Title: Computing Unconventional Quantum Phase Transitions

Date: Apr 24, 2008 03:30 PM

URL: http://pirsa.org/08040036

Abstract: Calculating universal properties of quantum phase transitions in microscopic Hamiltonians is a challenging task, made possible through large-scale numerical simulations coupled with finite-size scaling analyses. The continuing advancement of quantum Monte Carlo technologies, together with modern high-performance computing infrastructure, has made amenable a new class of quantum Heisenberg Hamiltonian with four-spin exchange, which may harbor a continuous NÃ©el-to-Valence Bond Solid quantum phase transition. Such an exotic quantum critical point would necessarily lie outside of the standard Landau-Ginzburg-Wilson paradigm, and may contain novel physical phenomena such as emergent topological order and quantum number fractionalization. I will discuss efforts to calculate universal critical exponents using large-scale quantum Monte Carlo simulations, and compare them to theoretical predictions, in particular from the recent theory of deconfined quantum criticality.

Computing Unconventional Quantum Phase Transitions

Roger Melko, University of Waterloo

Ribhu Kaul, Harvard University

- Quantum Monte Carlo: Phys. Rev. Lett. **100**, 017203 (2008)

- Large-N: arXiv:0804.2279

SUPPORT: DOE DE-AC05-00OR22725, NSF DMR-0132874, DMR-0541988, DMR-0132874

COMPUTING: NERSC (DOE DE-AC02-05CH11231), NCSS, SHARCNET, DEAS and NINN

THANKS: S. Chandrasekharan, A. Del Maestro, T. Senthil, S. Sachdev, A. Sandvik

outline

- Heisenberg models with four-spin exchange

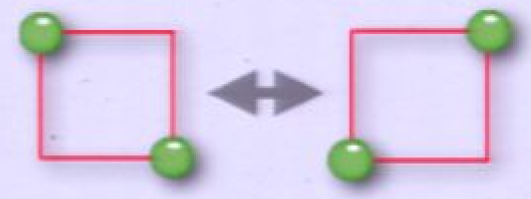
- Quantum Monte Carlo and the sign problem

- Simulations of the J-Q model $H = J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j - Q\sum_{\langle ijkl\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j)(\mathbf{S}_k\cdot\mathbf{S}_l)$

- Universal critical exponents and numbers $z\ \ \nu\ \ \eta$

outline

- Heisenberg models with four-spin exchange



- Quantum Monte Carlo and the sign problem

- Simulations of the J-Q model

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

- Universal critical exponents and numbers

$z \quad \nu \quad \eta$

microscopic models: 2D spin 1/2

goal: destabilize conventional Néel order, and realize interesting quantum phases and phase transitions...

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \cdots$$

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in models *without* the sign problem: quantum monte carlo

- allows for exact (unbiased) solutions
- very large systems sizes $\leq 10^7$

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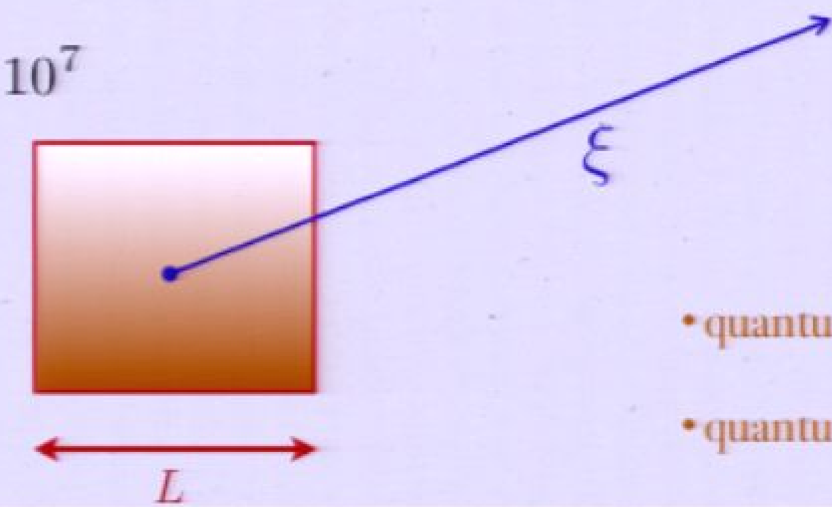


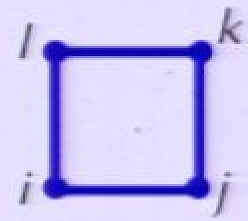
- quantum phases
- quantum phase transitions

Heisenberg "ring exchange" models

CUPRATES: low-energy effective theory of Hubbard model

$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle i,j_2 \rangle} \mathbf{S}_i \cdot \mathbf{S}_{j_2} + J_3 \sum_{\langle i,j_3 \rangle} \mathbf{S}_i \cdot \mathbf{S}_{j_3}$$

$$+ J_c \sum_{\langle i,j,k,l \rangle} \left[(\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) + (\mathbf{S}_i \cdot \mathbf{S}_l)(\mathbf{S}_j \cdot \mathbf{S}_k) - (\mathbf{S}_i \cdot \mathbf{S}_k)(\mathbf{S}_j \cdot \mathbf{S}_l) \right]$$



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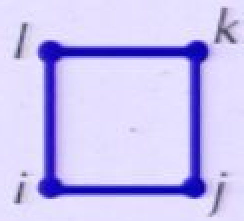
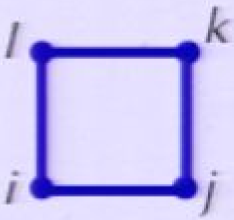


TOY MODEL:

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

Sandvik's J-Q model

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



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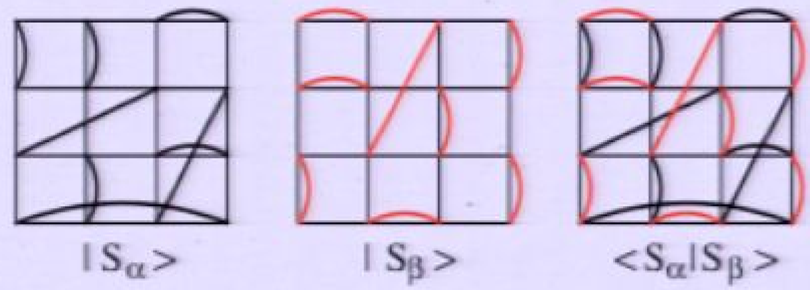
Valence Bond Basis
Sandvik
Phys. Rev. Lett. **95**, 207203 (2005)



T=0 projector Quantum Monte Carlo up to L=32

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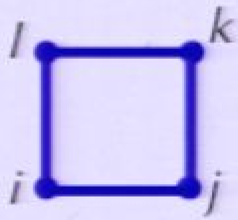

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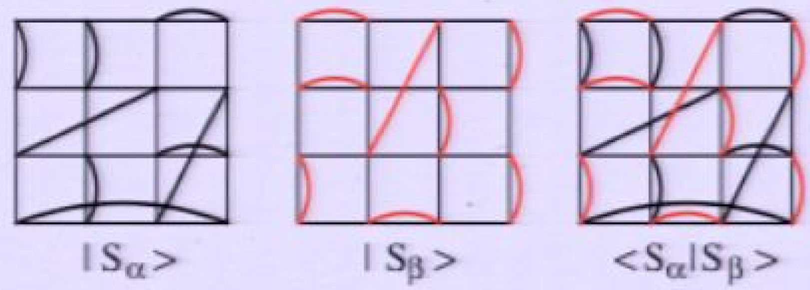

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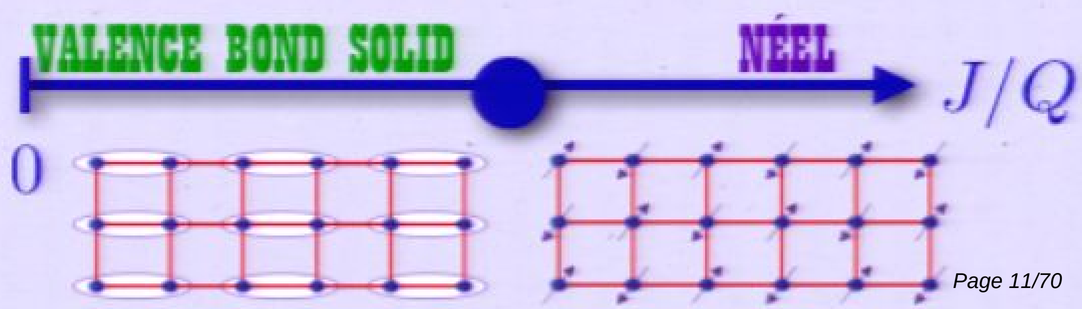

 $= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

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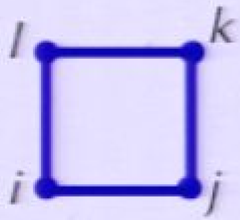

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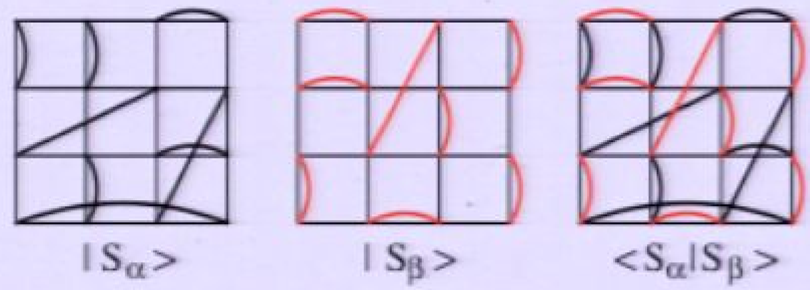
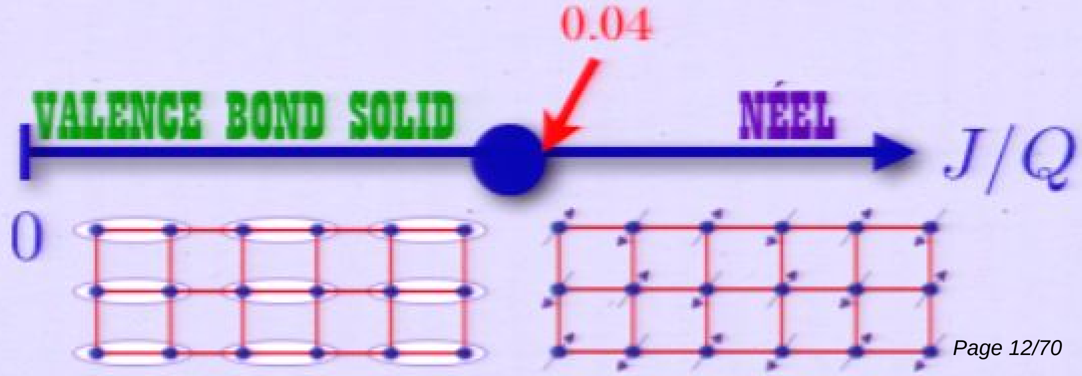


T=0 projector Quantum Monte Carlo up to L=32

Good numerical evidence for a direct (!) continuous quantum critical point



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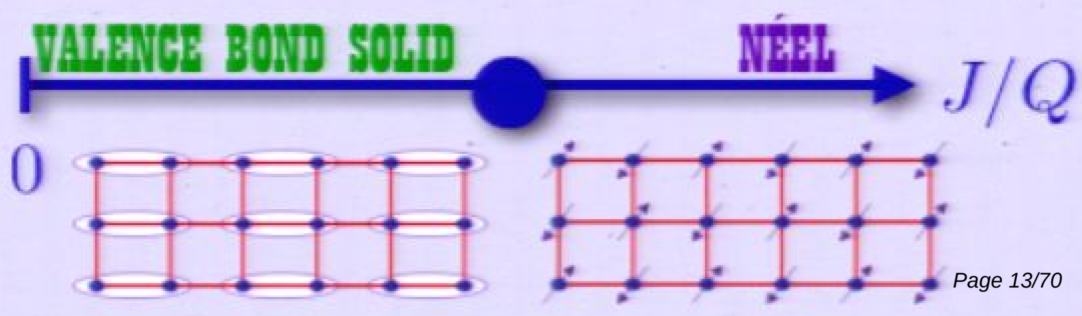
Sandvik's J-Q model

can we study via a finite-T QMC formalism in the S^z basis?



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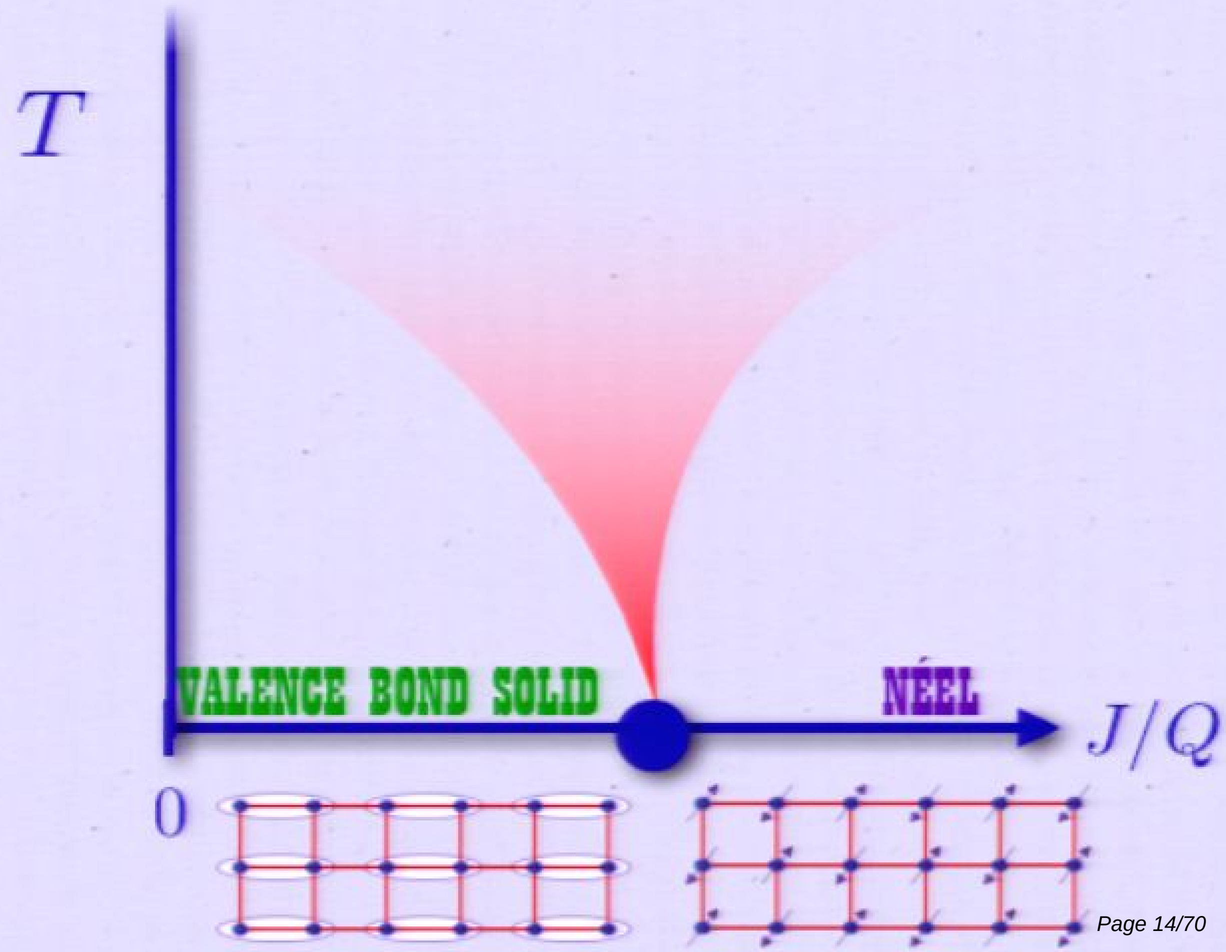

