Unconventional Quantum Criticality in 2D Dimerized Quantum Magnets

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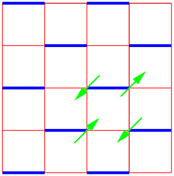
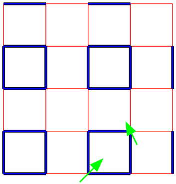
Stefan Wessel (Stuttgart)

ComPhys08, November 2008





Outline

SW, L. Bogacz, W. Janke, Phys. Rev. Lett. **101**, 127202 (2008).

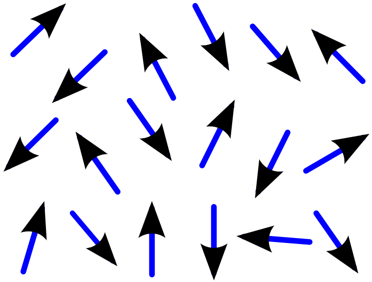
SW, W. Janke, Phys. Rev. B (in print); `arXiv:0808.1418`

Agenda:

- Dimerized Heisenberg Models
- Quantum Phase Transitions (Phenomenology)
- QMC: Critical Exponents
- QMC: Thermodynamics at Criticality

Dimerized quantum magnets: Ingredients

- take a **bunch** of (molecules with) **spins** S
- lattice + interaction $H = J \sum_{\langle i,j \rangle} S_i S_j$ + $T = 0K$
- add **deformation** / **perturbation** / **modulation** α



The cuprates, magnetism, ...

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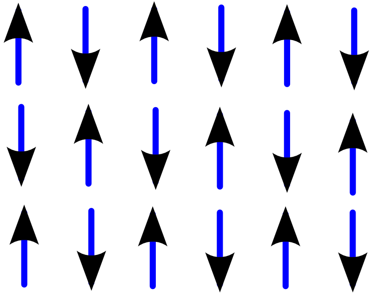
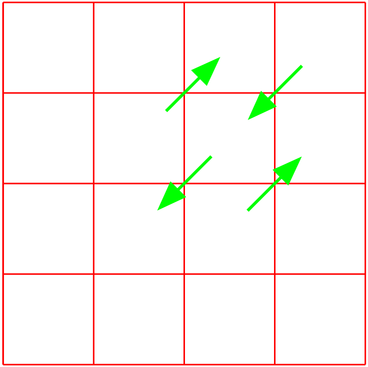
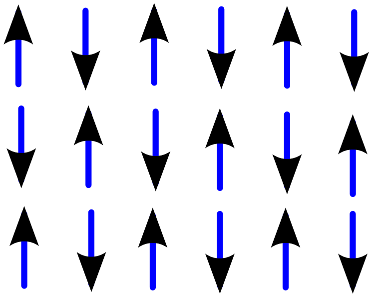


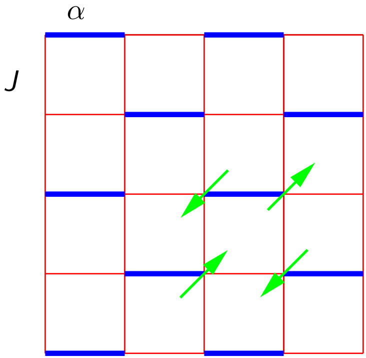


The cuprates, magnetism, ...

Dimerized quantum magnets: Ingredients

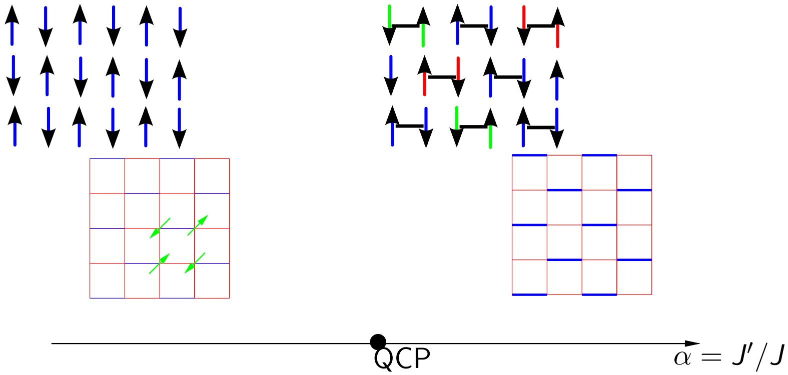
- take a **bunch** of (molecules with) **spins** S
- interaction $H = J\sum_{\langle i,j\rangle} S_i S_j + \alpha \sum_{\langle i,j\rangle'} S_i S_j$
- add **deformation** / **perturbation** / **modulation** α





The cuprates, magnetism, ...

