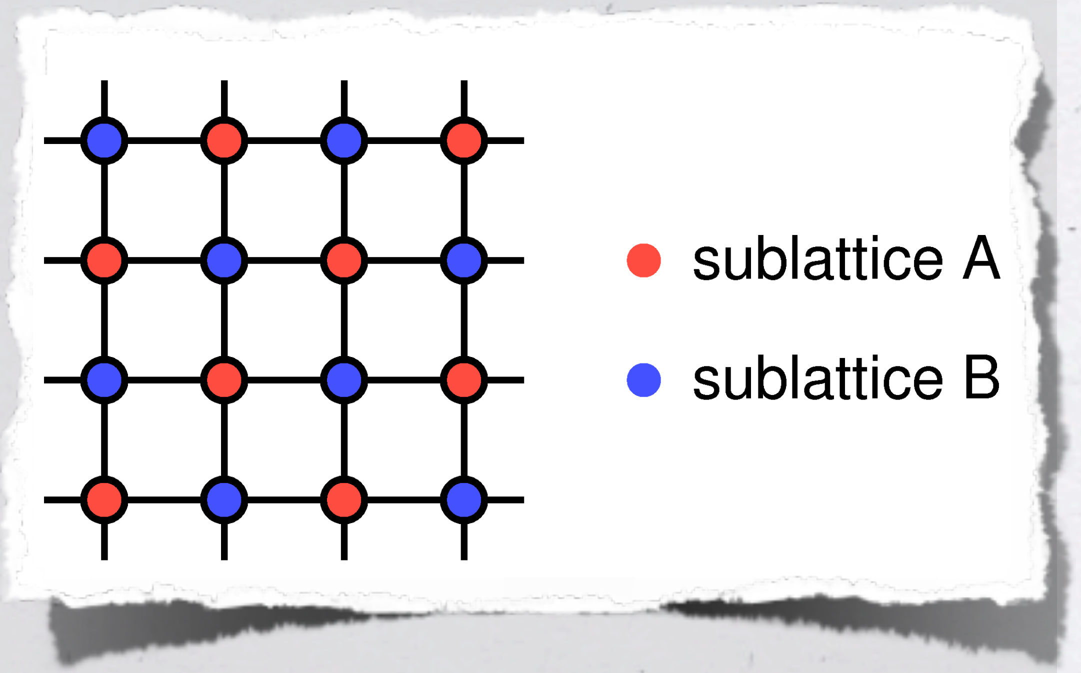

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$$H_{2,a} \to J/2(S_i^+ S_j^- I_{k,l})$$

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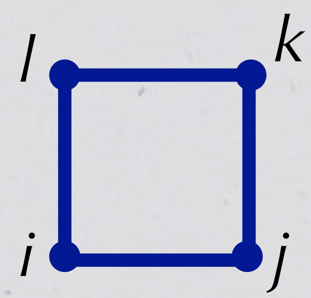
$$H_{4,a} \to -Q/2(S_i^z S_j^z - 1/4)(S_k^+ S_l^- + S_k^- S_l^+)$$

$$H_{5,a} = Q/4(S_i^+ S_j^- + S_i^- S_j^+)(S_k^+ S_l^- + S_k^- S_l^+)$$

Sandvik's J-Q model

RGM and Kaul, Phys. Rev. Lett. (2007)



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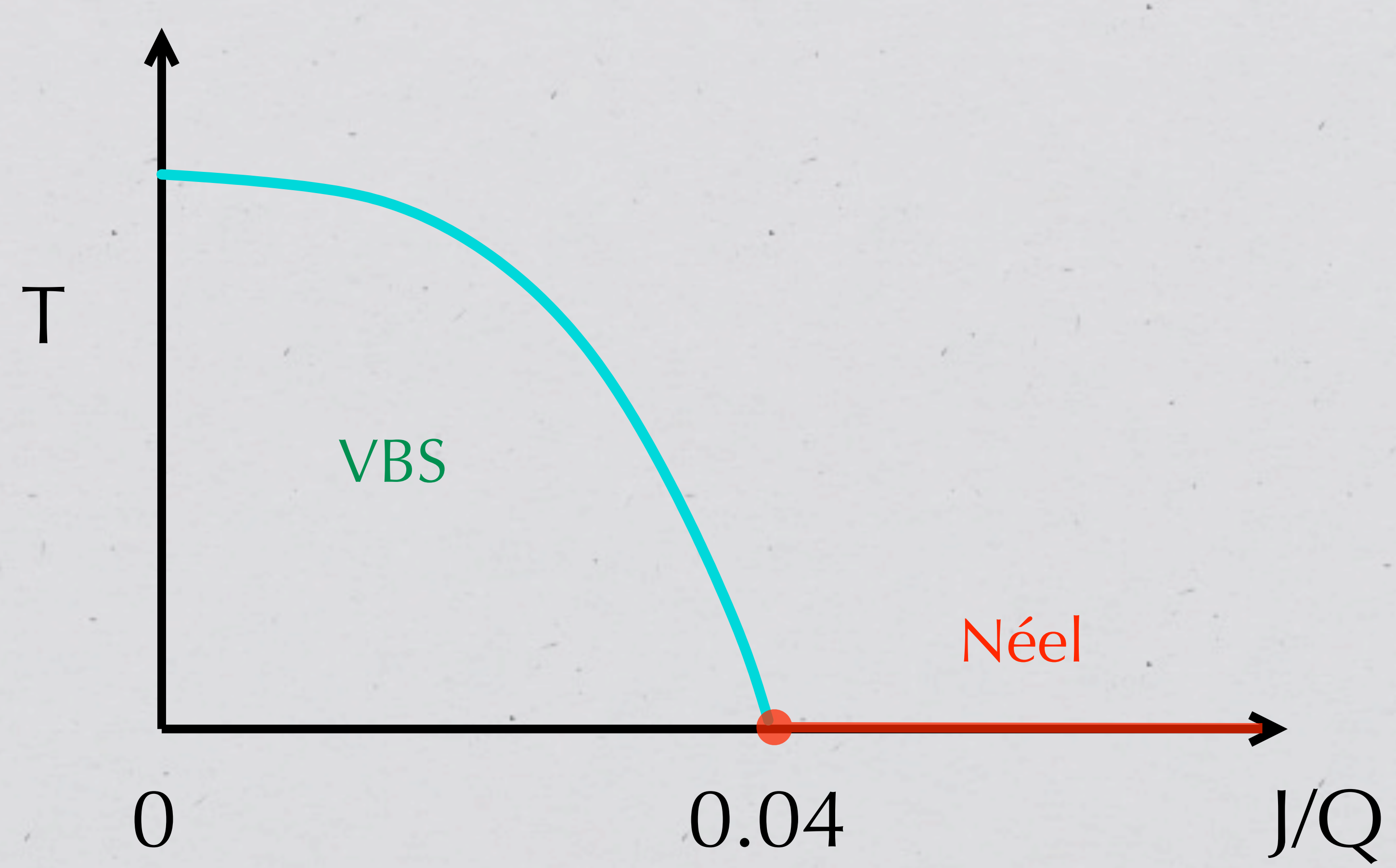


correlation functions:

