

# Quantum Phase Transitions and Hidden Orders in Low-Dimensional Spin Systems

Gennady Y. Chitov  
*Laurentian University*  
*Sudbury, Canada*  
*and*  
*KIT, Germany*

**Collaborators: (all at LU)**

*Prof. Ralf Meyer*

*Prof. Mohamed Azzouz*

*Students:*

*Sandra J. Gibson*

*Brandon Ramakko*

*Khalada Shahin*

**Supported by:**



# Outline:

- **Motivation: Phase Transitions without Conventional Landau Local Order Parameters -- Examples**
- **Two- & Three-Leg Ladders – More Motivation**
- **Staggering Patterns & Quantum Criticality**
- **Ground State Energies and Gaps**
- **String Order Parameters**
- **Conclusions**

# Motivation:

## Phase transitions without local order parameter

### 1. Berezinskii-Kosterlitz-Thouless Transition.

2D classical XY model

$$H = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j)$$

$$\langle S_i \rangle = 0 \quad \text{No long-range order}$$

$$\exists \text{ finite } T_C \quad \langle S_i S_j \rangle \longrightarrow \text{exponential}$$

$$\downarrow$$

**power-law**

Binding-Unbinding of vortices

Conventional Landau Theory

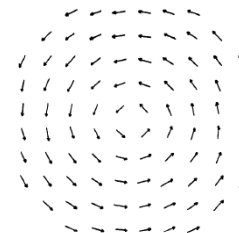
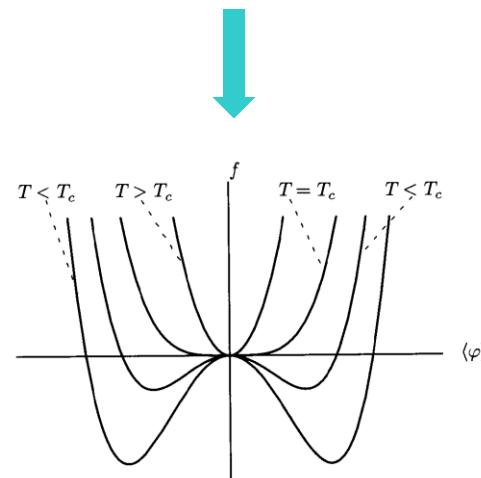


Figure 1. An isolated vortex in the xy model.

J M Kosterlitz and D J Thouless  
J. Phys. C: Solid State Phys., Vol. 6, 1973.

## 2. Solid-on-Solid Models. Surface Roughening Transitions

Den Nijs & Rommelse  
PRB 1989

$$H_{\text{RSOS}} = \sum_R \{ K[\delta(|h_1 - h_2| - 1) + \delta(|h_2 - h_3| - 1)] + L_1^{(x)}\delta(|h_1 - h_3| - 1) + L_2^{(x)}\delta(|h_1 - h_3| - 2) \\ + L_1^{(t)}\delta(|h_2 - h_4| - 1) + L_2^{(t)}\delta(|h_2 - h_4| - 2) + Q\delta(|h_1 - h_3| - 1)\delta(|h_2 - h_4| - 1) \} ,$$

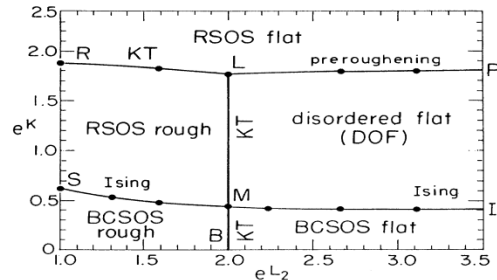


FIG. 2. Phase diagram of the RSOS model with nearest-neighbor interactions  $K$  and step repulsion  $L_2 = L_2^{(x)} = L_2^{(t)}$ , and the coupling constants  $Q = L_1^{(x)} = L_2^{(t)} = 0$ .

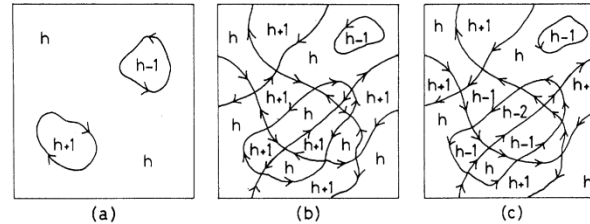


FIG. 3. Typical configurations in the RSOS flat phase (a), the disordered flat (DOF) phase (b), and RSOS rough phase (c).

No long-range order

Mapping: SOS  $\implies$  6-vertex model

Ising spin

$$\sigma_r = \exp(i\pi h_r).$$

$$G_H(\mathbf{r}_n - \mathbf{r}_0) = \langle \sigma_{\mathbf{r}_n} \sigma_{\mathbf{r}_0} \rangle = \langle \exp[i\pi(h_{\mathbf{r}_n} - h_{\mathbf{r}_0})] \rangle . \quad (2.4)$$

The Ising spins are disordered in the DOF phase and the RSOS rough phase, but ordered in the RSOS flat phase.  $G_H$  decays exponentially to zero in the DOF phase and to zero as a power law in the RSOS rough phase, but decays exponentially to the square of the Ising magnetization,

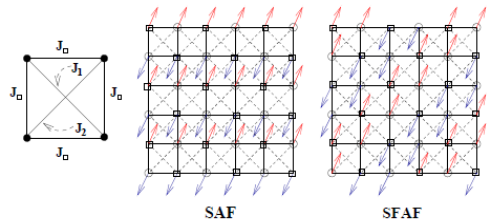
$$\rho = \langle \exp(i\pi h_r) \rangle , \quad (2.5)$$

in the RSOS flat phase. The Ising spins are AF ordered in the BCSOS flat and rough phase. There,  $G_H$  decays exponentially to the square of the staggered magnetization

More Mapping  $\implies$   
 quantum spin model  
 String Order Parameter (SOP)  
 Hidden (Topological) Order

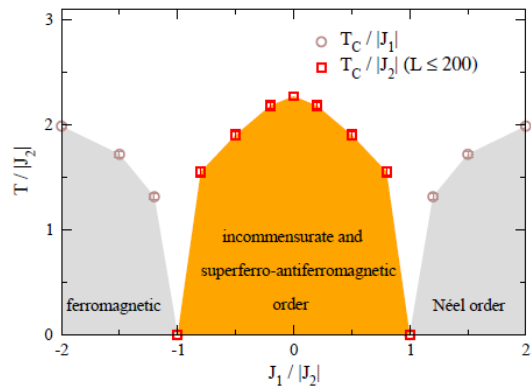
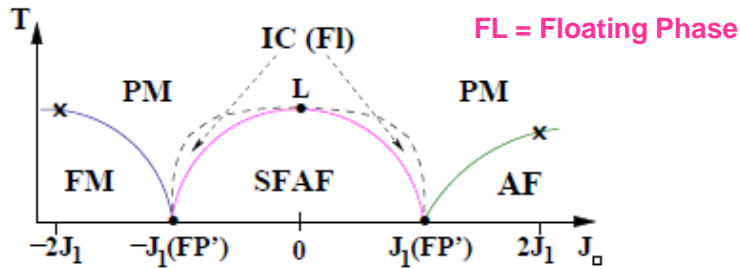
# 3. Frustrated 2D nn+nnn Ising Model