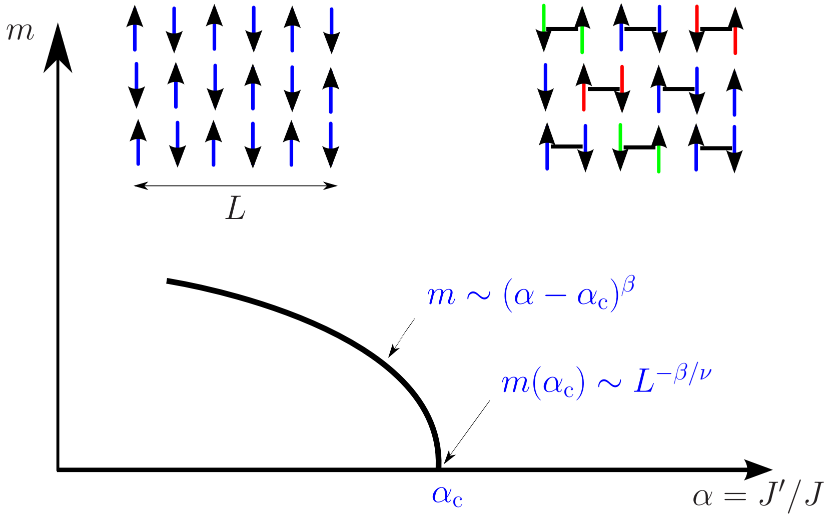
Driving a Phase Transition: Quantum Melting



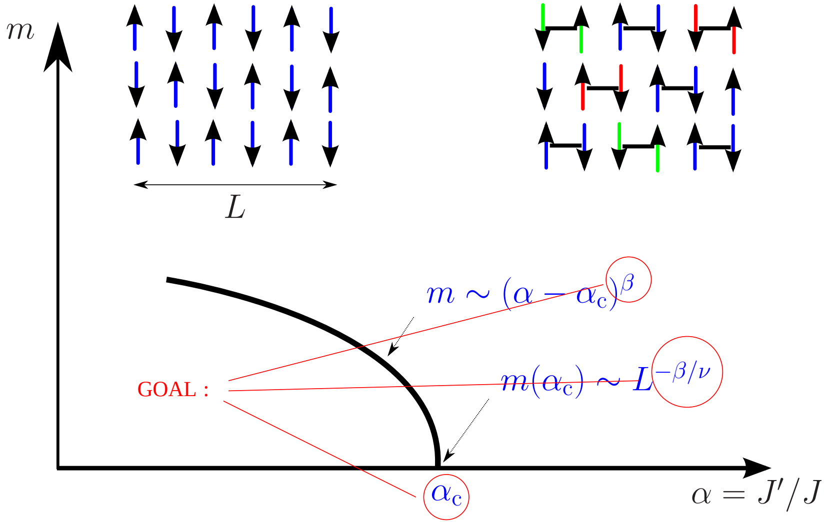
finite staggered magnetization
no excitation gap
$O(3)$ symmetry broken

gas of singlets
finite excitation gap Δ
no symmetry broken

Characterizing the Phase Transition



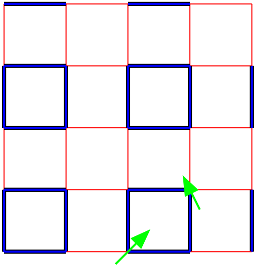
Objectives:



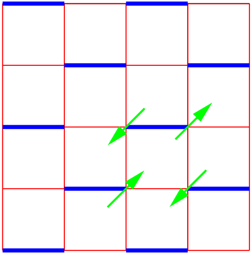
m
L
$m \sim (\alpha - \alpha_c)^\beta$
GOAL :
$m(\alpha_c) \sim L^{-\beta/\nu}$
α_c
$\alpha = J'/J$

Universality?

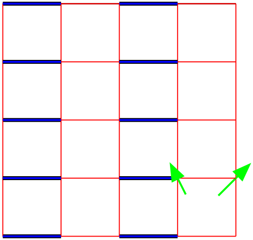
plaquette



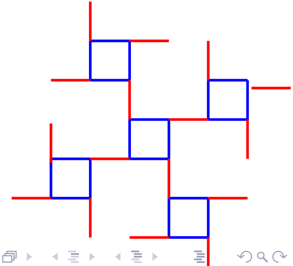
staggered



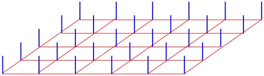
ladder



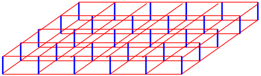
CaVO lattice



inc. bilayer



bilayer



Universality?