Neel $C^z_{\rm N}(\mathbf{r},\tau) = \langle S^z(\mathbf{r},\tau) S^z(0,0)\rangle$

VBS $C^z_{\rm V}(\mathbf{r},\tau) = \langle [S^z(\mathbf{r},\tau) S^z(\mathbf{r}+\hat{\mathbf{x}},\tau)][S^z(0,0)S^z(\hat{\mathbf{x}},0)]\rangle$

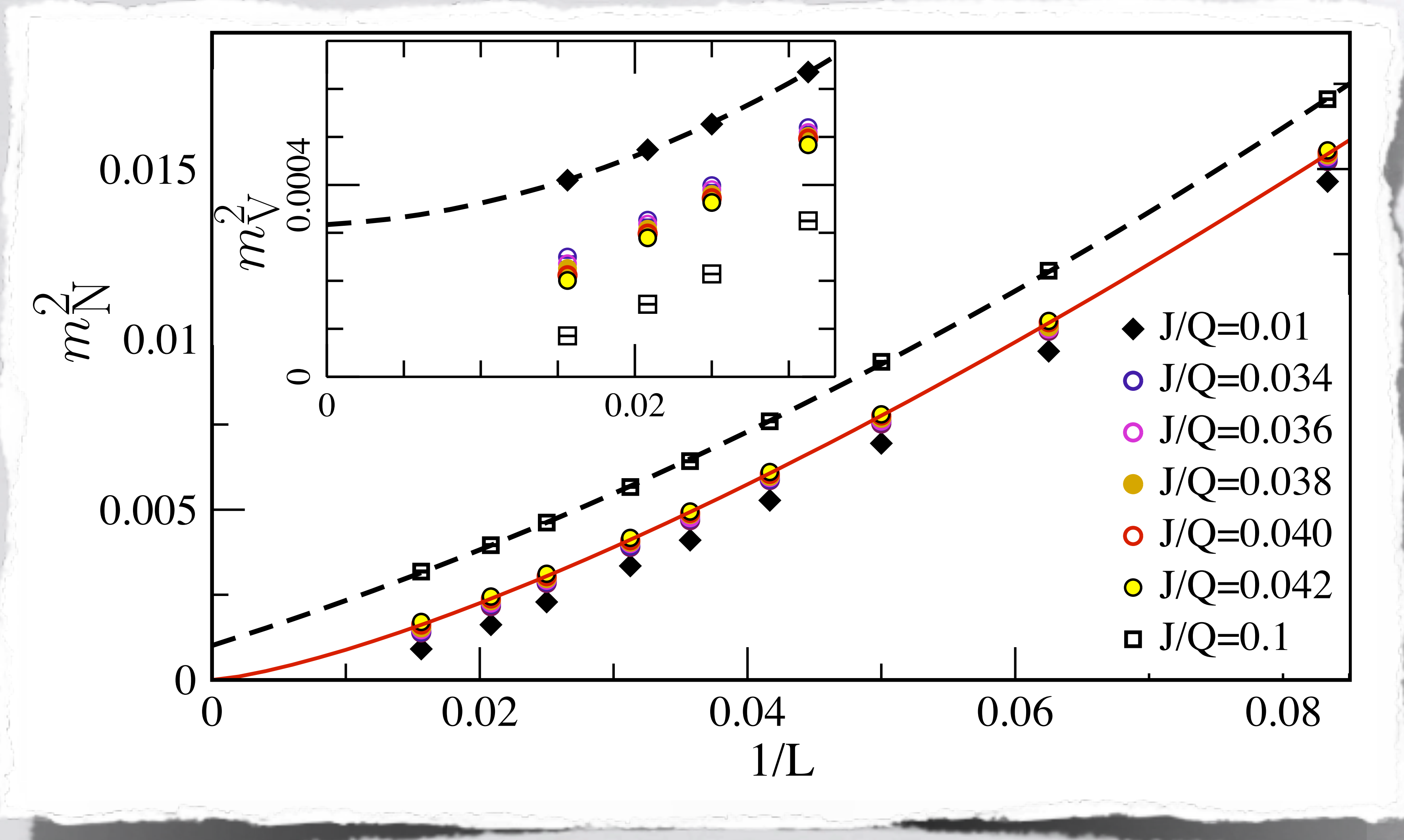
$$S_{\rm N,V}[\mathbf{q}] = \sum_{\mathbf{r}} [\exp(-i\mathbf{q}\cdot\mathbf{r}) C^z_{\rm N,V}(\mathbf{r},\tau=\mathbf{0})]/N_{\rm spin}$$

