DMRG applied to Diagonal Ladders

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Contribution to the Leiden Workshop on Density-Matrix Renormalization – August 2004

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Preview of Main Results
The Diagonal Ladders Universality Classes.

From Cuprates to Rectangular Ladders
A quick review of the main points in ladder physics.

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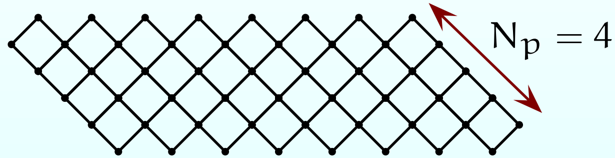
The Diagonal Ladders Universality Classes



AntiFerromagnetic $S = 1/2$ Heisenberg Model on...

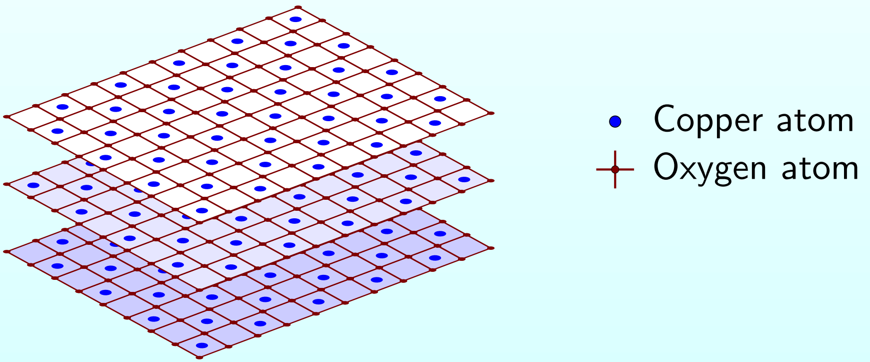
Rectangular Ladders
- Odd n_l — AF, Gapless
- Even n_l — AF, Gapped, Haldane Phase

Diagonal Ladders
- Odd N_p — Ferrimagnetic, Gapless (F), Gapped (AF)
- Even N_p
  - $N_p = 2 \pmod 4$ — AF, Gapped, Haldane Phase
  - $N_p = 0 \pmod 4$ — AF, Gapless

From Cuprates...

MOTIVATION:

High T_c superconductivity → Cuprate Planes → ANTIFERROMAGNETISM (AF)



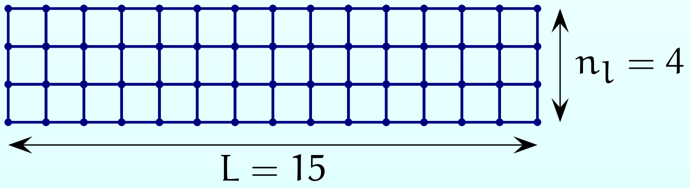
ANTIFERROMAGNETIC HEISENBERG MODEL

- 2D: All S, Long Range Order, Gapless
- 1D:
  - Half Integer S: Quasi Long Range Order (QLRO): Critical, Gapless ($S = 1/2 \rightarrow$ Bethe Ansatz)
  - Integer S: Finite correlation length, Gapped

...to Rectangular Ladders

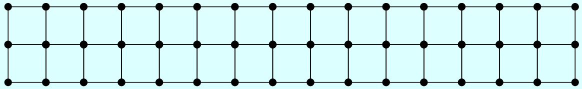
Surprises in the Route 1D → 2D.

Rectangular Spin Ladders

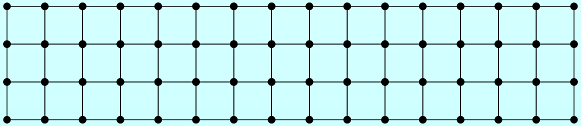


Universality Classes:

n_l odd: QLRO, gapless, critical.



n_l even: gapped, finite correlation length, **Haldane phase**.

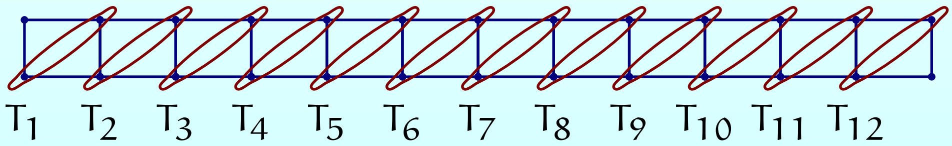


The Haldane Phase

- Dynamical Mass Generation.
- Perhaps some Hidden Order Parameter? YES.

The String Order Parameter

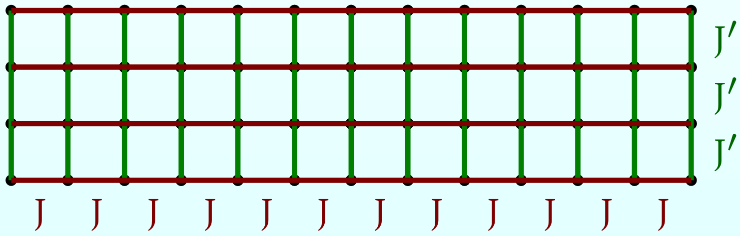
$$\left\langle T_1 \, \exp\left[i\pi \sum_{i=2}^{L-1} T_i \right] T_L \right\rangle \not\to 0$$



- $e^{i\pi T}$ trick maps eigenvalues $\{-1, 0, 1\}$ into $\{-1, 1, -1\}$.

Strong and Weak Coupling Limits

Let's attach different coupling constants J and J' along each axis:



WEAK COUPLING LIMIT: $J'/J \to 0$, n_l independent chains.

STRONG COUPLING LIMIT: $J'/J \to \infty$, L weakly coupled rungs.

- If n_l even: equivalent to integer S Heisenberg AF chain.
- If n_l odd: equivalent to half integer S Heisenberg AF chain.

An Unexpected Application...

Den Haag, Aug 7 2004, An unexpected application: the JACKET LADDER.

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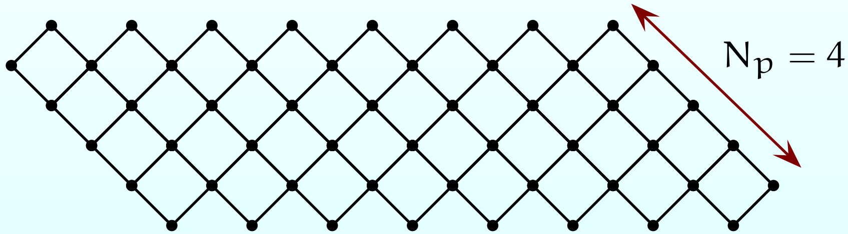
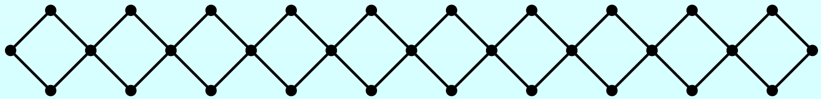
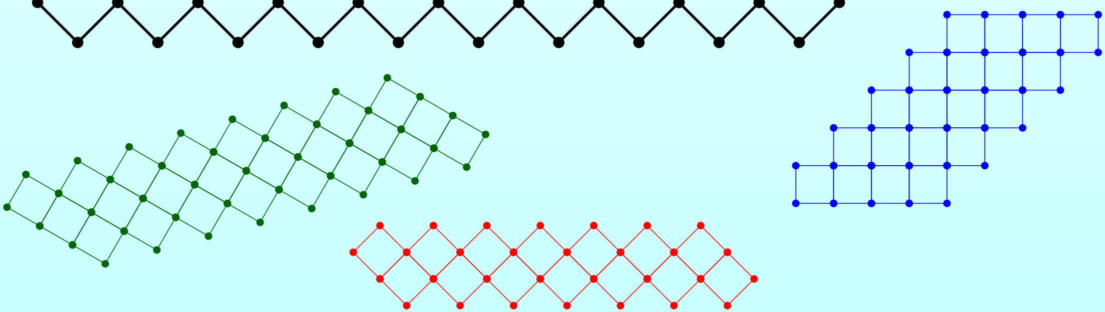
Diagonal Ladders: What?