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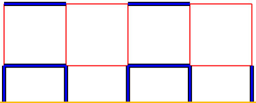

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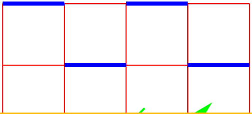
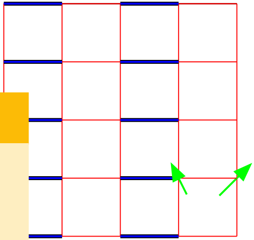


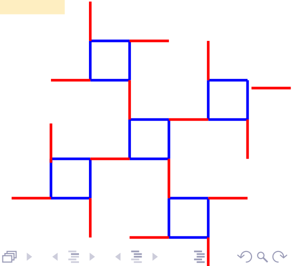
ladder



=> Predictions (from key principles):

- **universality**: all magnets have **same** β, ν
- **in fact:** $\beta = 0.369$, $\nu = 0.711$ (3D O(3) universality class)

O lattice



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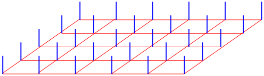
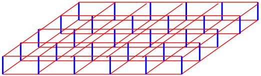


bilayer



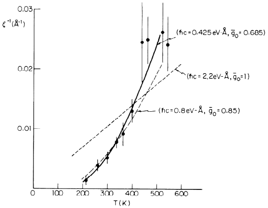
Criticality: Field theoretic predictions and the NLSM

express magnetic order in terms of a field $\hat{n}(r)$

Action of field theory

$$S_n = \frac{1}{2g}\int \mathrm{d}\tau \int \mathrm{d}^2 r \left[\frac{1}{c^2}\left(\frac{\partial n}{\partial \tau}\right)^2 + (\nabla_r n)^2\right] (NLSM)$$

$+ iS_B$ Berry phase terms



La_2CuO_4

Haldane (1983), Chakravarty *et al.*(1989), Chubukov *et al.*(1993), ...

NLSM is in 3D O(3) universality class!

d-dimensional quantum system $\rightarrow$ $d+1$ - dim class. system

$z = 1$

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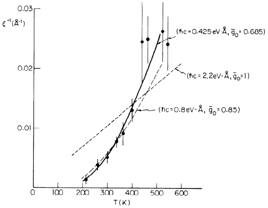

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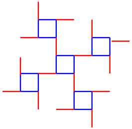
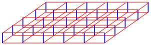
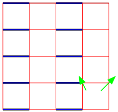
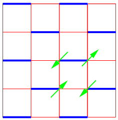
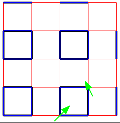
What has been done?

Model	crit. J'/J, exponent ν	who, method
	$0.939(1)$, $\nu = 0.695(30)$	Troyer *et al.* 1997; QMC
	$2.5220(1)$, $\nu = 0.7106(9)$	Wang *et al.* 2006; QMC
	$1.909(1)$, $\nu = 0.71(3)$	Matsumoto *et al.* 2001; QMC
	$\approx 2.56(7)$, ν?	R. Singh *et al.* 1988; Series Exp.
	$\approx 1.82(1)$, ν?	A. Läuchli *et al.* 2002; (QMC)

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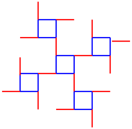
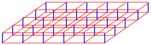
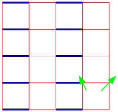
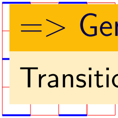
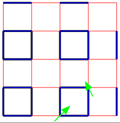
	$0.939(1)$, $\nu = 0.695(30)$	Troyer *et al.* 1997; QMC
	$2.5220(1)$, $\nu = 0.7106(9)$	Wang *et al.* 2006; QMC
	$1.909(1)$, $\nu = 0.71(3)$	Matsumoto *et al.* 2001; QMC
		
	$\approx 1.82(1)$, $\nu?$	A. Läuchli *et al.* 2002; (QMC)

=> Generally Accepted:

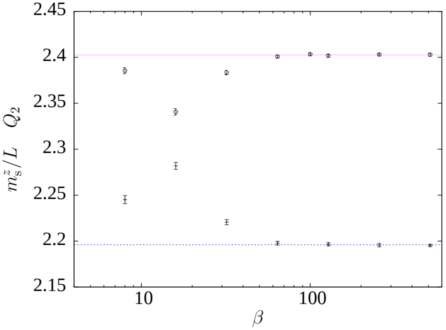
Transition is indeed in 3D $O(3)$ universality class! **??**

Computer Experiments: Expectations vs Reality

- perform **quantum Monte Carlo** investigations
- scan couplings, measure stagg. magnetization

$$m_s^z = \frac{1}{N} \sum_j (-1)^{x+y} S_j^z$$

- access ground state (β large enough)



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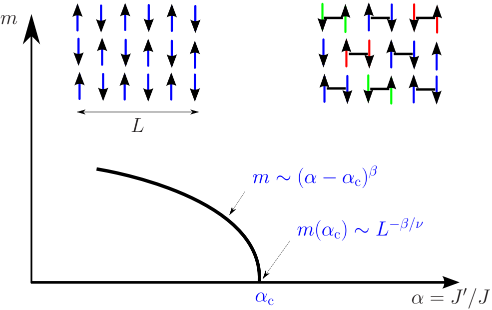
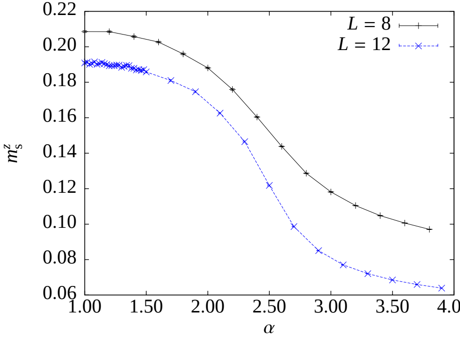