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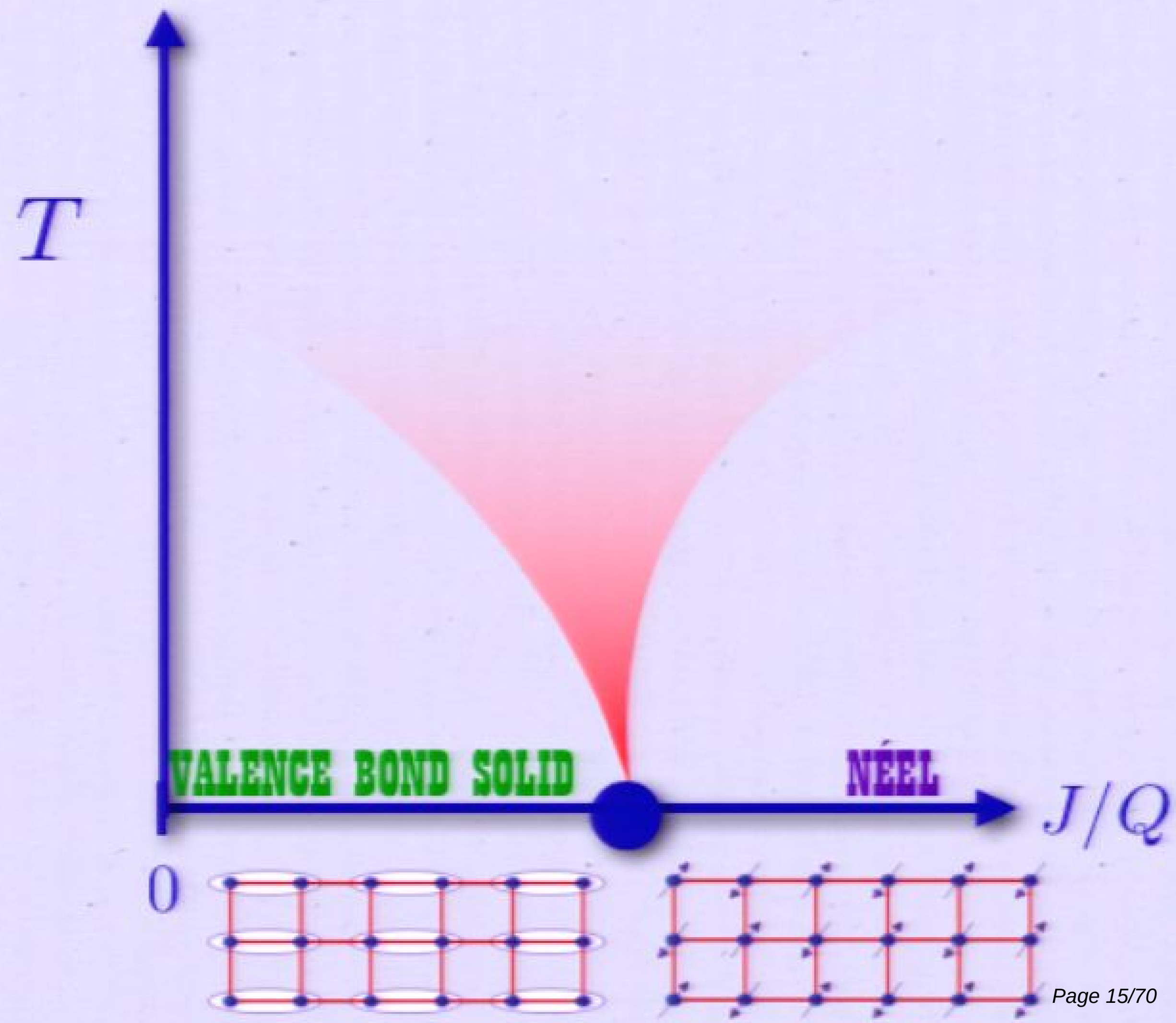

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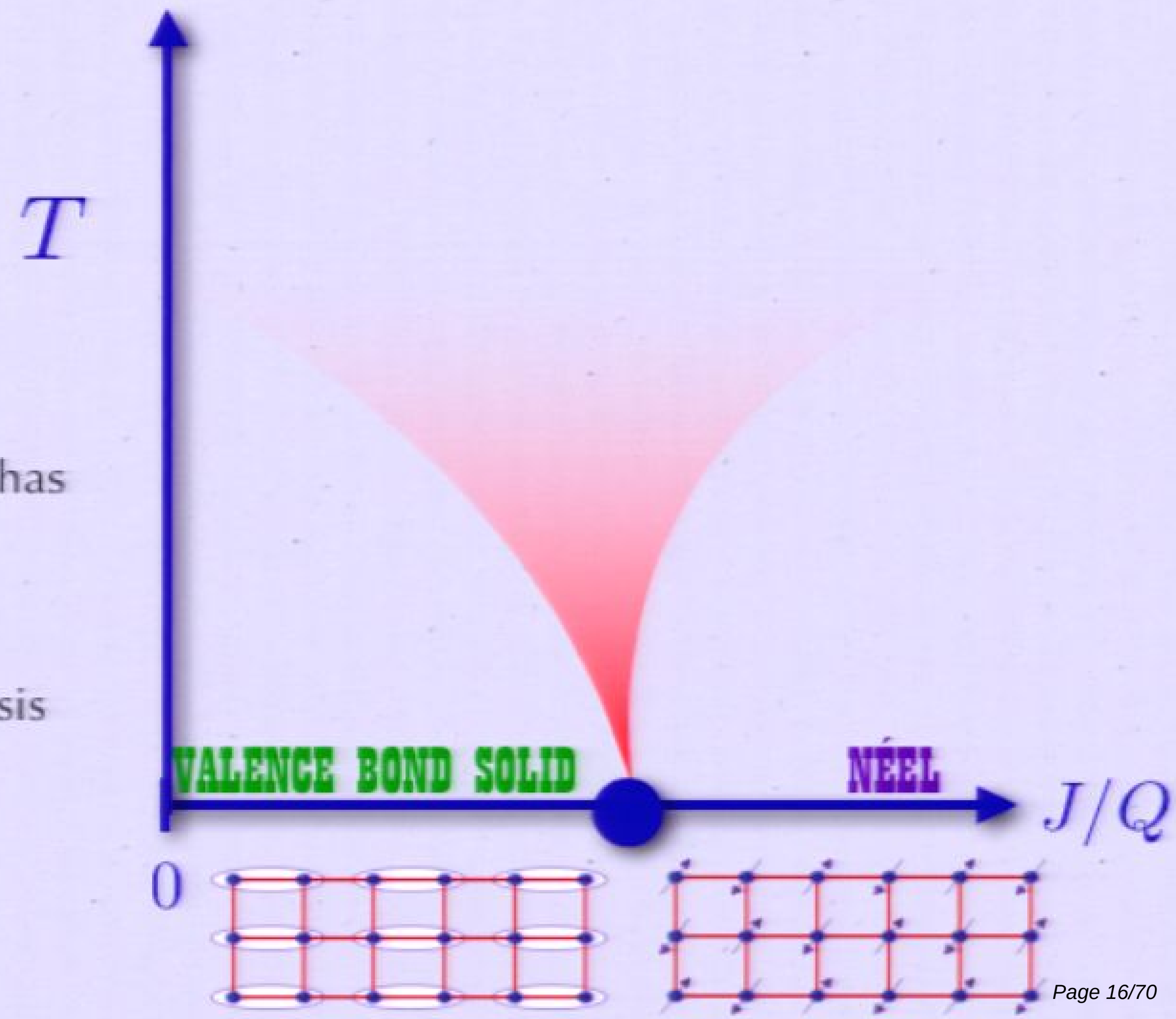


- the overcomplete VB-basis has no sign problem

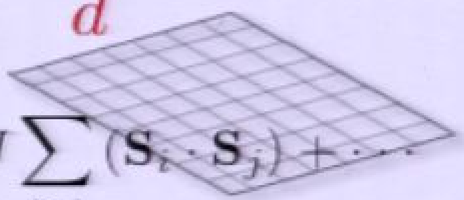
- the more powerful finite-T formalism based on the Sz basis does (naively)

Quantum Monte Carlo

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

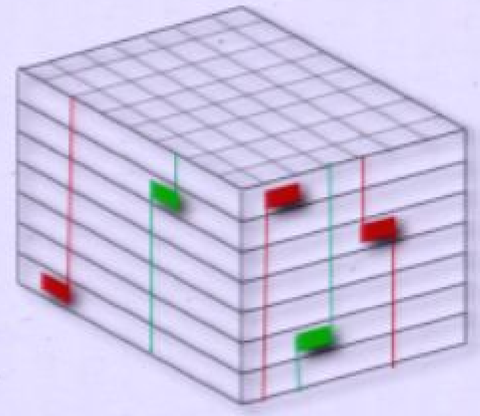
map to higher dimensional classical system

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:

-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:

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

trace over standard basis

● = ↑
○ = ↓

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

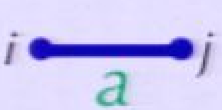
power series expansion

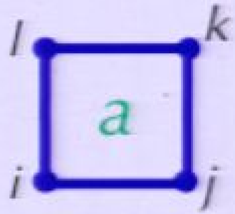
$$= \sum_{\{\alpha_i\}} \sum_{n=0}^{\infty} \frac{(-1)^n \beta^n}{n!} \prod_{i=0}^{n} \langle \alpha_i \,|H|\, \alpha_{i+1} \rangle$$

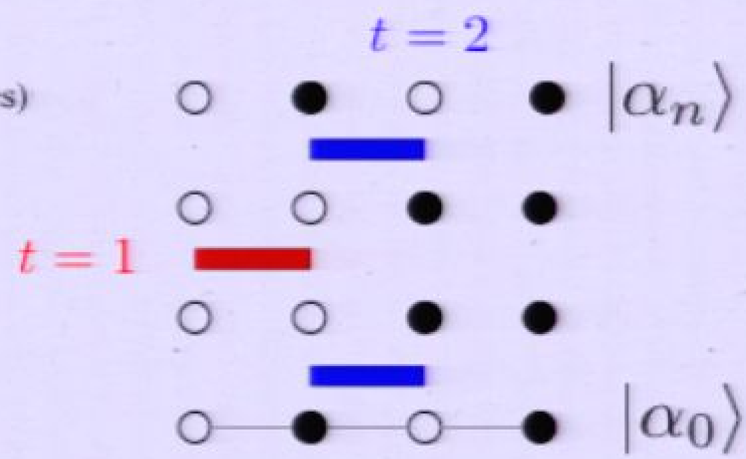
matrix elements = real numbers

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

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



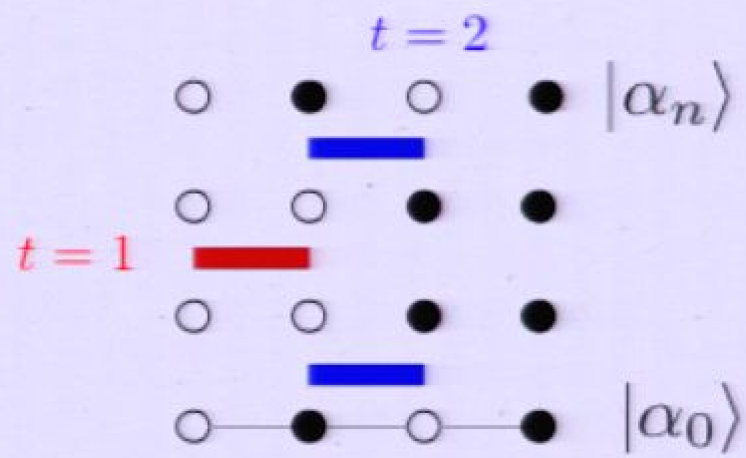




Stochastic Series Expansion QMC

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

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



- construct weights from partition function

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

- Metropolis algorithm (attempted operator change)

$$r \leq \frac{W_i'}{W_i} \qquad 0 < r < 1$$

need positive definite weights

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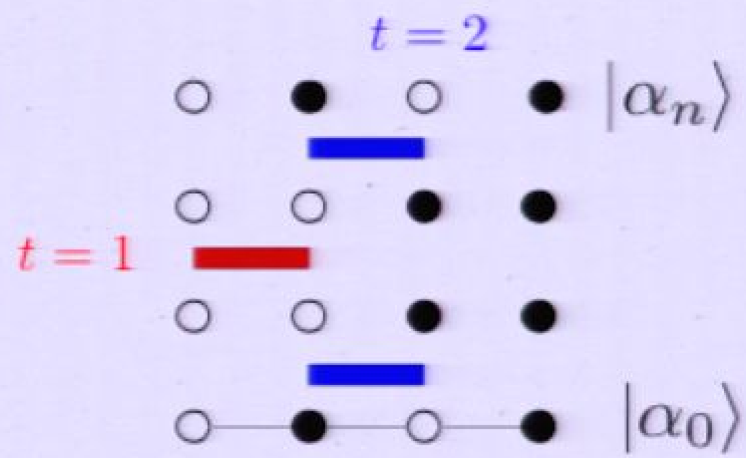

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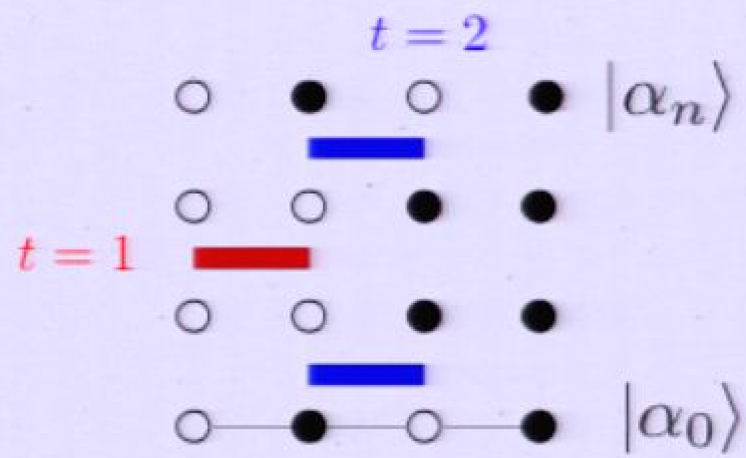