DIAGONAL LADDERS are defined by the **number of plaquettes** N_p.



- They are all bipartite (non-frustrated). If N_p is odd, they are FERRIMAGNETIC.
- The $N_p = 1$ is a special case, known as the necklace ladder.





Diagonal Ladders. Why?

REASON # 1.- Because they are there.

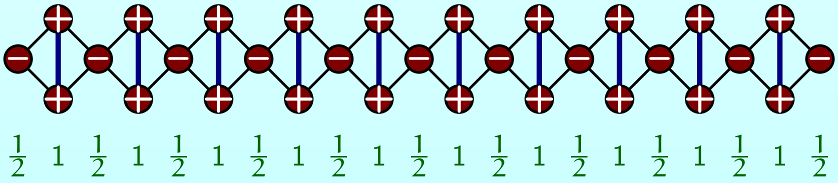
REASON # 2.- They provide an alternative 1D → 2D route.

REASON # 3.- They appear in:

- Stripes in cuprates (e.g. $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$) [Tranquada, Nature 1995]
- Numerical simulations of $t-J$ model on AF planes [White and Scalapino, PRL 1998]
- Necklace appears in polymer compounds [Raposo and Coutinho-Filho, PRB 1999]

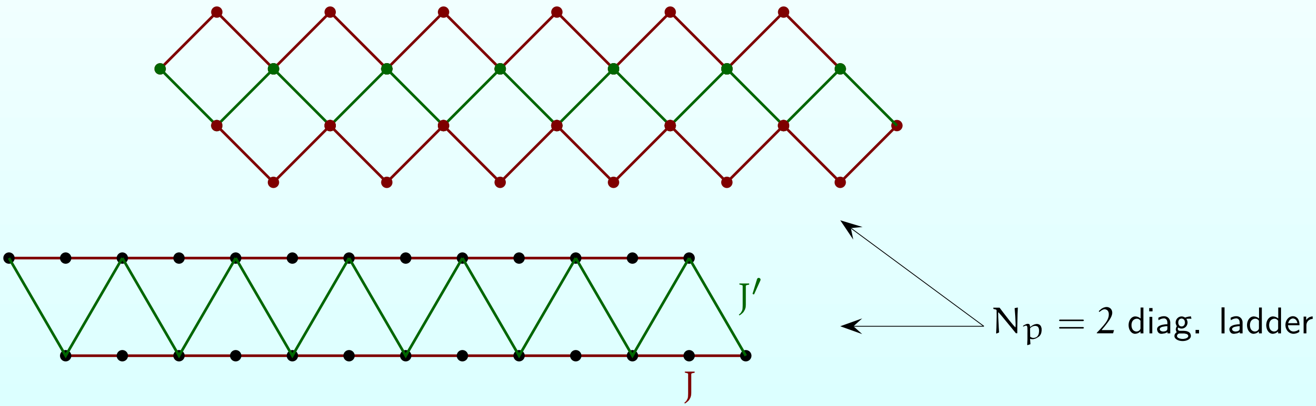
(e.g.: metal-free poly(m-aniline) or poly[1,4-bis-(2,2,6,6-tetramethyl 1-4-oxy-4-piperidyl-1-oxyl)-butadiyne])

NECKLACE PHYSICS: Equivalent to alternating 1-1/2 behaviour, [Sierra, Martín-Delgado, White, Scalapino and Dukelsky, PRB 1999]



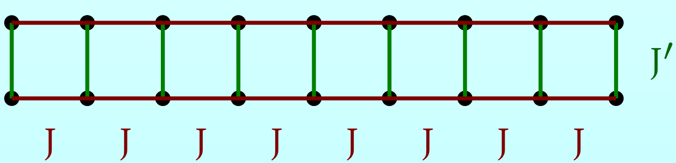
Topological Deformation of the Np=2 Ladder

Case $N_p = 2$: Flatten the "outer links".



In this new disguise, we shall call it DECORATED ZIG-ZAG LADDER.

Differences with Rectangular Ladders:



- No Strong Coupling Limit.
- Perturbation Theory is impossible.
- Mean Field Theory is impossible (à la Gopalan et al., PRB 1994).

It seems to be a hard problem...

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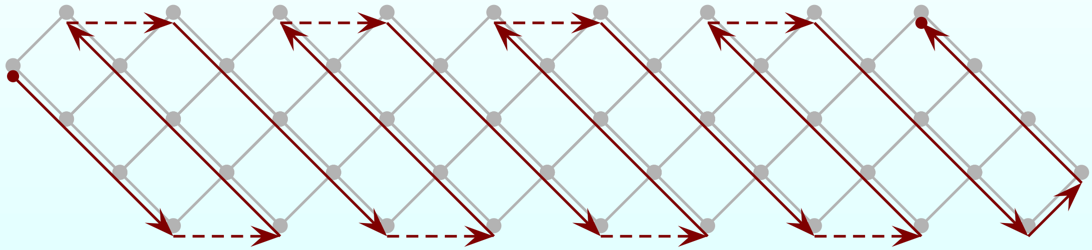
DMRG for Diagonal Ladders

Sweeping Path: For arbitrary N_p.



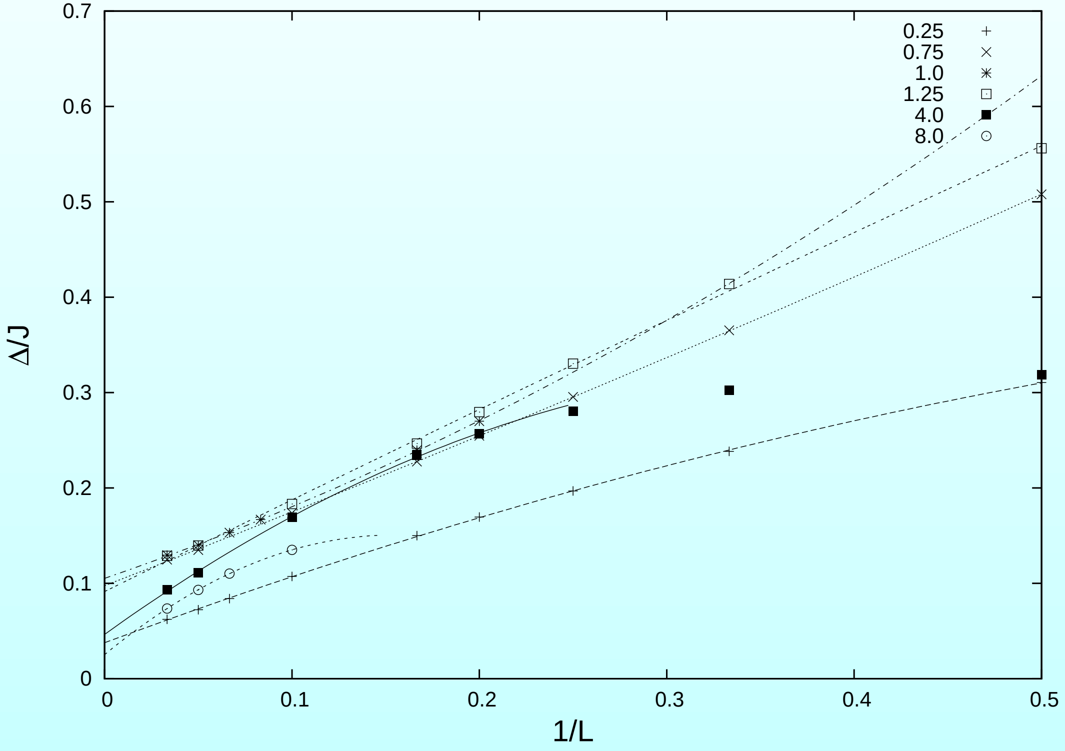
Diagonal Ladder, Some Technical Details

- C++
- Finite algorithm
- Truncation Error always below 10^{-8}
- Fixed digits in energy above 6
- $N_p = 2$: L up to 30 (122 sites), $m = 120$!
- $N_p = 4$: L up to 15 (92 sites)
- Improvements are Under Progress...