G. Y. Chitov and C. Gros Low Temp. Phys. 31 (8-9), August-September 2005

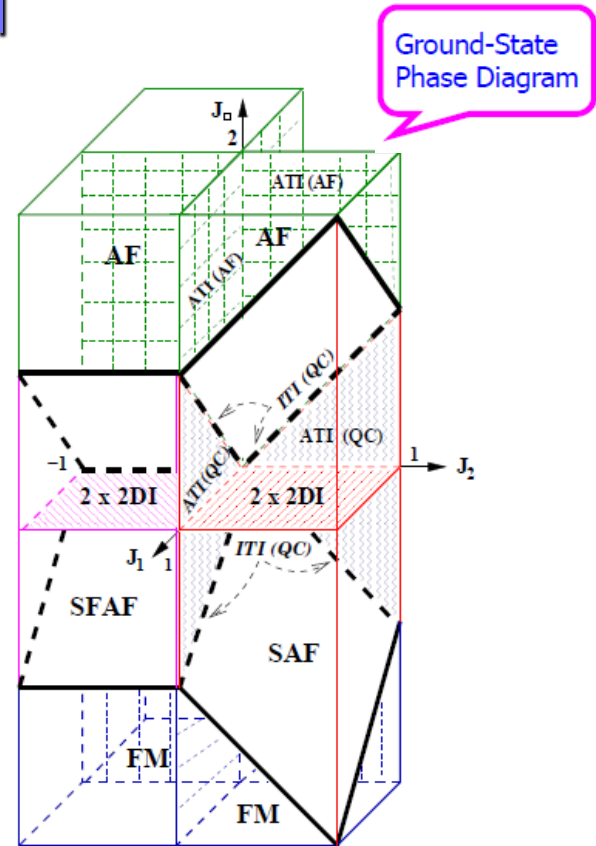


Super-Antiferromagnetic

4x4



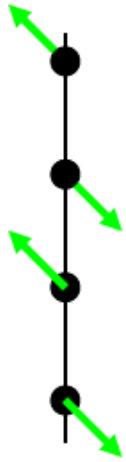
A. Kalz and G.Y.C., in preparation



PM to FL transition =  
 BKT transition ->  
 NO local Order Parameter  
 Power-Law Correlation function  
 Analogue: 2D ANNNI model  
 P. Bak, Rep. Prog. Phys. (1982)

FIG. 2. Phase diagram of the anisotropic Ising model for varying nearest-neighbor interactions  $J_1/J_2$ . Critical temperatures are determined using Binder cumulants for  $|J_1| > |J_2|$  and estimated from energies and specific heats for  $|J_1| < |J_2|$ , and strongly depend on the system size - here  $L \leq 200$  (see text for more details). The agreement with a qualitative sketch in<sup>1</sup> is very good.

## 4. Spin Chain

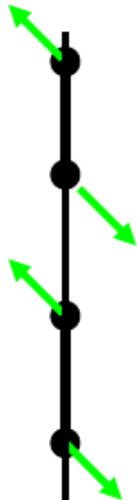


$$\mathcal{H} = J \sum_n \mathbf{S}_n \mathbf{S}_{n+1}$$

Heisenberg Chain:

Gapless State (Luttinger Liquid Universality Class)

No Magnetic LRO



$$\mathcal{H} = J \sum_n [1 + (-)^n \delta] \mathbf{S}_n \mathbf{S}_{n+1}$$

Dimerized Heisenberg Chain:

Gapped GS

No Magnetic LRO

Crossover between the Haldane-gap phase and the dimer phase  
in the spin- $\frac{1}{2}$  alternating Heisenberg chain

Kazuo Hida

$$O_{\text{str}}(i-j) = \langle \exp[i\pi(S_{2i}^z + S_{2i+1}^z + \cdots + S_{2j-1}^z)] \rangle$$

$$H = 2J' \sum_{i=1} \mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i} + 2J \sum_{i=1} \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1},$$

## Bosonization



The string order parameter is given by

$$\begin{aligned} O_{\text{str}} &= \lim_{|x-x'| \rightarrow \infty} O_{\text{str}}(x-x') \\ &= \lim_{|x-x'| \rightarrow \infty} \exp \left\{ -\frac{1}{8} \langle [\phi(x) - \phi(x')]^2 \rangle \right\} \\ &= (\pi/ma)^{1/4} \sim (1-J'/J)^{1/6}. \end{aligned}$$

for  $J'=J$ ,

$$O_{\text{str}}(x-x') \sim |x-x'|^{-1/4}$$

Baxter's 2D 8-vertex model

$$(\mu = 3\pi / 4)$$

$$\alpha = 2/3$$

$$\beta = 1/12$$

$$\nu = 2/3$$

$$\eta = 1/4$$

+ log corrections



# 5. Kitaev Model (exactly solvable, free Majorana fermions)

$$H = \sum_{j+l=\text{even}} (J_1 \sigma_{j,l}^x \sigma_{j+1,l}^x + J_2 \sigma_{j-1,l}^y \sigma_{j,l}^y + J_3 \sigma_{j,l}^z \sigma_{j,l+1}^z)$$

Kitaev, *Ann. Phys.*, 2003, 2006  
Feng, Zhang & Xiang, *PRL* 2007

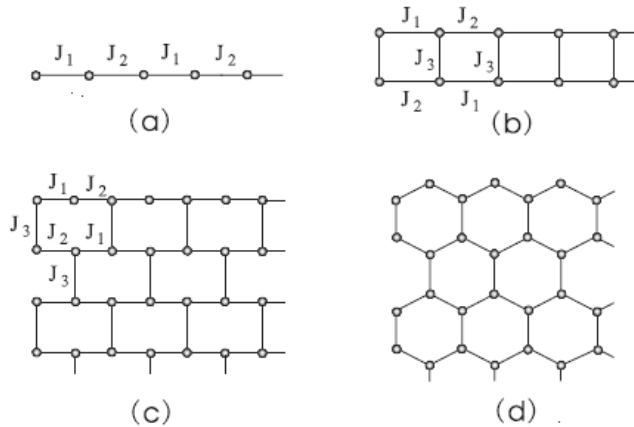


FIG. 1. A brick-wall lattice (c) with its equivalent honeycomb lattice (d). (a) and (b) are the one- and two-row limits of the brick-wall lattices, respectively.

*PRL* 98, 087204 (2007) © 2007 The American Physical Society

**Kitaev Model (SOP)**

↓

**Jordan Wigner Majorana Fermions**

↓

**XY spin chain in transverse field  
(local Order Parameter)**

20

*A. Kitaev / Annals of Physics 321 (2006) 2–111*

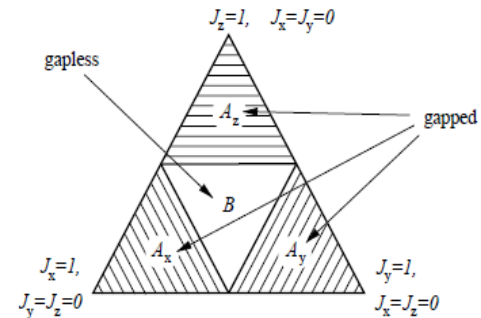
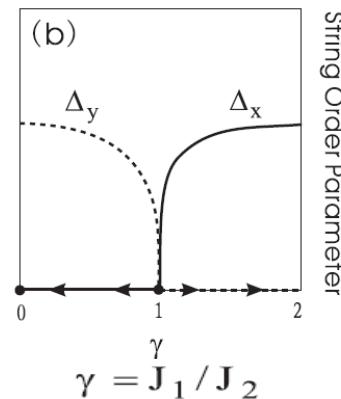


Fig. 5. Phase diagram of the model. The triangle is the section of the positive octant ( $J_x, J_y, J_z \geq 0$ ) by the plane  $J_x + J_y + J_z = 1$ . The diagrams for the other octants are similar.