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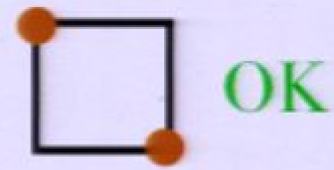
if $H_{t,a} < 0$ (antiferromagnetic) and...

an EVEN number is required to satisfy PBC:



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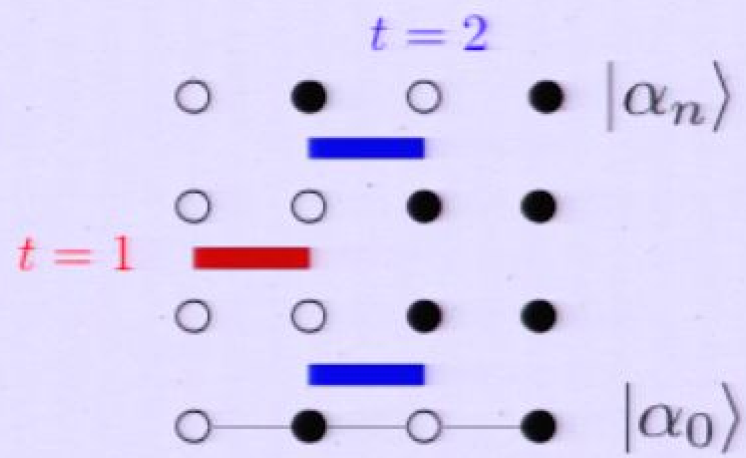

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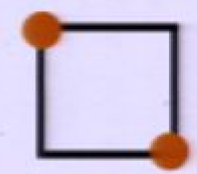
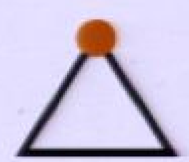


OK

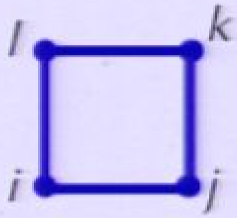
an ODD number can satisfy PBC:



sign problem

Sandvik's J-Q model

RGM and Kaul, Phys. Rev. Lett. 100, 017203



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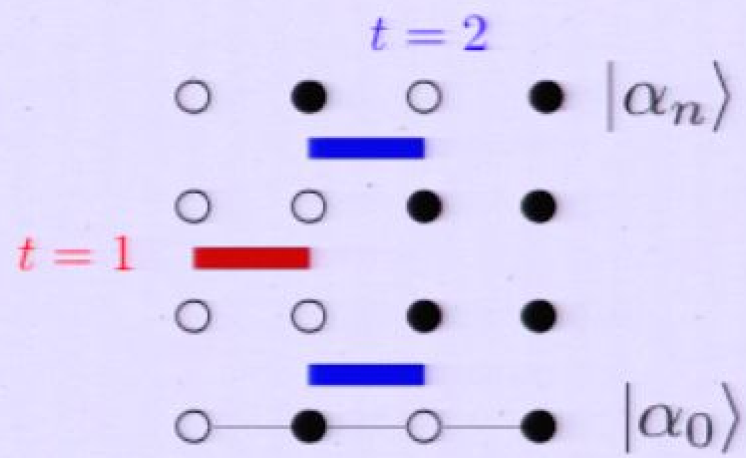

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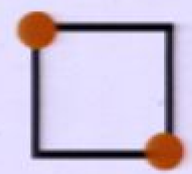

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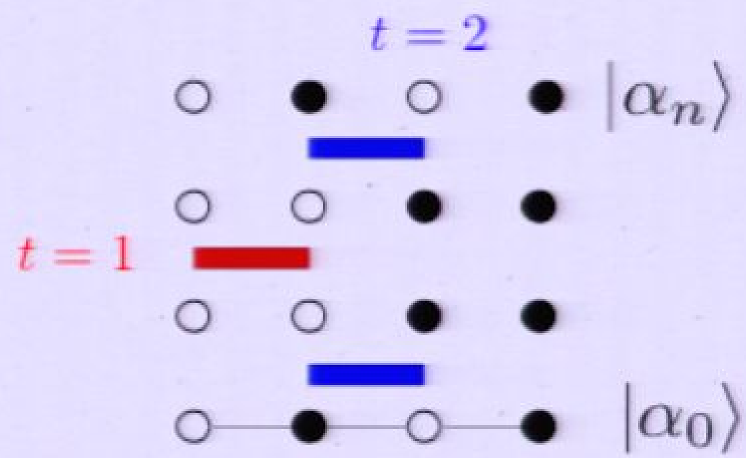

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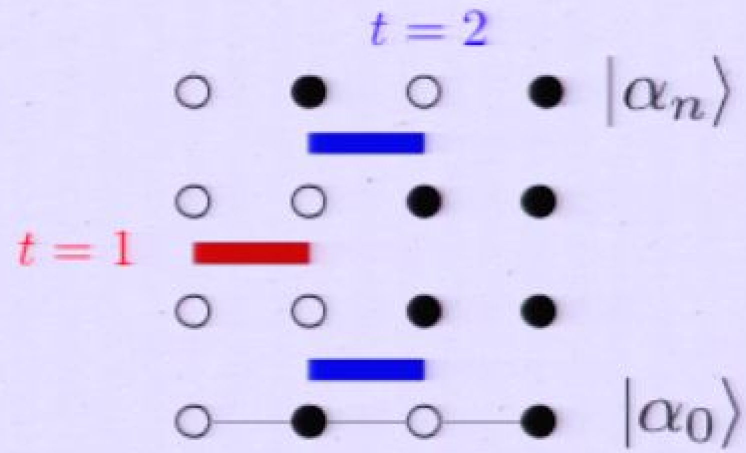

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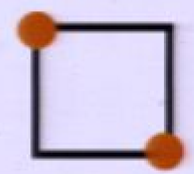

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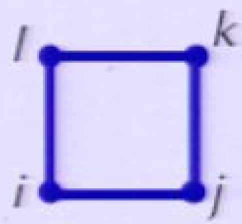
Sandvik's J-Q model

RGM and Kaul, Phys. Rev. Lett. 100, 017203



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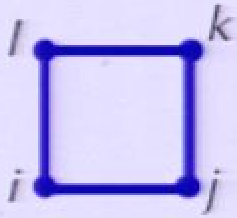

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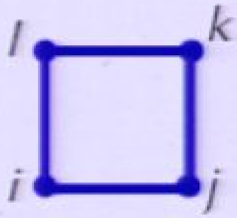
$$
\begin{aligned}
H_{1,a} &= -J(S_i^z S_j^z I_{k,l}) \\
H_{2,a} &= -J/2(S_i^+ S_j^- I_{k,l}) \\
H_{3,a} &= Q(S_i^z S_j^z - 1/4)(S_k^z S_l^z - 1/4) \\
H_{4,a} &= Q/2(S_i^z S_j^z - 1/4)(S_k^+ S_l^- + S_k^- S_l^+) \\
H_{5,a} &= Q/4(S_i^+ S_j^- + S_i^- S_j^+)(S_k^+ S_l^- + S_k^- S_l^+)
\end{aligned}
$$

$I_{k,l} =$ identity operator

Sandvik's J-Q model

RGM and Kaul, Phys. Rev. Lett. 100, 017203



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

What about the S^z basis?

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

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

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

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

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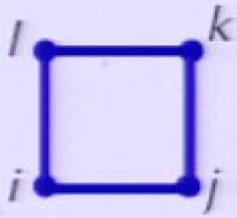

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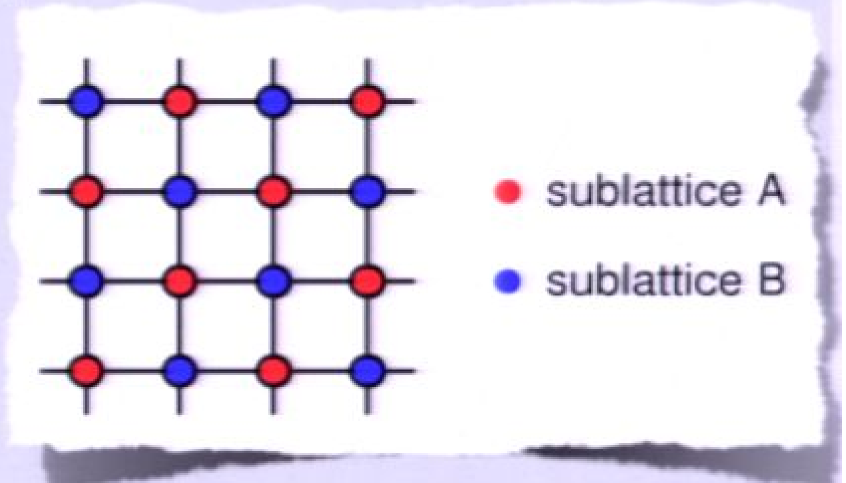
What about the S^z basis?



rotate sublattice B by π around the z axis

$$H_{1,a} = -J(S^z_i S^z_j I_{k,l})$$

$$H_{2,a} \to J/2(S^+_i S^-_j I_{k,l})$$

$$H_{3,a} = Q(S^z_i S^z_j - 1/4)(S^z_k S^z_l - 1/4)$$

$$H_{4,a} \to -Q/2(S^z_i S^z_j - 1/4)(S^+_k S^-_l + S^-_k S^+_l)$$

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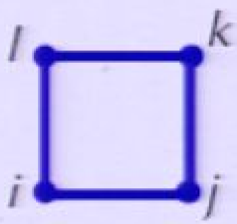
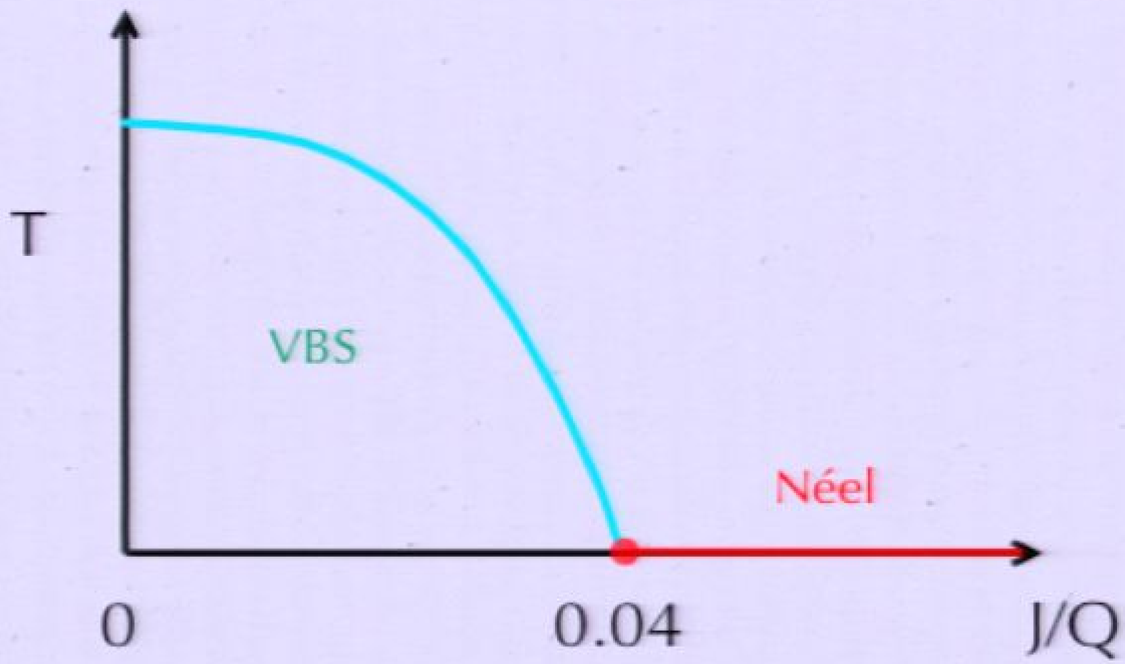
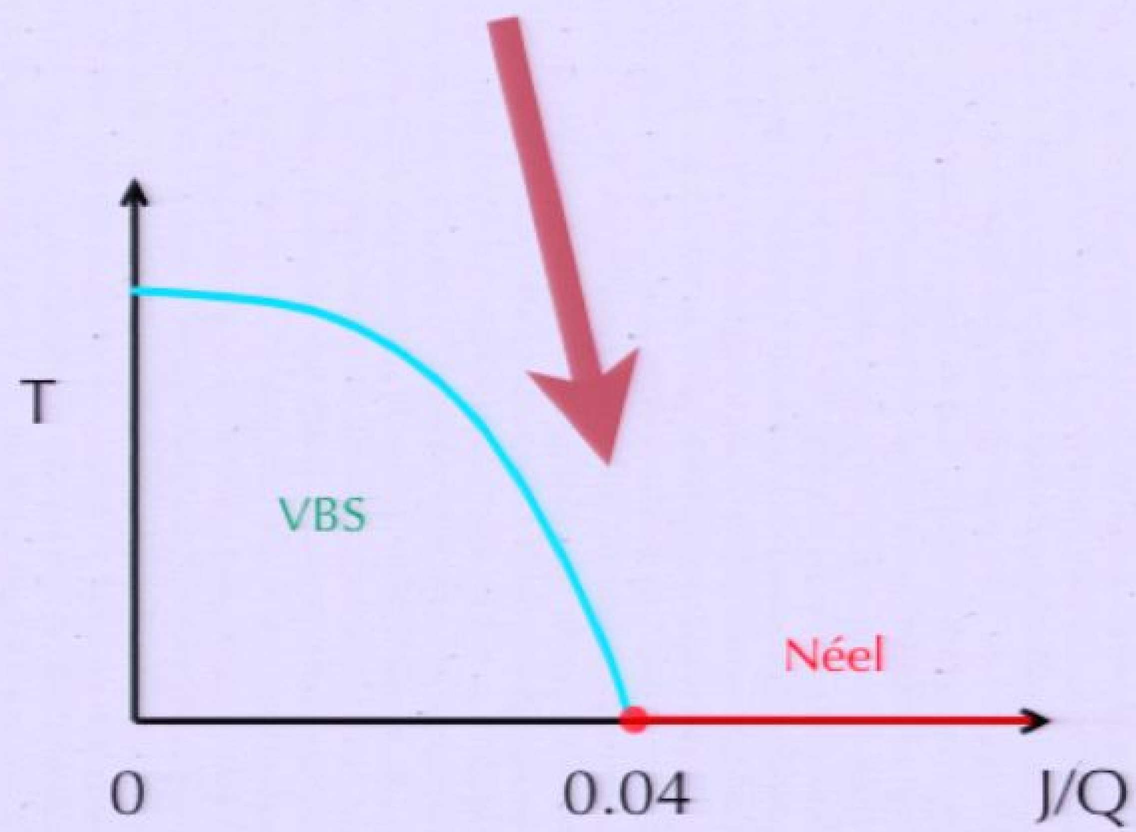


