

(Topological Aspects of) Quantum Spin Nanotubes -S=1/2 Three-Leg Spin Tube-

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Review : T.Sakai et al. , J. Phys. Condensed Matter 22 (2010) 403201

R&D Centers of JAEA

Tsuruga

Prototype fast breeder Monju,
Decommissioning of Advanced Thermal
Reactor Fugen



Tono

High-level rad-waste
research



Horonobe

High-level rad-waste
research



Mutsu

Decommissioning of
nuclear ship



Ningyotoge

Decommissioning of
uranium enrichment
plants



Kansai

Photon & Synchrotron
Radiation Science



Takasaki

Radiation application



Tokai

Basic research, Safety
studies, Neutron
Science, Nuclear fuel-
cycle technologies,
Rad-waste management
and disposal, etc.



Oarai

Experimental reactors
Joyo, HTTR and JMTR;
Advanced reactor R&D
including FBR cycle
commercialization



Naka

Fusion R&D, ITER
support



SPring-8 (Super Photon Ring 8Gev)

SACLA(SPring-8 Angstrom Compact Free Electron Laser)



Contents

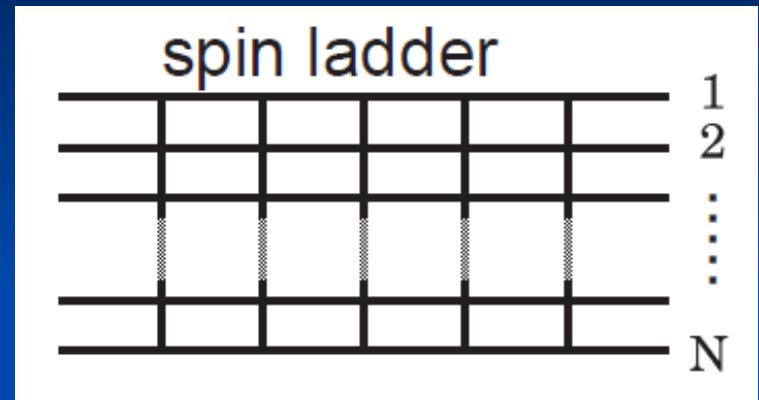
- Introduction
- Quantum Phase Transition between 3-leg tube and ladder
- Real Spin Tubes
- 1/3 Magnetization Plateau
- Carrier doped spin tubes

Introduction

Spin Ladder

Two (even) legs : Spin gap

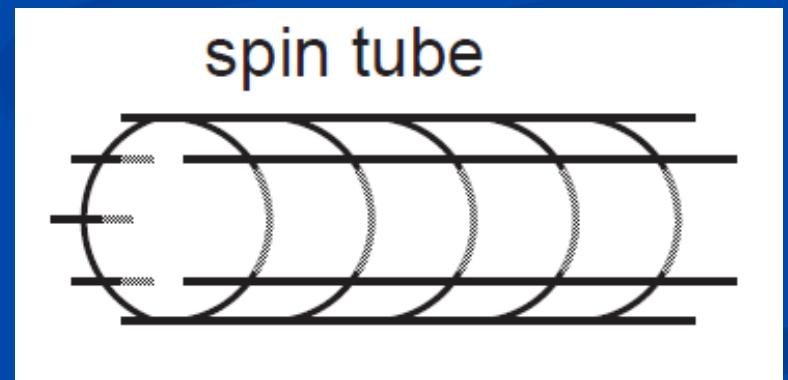
Three (odd) legs : Gapless



Spin Tube

Two (even) legs : Spin gap

Three (odd) legs : **Spin gap**



$$H = J_r \sum_{i=1}^N \sum_{j=1}^L S_{i,j} \cdot S_{i+1,j} + J_l \sum_{i=1}^N \sum_{j=1}^L S_{i,j} \cdot S_{i,j+1}$$