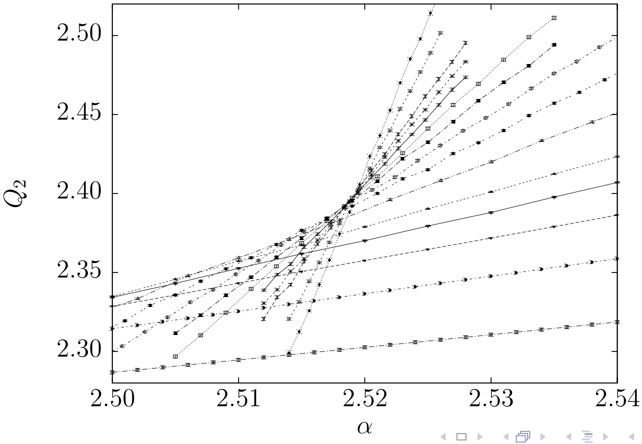


The critical coupling from the Binder parameter Q_2

- to obtain the critical coupling, best to use Binder parameter

$$Q_2 = \frac{\langle (m_s^z)^4 \rangle}{\langle (m_s^z)^2 \rangle^2}$$

should cross at the critical point (for different lattice sizes)

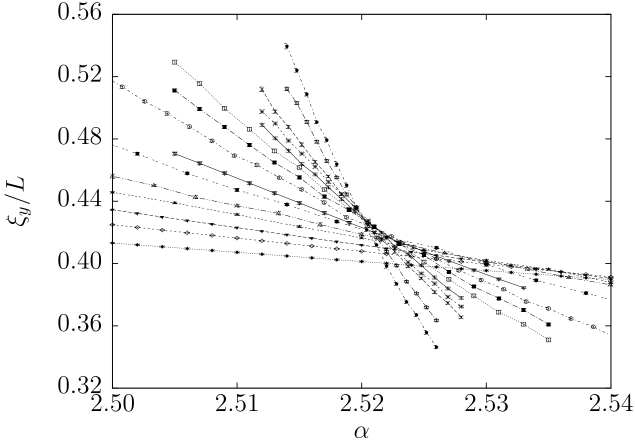


The critical coupling from the correlation length ξ_y/L

- similar for correlation length

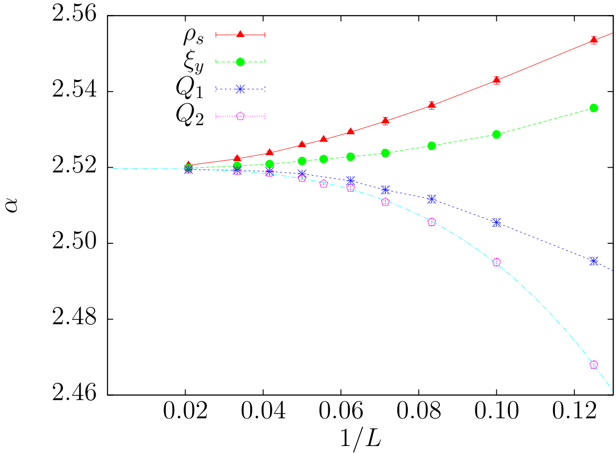
$$\xi_y = \frac{L_y}{2\pi}\sqrt{\frac{S(\pi,\pi)}{S(\pi,\pi+2\pi/L_y)} - 1}$$

- here from L=8 to L=96 (ca 9216 quantum spins)



Bracketing the critical coupling

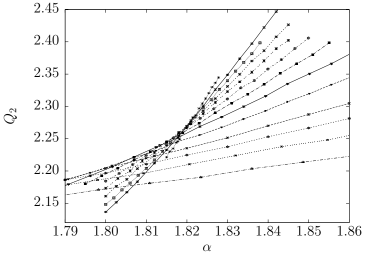
take intersection points for curves from L and $2L$



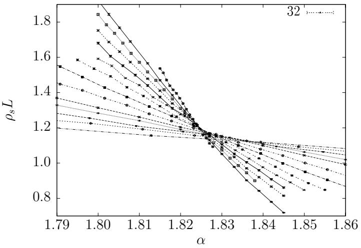
fit $\alpha_c(L, 2L) = \alpha_c + cL^{-1/\nu-\omega}$ $\alpha_c = 2.5198(3)$