$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - Q \sum_{\langle ijkl \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4})(\mathbf{S}_k \cdot \mathbf{S}_l - \tfrac{1}{4})$$



some results....



correlation functions:

Neel $C_{\mathrm{N}}^{z}(\mathbf{r},\tau) = \langle S^{z}(\mathbf{r},\tau) S^{z}(0,0)\rangle$

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

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

correlation functions:

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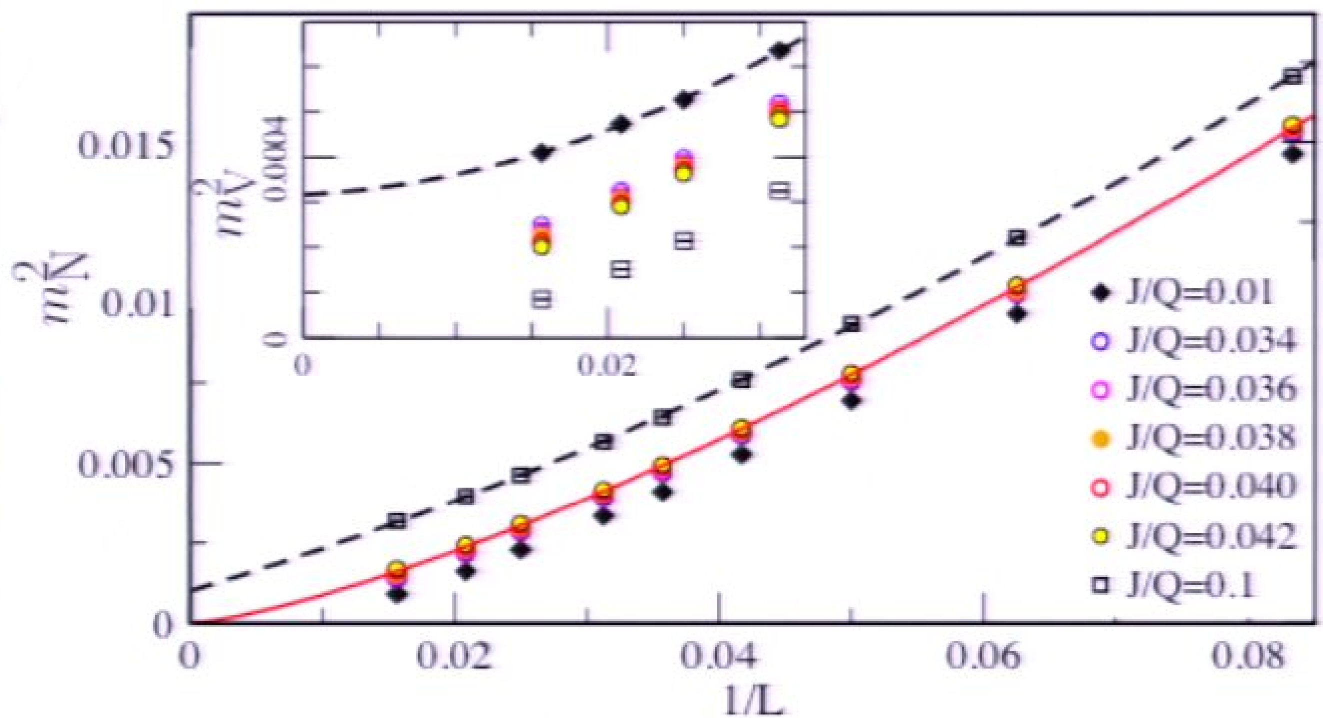
order parameters

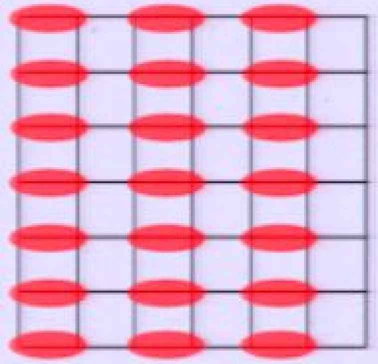
$$m^2_{\mathrm{N,V}} = \frac{S_{\mathrm{N,V}}[\mathbf{q}_{\mathrm{N,V}}]}{N_{\mathrm{spin}}}$$

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

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



the VBS phase exists in the thermodynamic limit



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

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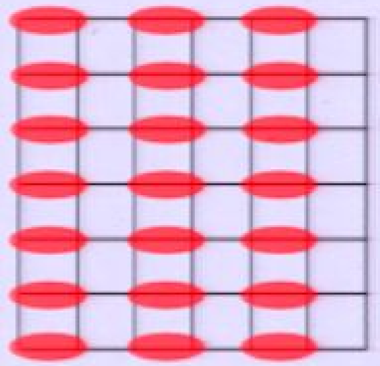
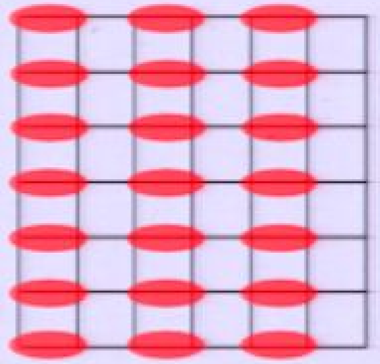


$\mathbf{q}_V = (\pi, 0)$

what about the apparent quantum critical point?

$$\left(\frac{J}{Q}\right)_c \approx 0.04$$

the VBS phase exists in the thermodynamic limit



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

what about the apparent quantum critical point?

$$\left(\frac{J}{Q}\right)_c \approx 0.04$$

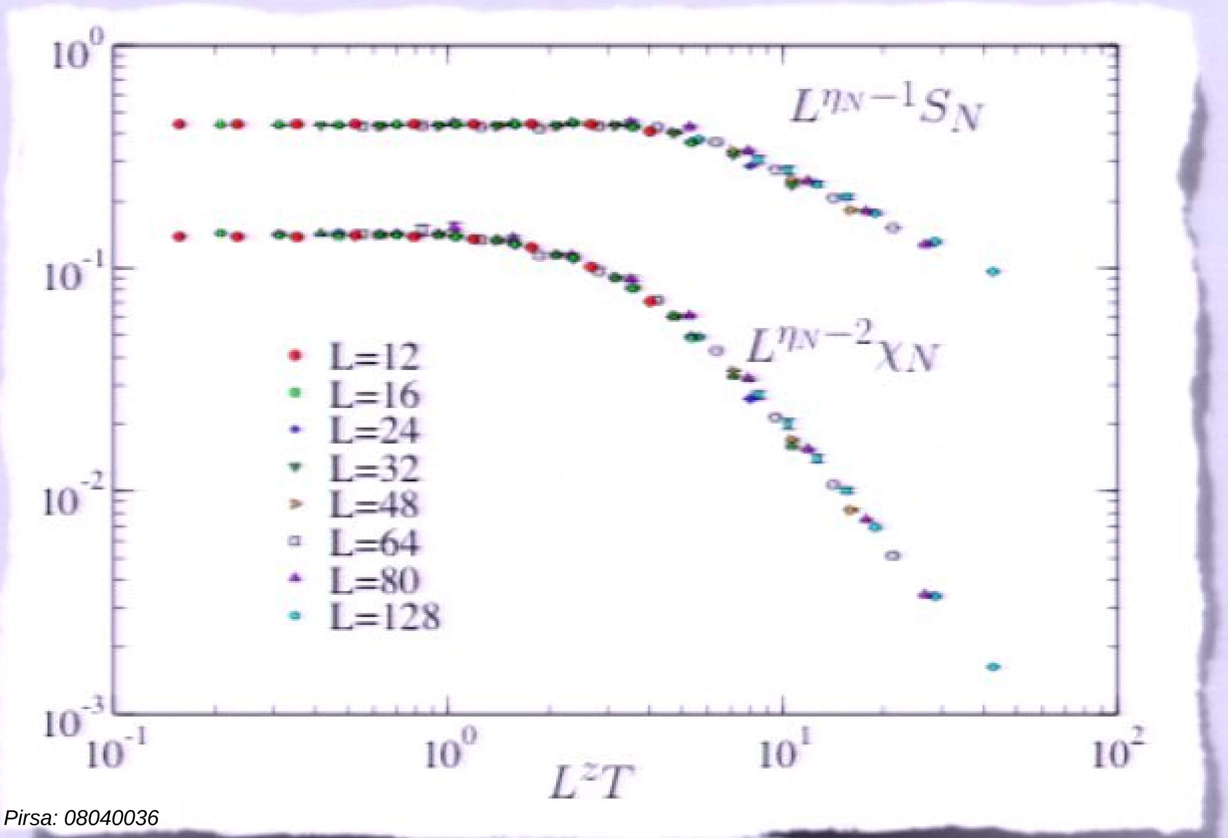
look at scaling and universal quantities: z ν η ....

staggered structure factor and susceptibility

$$S_{\rm N}[\mathbf{q}] = \frac{1}{N_{\rm spin}} \sum_{\mathbf{r}} e^{(-i\mathbf{q}\cdot\mathbf{r})} C^z_{\rm N}(\mathbf{r}, \tau = \mathbf{0})$$

$$\chi_{\rm N}[\mathbf{q}] = \frac{1}{N_{\rm spin}} \sum_{\mathbf{r}} e^{(-i\mathbf{q}\cdot\mathbf{r})} \int_0^\beta C^z_{\rm N}(\mathbf{r}, \tau) d\tau$$

$\mathbf{q} = (\pi, \pi)$



$S_N \propto L^{1-\eta_N} \mathbb{X}_{\rm S}(L^z T/c)$

$\chi_N \propto L^{2-\eta_N} \mathbb{X}_{\chi}(L^z T/c)$

assume z=1

$\eta_N = 0.35$

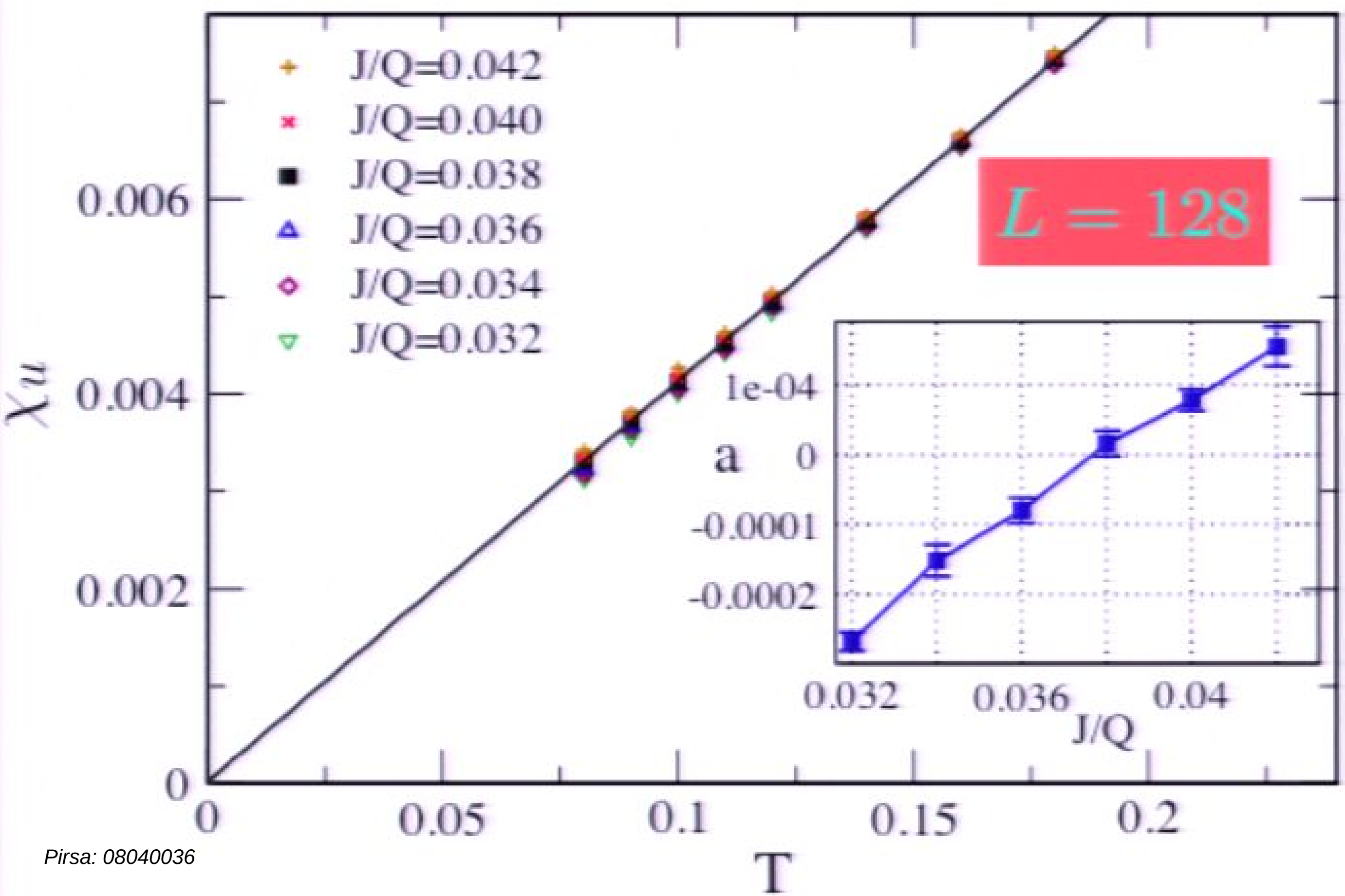
$J/Q = 0.038$

exponent z: uniform spin susceptibility

$$\chi_u = \frac{1}{TN}\left\langle \left(\sum_{i=1}^{N} S_i^z \right)^2 \right\rangle$$

$$\chi_u = a + bT^{d/z-1}$$

Chubukov *et al.* PRB 49, 11919 (1994)