$$\hat{\Delta}_x(j) = \tau_0^x \tau_{2j}^x = \prod_{k=1}^{2j} \sigma_k^x = (-1)^j \prod_{k=1}^{2j} c_k \quad \Delta_x = \lim_{j \rightarrow \infty} \langle \hat{\Delta}_x(j) \rangle$$

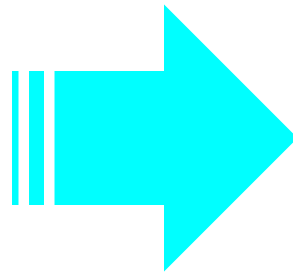
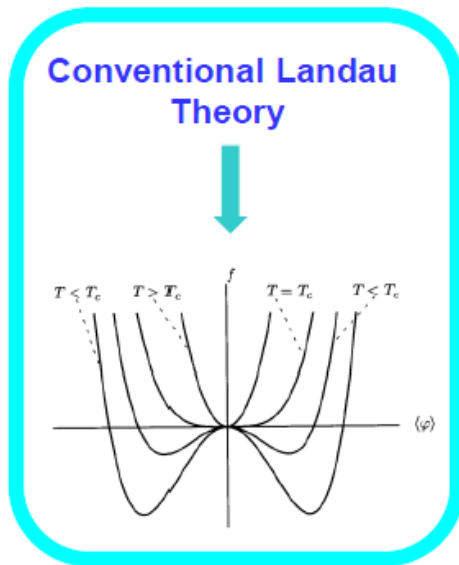
$$\Delta_y = \lim_{j \rightarrow \infty} \langle \prod_{k=2}^{2j+1} \sigma_k^y \rangle = (-1)^j \lim_{j \rightarrow \infty} \langle \prod_{k=2}^{2j+1} c_k \rangle$$



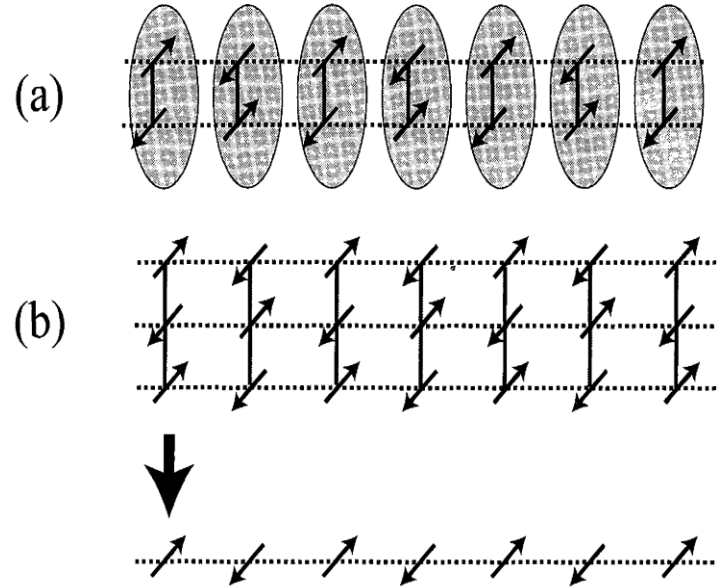
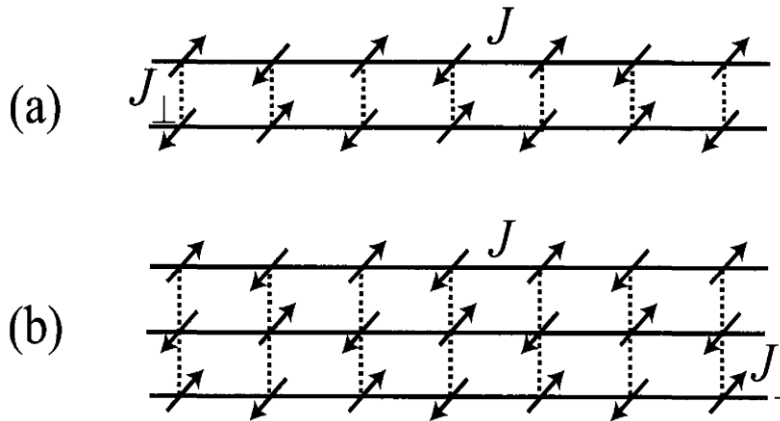
$\alpha = 0, \beta = 1/8, \nu = 1, \eta = 1/4$

**Critical indices of the 2D Ising Model**

Here we need to pause  
and share some  
(deep !!!)  
thoughts



# More Motivation: n-Leg Spin-1/2 Ladders (No Dimerization)



See, e.g., T. Giamarchi, *Quantum Physics in One Dimension*, 2004

FIG. 6.17. (a) In an even leg antiferromagnetic ladder, the spins on a rung are locked into a singlet state. The ground state is essentially a collection of singlets. (b) For an odd leg antiferromagnetic ladder, one of the spins on the rung remains free. The system is thus essentially equivalent to a spin 1/2 system.