48	-66.19208344
49	-66.19207816
50	-66.19207764
51	-66.19207764
55	-66.19207764
54	-66.19207816
53	-66.19208345
52	-66.19207816
56	-66.19207764
57	-66.19207764
58	-66.19207764
59	-66.19207816
63	-66.19208346

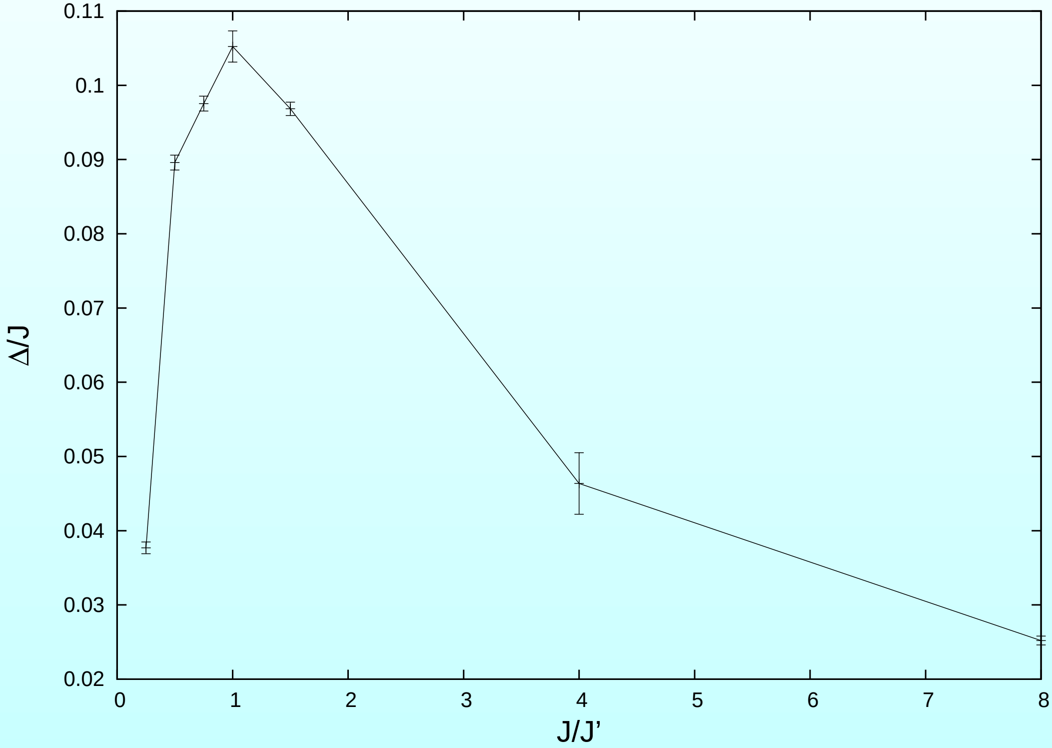
Gap of the Np=2 Diagonal Ladder

Δ/J is shown as a function of L for different values of J/J'.



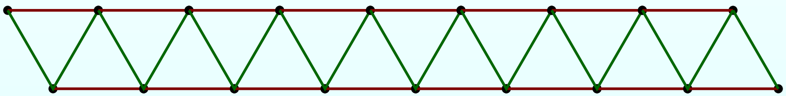
Gap of the Np=2 Diagonal Ladder

The thermodynamical limit of Δ/J is now shown as a function of J/J'.

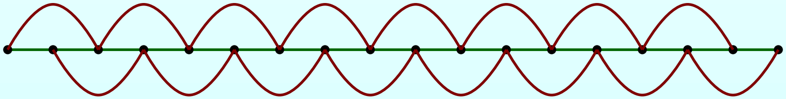


The Zig-Zag Ladder

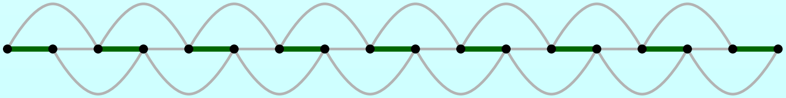
The last plot recalls a close relative of our ladders, the ZIG-ZAG LADDER:

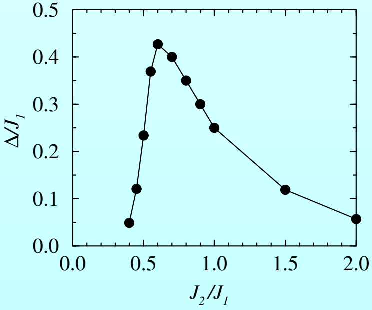


It is equivalent to a next-nearest-neighbours (NNN) linear chain: FRUSTRATION



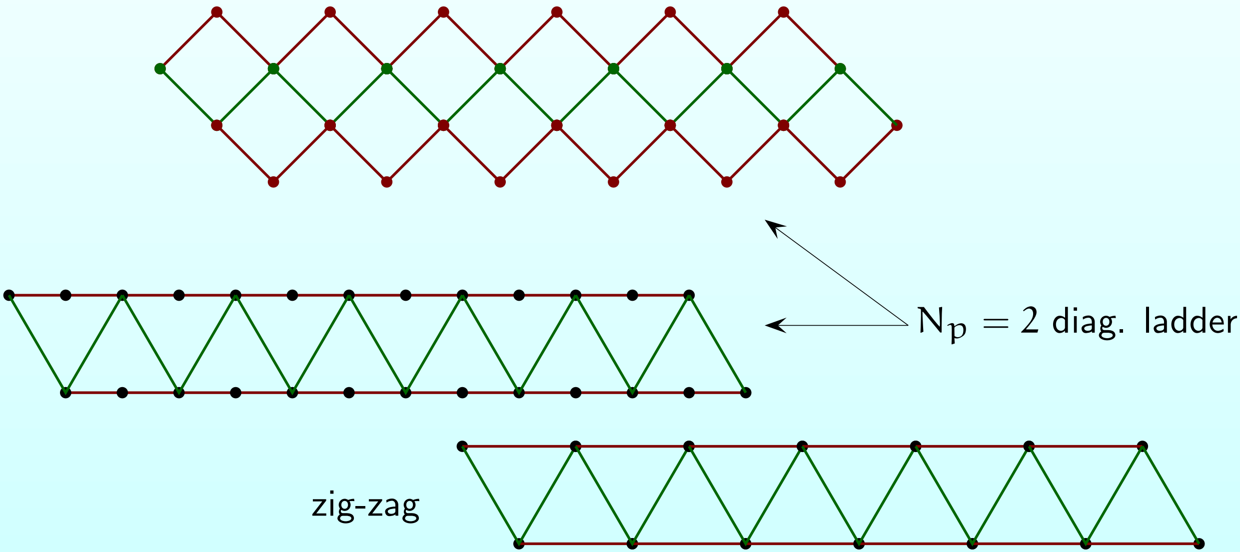
If $J_2/J_1 = 1/2$, Majumdar-Ghosh point, gapped and **fully dimerized**.
Phase Transition: If $J_2/J_1 < 0.24$, gap $\rightarrow 0$, QLRO [White and Affleck, PRB 1996]





Decorated Zig-Zag Ladder

Our Topological Deformation of the $N_p = 2$ diagonal ladder:



The main effect of the decoration → Remove Frustration

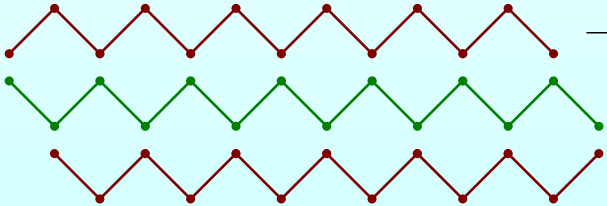
Dimerization

Might the Ground State be dimerized, as in the Zig-Zag ladder?