$z = 1$

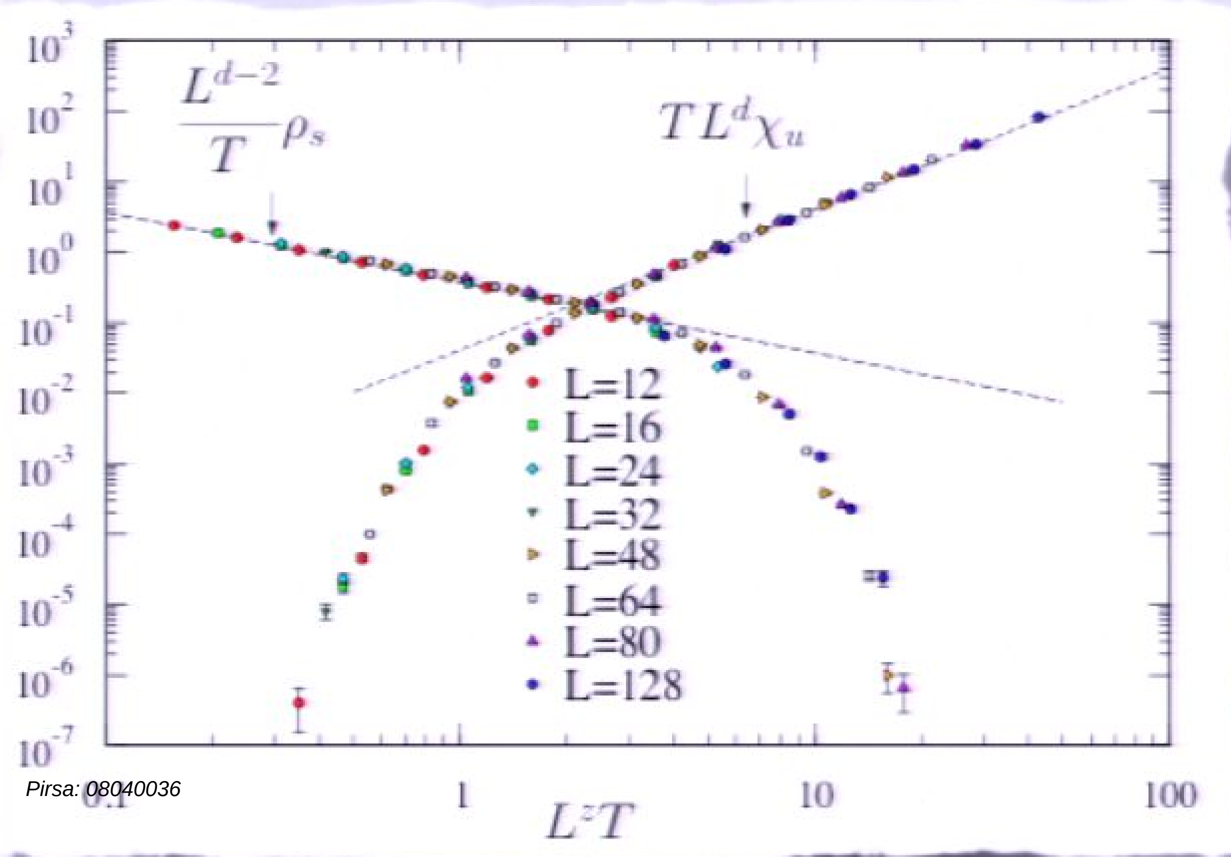
$J/Q = 0.038$

susceptibility and stiffness

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

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

$$\rho_s = \frac{\langle W_x^2 + W_y^2\rangle}{2\beta}$$



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

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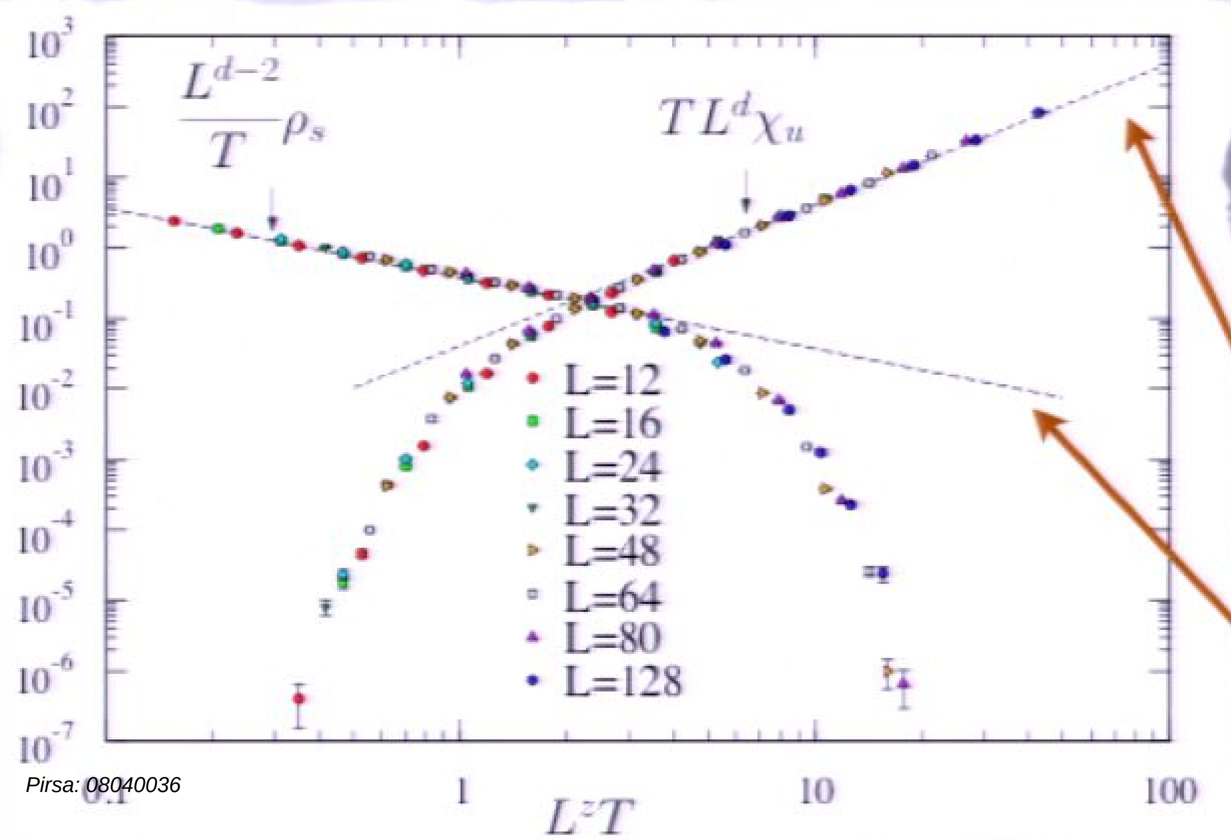

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$z = 1$

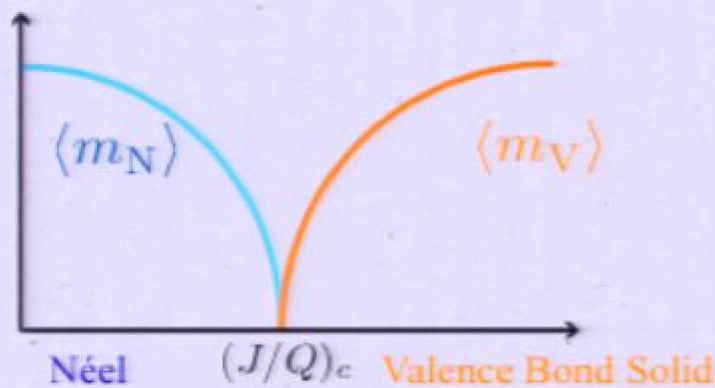
$J/Q = 0.038$

$A_\chi (LT/c)^2$

$\frac{A_\rho}{LT/c}$

A continuous Néel to VBS phase quantum critical point...?

Landau-forbidden (requires fine-tuning)



A continuous Néel to VBS phase quantum critical point...?

Landau-forbidden (requires fine-tuning)

- Theory for a generic Néel-VBS transitions proposed by Senthil et al. Science 303, 1490 (2004):
  - ∗ "Deconfined" quantum criticality
  - ∗ Dynamical scaling exponent $z = 1$
  - ∗ Anomalous dimension "large" $\eta > 0.038$
  - ∗ Emergent global U(1) symmetry
  - ∗ Deconfined fractionalized excitations (spinons)

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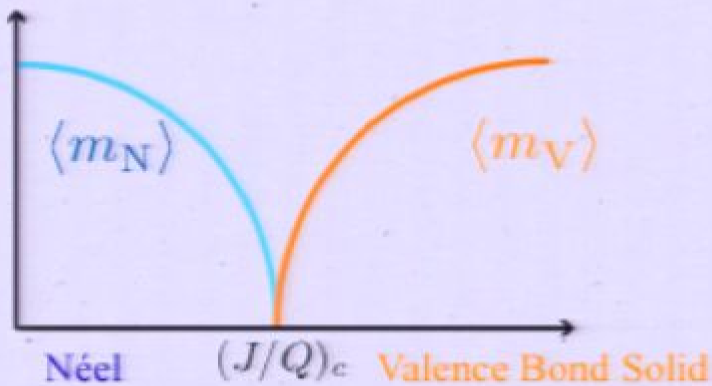
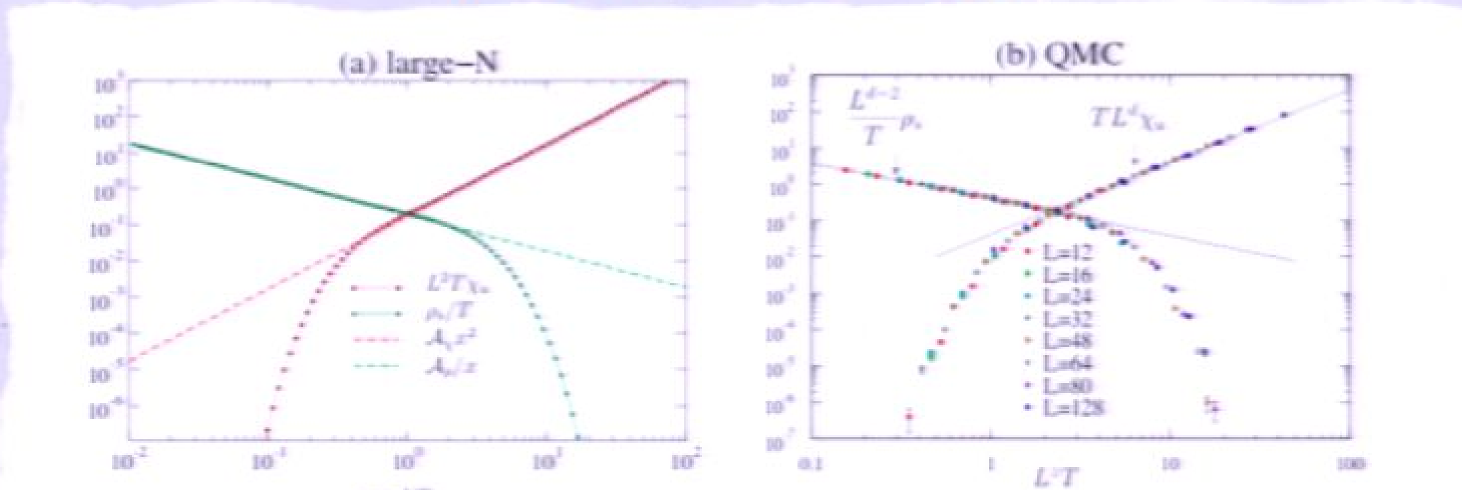


- non-compact CP^1 field theory of two complex bosonic spinons

- look at large-N limit: $ncCP^{N-1}$ (Ribhu K. Kaul, RGM, arXiv:0804.2279)



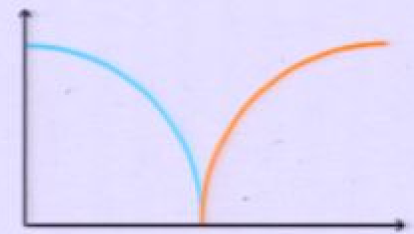
	this work	Sandvik	DQCP / ncCP^{N-1}
$(J/Q)_c$	0.038	<0.04	N/A
z	1.00	1	1
η	0.35	0.26(3)	“large” (>0.038)
ν	0.68	0.78(3)	?
$A_\rho \sqrt{A_\chi}$	0.075	?	0.0766
$\frac{T\chi_u}{C_v} = \frac{A_\chi}{A_{C_v}}$	0.055	?	0.0466

Discussion

* We have the QMC technology to solve the general "class" of the JQ Hamiltonian without the sign problem

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

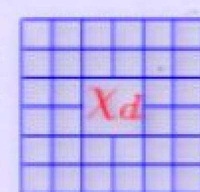
* Neel-VBS quantum phase appears continuous (up to L=128)



* scaling "well behaved" and consistent with predictions from deconfined quantum criticality

$$A_\rho \sqrt{A_\chi}$$

* Current/future work: search for emergent U(1) symmetry, deconfined spinons



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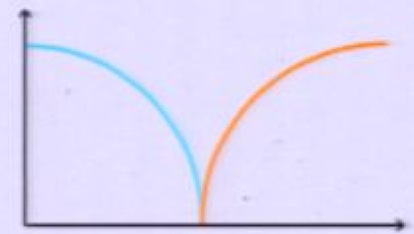
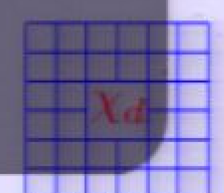


- scaling “well … l con… redic… deconfined c… ality

$$A_\rho\sqrt{A_\chi}$$

29 30 31

- Current/future w… : search f… (1) symmetry, deconfined spinons



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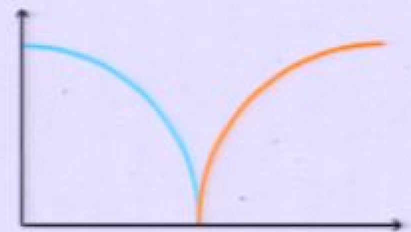

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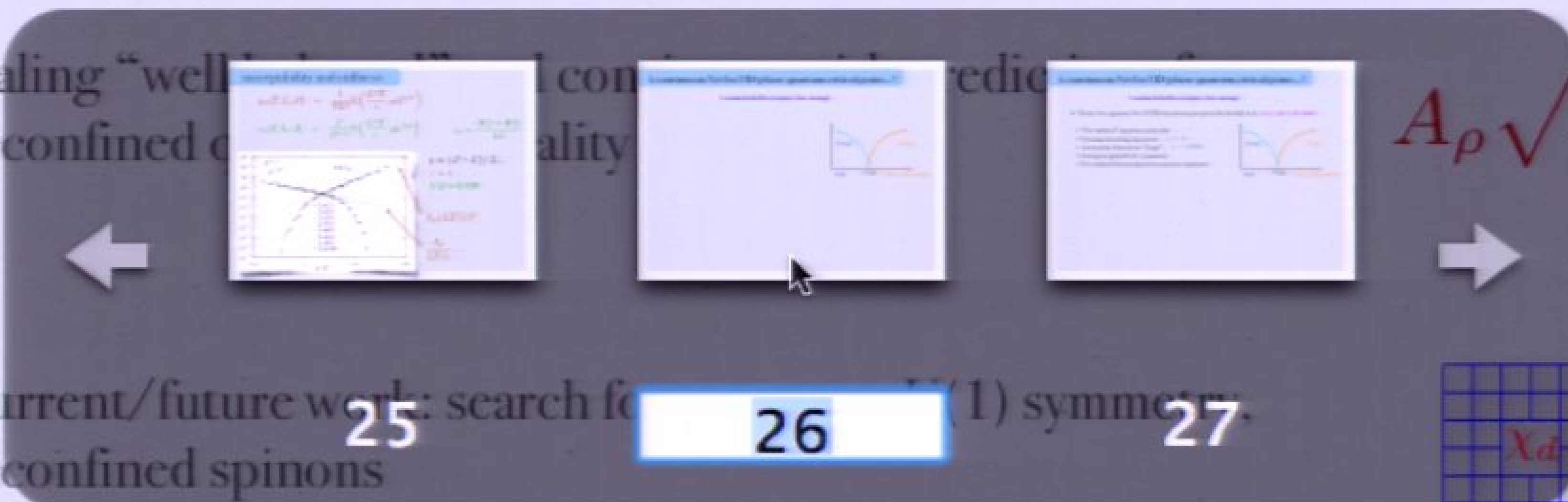