**Spin-1/2 Ladders**

**Even number of legs**



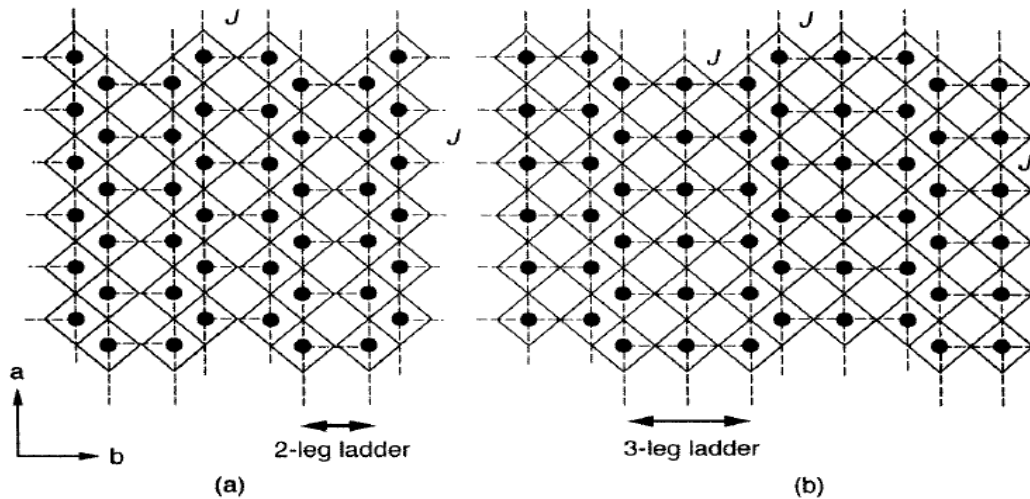
**GAPPED**

**Odd number of legs**

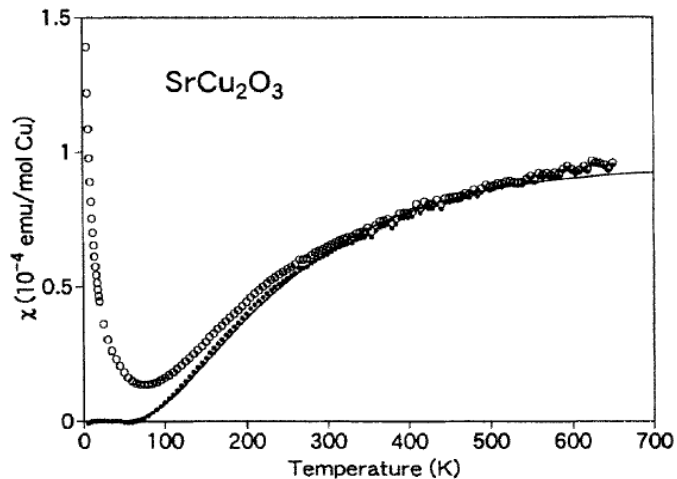


**GAPLESS**

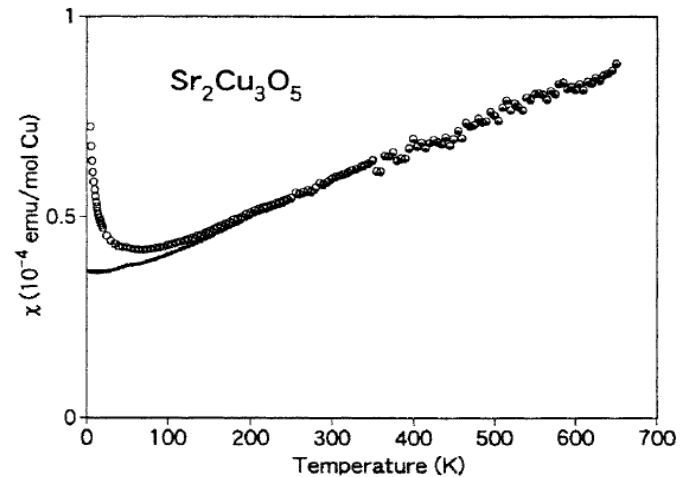
# Two- & Three-Leg Ladders: Experiments



**Figure 6.** Schematic representation of (a) the  $\text{Cu}_2\text{O}_3$  sheets of  $\text{SrCu}_2\text{O}_3$  (from Azuma *et al* 1994). The three-leg ladder  $\text{Sr}_2\text{Cu}_3\text{O}_5$  is also shown in (b). The filled circles are  $\text{Cu}^{2+}$  ions, and  $\text{O}^{2-}$  ions are located at the corners of the squares drawn with solid lines.

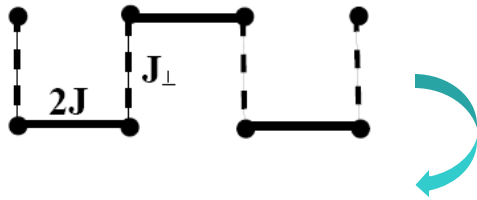
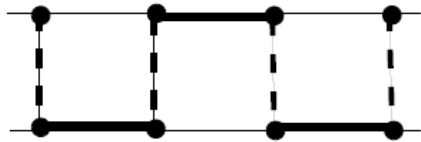


**Figure 7.** The temperature dependence of the magnetic susceptibility of  $\text{SrCu}_2\text{O}_3$  (from Azuma *et al* 1994). Details can be found in the text.



**Figure 8.** As figure 7 but for the three-leg compound  $\text{Sr}_2\text{Cu}_3\text{O}_5$  (from Azuma *et al* 1994). In this case a large susceptibility is observed even at low temperatures, indicative of the absence of a spin gap, in agreement with theoretical expectations.

# Dimerized 2-leg Ladders:



Completely dimerized ladder,  $\delta = 1$ .

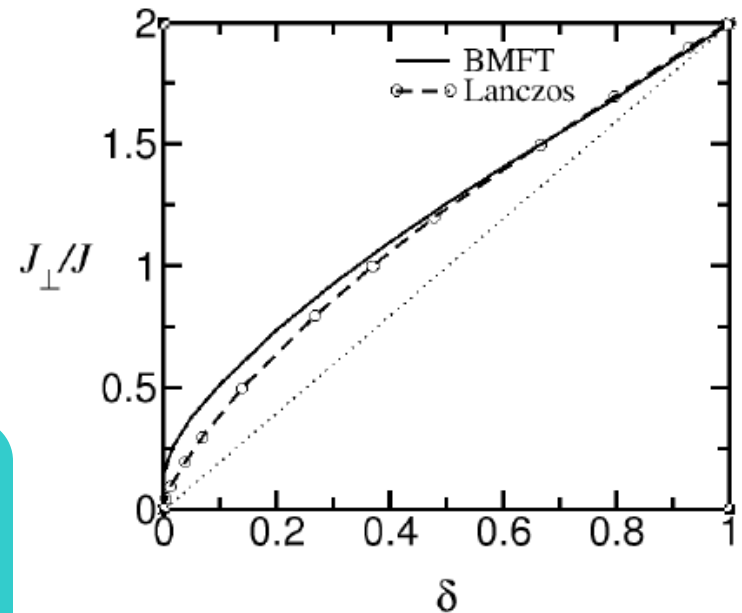
**Conjecture:**

**Martin-Delgado, Shankar, Sierra, PRL 1996**

- Line of Quantum Criticality = No Gap (Mass)
- QCP & No (Apparent) Symmetry Change or SSB
- Non-Local String (Topological) Order Parameter (to discuss)

$$H_{2L} = \sum_{\alpha=1,2} \sum_{n=1}^N J_{\alpha}(n) \mathbf{S}_{\alpha}(n) \cdot \mathbf{S}_{\alpha}(n+1) + J_{\perp} \sum_{n=1}^N \mathbf{S}_1(n) \cdot \mathbf{S}_2(n).$$

$$J_{\alpha}(n) = J[1 + (-1)^{n+\alpha}\delta]$$



**NB:** 3-Leg Ladders, Similar Properties, omitted for brevity

# Dimerization Patterns:

(Chitov, et al, PRB 08)

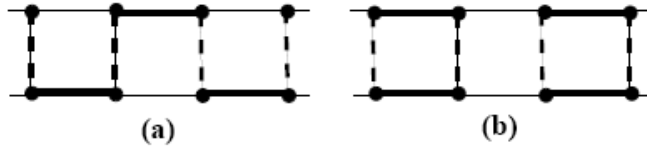


FIG. 1: Dimerized two-leg ladder. Bold/thin/dashed lines represent the stronger/weaker chain coupling  $J(1 \pm \delta)$  and rung coupling  $J_{\perp}$ , respectively. Dimerization patterns: (a) - staggered; (b) - columnar.

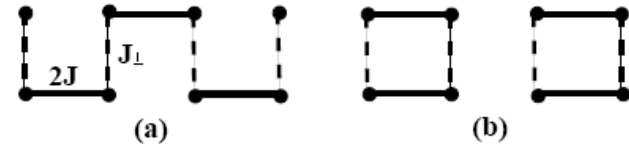


FIG. 2: Completely dimerized ladder,  $\delta = 1$ . (a): Alternated staggering reduces the model (1) to a snake-like dimerized Heisenberg chain of  $2N$  spins; (b): Columnar order degenerates into a set of  $N/2$  decoupled plaquettes.

**Staggered**



**Quantum Critical (line)**

**Columnar**



**Always Gapped**

**Hints:** 3-leg Spin-Peierls Ladder, Azzouz, Shahin, Chitov, PRB 07

# Methods & Results:

## Methods-I: Jordan-Wigner Transformation Mean-Field Theory; Azzouz, PRB 93

CHITOV, RAMAKKO, AND AZZOUZ  
PHYSICAL REVIEW B 77, 1 (2008)

$$S \Rightarrow c^*c, \quad c^*cc^*c \Rightarrow \langle c^*c \rangle c^*c$$

## Methods-II: Exact Diagonalization, Finite-Size Scaling

Gibson, Meyer & Chitov PRB 2011  
Gibson, M.Sc. Thesis, Laurentian, 2010

# Ground State Energies & Gaps:

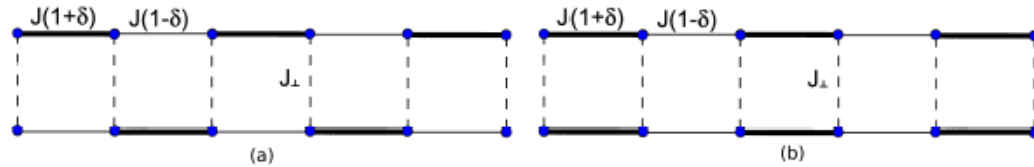


FIG. 1: Dimerized two-leg Heisenberg ladder. Thick and/or thin lines represent stronger and/or weaker intra-chain coupling  $J(1 \pm \delta)$ , while dashed lines represent the rung coupling  $J_{\perp}$ . The staggered and columnar dimerization patterns are shown in (a) and (b) respectively.