order parameter

$$m^2_{\rm N,V} = \frac{S_{\rm N,V}[\mathbf{q}_{\rm N,V}]}{N_{\rm spin}}$$

$$\mathbf{q}_{\rm N} = (\pi,\pi)$$

$$\mathbf{q}_{\rm V} = (\pi,0)$$

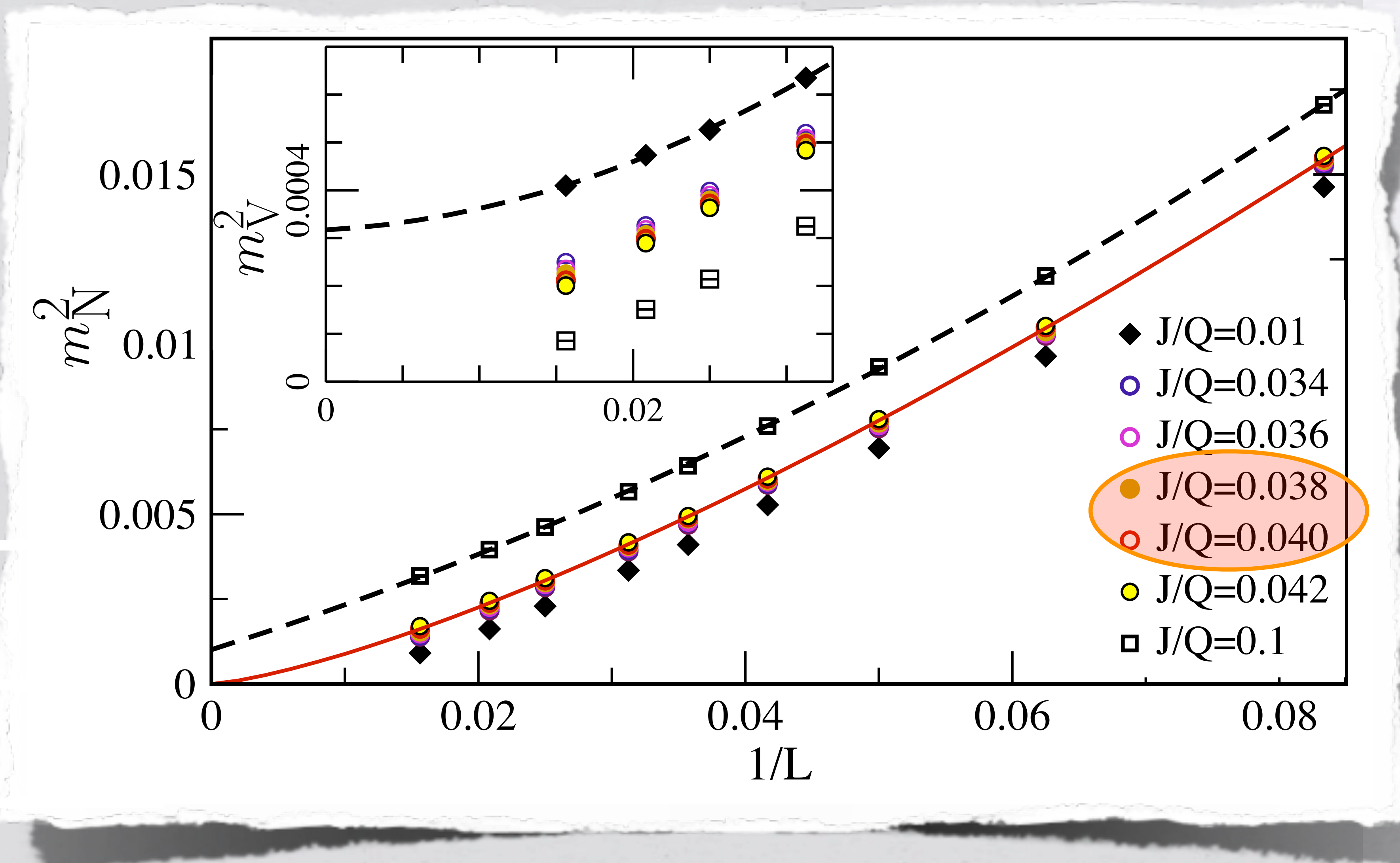


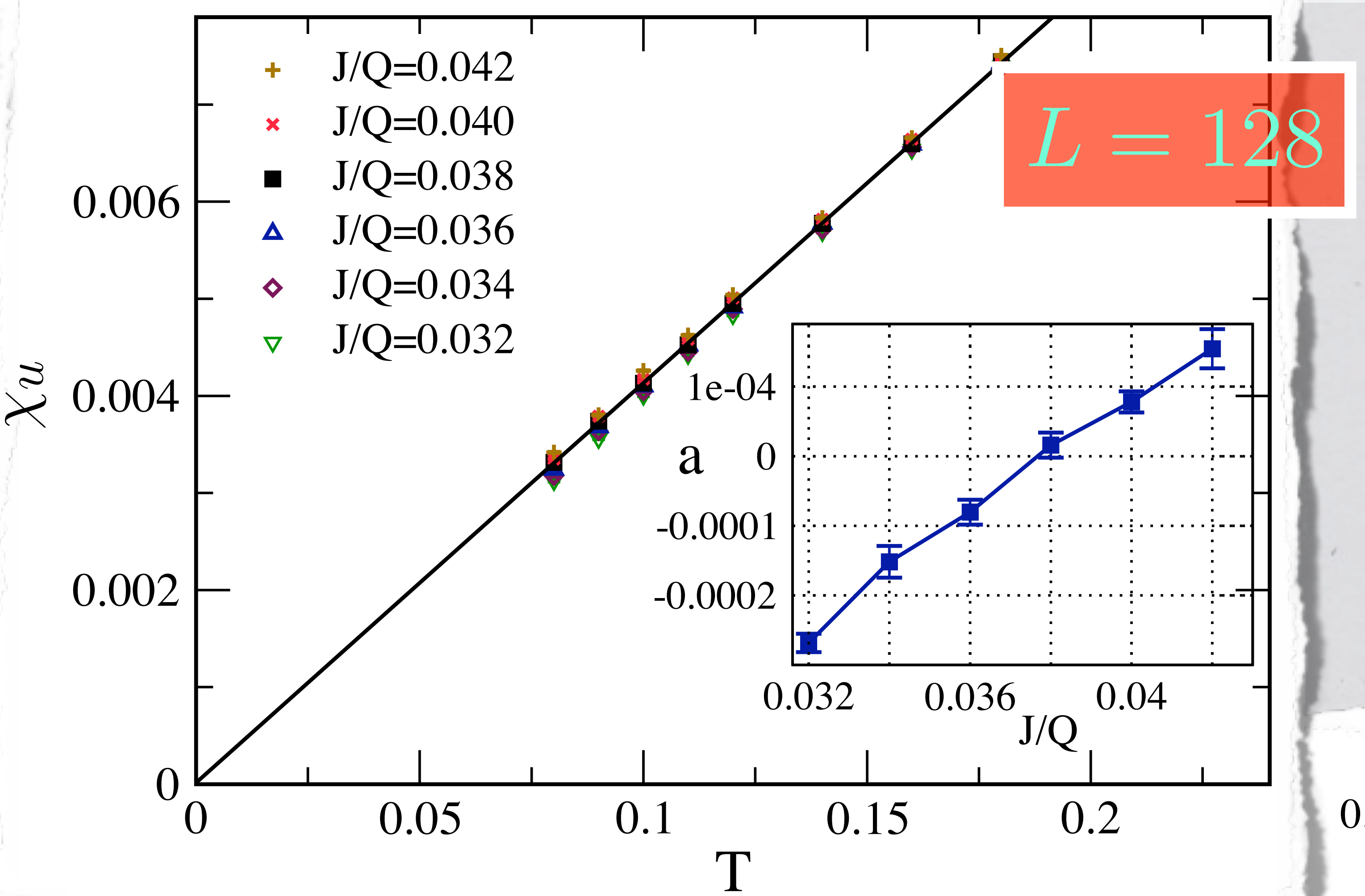
finite size scaling:

$$m_{\mathrm{N}}^2 \sim L^{-(d+z-2+\eta)}$$

$$y = c_1 x^{c_2} \qquad c_2 = z + \eta_{\mathrm{N}}$$

J/Q	c_2
0.038	1.37(1)
0.040	1.35(1)