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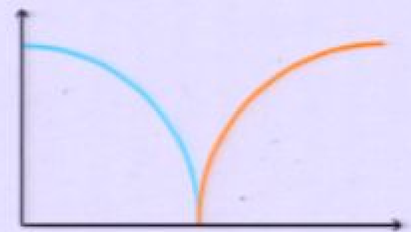

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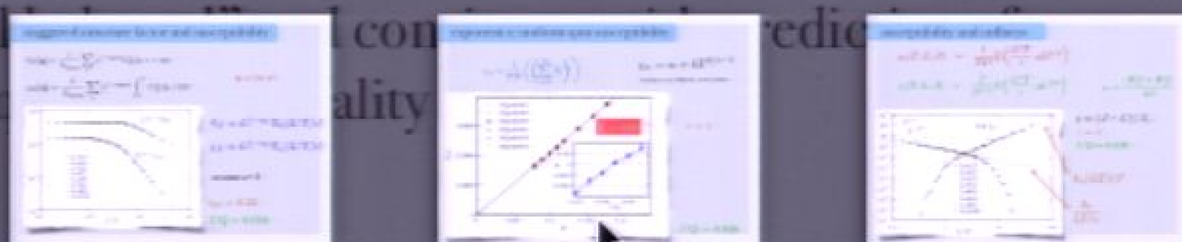

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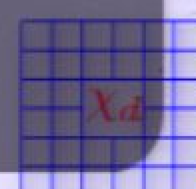

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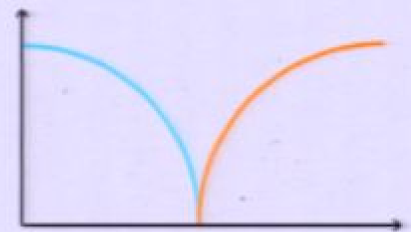

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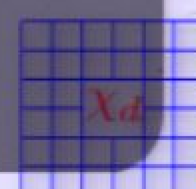

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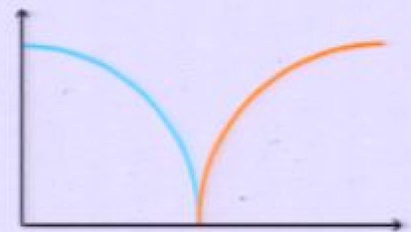
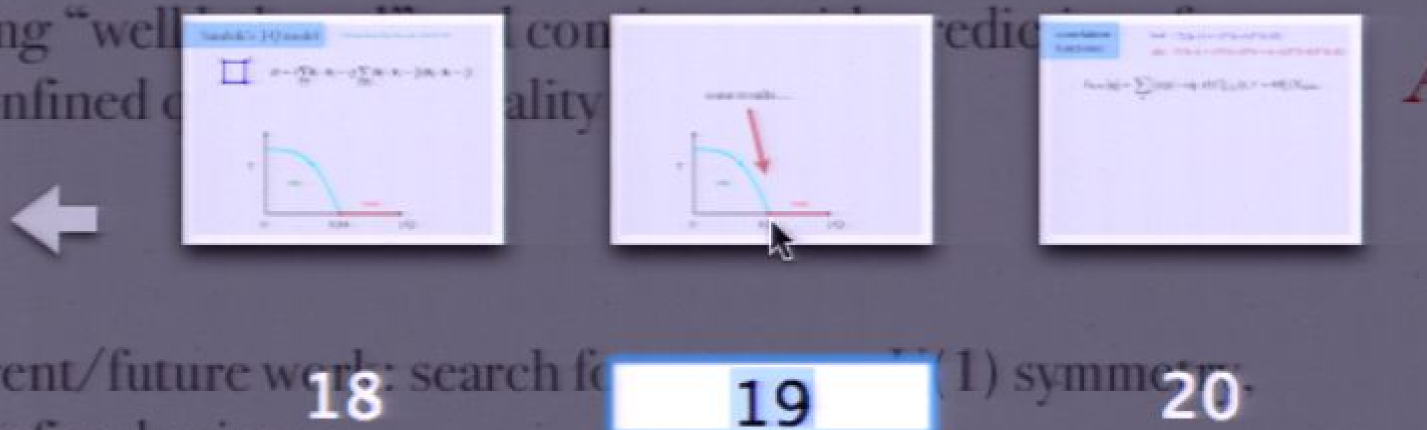


- sc... "wel... ...l con... ...redic... de... ...ality



$$A_\rho \sqrt{A_\chi}$$

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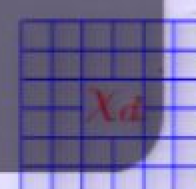

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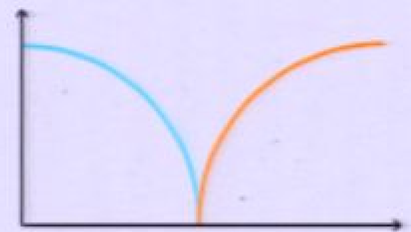

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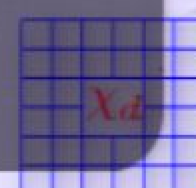

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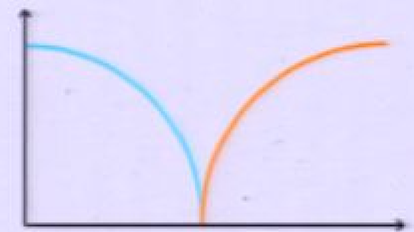

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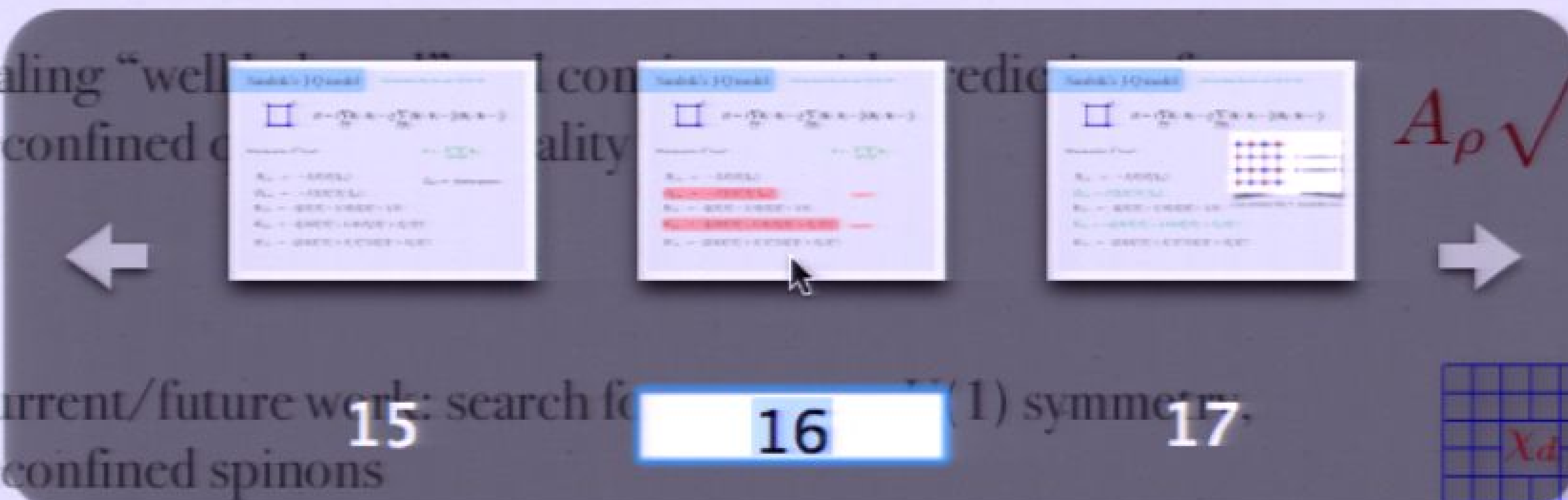

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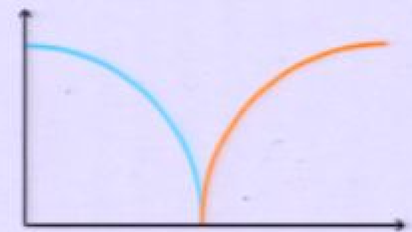

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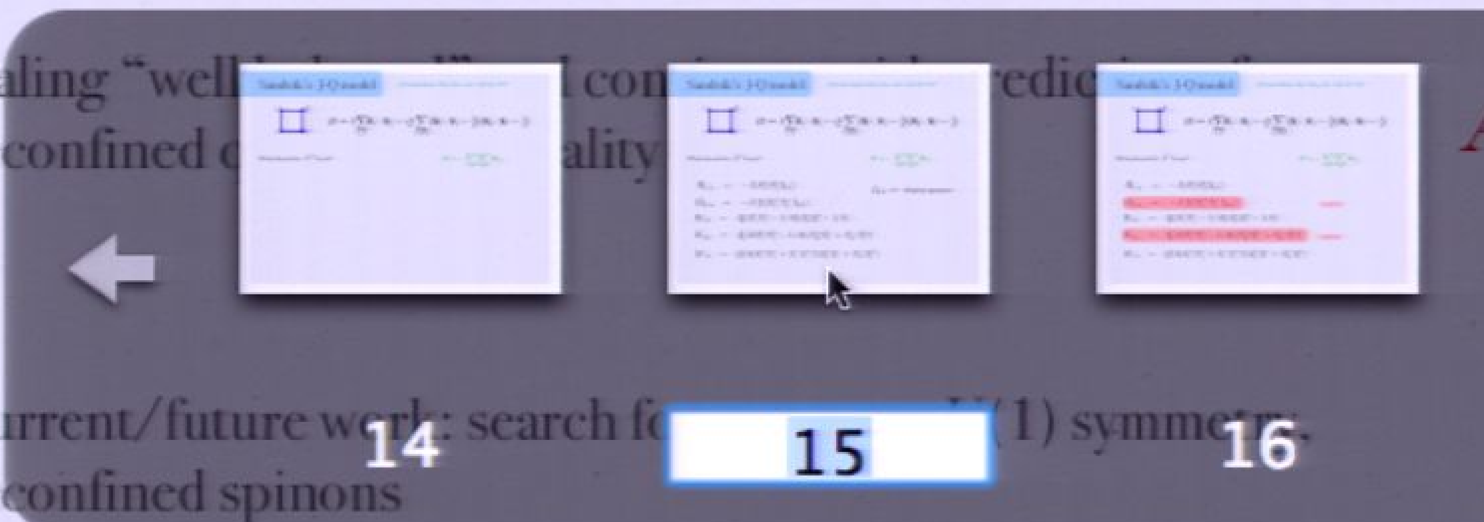

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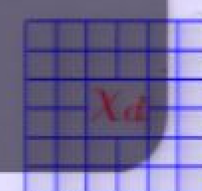

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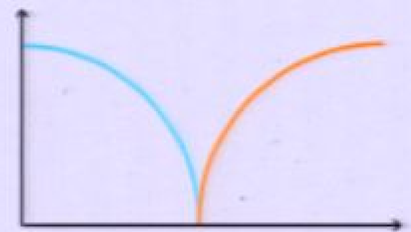
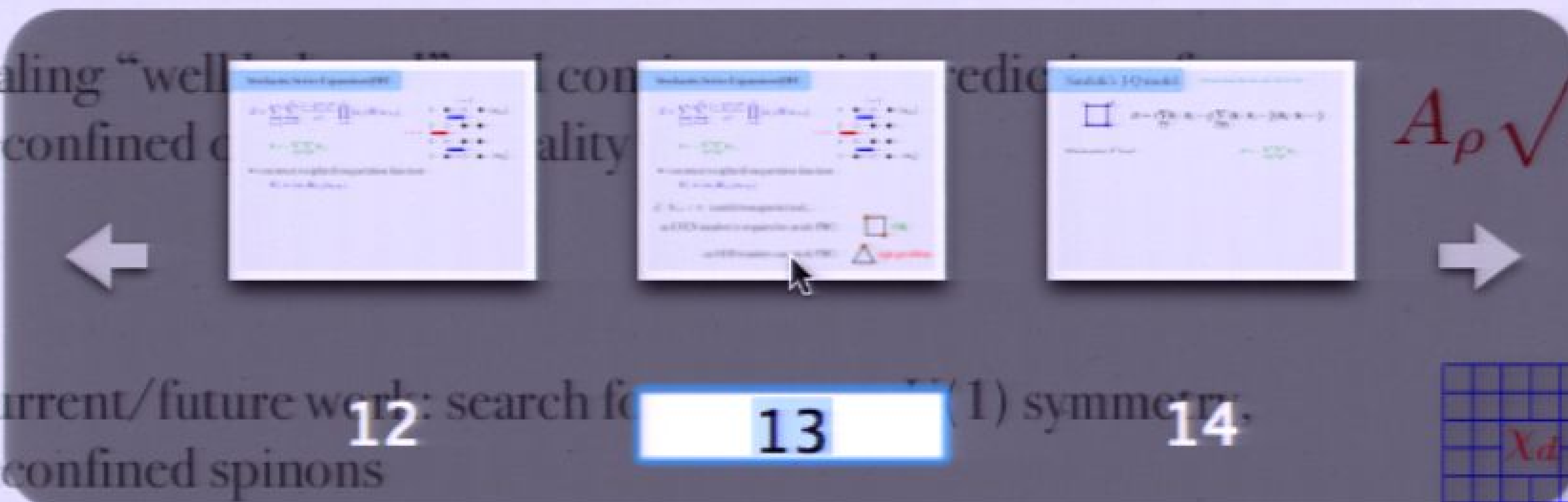
$$H = J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j - Q\sum_{\langle ijkl\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j)(\mathbf{S}_k\cdot\mathbf{S}_l)$$