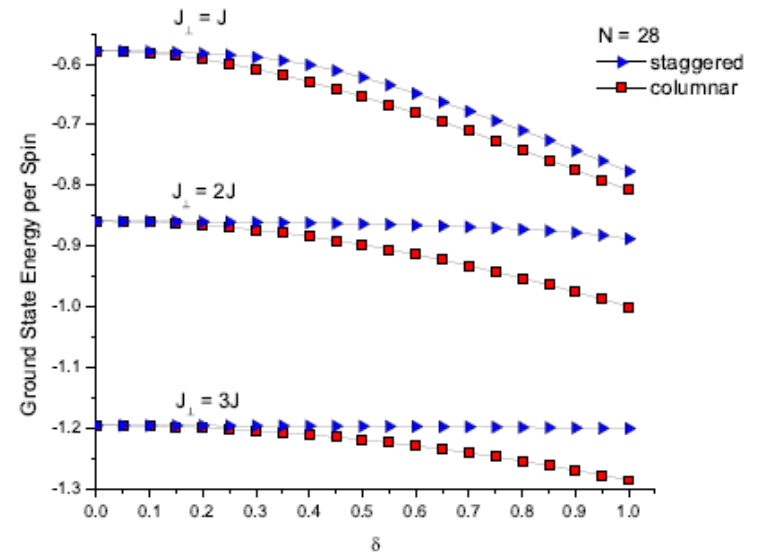
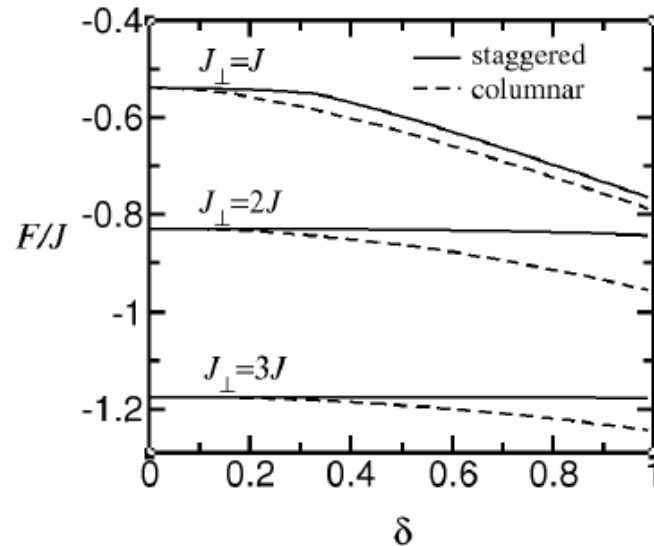


FIG. 2: Ground state energies per spin for the dimerized two-leg ladder calculated by the mean-field theory [11] (left) and by the exact diagonalization for  $N = 28$  (right).



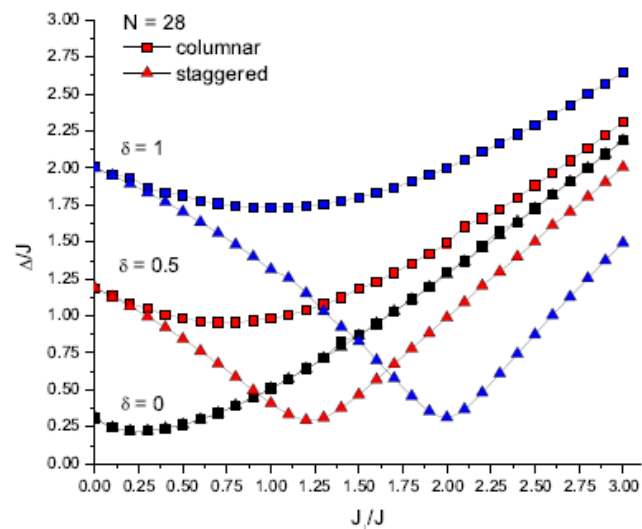
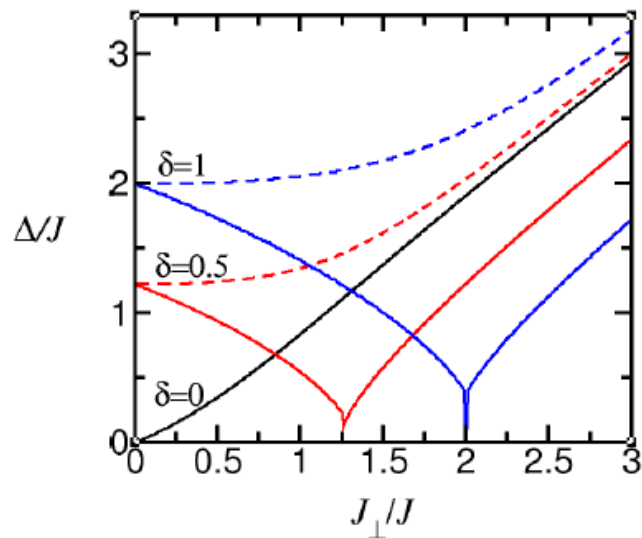


FIG. 3: Energy gaps for the staggered and columnar two-leg ladder dimerization patterns calculated by the mean-field theory [11] (left) and by the exact diagonalization for  $N = 28$  (right).

# Staggered Gaps: Finite-Size Scaling

$$\Delta_L(g) = L^{-1} f\left(gL^{\frac{1}{\nu}}\right)$$

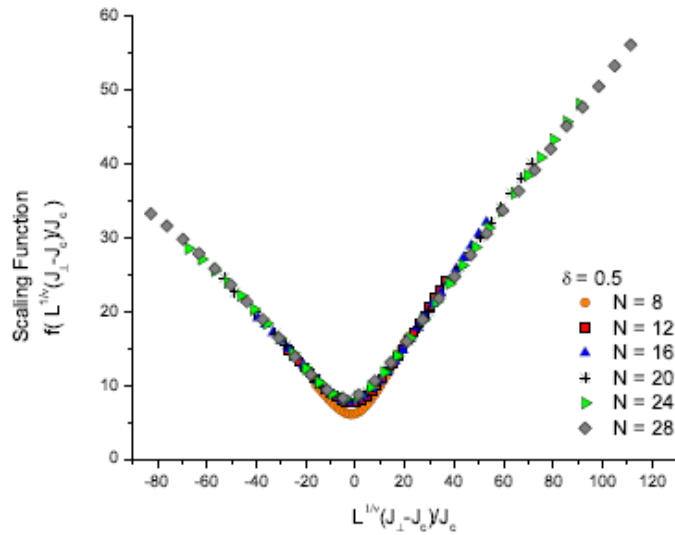


FIG. 4: Fitted scaling function for the gap in the staggered two-leg ladder with  $\delta = 0.5$ . The data collapse for the scaling parameters  $\nu = 0.755$  and  $J_c = 1.27$ .