Dimerization measures

$$D_i \equiv \left|\langle S_{i-1} \cdot S_i \rangle - \langle S_i \cdot S_{i+1} \rangle\right|$$

(Deconstruction of a Diagonal Ladder)

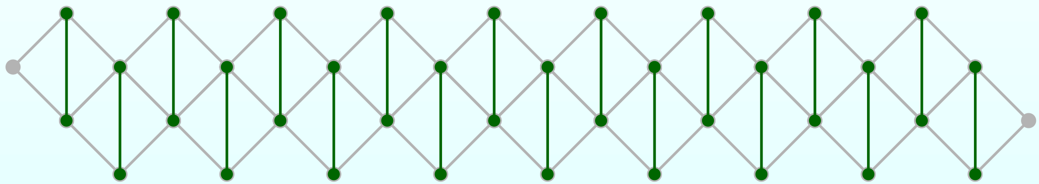


$\longrightarrow$ L=25, $D \approx 4 \cdot 10^{-6}$

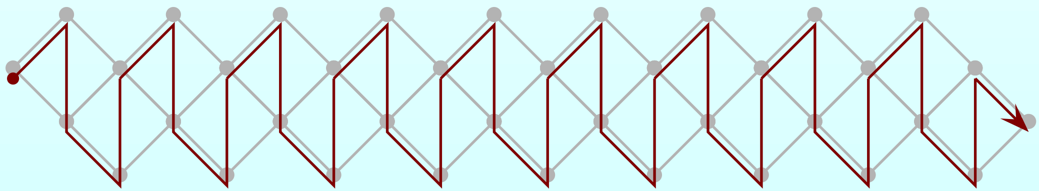
$\longrightarrow$ L=25, $D \approx 2 \cdot 10^{-5}$

String Order Parameter

- To ensure the existence of the HALDANE PHASE for the $N_p = 2$ diagonal ladder.



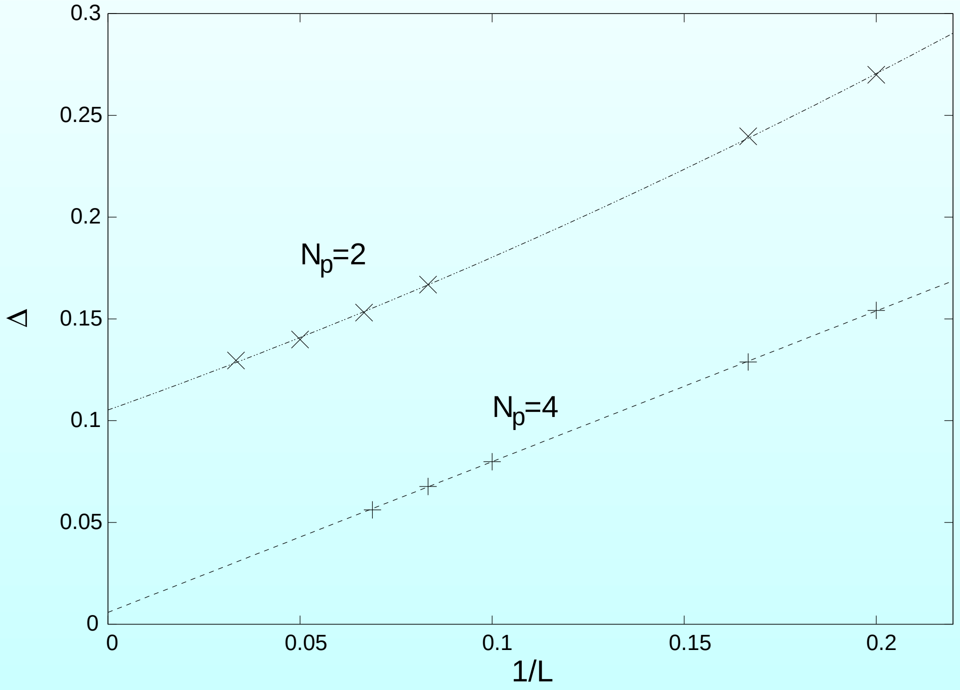
- A different SWEEPING PATH should be used.



DMRG implementation under current work...

DMRG for the Np=4 Diagonal Ladder

Comparison of $\Delta(1/L)$ for $N_p = 2$ and $N_p = 4$.



This points to a negligible gap for $N_p = 4$.

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The Non-Linear Sigma Model

The Non-Linear σ-Model (NLσM) provides an

EFFECTIVE FIELD THEORY for Heisenberg chains [Haldane, PRL 1983]

- ACTION: $S = \int dxdt \left[-\frac{1}{2g} \left(\partial_\mu \vec{\phi}\right)^2 + \frac{\theta}{8\pi} \epsilon_{\mu\nu} \vec{\phi} \cdot \left(\partial_\mu \vec{\phi} \times \partial_\nu \vec{\phi}\right) \right]$

  Kinetic term — Topological term

- CONFIGURATION SPACE: 1+1D; FIELD: $\vec{\phi} \in S^2$.
- COUPLING CONSTANTS: g and θ. If parity is conserved, $\theta \in \{0, \pi\}$.
- Because of Topological Arguments:

$\theta = 0 \rightarrow$ Dynamic Mass Generation, i.e.: GAPPED SPECTRUM.

$\theta = \pi \rightarrow$ Massless Excitations, i.e.: GAPLESS SPECTRUM.

HAMILTONIAN FORMALISM:

- Hamiltonian: $\mathcal{H} = \frac{v}{2} \int dx \left[g \left(\vec{\ell} - \frac{\theta}{4\pi} \vec{\phi}' \right)^2 + \frac{1}{g} \vec{\phi}'^2 \right]$

Where v is the "speed of light", $\vec{\phi}' = \partial_x \vec{\phi}$ and $\vec{\ell}$ is the conjugate momentum of $\vec{\phi}$.

The Non-Linear Sigma Model

The Haldane Mapping (à la Affleck)

1.- Select a classical vacuum state (Néel state).

2.- Split the system into blocks.

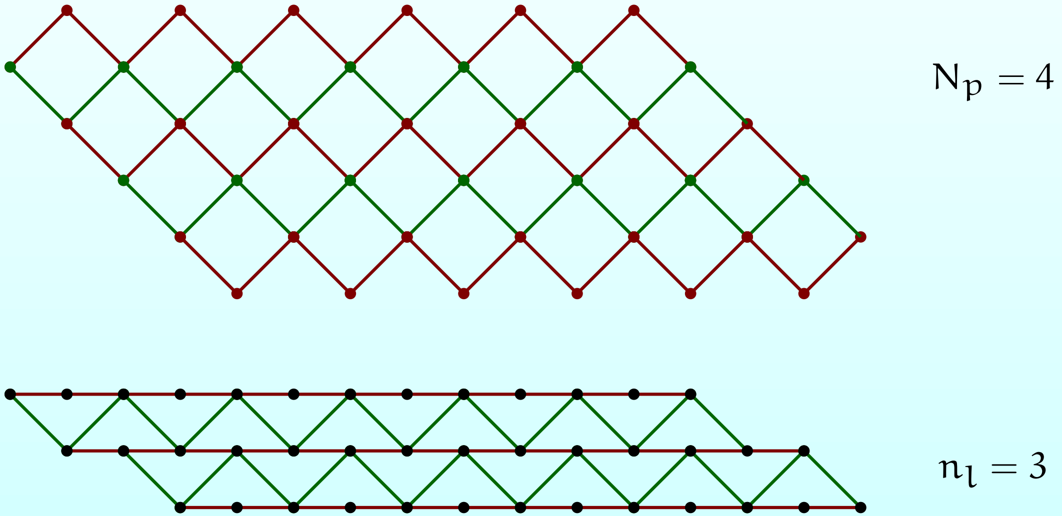
3.- Select $\vec{\phi}$ and $\vec{\ell}$ within each block
Using spin-wave theory, so as they fulfill commutation relations and constraints.