- Neel-VBS quantum phase appears continuous (up to L=128)



- scaling “well ... l con ... redic ... deconfined c ... ality

$$A_\rho\sqrt{A_\chi}$$



- Current/future w ... : search fo ... (1) symmetry, deconfined spinons

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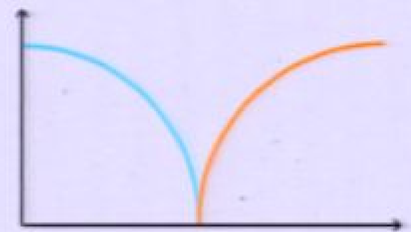

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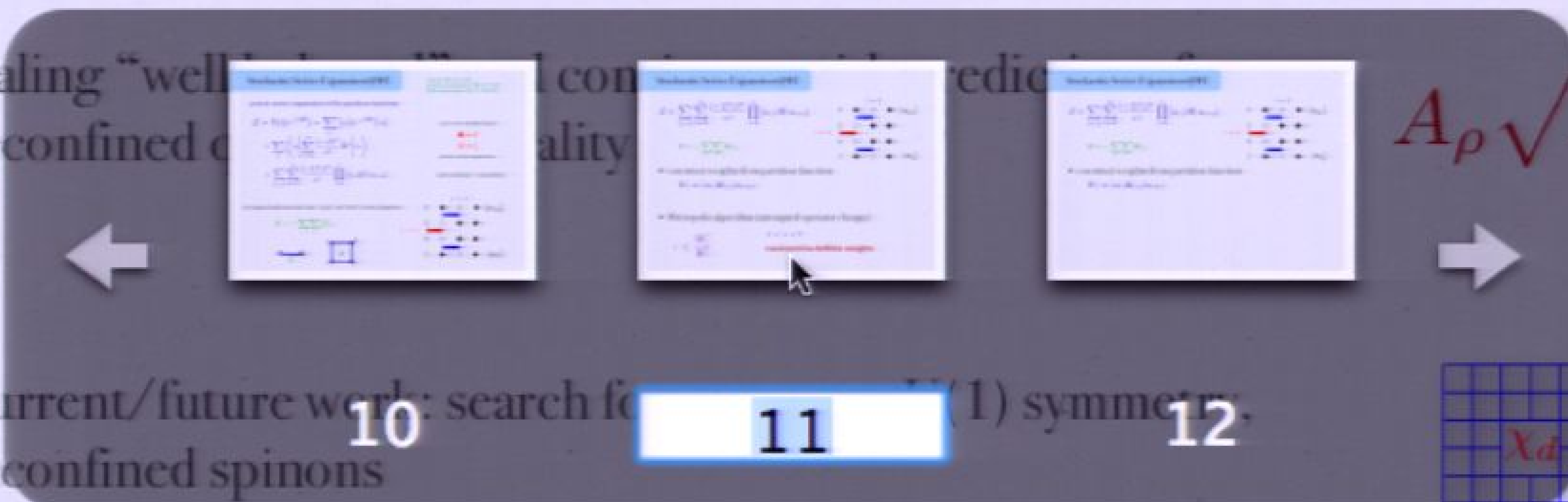

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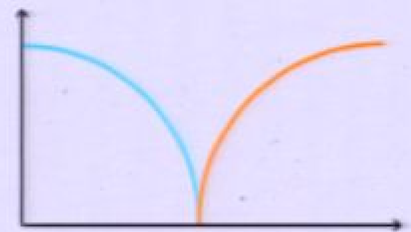

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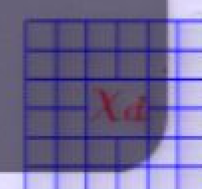
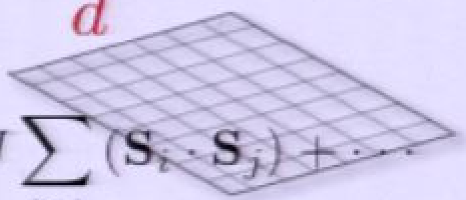


Quantum Monte Carlo

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

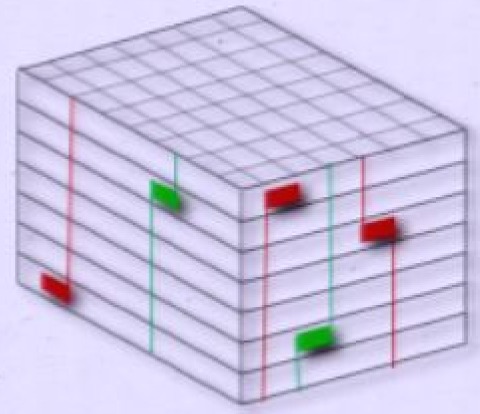
map to higher dimensional classical system

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:

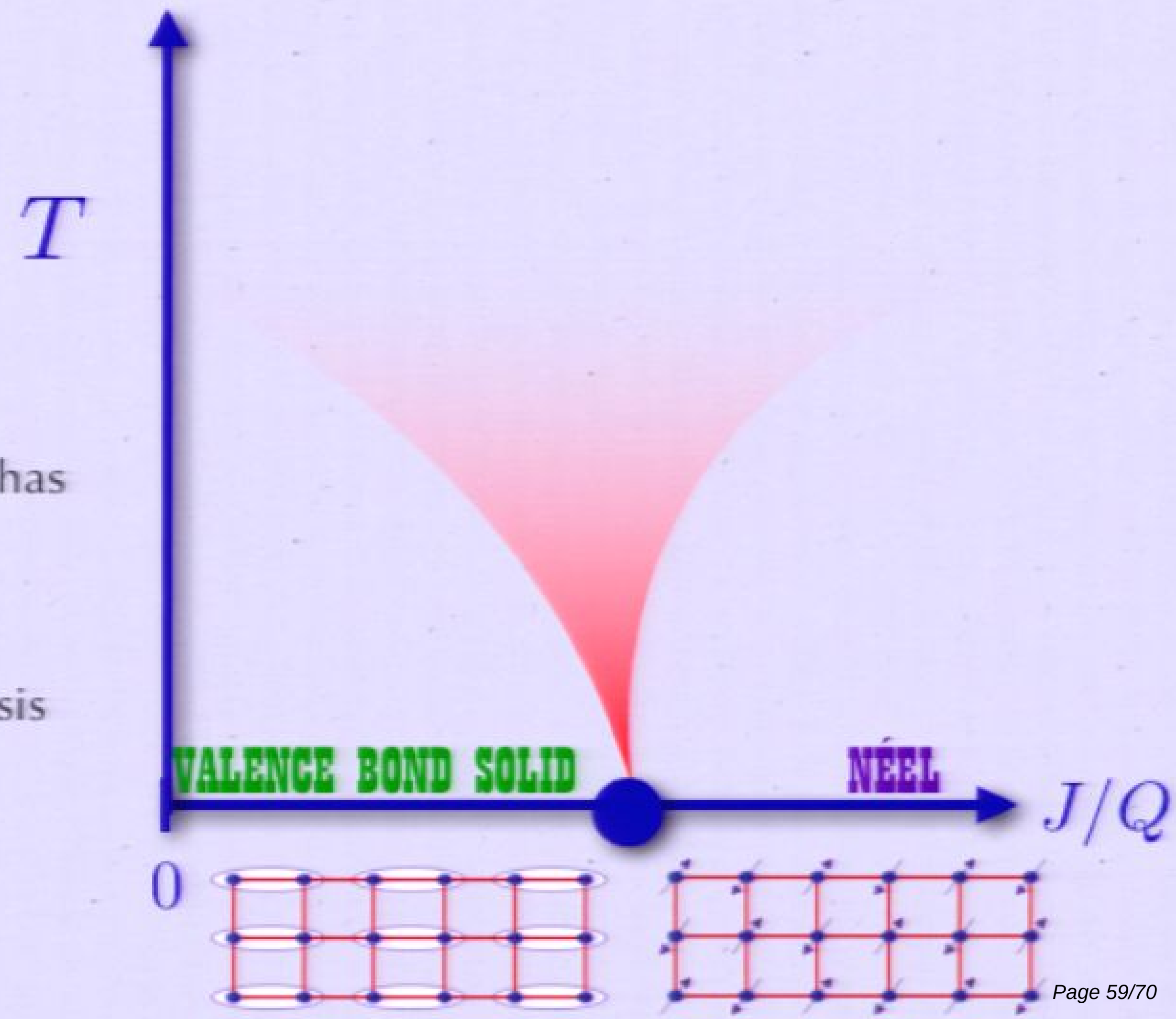
- -sign problem
- -ergodicity/freezing problems

Sandvik's J-Q model

can we study via a finite-T QMC formalism in the S^z basis?

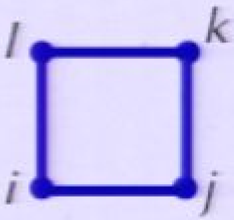
- the overcomplete VB-basis has no sign problem

- the more powerful finite-T formalism based on the Sz basis does (naively)



Sandvik's J-Q model

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



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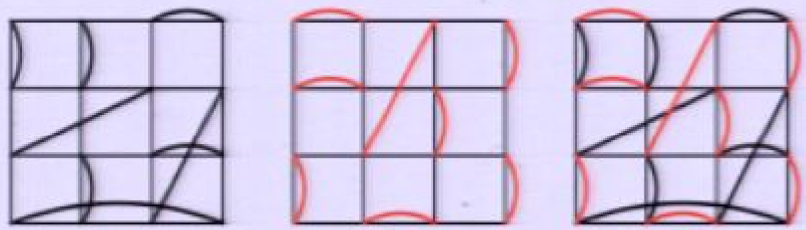
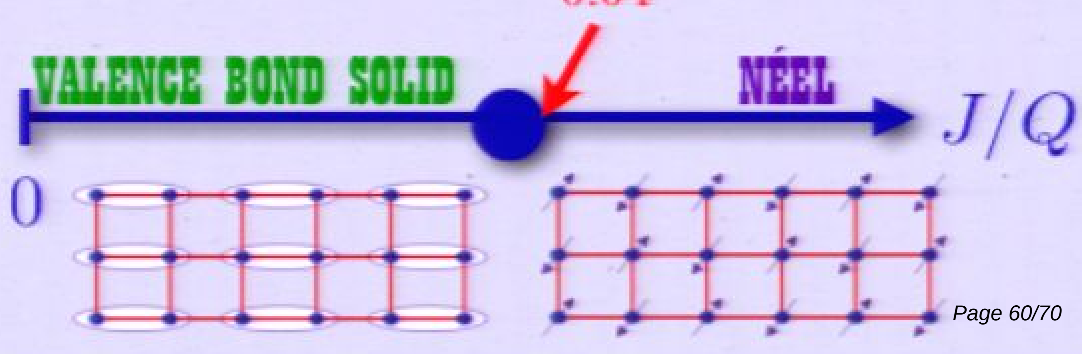
Valence Bond Basis
Sandvik
Phys. Rev. Lett. **95**, 207203 (2005)



$|S_\alpha\rangle$ $|S_\beta\rangle$ $\langle S_\alpha|S_\beta\rangle$

T=0 projector Quantum Monte Carlo up to L=32

Good numerical evidence for a direct (!) continuous quantum critical point



 $= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

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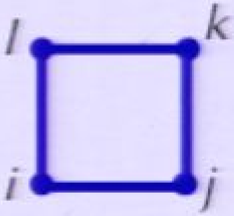

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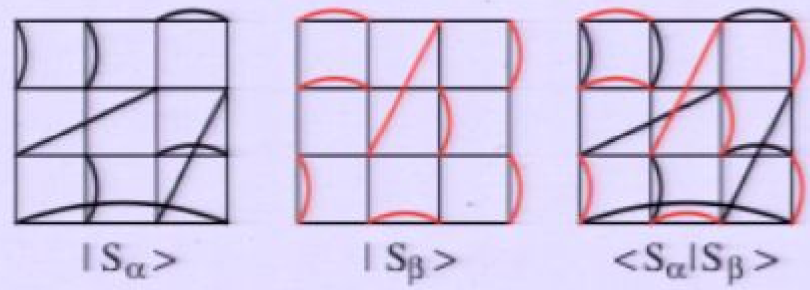

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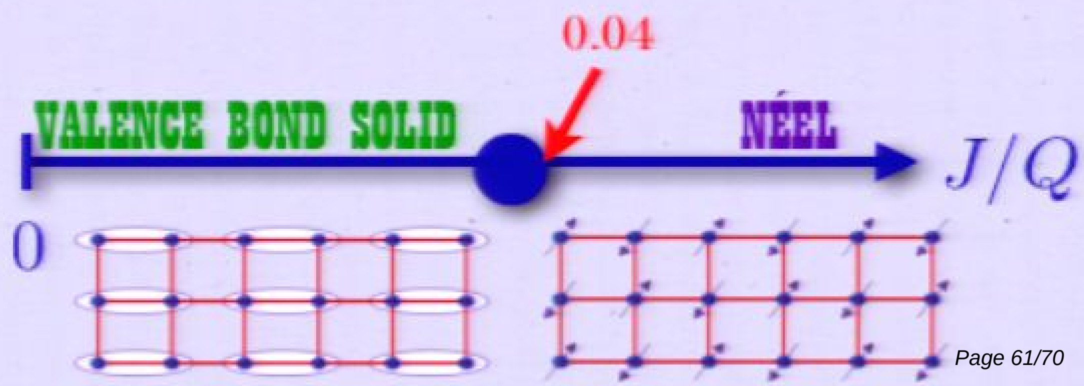


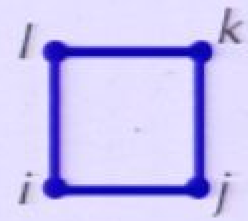
 $= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

Heisenberg "ring exchange" models

CUPRATES: low-energy effective theory of Hubbard model

$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle i,j_2 \rangle} \mathbf{S}_i \cdot \mathbf{S}_{j_2} + J_3 \sum_{\langle i,j_3 \rangle} \mathbf{S}_i \cdot \mathbf{S}_{j_3}$$

$$+ J_c \sum_{\langle i,j,k,l \rangle} [(\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) + (\mathbf{S}_i \cdot \mathbf{S}_l)(\mathbf{S}_j \cdot \mathbf{S}_k) - (\mathbf{S}_i \cdot \mathbf{S}_k)(\mathbf{S}_j \cdot \mathbf{S}_l)]$$



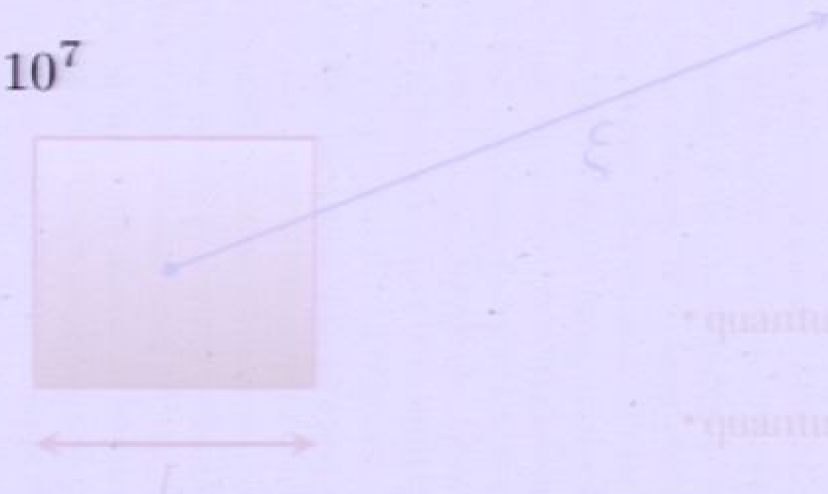
microscopic models: 2D spin 1/2

goal: destabilize conventional Néel order, and realize interesting quantum phases and phase transitions...