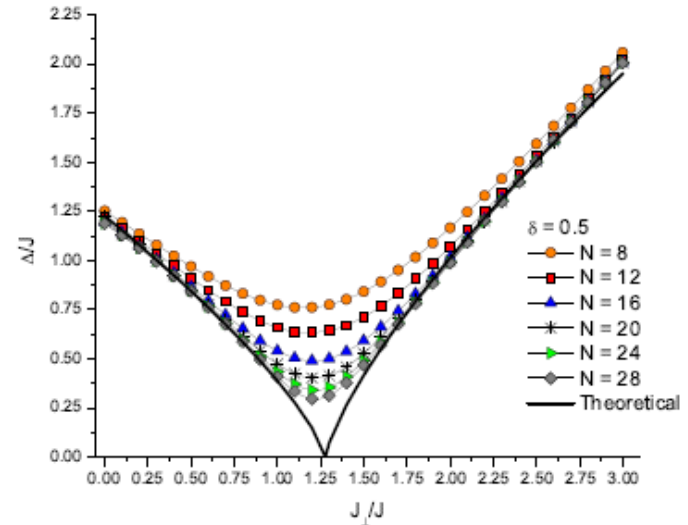


FIG. 5: The gap for the staggered two-leg ladder with  $\delta = 0.5$ , calculated for  $N = 8$  through 28 along with the theoretical fit with critical parameters  $\nu \approx 0.755$  and  $J_c \approx 1.27$ .

# (Hidden) String Order Parameters: Definition

$$\begin{aligned}
 O_{odd}^z &= \lim_{|i-j| \rightarrow \infty} O_{odd}^z(|i-j|) = \\
 &- \left\langle \left( \hat{S}_{1,i}^z + \hat{S}_{2,i}^z \right) \exp \left( i\pi \sum_{l=i+1}^{j-1} \left( \hat{S}_{1,l}^z + \hat{S}_{2,l}^z \right) \right) \left( \hat{S}_{1,j}^z + \hat{S}_{2,j}^z \right) \right\rangle \\
 O_{even}^z &= \lim_{|i-j| \rightarrow \infty} O_{even}^z(|i-j|) = \\
 &- \left\langle \left( \hat{S}_{1,i}^z + \hat{S}_{2,i+1}^z \right) \exp \left( i\pi \sum_{l=i+1}^{j-1} \left( \hat{S}_{1,l}^z + \hat{S}_{2,l+1}^z \right) \right) \left( \hat{S}_{1,j}^z + \hat{S}_{2,j+1}^z \right) \right\rangle
 \end{aligned}$$

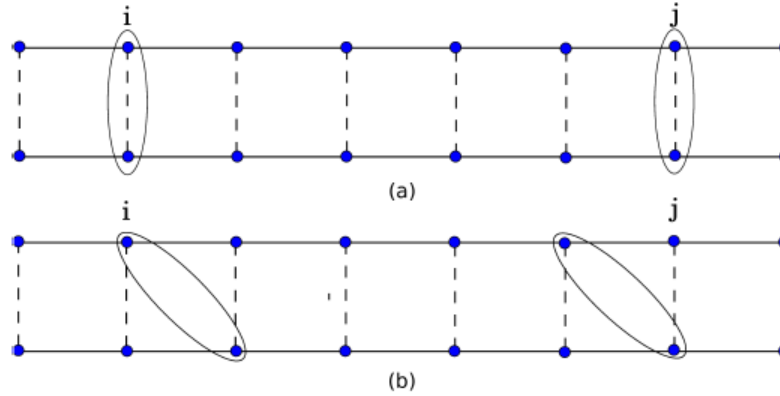


FIG. 3: An illustration of the extended (a) odd and (b) even string order parameters calculated here for a two-leg ladder. In the odd string order (a), spin operators are summed along a rung between the  $i$  and  $j$  limits, whereas the even string order (b) sums along the diagonals.

## References:

- M. den Nijs and K. Rommelse, Phys. Rev. B **40**, 4709 (1989).
- D. G. Shelton, A. A. Nersisyan, and A. M. Tsvelik, Phys. Rev. B **53**, 8521 (1996).
- M. Oshikawa, J. Phys. Condens. Matt. **4**, 7469 (1992).
- E.H. Kim, G. Fath, J. Solyom, and D. J. Scalapino, Phys. Rev. B **62**, 14965 (2000).
- E.H. Kim, O. Legeza, and J. Solyom, Phys. Rev. B **77**, 205121 (2008).
- G. Fath, O. Legeza, J. Solyom, Phys. Rev. B **63**, 134403 (2001).

# String Order Parameters (Ladders) :

## References:

M. Oshikawa, *J. Phys. Condens. Matter* **4**, 7469 (1992).

Y. Nishiyama, N. Hatano, and M. Suzuki, *J. Phys. Soc. Jpn.* **64**, 1967 (1995).

D. G. Shelton, A. A. Nersisyan, and A. M. Tsvelik, *Phys. Rev. B* **53**, 8521 (1996).



transparent representation for the string operator:

$$O^z(x,y) = \exp\{i\sqrt{\pi}[\phi_+(x) - \phi_+(y)]\}. \quad (83)$$

Using Eq. (31),

$$\exp(i\sqrt{\pi}\phi_+(x)) \sim \mu_1\mu_2 + i\sigma_1\sigma_2, \quad (84)$$

we find that the string operator is expressed in terms of the Ising order and disorder operators. For either sign of  $J_{\perp}$ , we find that, in the limit  $|x-x'| \rightarrow \infty$ , the vacuum expectation value of  $O^z(x,y)$  is indeed nonzero:

$$\lim_{|x-x'| \rightarrow \infty} \langle O^z(x,y) \rangle \sim \langle \sigma_1 \rangle^2 \langle \sigma_2 \rangle^2 = \langle \sigma \rangle^4 \neq 0, \quad J_{\perp} < 0, \quad (85)$$

$$\lim_{|x-x'| \rightarrow \infty} \langle O^z(x,y) \rangle \sim \langle \mu_1 \rangle^2 \langle \mu_2 \rangle^2 = \langle \mu \rangle^4 \neq 0, \quad J_{\perp} > 0. \quad (86)$$

**SOP  $\neq 0$**



**What Symmetry is Broken?**



**$Z_2 \times Z_2$**

# String Order Parameters: Columnar Dimerization

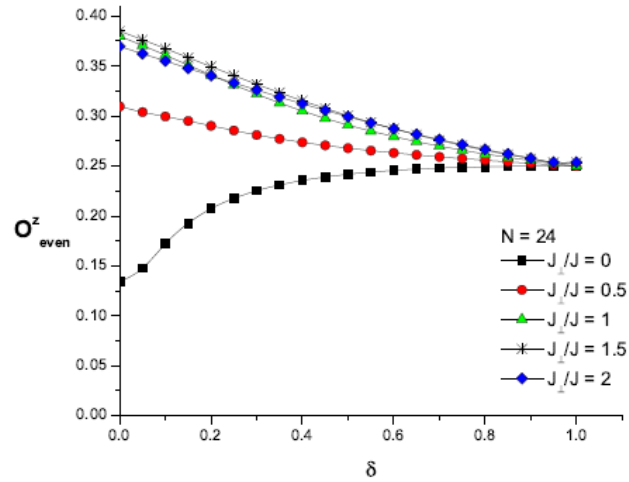


FIG. 25: Calculated even string order parameter for the two-leg ladder with the columnar dimerization pattern and  $N = 24$ . Here  $|i - j| = 7$