Results for plaquette model

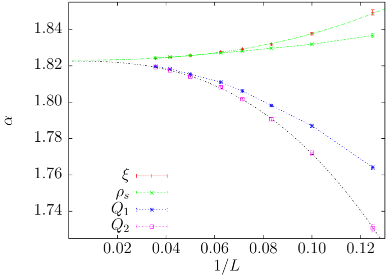
Binder parameter:



spin stiffness:



Scaling of crossing points:



Estimate for the critical coupling:

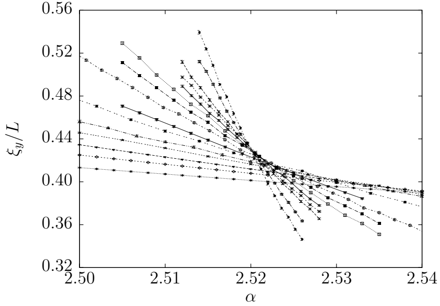
$\alpha_c = 1.8229(3)$

Finite-size scaling: Data collapsing

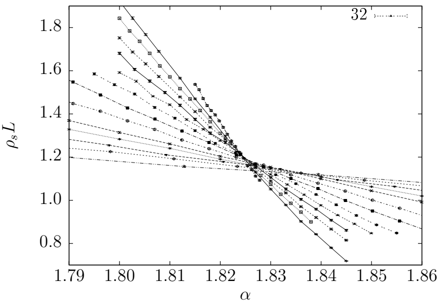
Scaling assumption:

$$A_L = L^{\lambda/\nu}(1 + cL^{-\omega})f_A\left(|t|L^{1/\nu}\right)$$

staggered model



plaquette model



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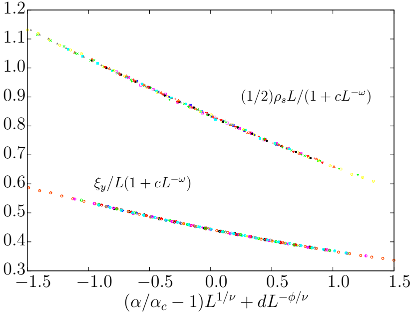

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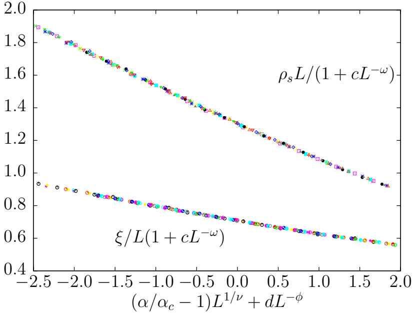


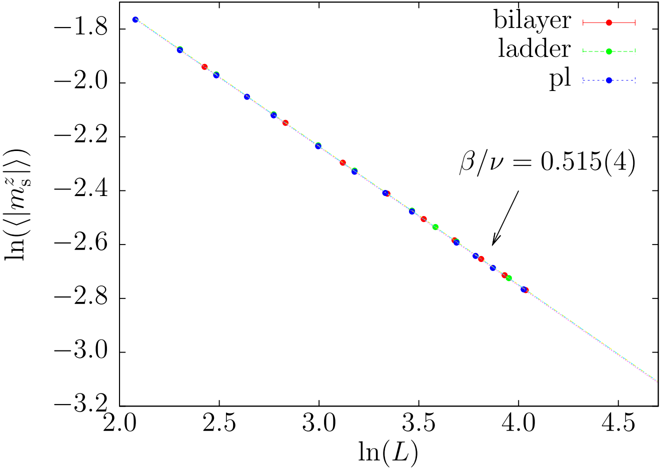
$\nu = 0.689(5)$

$\nu = 0.714(5)$

Is there a difference?

Magnetization at criticality: exponent β/ν

$$|m_s^z| \sim L^{-\beta/\nu}$$



O(3): $\beta/\nu = 0.5188(3)$ Campostrini, Rossi, Vicari, Hasenbusch, Pelisseto (2002)

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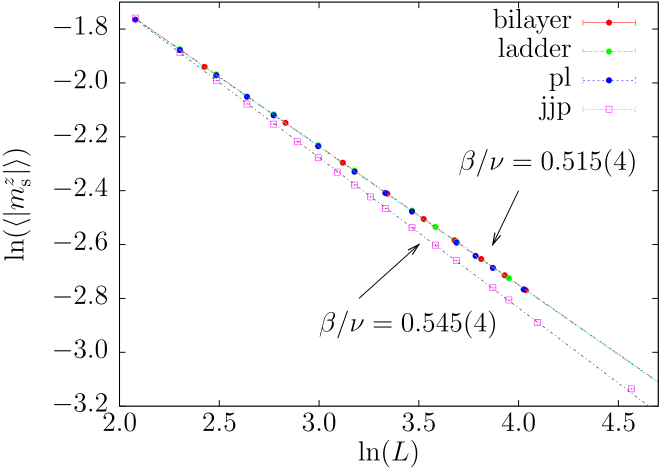