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \cdots$$

in models *without* the sign problem: quantum monte carlo

- allows for exact (unbiased) solutions
- very large systems sizes $\leq 10^7$



- quantum phases
- quantum phase transitions

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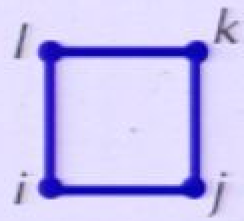
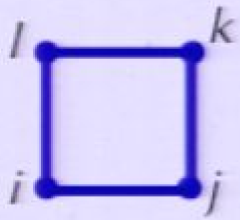


TOY MODEL:

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

Sandvik's J-Q model

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



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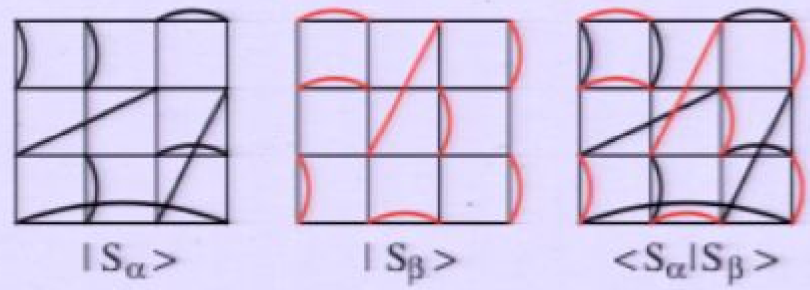

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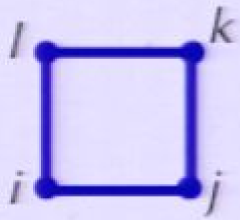

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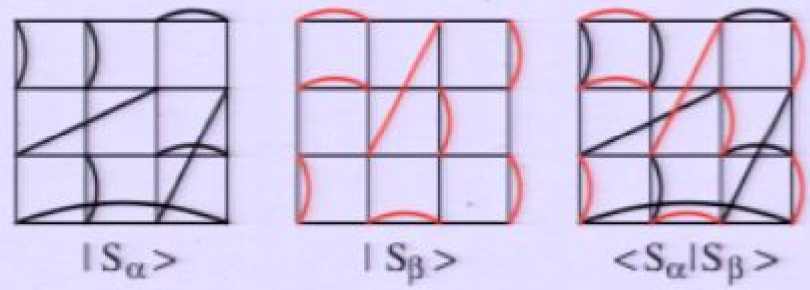

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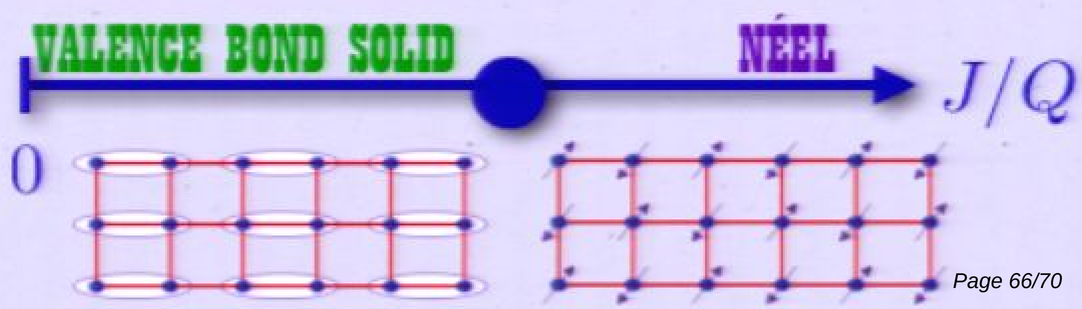

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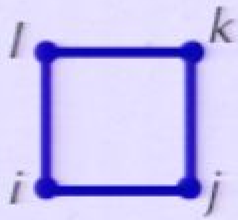

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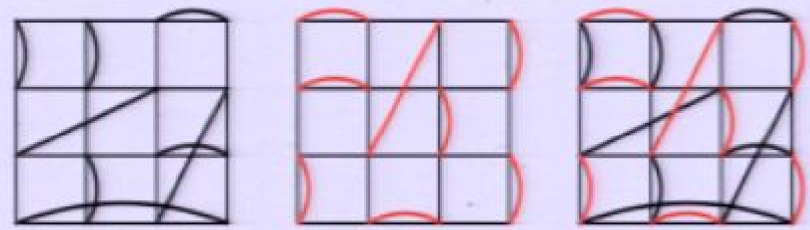

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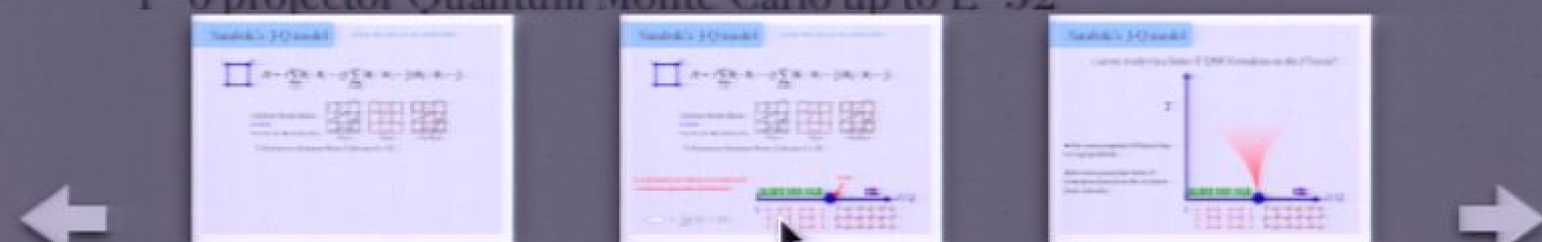

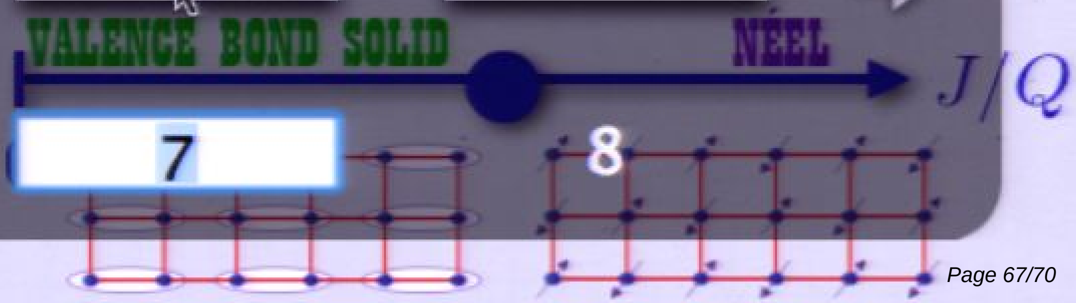

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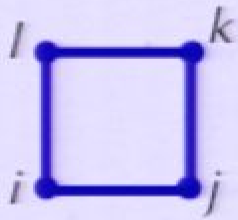

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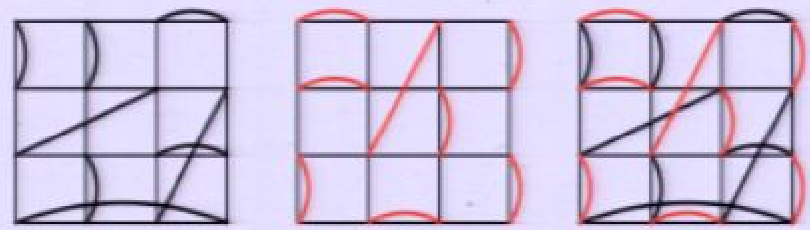

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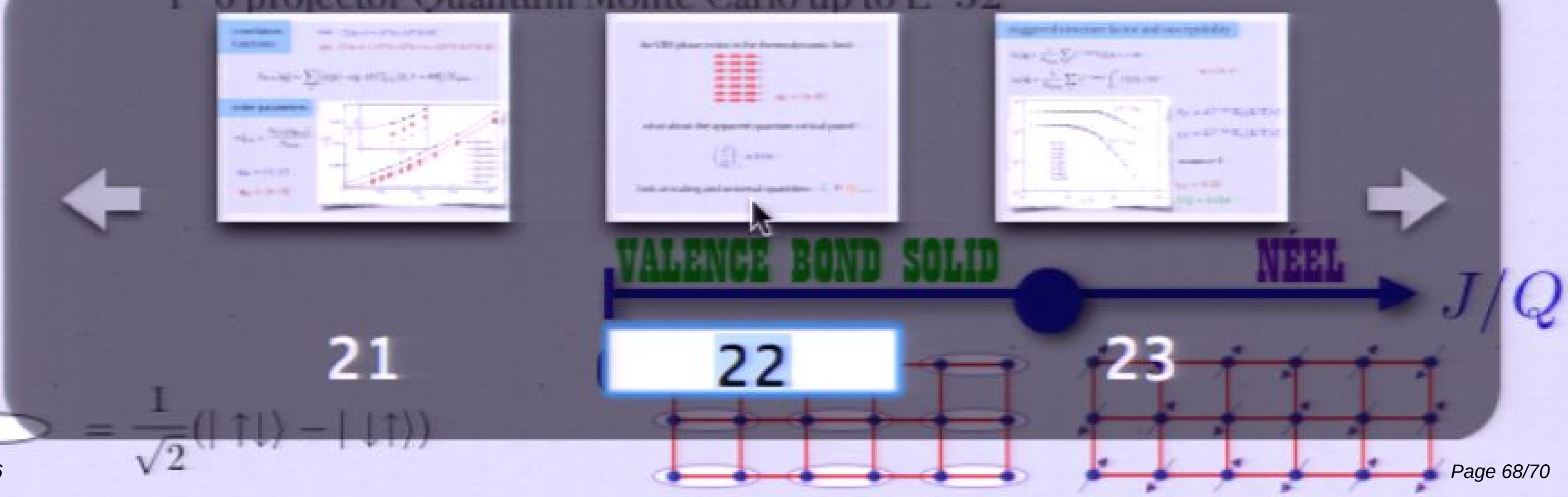

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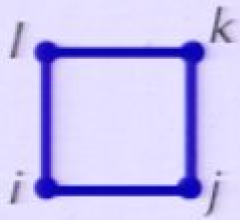

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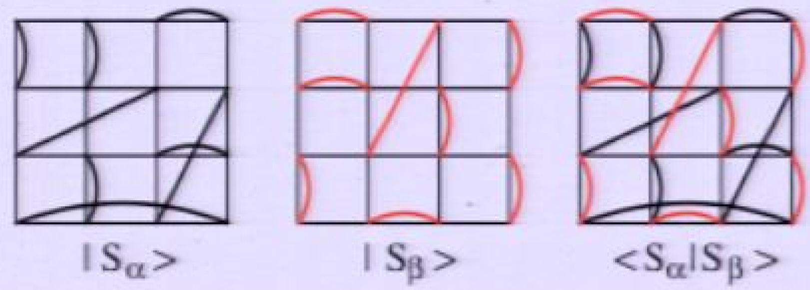

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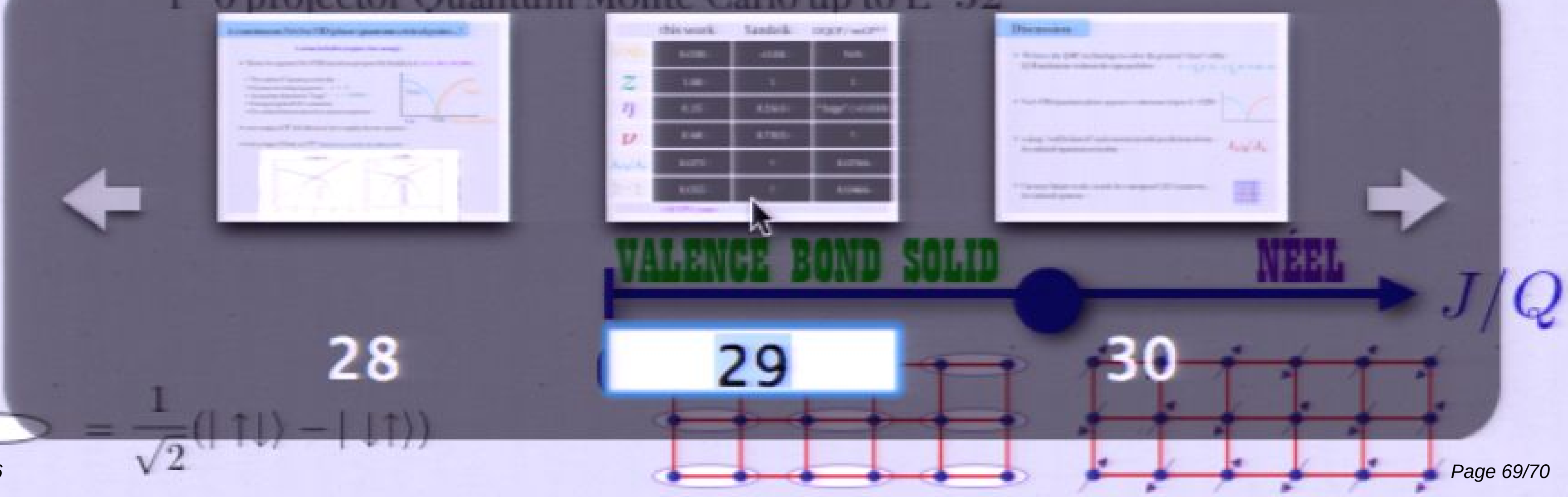

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	this work	Sandvik	DQCP / ncCP^{N-1}
$(J/Q)_c$	0.038	<0.04	N/A
z	1.00	1	1
η	0.35	0.26(3)	"large" (>0.038)
ν	0.68	0.78(3)	?
$A_\rho \sqrt{A_\chi}$	0.075	?	0.0766
$\frac{T\chi_u}{C_v} = \frac{A_\chi}{A_{C_v}}$	0.055	?	0.0466