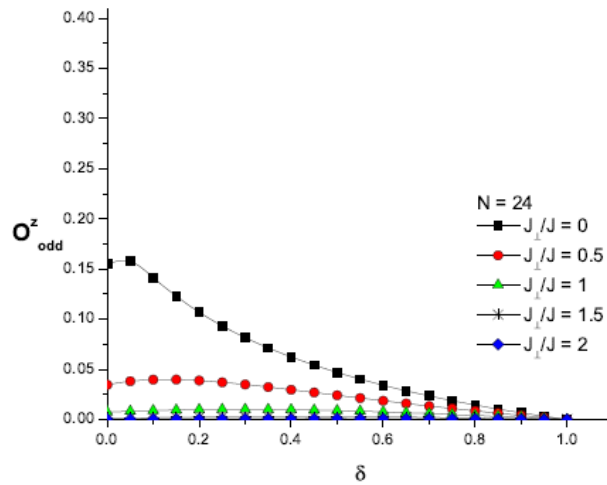


FIG. 26: Calculated odd string order parameter for the two-leg ladder with the columnar dimerization pattern and  $N = 24$ . Here  $|i - j| = 8$

# String Order Parameters: Staggered Dimerization

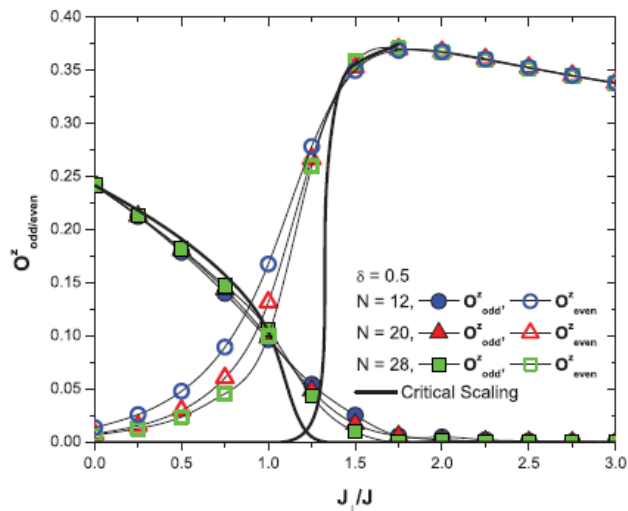
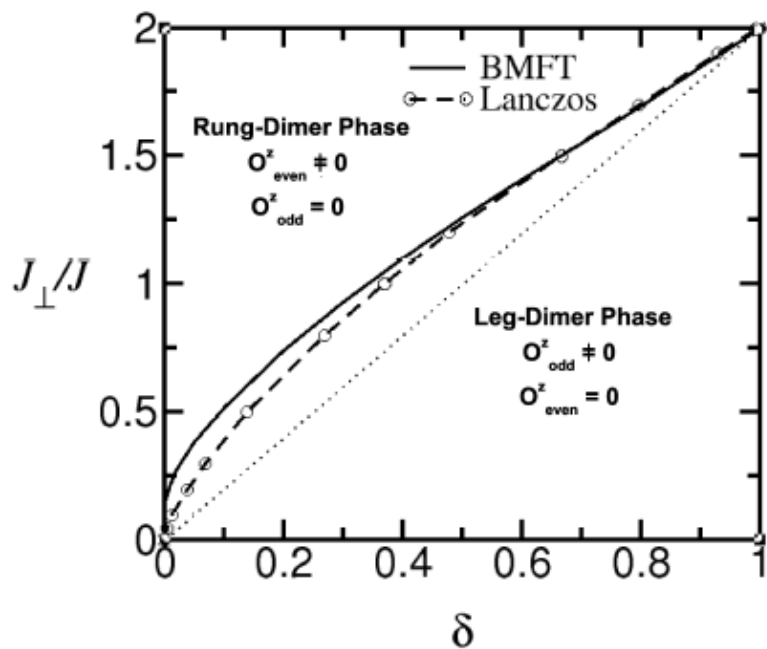


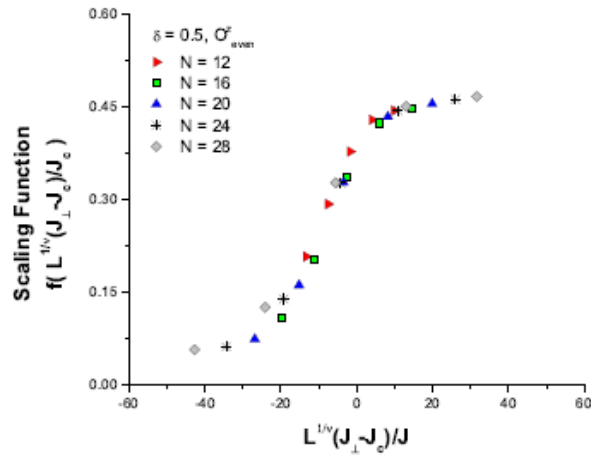
FIG. 6. (Color online) The odd and even SOPs of the staggered two-leg ladder with  $\delta = 0.5$ . The ED data for ladders with number of spins  $N = 12$  to 28 are shown, along with the critical scaling curves.



See also:

J. Almeida, M. A. Martin-Delgado, and G. Sierra, *Phys. Rev. B* **76**, 184428 (2007); **77**, 094415 (2008); *J. Phys. A* **41**, 485301 (2008).

# String Order Parameters: Finite-Size Scaling



$$O_L^z(g) = L^{-\frac{2\beta}{\nu}} f\left(gL^{\frac{1}{\nu}}\right)$$

FIG. 38: Calculated scaling function values for  $O_{even}^z$ , shown for the staggered two-leg ladder configuration with  $\delta = 0.5$ . This figure shows the collapse of the data for  $\beta = 0.0251$  and  $\nu = 0.736$  and  $J_c/J = 1.32$ .

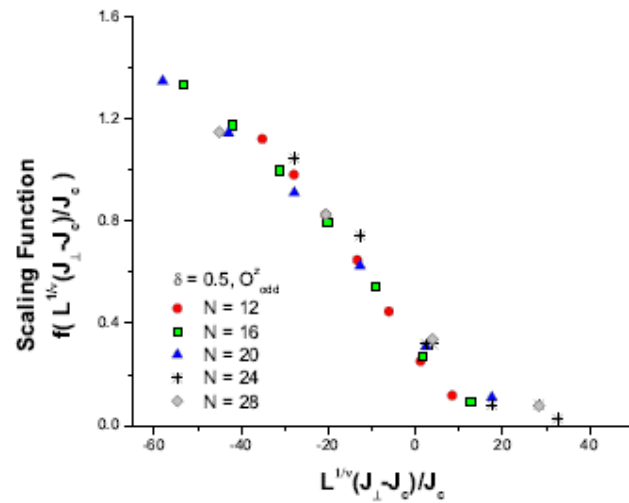


FIG. 40: Calculated scaling function values for  $O_{odd}^z$ , shown for the staggered two-leg ladder configuration with  $\delta = 0.5$ . This figure shows the collapse of the data for  $\beta = 0.251$ ,  $\nu = 0.6979$ , and  $J_c/J = 1.21$ .

# Critical Properties. Universality Class

TABLE I: Critical Scaling Indices of the Two-Leg Ladder

Critical Scaling				
$\delta$	even/odd	$\beta$	$\nu$	$J_c/J$
0.25	even	0.05294	0.758	0.775
0.25	odd	0.285	0.787	0.759
0.5	even	0.0251	0.726	1.32
0.5	odd	0.215	0.698	1.21
0.75	even	0.0687	0.764	1.62
0.75	odd	0.235	0.648	1.64
1.0	even	0.0124	0.7306	2.08
1.0	odd	0.227	0.7013	1.98

$$\alpha = 0, \beta = 1/8, \nu = 1, \eta = 1/4$$

Critical indices of  
the 2D Ising Model

Conjecture: Martin-Delgado et al, 96,98  
Wang & Nersesyan, 2000



Dimerized Heisenberg chain  
Hida, PRB 1992



Baxter's 2D 8-vertex model

$$(\mu = 3\pi / 4)$$

$$\alpha = 2/3$$

$$\beta = 1/12$$

$$\nu = 2/3$$

$$\eta = 1/4$$

+ log corrections



# Dimerized 3-leg Ladders: (Similar Properties)

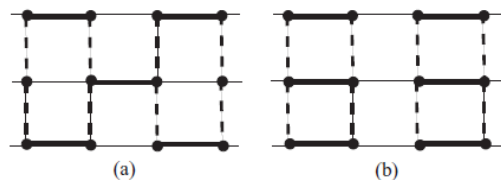


FIG. 8. Dimerized three-leg ladder. Bold, thin, and dashed lines represent the stronger or weaker chain coupling  $J(1 \pm \delta)$  and rung coupling  $J_{\perp}$ , respectively. Dimerization patterns: (a) staggered; (b) columnar.