4.- Rewrite the Heisenberg Hamiltonian.
Then, identify μ-scopic and phenomenological parameters.

If the final hamiltonian does not have the NLσM form, then it has not worked for our problem.

The Non-Linear Sigma Model

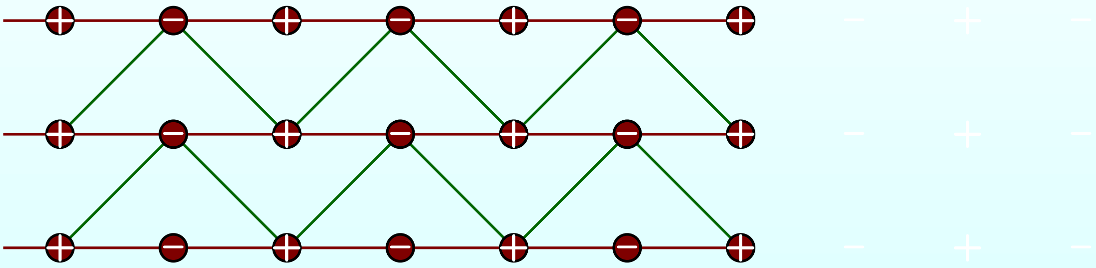
Topological Deformation of an Arbitrary Diagonal Ladder



In general, $n_l = \left(\frac{N_p}{2} + 1\right)$.

The Non-Linear Sigma Model

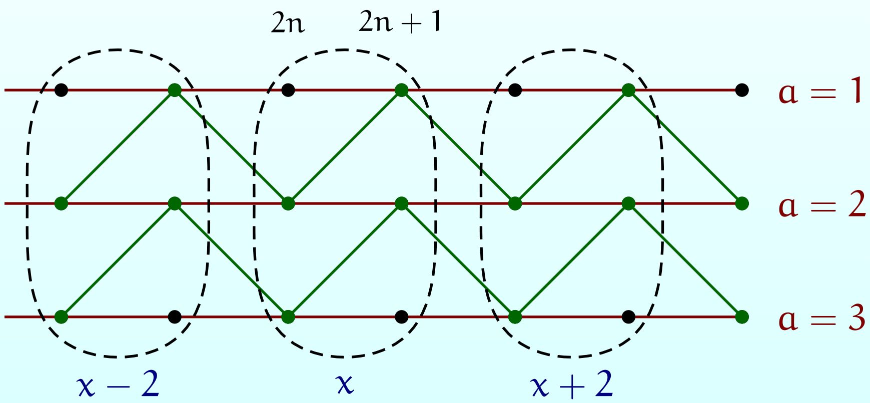
The Néel State in Diagonal Ladders



AF in one direction, but Ferromagnetic in the other!

The Non-Linear Sigma Model

Blocking Scheme



$$\begin{cases} \vec{S}_a(2n) & = & A_a^e \vec{\ell}(x) + \vec{\ell}_a(x) + S\,(\vec{\phi}(x) + \vec{\phi}_a(x)) \\ \vec{S}_a(2n+1) & = & A_a^o \vec{\ell}(x) + \vec{\ell}_a(x) - S\,(\vec{\phi}(x) + \vec{\phi}_a(x)) \end{cases}$$

with constraints $\sum_a A_a^e = \sum_a A_a^o = 1, \quad \sum_a \vec{\ell}_a = 0, \sum_a \vec{\phi}_a = 0.$

The Non-Linear Sigma Model

Main Result

$$\theta = 2\pi S n_l = 2\pi S \left(\frac{N_p}{2} + 1 \right)$$

Independent of J and J'! Hence, the Universality Classes:

$$\text{Diagonal Ladders} \begin{cases} \text{Odd } N_p & \text{Ferrimagnetic, Gapless (F), Gapped (AF)} \\ \text{Even } N_p & \begin{cases} N_p = 2 \pmod 4 & \text{AF, Gapped, Haldane Phase} \\ N_p = 0 \pmod 4 & \text{AF, Gapless} \end{cases} \end{cases}$$

The Non-Linear Sigma Model

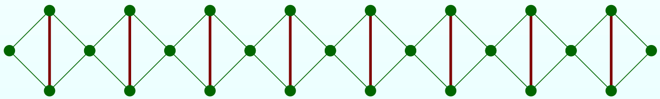
More Results...

	$n_l = 2$ Rectangular Ladder	$N_p = 2$ Diagonal Ladder
θ	$4\pi S$	$4\pi S$
g	$\frac{1}{S\sqrt{2}}\left(1+\frac{J'}{2J}\right)^{1/2}$	$\frac{1}{S}\left(1+\frac{J'}{J}\right)^{-1/2}$
v	$2\sqrt{2}SJ\left(1+\frac{J'}{2J}\right)^{1/2}$	$2SJ\left(1+\frac{J'}{J}\right)^{1/2}$

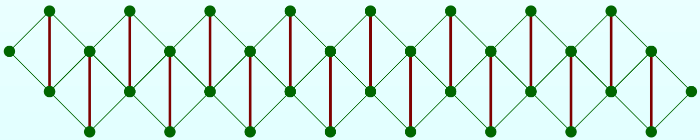
	$n_l = 3$ Rectangular Ladder	$N_p = 4$ Diagonal Ladder
θ	$6\pi S$	$6\pi S$
g	$\frac{2}{S}\left(\frac{1+\frac{3J'}{4J}}{17+\frac{3J'}{4J}}\right)^{1/2}$	$\frac{2}{3S}\left(1+\frac{4J'}{3J}\right)^{-1/2}$
v	$\frac{2JS}{3}\frac{\sqrt{1+\frac{3J'}{4J}}\sqrt{17+\frac{3J'}{4J}}}{1+\frac{J'}{12J}}$	$v = 2JS\left(1+\frac{4J'}{3J}\right)^{1/2}$

A Global Picture

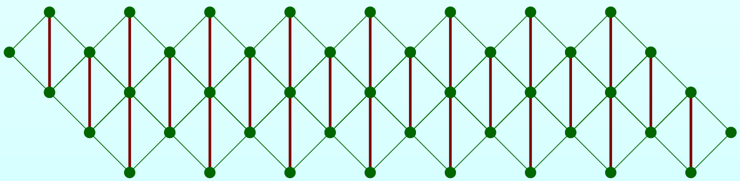
The NLσM result allows us to present this global picture:



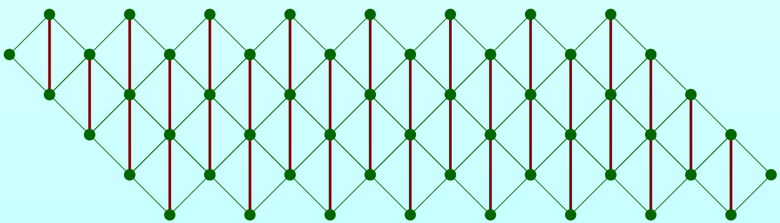
$$\cdots - \tfrac{1}{2} - 1 - \tfrac{1}{2} - 1 - \cdots$$



$$\cdots - 1 - 1 - 1 - 1 - \cdots$$



$$\cdots - 1 - \tfrac{3}{2} - 1 - \tfrac{3}{2} - \cdots$$



$$\cdots - \tfrac{3}{2} - \tfrac{3}{2} - \tfrac{3}{2} - \tfrac{3}{2} - \cdots$$

Bosonization for 2-leg Ladders

- ABELIAN BOSONIZATION: A different FIELD THEORETIC APPROACH.
- Valid for $S = 1/2$.
- Weak coupling limit for the rungs.

$$\vec{S}_i(x) = (\vec{J}_{L,i}(x) + \vec{J}_{R,i}(x)) + (-1)^{\lfloor x/a \rfloor}\, \vec{n}_i(x)$$

where $i \in \{1, 2\}$ is the leg index, $\vec{J}_L$, $\vec{J}_R$ and $\vec{n}$ are slowly varying fields.

$$n^z = -\frac{\lambda}{\pi a} \sin\left(\sqrt{2\pi}\phi(x)\right) \qquad n^{\pm} = \frac{\lambda}{\pi a} e^{\pm i\sqrt{2\pi}\theta(x)}$$

where $\theta(x) = \int_{-\infty}^{x} dy \Pi(y)$ and $\Pi(x)$ is the conjugate momentum of $\phi(x)$.