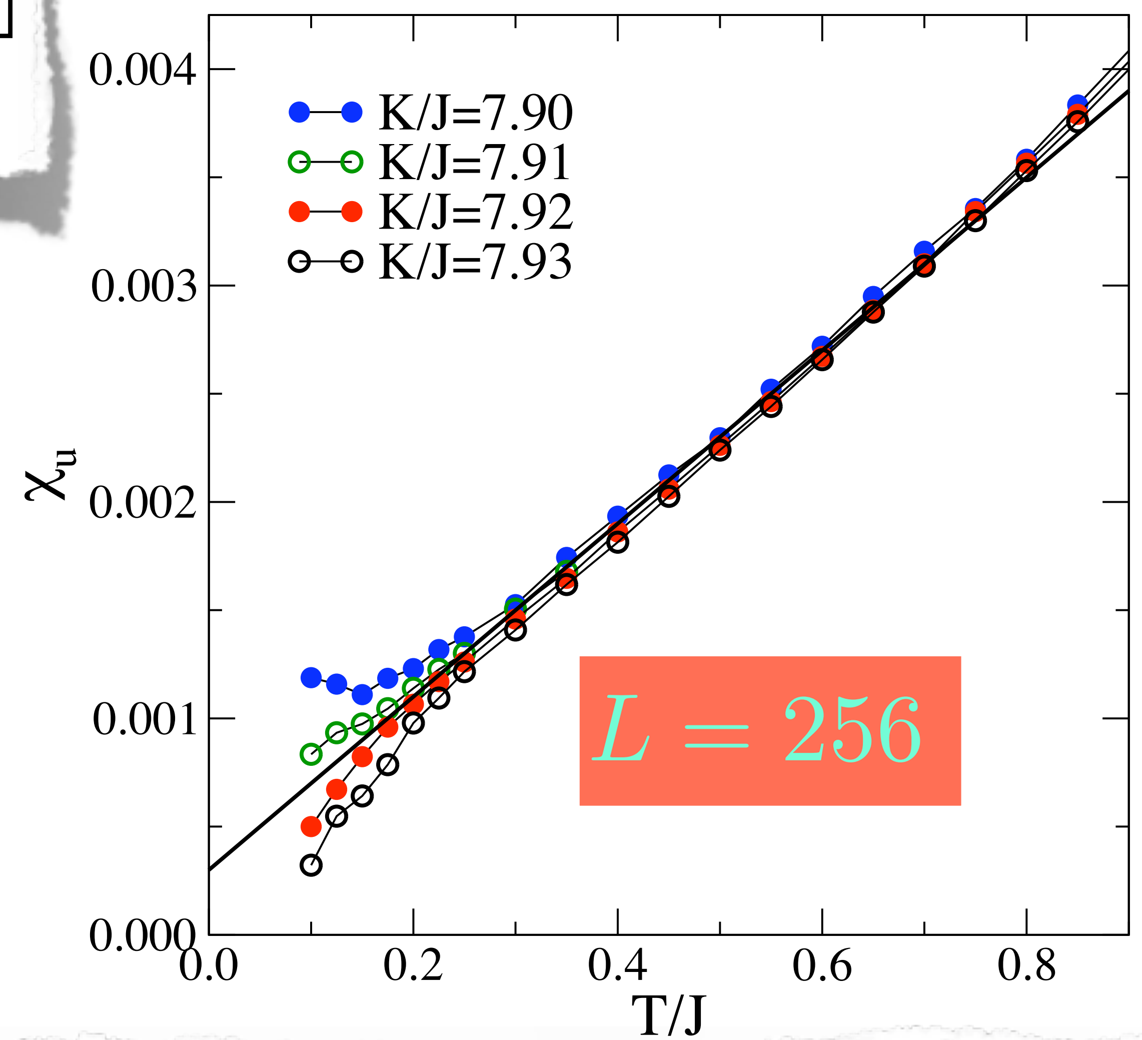


uniform susceptibility

J-Q model

$$\chi_u \propto T^{d/z-1}$$

J-K model

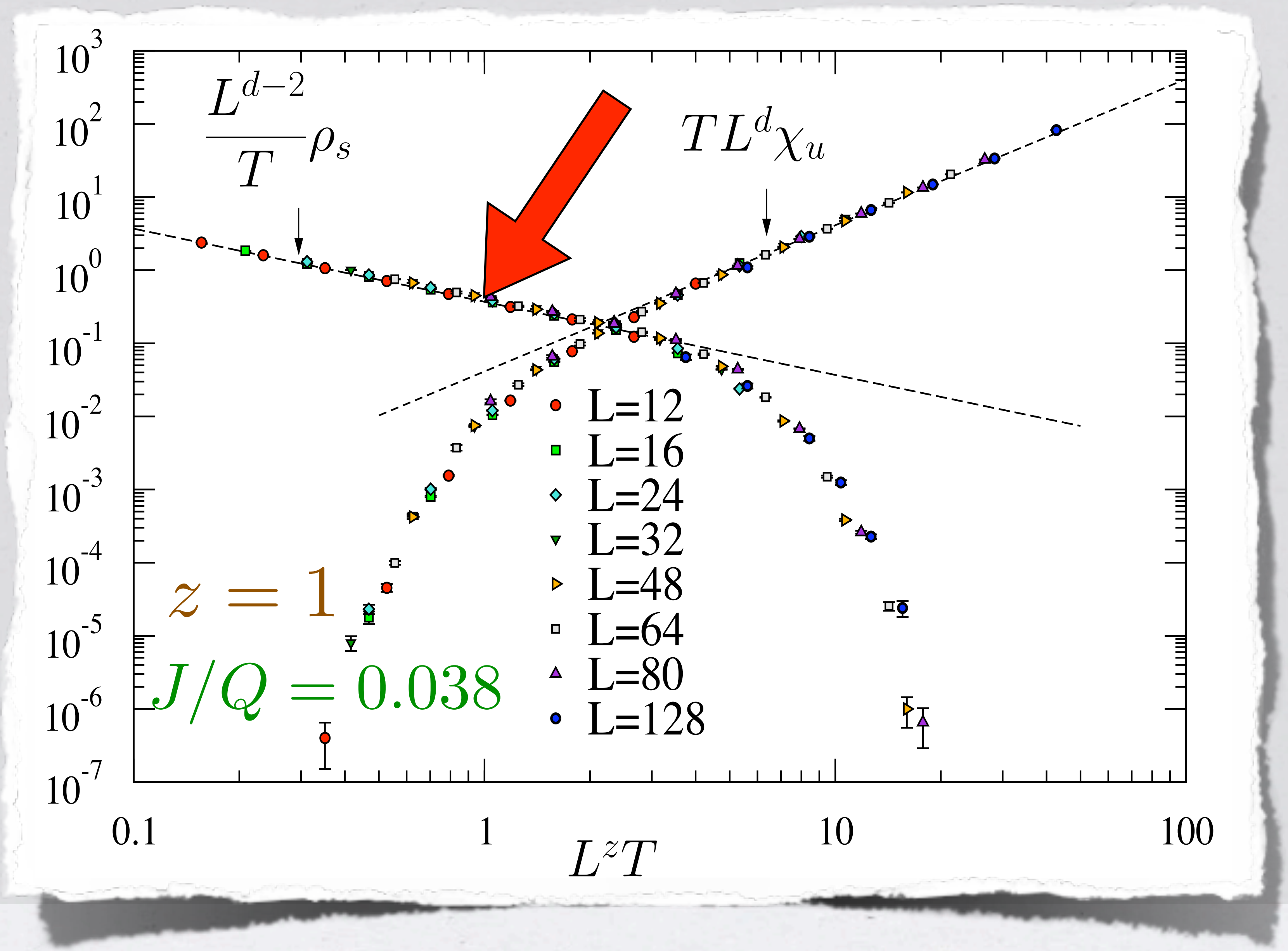


stiffness scaling: J-Q model

$$\chi_u(T, L, J) = \frac{1}{TL^d}\mathbb{Z}\left(\frac{L^z T}{c}, gL^{1/\nu}\right)$$