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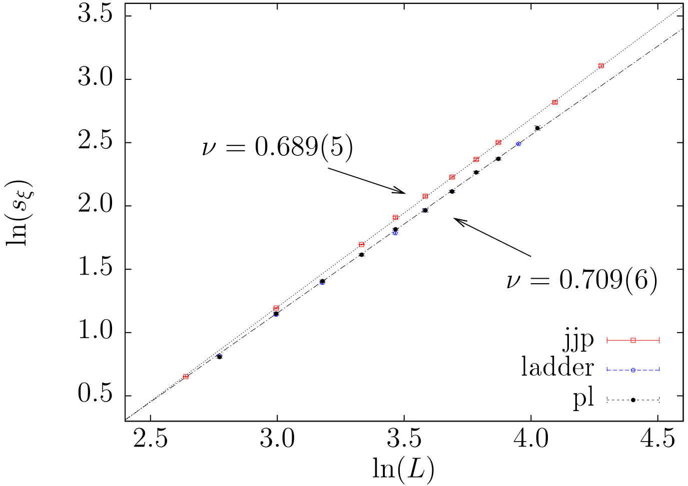
$\beta/\nu = 0.5188(3)$ Campostrini, Rossi, Vicari, Hasenbusch, Pelisseto (2002)

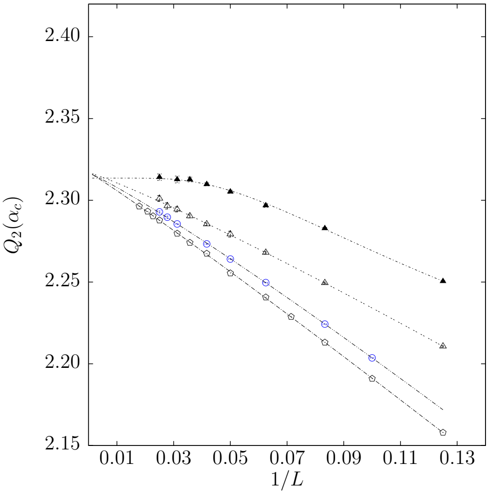
Scaling at criticality: exponent ν

$$s_\xi = \frac{\partial}{\partial \alpha}(\xi/L) \restriction_{\alpha_c} \sim L^{1/\nu}$$



O(3): $\nu = 0.7112(5)$ Campostrini *et al.*(2002)

The critical Binder parameter



$$Q_2 = \frac{\langle (m_s^z)^4 \rangle}{\langle (m_s^z)^2 \rangle^2}$$

- (a) plaquette
- (b) ladder
- (c) bilayer
- (d) inc. bilayer
- (e) classical O(3) model in 3D
- (f) the staggered model

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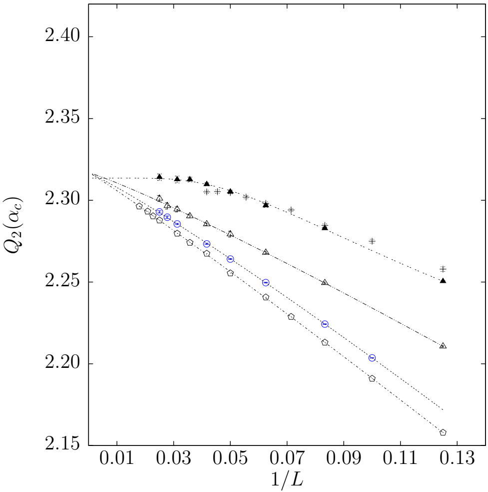

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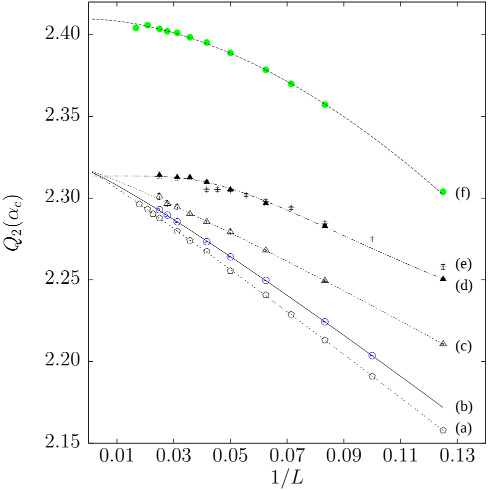

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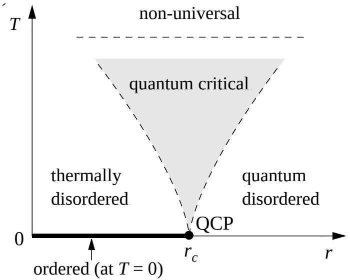
- (f) the staggered model