Bosonization for 2-leg Ladders

- RECTANGULAR LADDER with $n_l = 2$.

$$H_{int} = J' \sum_n \vec{S}_1(n) \cdot \vec{S}_2(n) \approx J' \vec{n}_1(x) \cdot \vec{n}_2(x)$$

Introducing $\phi_\pm = \frac{1}{\sqrt{2}}(\phi_1 \pm \phi_2)$

$$H_{int} \approx \frac{J'\lambda^2}{2\pi^2 a^2} \left[\cos\sqrt{4\pi}\,\phi_- \cos\sqrt{4\pi}\,\phi_+\right] + \frac{J'\lambda^2}{\pi^2 a^2} \cos\sqrt{4\pi}\,\theta_-$$

Terms of the form $\cos\sqrt{4\pi}\phi$ lead to a mass gap.

- ZIG-ZAG LADDER

$$H_{int} = J' \sum_n [\vec{S}_1(n) + \vec{S}_1(n+1)] \cdot \vec{S}_2(n) \approx \vec{n}_1 \partial_x \vec{n}_2 - \vec{n}_2 \partial_x \vec{n}_1$$

- DIAGONAL $N_p = 2$ LADDER

$$H_{int} = J' \sum_n [\vec{S}_1(2n+1) + \vec{S}_1(2n+3)] \vec{S}_2(2n+2) \approx -4\vec{n}_1 \cdot \vec{n}_2$$

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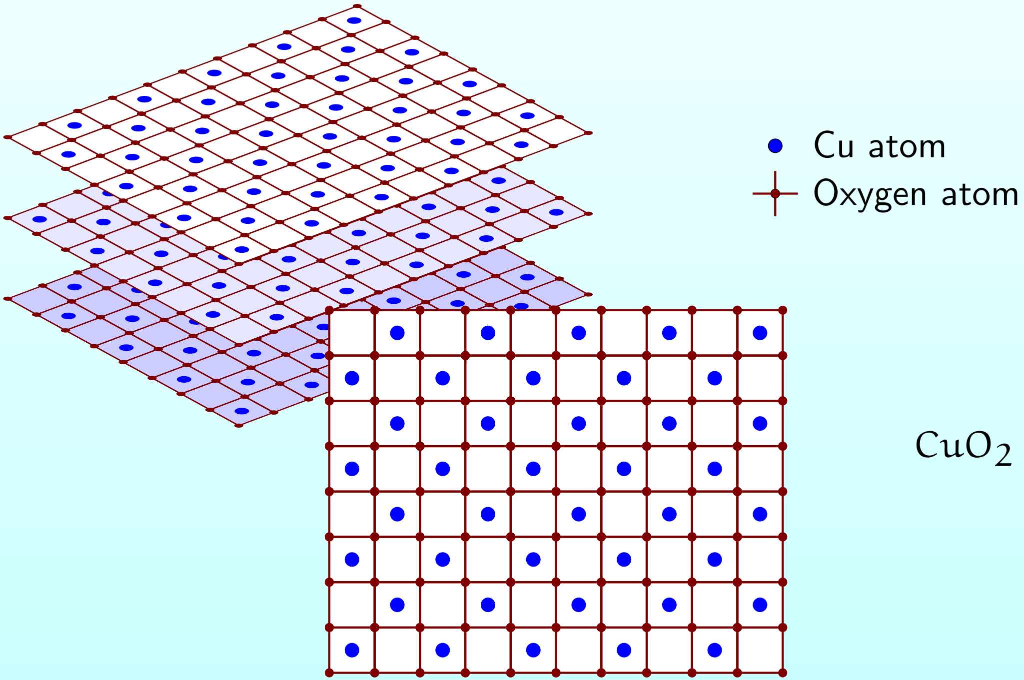
Proposal for Experimental Realization

Usual Cuprate Plane Structure:

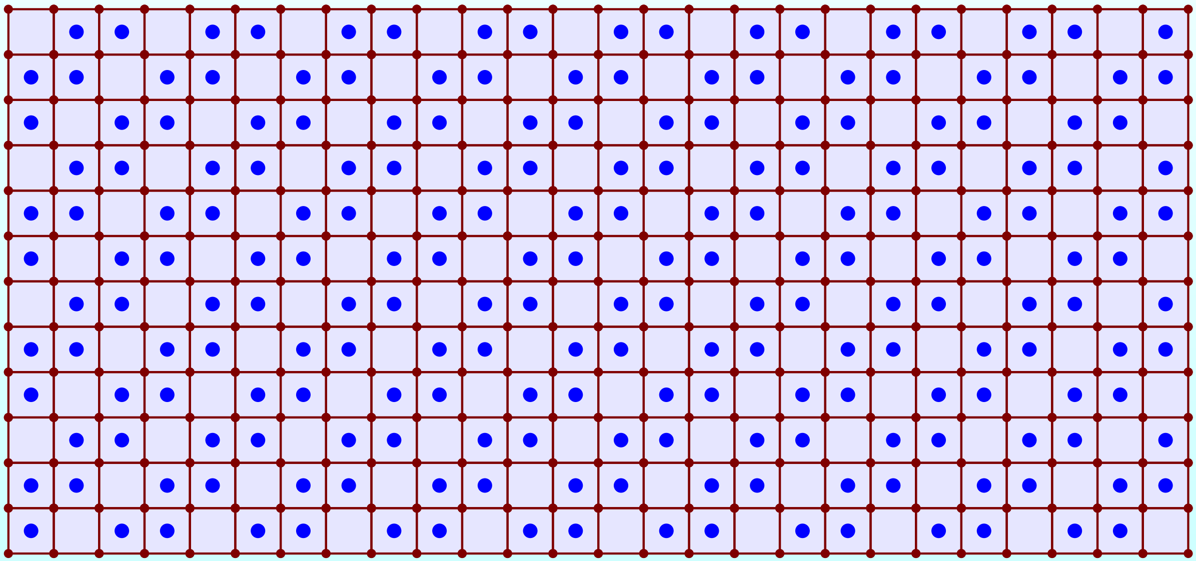


CuO_2

Proposal for Experimental Realization

Azuma, Hiroi, Takano, Ishida, Kitaoka, Phys. Rev. Lett. 1994.

Proposed compounds series $Sr_{n-1}Cu_{n+1}O_{2n}$ series, with $n \in \{3, 5, 7, \cdots\}$.