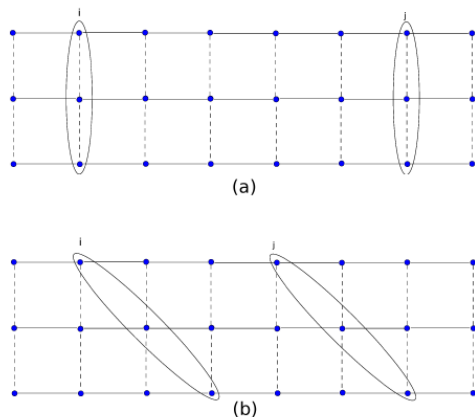


Figure 4.17: An illustration of the (a) odd and (b) even string order parameters. The chosen  $i$  and  $j$  limits used in the calculations are labeled.

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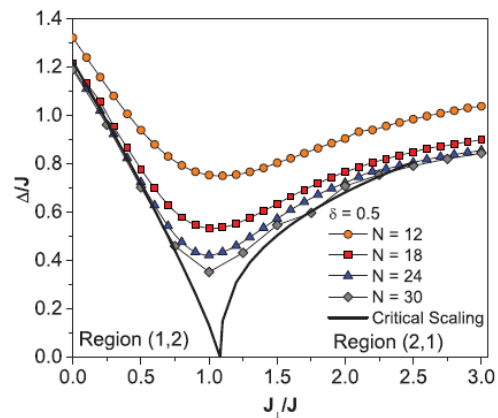


FIG. 12. (Color online) The collapsed scaling functions for the staggered three-leg ladder with  $\delta = 0.5$  in region (1,2) (left-hand panel) and region (2,1) (right-hand panel), calculated for  $N = 12$  through 30 with optimized parameters  $\nu_{(1,2)} \approx 0.863$ ,  $\nu_{(2,1)} \approx 0.385$ , and  $J_{\perp c} \approx 1.08$ .

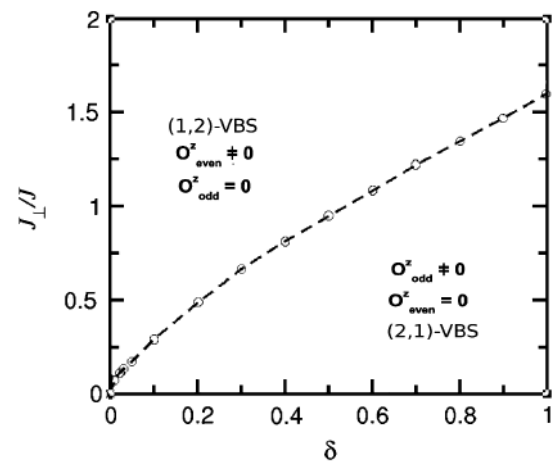


FIG. 10. Three-leg ladder; critical line  $J_{\perp c}(\delta)$  where the gap of the staggered phase vanishes. Adapted from Ref. 12, original data from Ref. 11.

# Dimerized 3-leg Ladders: (continued)

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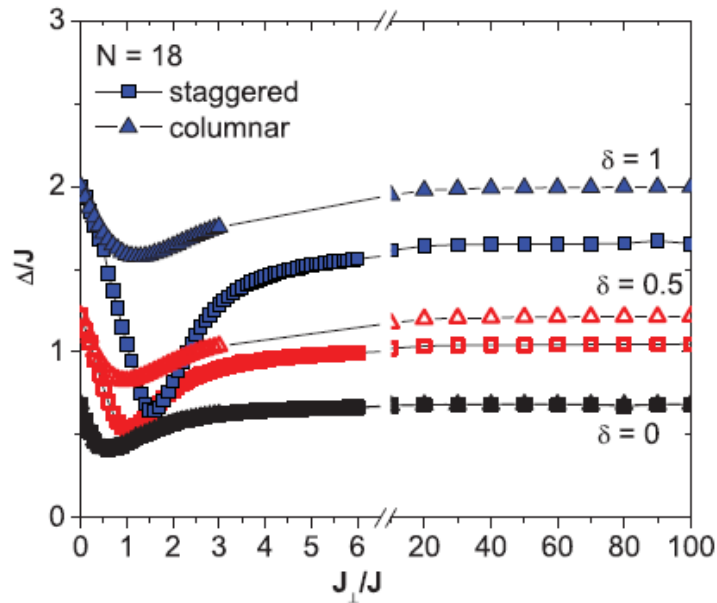


FIG. 13. (Color online) The ED data for the ground-state energy gap with  $\delta = 0.5$  for number of spins  $N = 12$  to  $30$ , along with the fit using optimized parameters  $v_{(1,2)} = 0.863$  in region  $(1,2)$ ,  $v_{(2,1)} = 0.385$  in region  $(2,1)$ , and  $J_{1c} = 1.08$ .

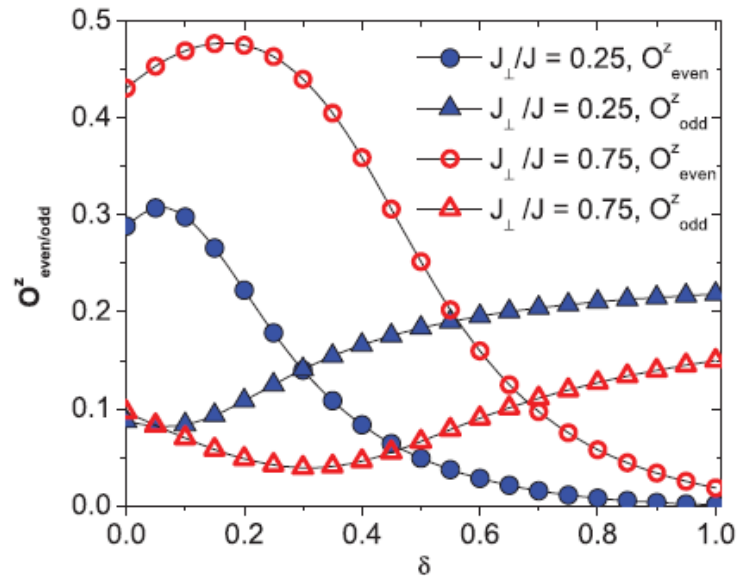


FIG. 14. (Color online) The odd and even string-order parameters of the staggered two-leg ladder with  $J_{\perp}/J = 0.25$  and  $0.75$  as functions of dimerization  $\delta$ . The ED data for ladders with  $N = 24$  total number of spins is shown.

**NB: Size makes limitations on scaling of SOP**

# Summary:

1. Critical properties of the dimerized ladders are investigated
2. Hidden string order parameters are identified and studied
3. Critical indices of the model are determined
4. What is next: Analytical work (FFA, RG, ?)

**THE END**

**THANK YOU!**