Experimentally detectable?: Thermodynamics of χ_u



M. Vojta (2003)

NLSM prediction for χ_{u} at critical point:

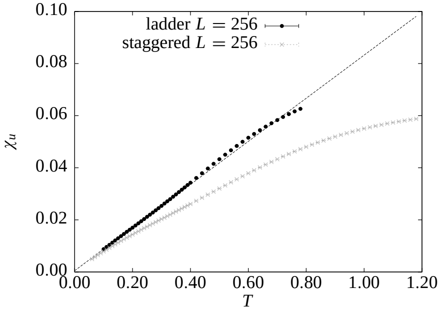
$$\begin{aligned}\chi_{\mathrm{u}} &= \mathrm{d}\langle M^z \rangle / \mathrm{d}H = \Omega T \\ &= \frac{\sqrt{5}}{\pi c^2} \ln\left(\frac{\sqrt{5}+1}{2}\right)\left(\frac{8\pi}{15}\rho_{\mathrm{s}} + 0.7937\, T\right)\end{aligned}$$

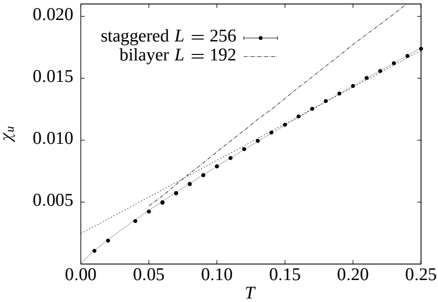
Chubukov, Sachdev, Yeh (1993)

Experimentally detectable?: Thermodynamics of χ_u

NLSM prediction for χ_{u} at critical point:

$$\chi_{\mathrm{u}} = \mathrm{d}\langle M^z \rangle / \mathrm{d}H = \Omega T$$





Experimentally detectable?: Thermodynamics of χ_u

NLSM prediction for χ_u at critical point:

$$\chi_\mathrm{u} = \mathrm{d}\langle M^z\rangle/\mathrm{d}H = \Omega T$$

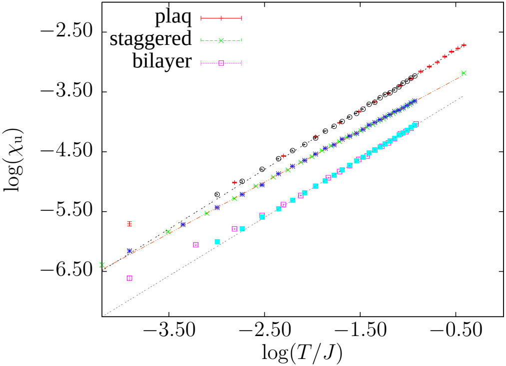
take $L = 128, 256$

assume $\chi_u \sim T^\kappa$

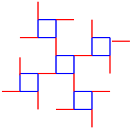
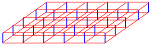
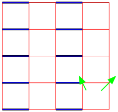
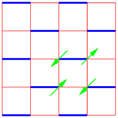
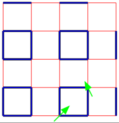
model	κ
bilayer	0.99(2)
plaquette	0.98(2)
staggered	0.89(2)

as $\kappa = d/z - 1$

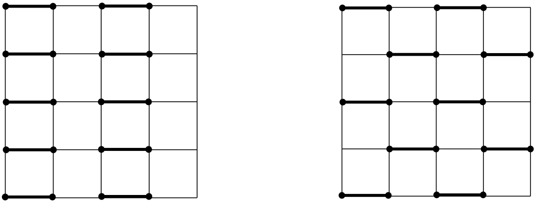
$\Rightarrow z \approx 1.05$



Summary: Overview

Model	crit. J'/J, exponent ν	who, method
	0.939(1), $\nu = 0.695(30)$	Troyer *et al.* 1997; QMC
	2.5220(1), $\nu = 0.7106(9)$	Wang *et al.* 2006; QMC
	1.9096(2), $\nu = 0.708(4)$	here
	2.5196(2), $\nu = 0.690(5)$	here
	1.8230(2), $\nu = 0.709(4)$	here

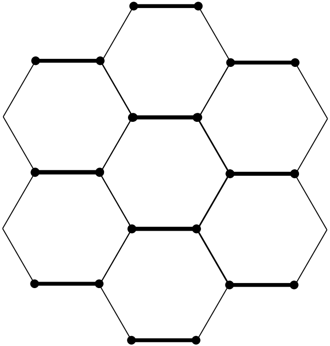
Summary: What you should take home

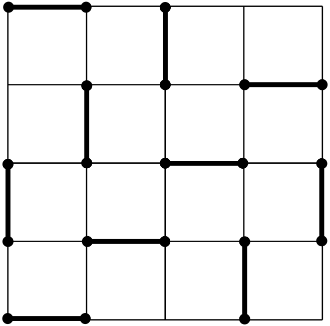


- are **completely different** quantum magnets (different critical exponents, thermodynamic behaviour).
- effects **not** captured by NLSM
- **universality** is **violated** due to suble quantum effects.
- conjecture: **geometry** of the staggered model leads to **resonating interference of topological terms** (iS_{top}) in the action that change criticality.