$Cu_2O_3 \qquad n = 3$

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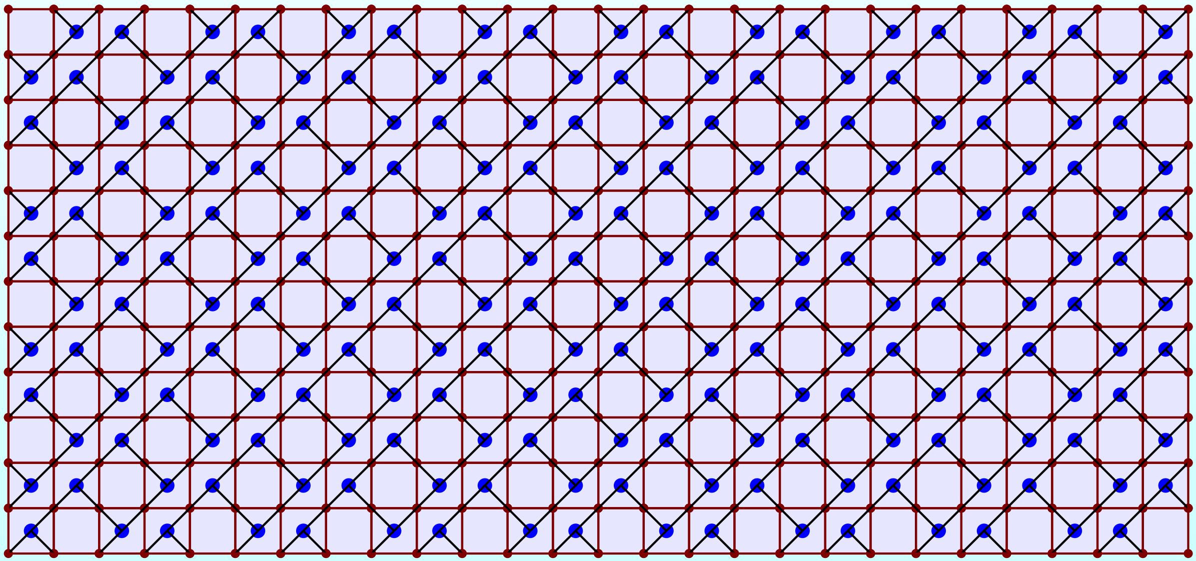

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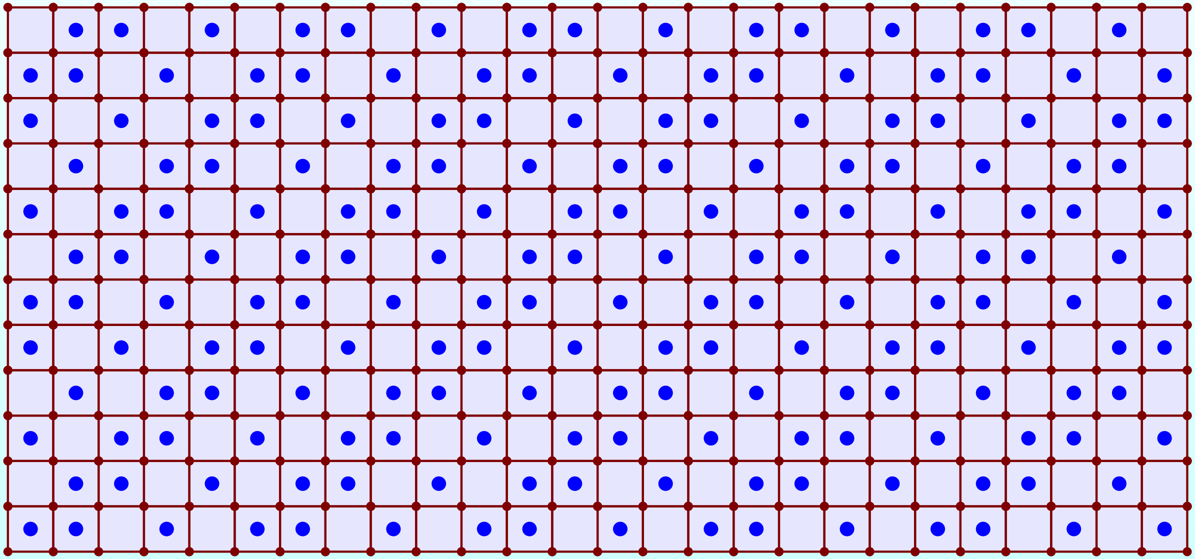

$Cu_3O_5 \qquad n = 5$

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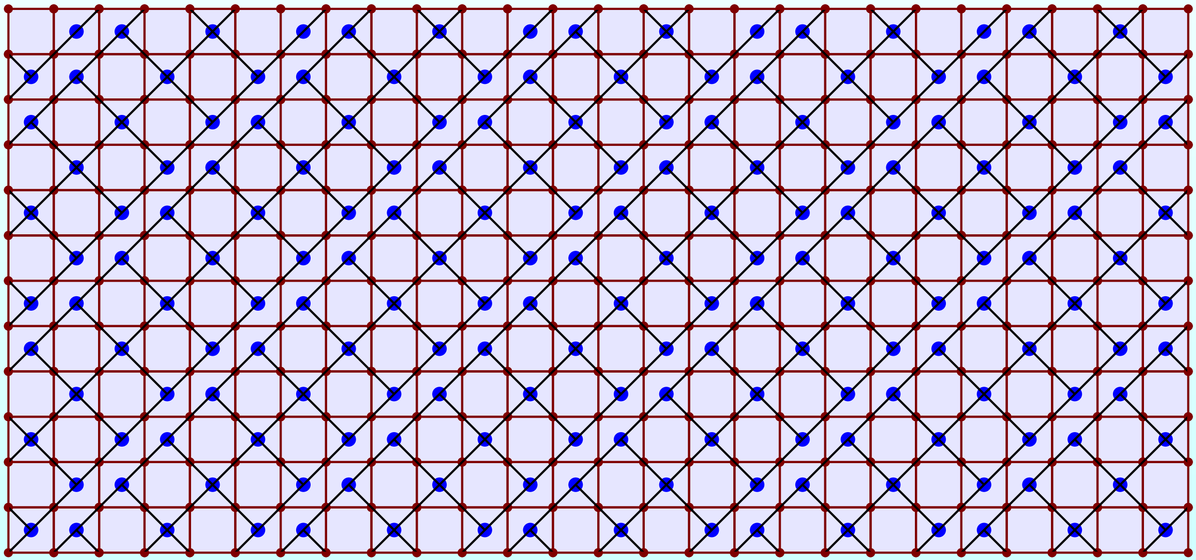
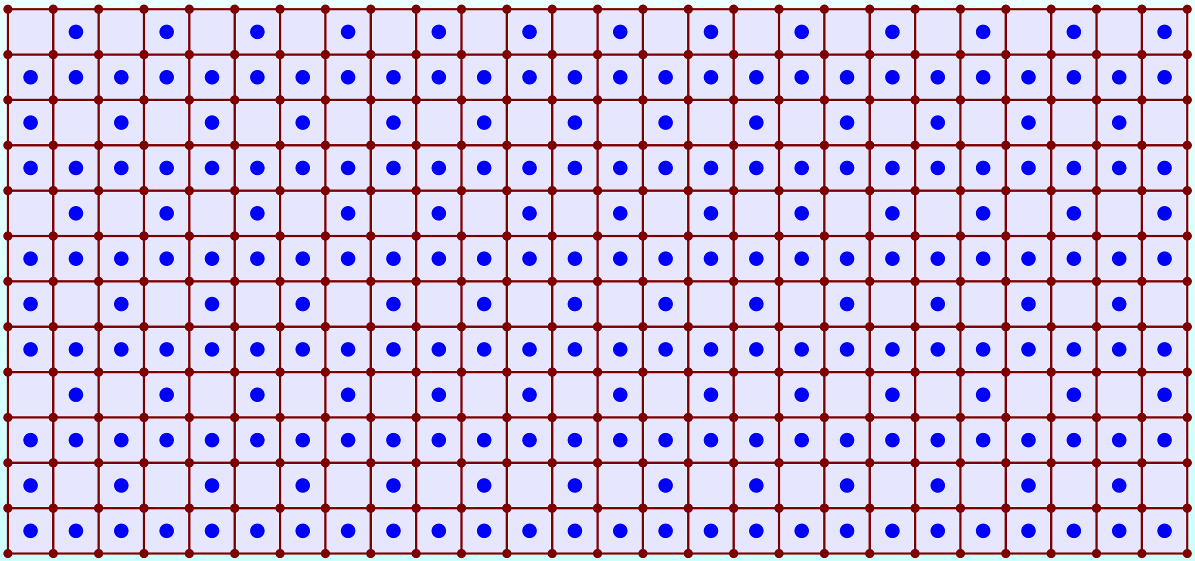


$Cu_3O_5 \qquad n = 5$

Proposal for Experimental Realization

We propose to study the **whole** series:

$Sr_{n-1}Cu_{n+1}O_{2n}$ series, with $n \in \{2, 3, 4, \cdots\}$.