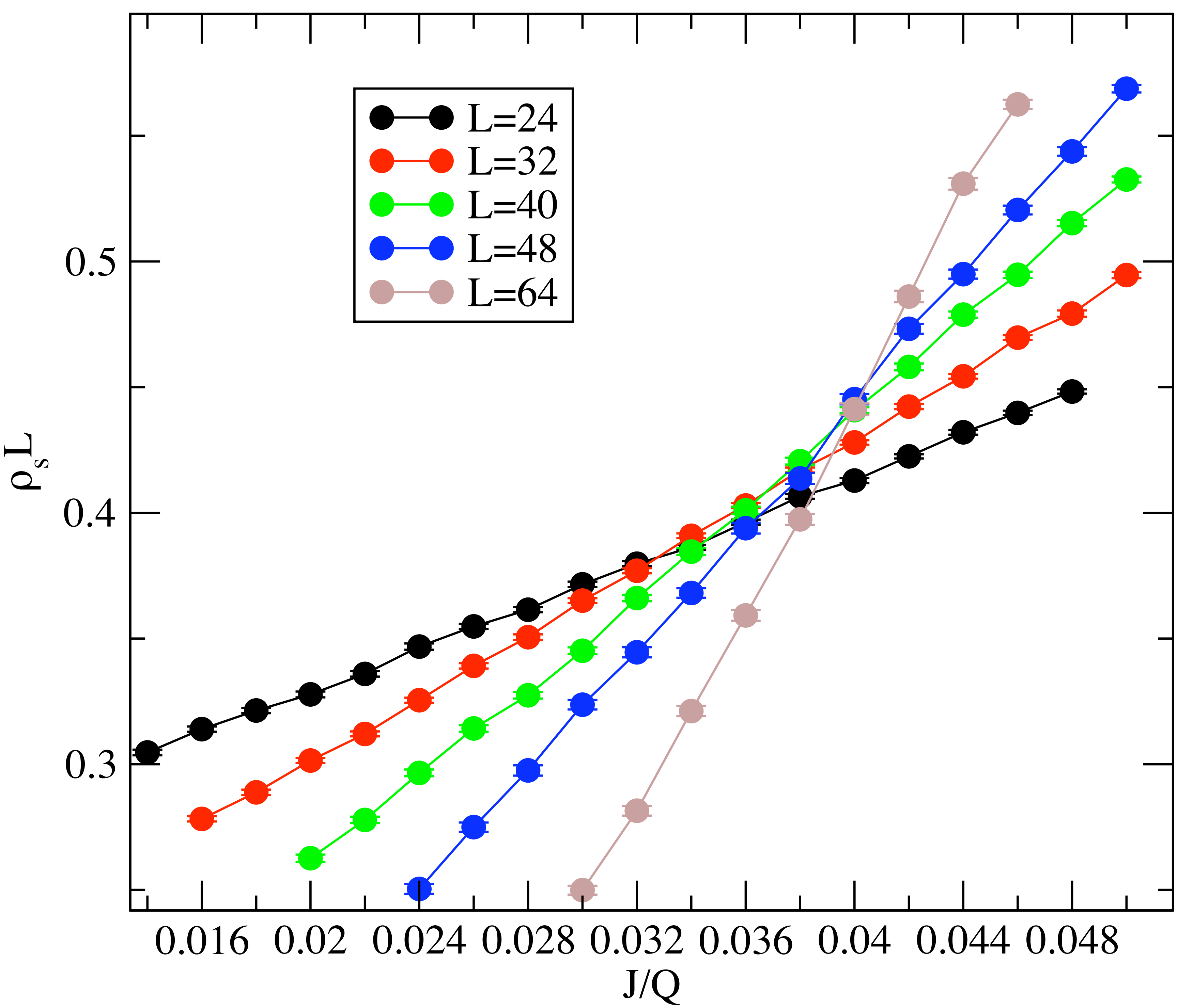
$$\rho_s(T, L, J) = \frac{T}{L^{d-2}}\mathbb{Y}\left(\frac{L^z T}{c}, gL^{1/\nu}\right)$$