Outlook

- field theoretical analysis (started)
- other quantities (dynamical correlation functions ?)
- extend to $S = 1$ and $S = 3/2$.
- experimental investigation of these systems (??)
- **honeycomb** and **herringbone** model (partly finished)





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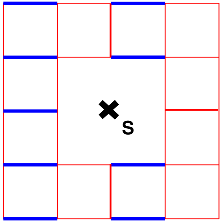
Literature:

1. SW, L. Bogacz, W. Janke, Phys. Rev. Lett. **101**, 127202 (2008).
2. SW, W. Janke, Phys. Rev. B (in print); `arXiv:0808.1418`

Thank You

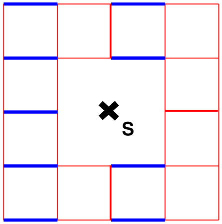
A critical vacancy



Sachdev, Buroghain, Vojta, Science **286**, 2479 (1999):

consider one vacancy ($\times$) in quantum critical system:

A critical vacancy



Sachdev, Buroghain, Vojta, Science **286**, 2479 (1999): consider one vacancy ($\times$) in quantum critical system:

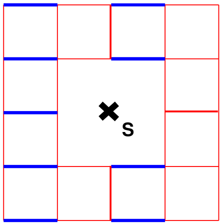
- $\chi_{-} = \chi_0 + \chi_{\rm imp}$

$$\chi_{\rm imp} = \frac{C^\star}{T}(1 + \dots)$$

$$C^\star = \frac{1}{4}(1 + (33\epsilon/40)^{1/2} + \dots)$$

- $C^\star$ **universal** within universality class

A critical vacancy



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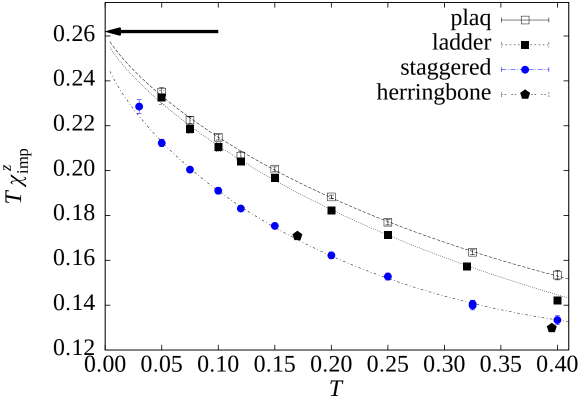
- $C^\star$ **universal** within universality class

so far 2 QMC studies for dimerized models:

- Troyer (2004): $C^\star = 1/4$ (no visible quantum effect)
- Höglund, Sandvik, PRL (2007): $C^\star = 0.262(2)$

A critical vacancy: Preliminary QMC results



- simulations **VERY** demanding (as $\chi_{\mathrm{imp}} = \chi_- - \chi_0$)
- can argue pro anomalous $C^\star > 0.25$
- staggered model again different, asymptotic $T \to 0$ difficult

Deconfined Excitations?

1. Senthil *et al.* (2004): Deconfined Quantum Criticality in 2D where Berry phases play decisive role.
2. Yoshioka *et al.* (2004): argued in favour of deconfinement in staggered model based on $\mathrm{CP}^1 + \mathrm{U}(1)$ (but: questioned by Senthil *et al.*)

FIG. 1. Numbering and dimer picture:cross symbol is odd site, and spot symbol is even site. Solid line means that its correlation is stronger than dotted lines.

Néel-Dimer Transition in Antiferromagnetic Heisenberg
and Deconfinement of Spinons at the Critical Point

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(August 6, 2006)

Quantum phase transition from the Néel to the dimer states in an antiferromagnetic(AF model on square lattice is studied. We introduce a control parameter α for the excha which connects the Néel ($\alpha = 0$) and the dimer ($\alpha = 1$) states. We employ the CP^1 re of the $s = \frac{1}{2}$ spin operator and integrate out the half of the CP^1 variables at odd sites CP^1 nonlinear σ model. The effective coupling constant is a function of α and at α = model is in the ordered phase which corresponds to the Néel state of the AF Heisenbe phase transition to the dimer state occurs at a certain critical value of α_C as α incre Néel state, the dynamical composite U(1) gauge field in the CP^1 model is in a Higg low-energy excitations are gapless spin wave. In the dimer phase, a confinement phase theory with $s = 1$ excitations is realized. For the critical point, we argue that a de phase, which is similar to the Coulomb phase in 3 spatial dimensions, is realized and s appear as low-energy excitations.