$Cu_3O_4 \qquad n = 2$

Proposal for Experimental Realization

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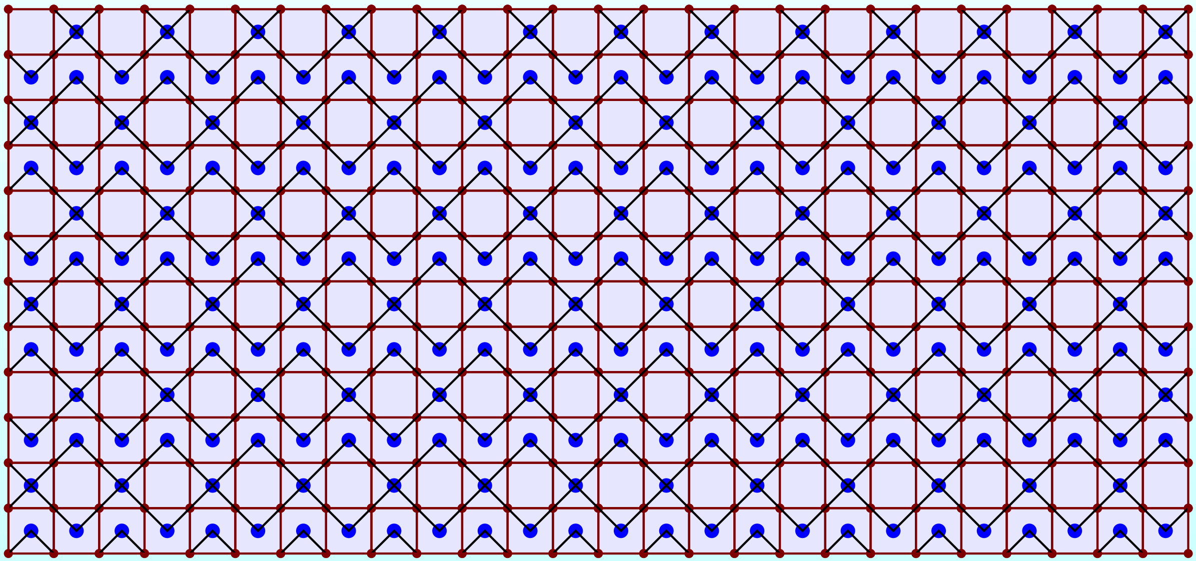

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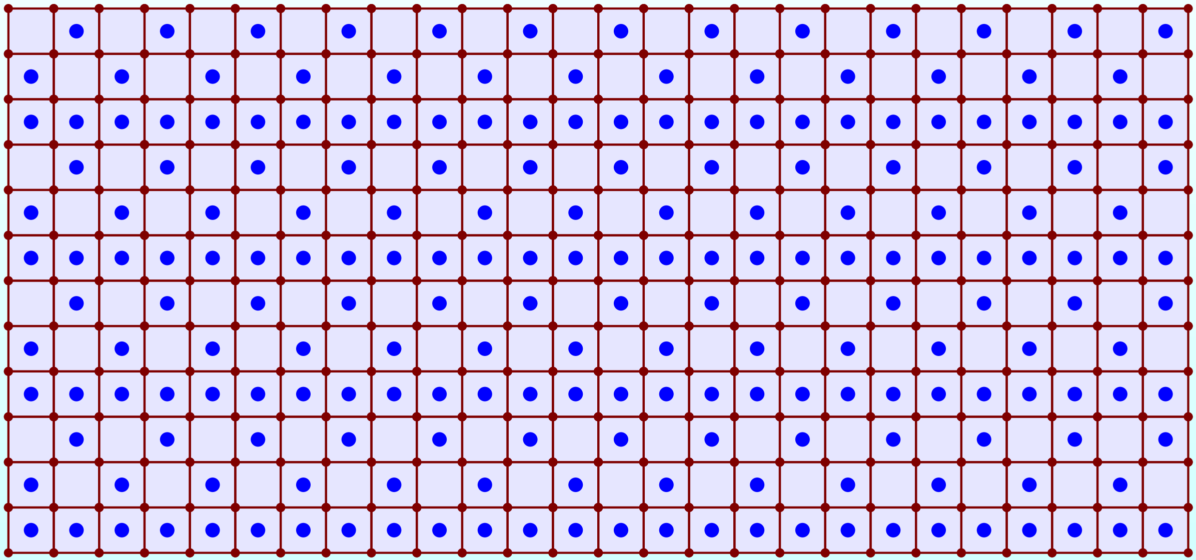
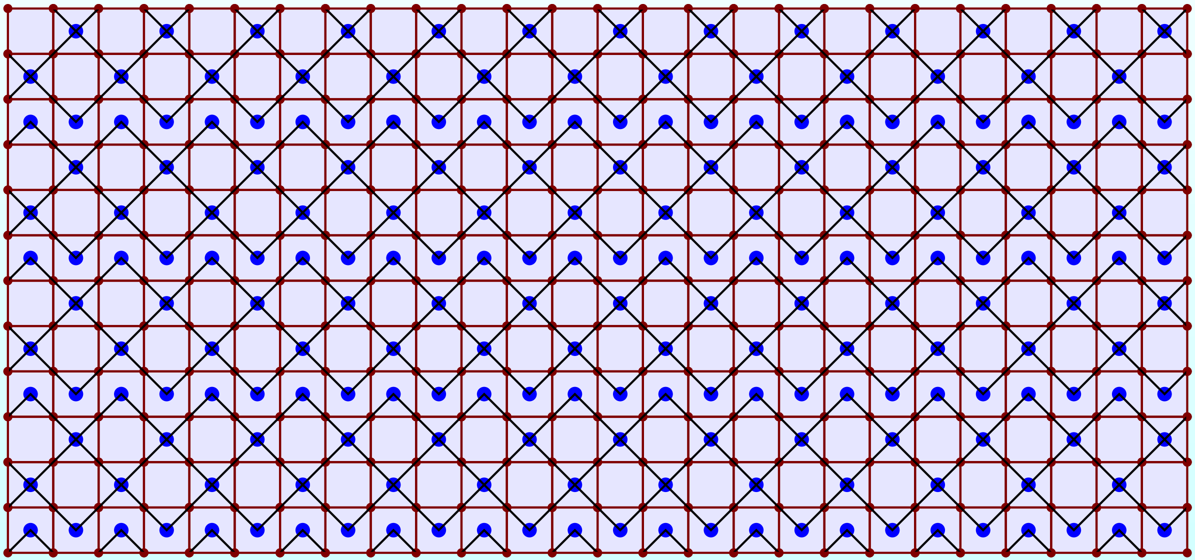
Proposal for Experimental Realization



$Cu_2O_3 \qquad n = 3$

Allomorphic to the $n_l = 2$ rectangular chain!

Proposal for Experimental Realization



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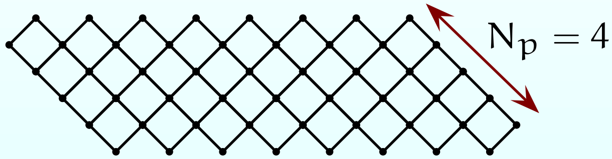
Allomorphic to the $n_l = 2$ rectangular chain!

Conclusions

The Diagonal Ladders Universality Classes



Diagonal Ladders:

- Odd N_p: Ferrimagnetic, Gapless (F), Gapped (AF)
- Even N_p:
  - $N_p = 2 \pmod 4$: AF, Gapped, Haldane Phase
  - $N_p = 0 \pmod 4$: AF, Gapless

- And a proposal for the experimentalists...
- Future work: $t - J$ model on diagonal ladders.

Thank You For Your Attention!