$$g \propto (J - J_c)/J_c$$



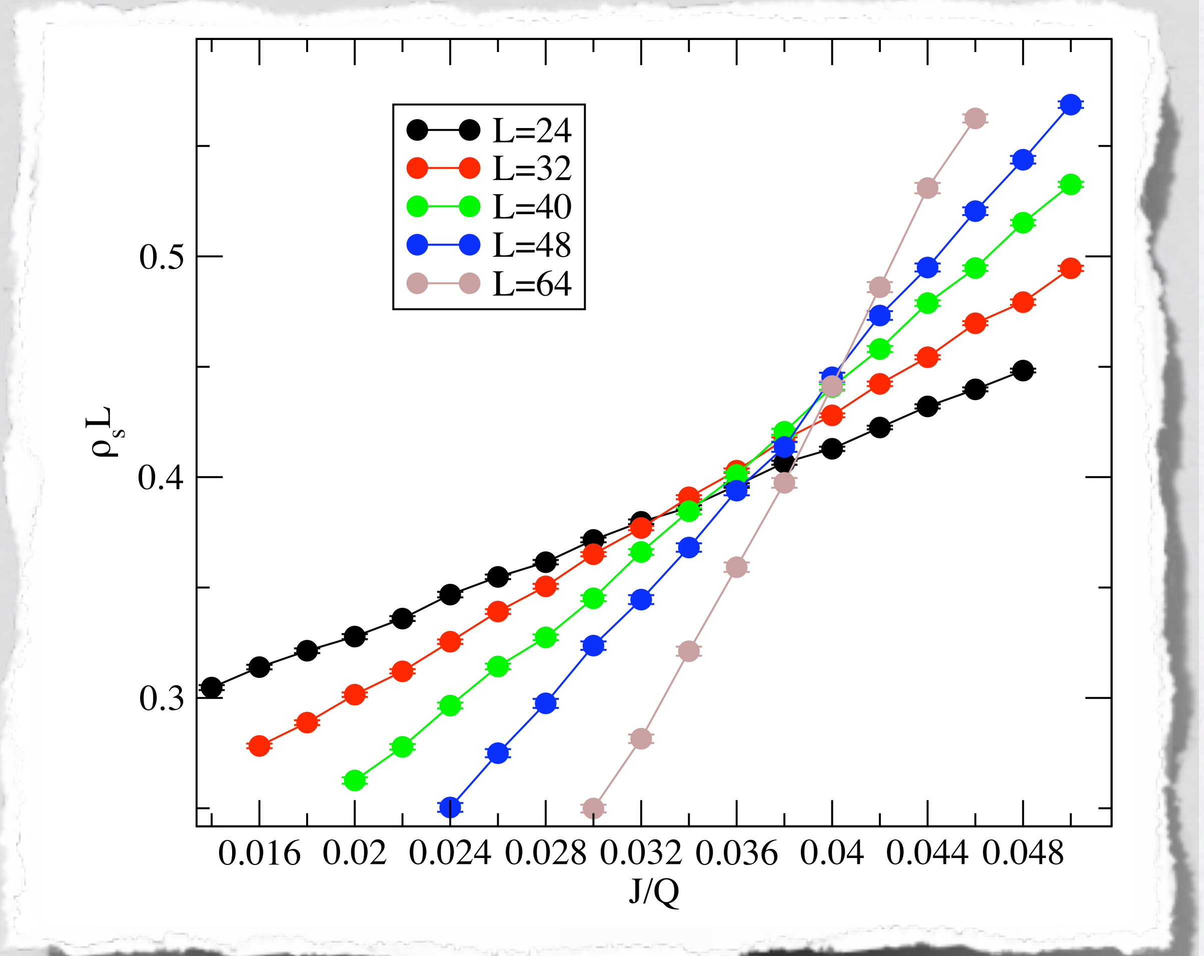
stiffness scaling: J-Q model

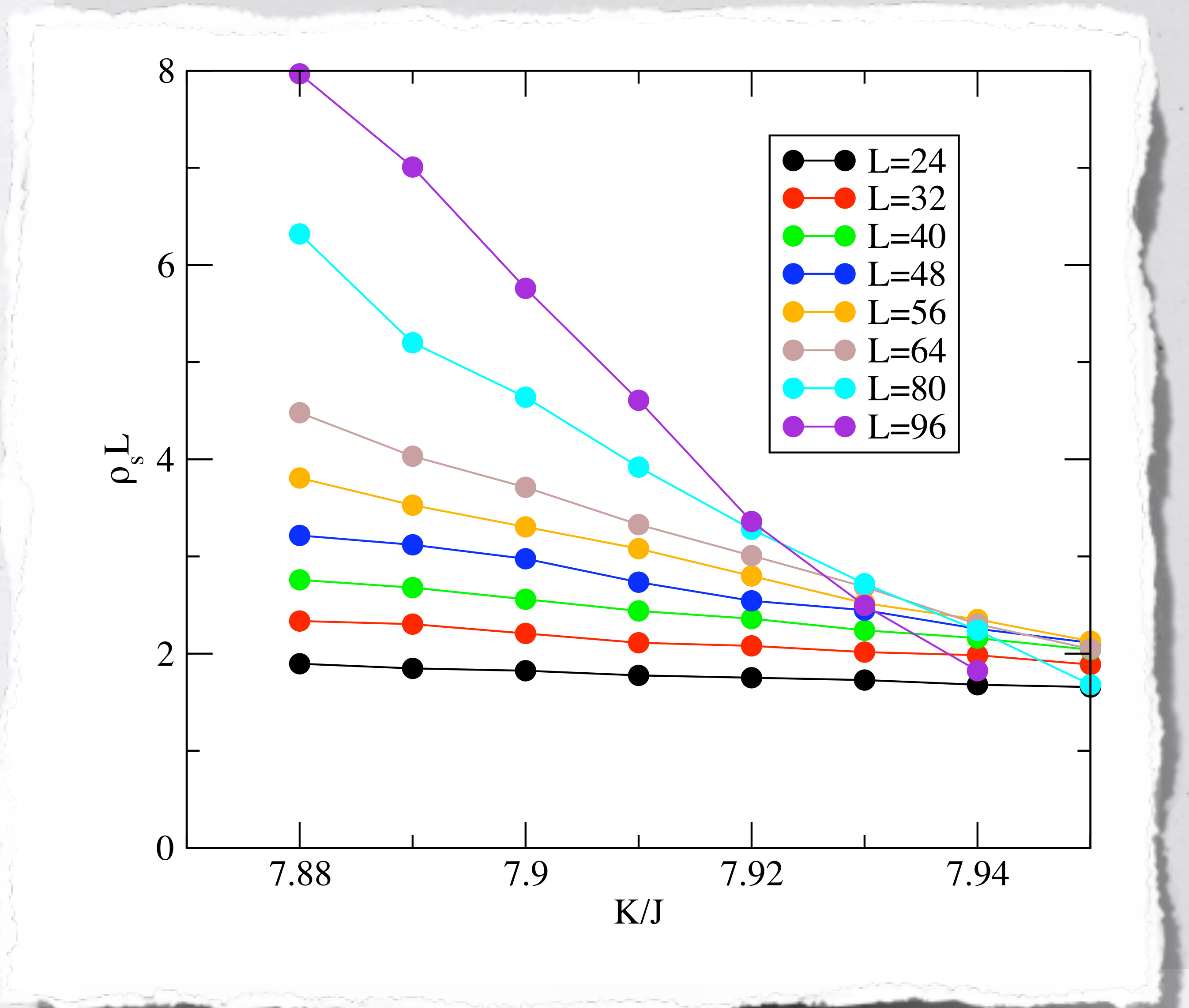
$LT = 1$



J-Q model

$LT = 1$





J-K model:

T=0 converged data

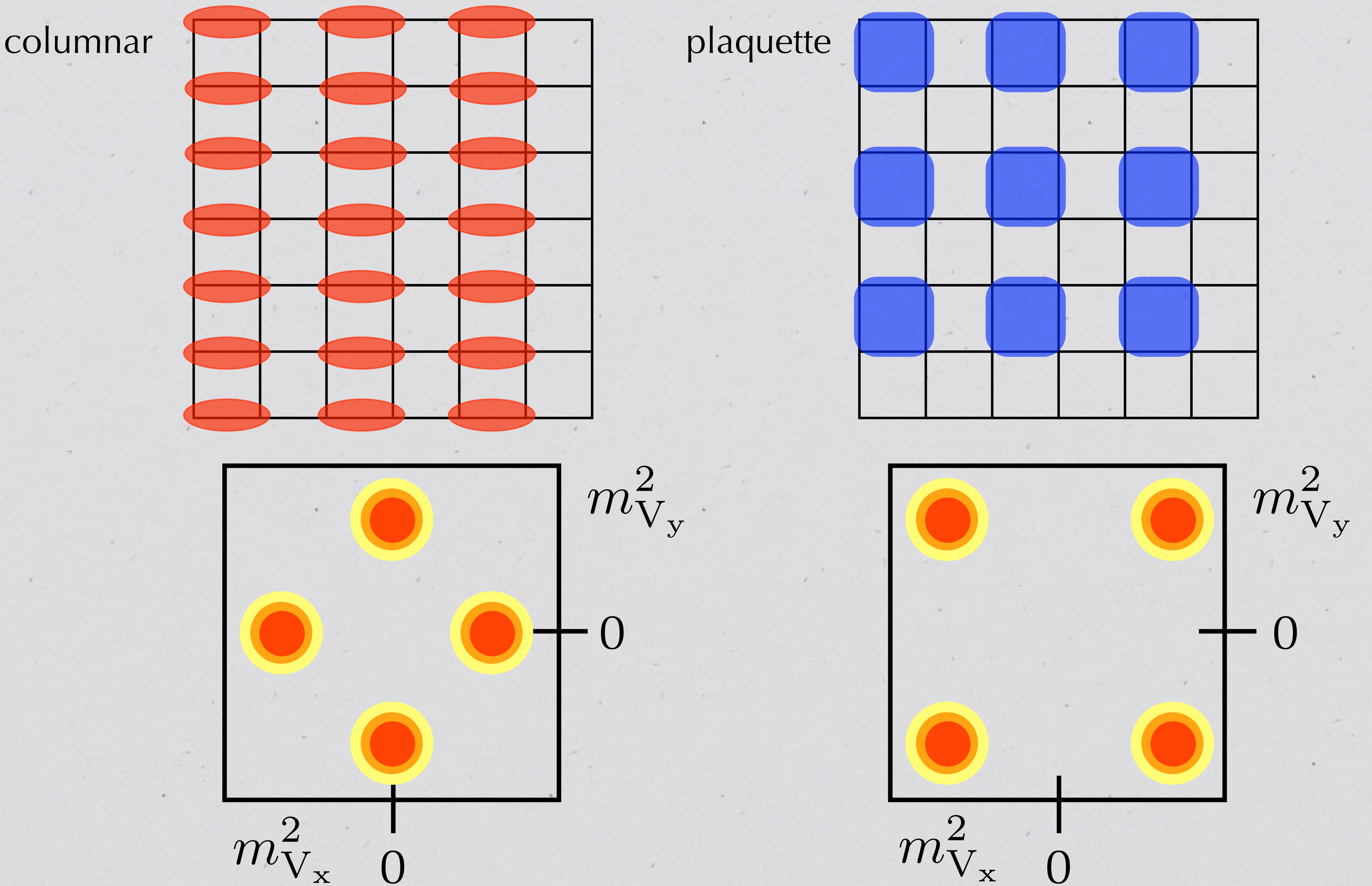
discussion: J-Q model scaling

- scaling exponent z=1 to high accuracy
- anomalous dimension is large and positive (0.35)
- Jiang et al. (arXiv:07103926): stiffness scaling suggests weak 1st order transition (?)

outline

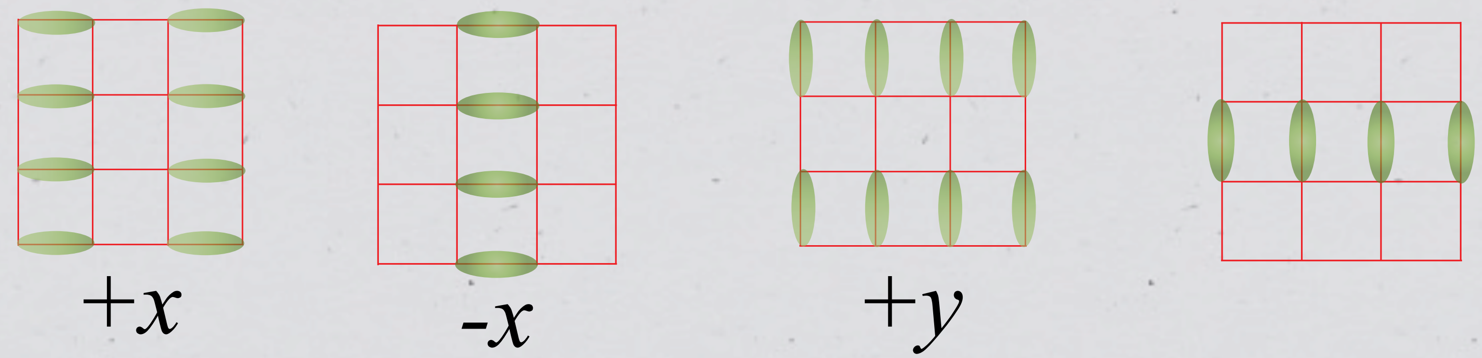
- Quantum Monte Carlo: SSE and the sign problem
- The J-K model, deconfined quantum criticality, and scaling
- The J-Q model: scaling in the quantum critical fan
- Emergent U(1) symmetries in the valence-bond-solid phases

probability distribution of VBS order parameter $P(m^2_{\mathrm{V_x}}, m^2_{\mathrm{V_y}})$

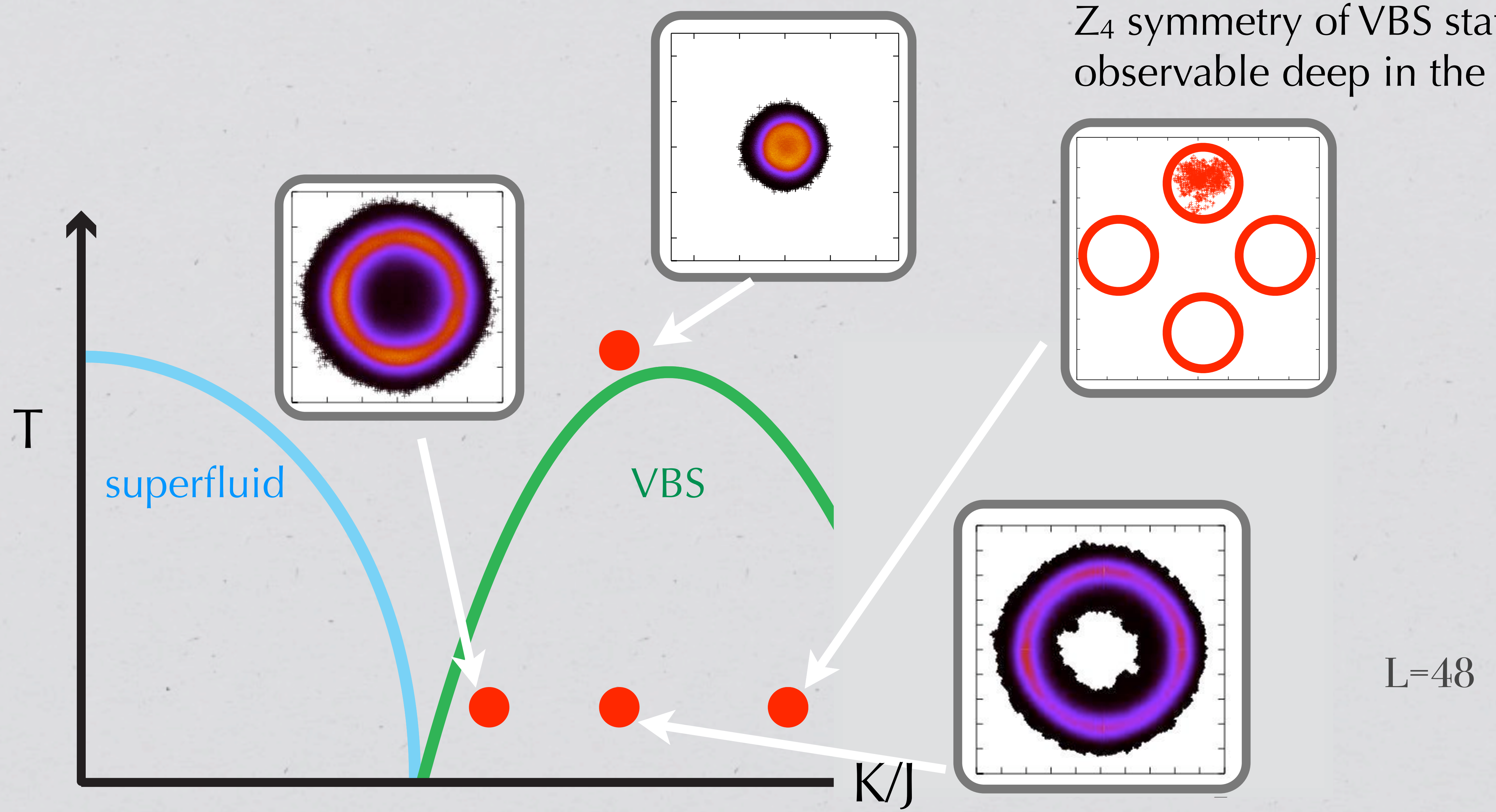


symmetry of columnar bond-order in J-K

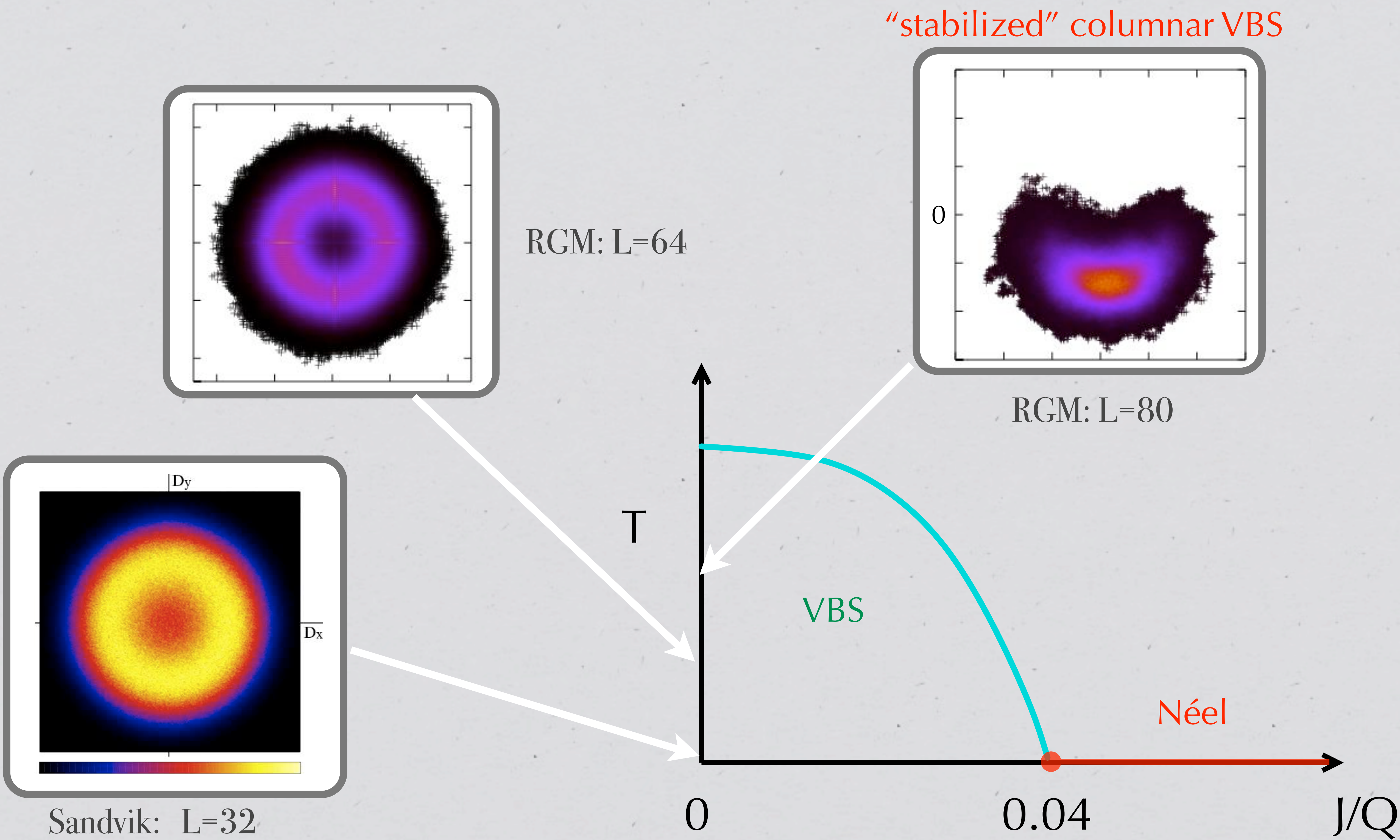
four possible VBS orderings:



Z_4 symmetry of VBS state observable deep in the phase



symmetry of VBS bond-order in J-Q model



Discussion:

- scaling in the J-Q model much more "well behaved" than the J-K model

$$z = 1 \qquad \eta = 0.35$$

- irrelevancy of the broken Z4 symmetry of the VBS phase observed in both models:
  - "deep" in the VBS phase
  - near the quantum phase transition
  - clear finite-L, finite-T effects
  - both models appear to harbor columnar VBS order