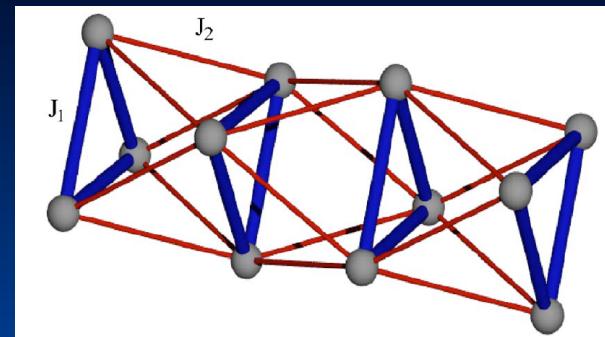
$$S=1/2$$

Real spin tubes

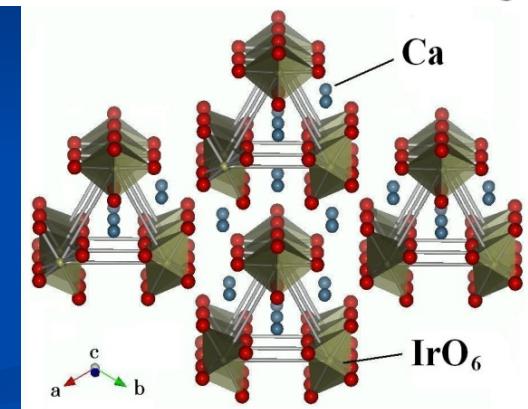
3-leg



J. Schnack, et al, PRB70, 174420 (2004).



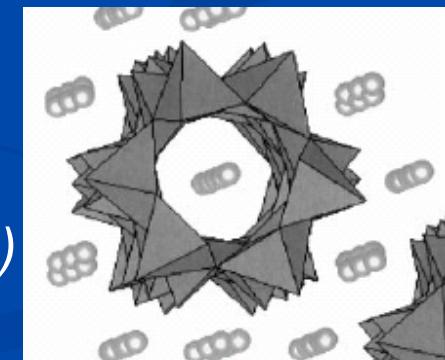
H. Sato, et al, (Chuo University)



9-leg



P. Millet, et al, J. Solid State Chem. 147, 676 (1999)



7-leg

Organic compounds

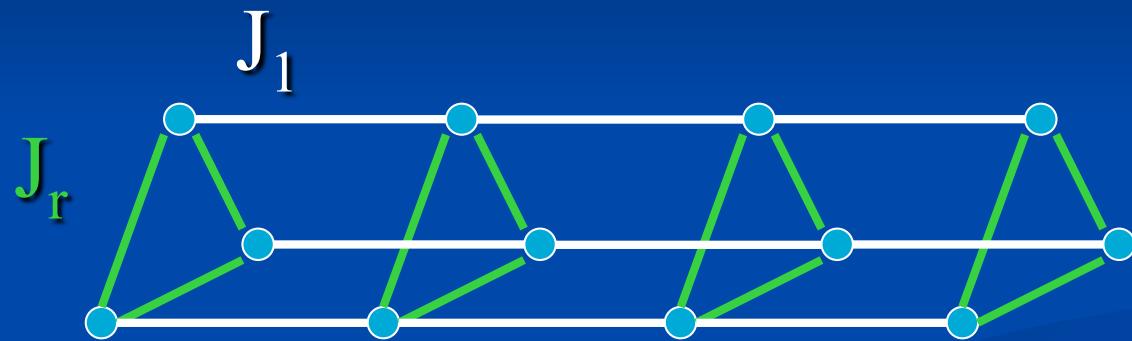
Unpublished (Tsukuba University)

Theories on 3-leg spin tubes

- Schulz 1996: $S=1/2$ Bosonization
- Kawano-Takahashi 1997: $S=1/2$, Spin gap $\sim 0.28J_\perp$
- Cabra-Honecker-Pujol 1998: $S=1/2, 1/3$ magnetization plateau
- Sato-TS 2007 : field-induced new phases
- TS-Sato-Okunishi-Okamoto-Itoi 2008, 2010: Isosceles triangle
- Nishimoto-Arikawa 2008: Isosceles triangle
- Charrier-Capponi-Oshikawa-Pujol 2010: Integer spin
- Nishimoto-Fuji-Ohta 2011: $S=3/2$, Spin gap
- Lajko-Sindzingre-Penc 2012: $S=1/2$, Multispin exchange
- Okunishi-Sato-TS-Okamoto-Itoi 2012: new phase at $m=1/3$

$S=1/2$ Three-leg spin tube

Model



S=1/2 Three-leg spin tube

Kawano-Takahashi: JPSJ 66 (1997) 4001

Effective model based on Chirality operators

Density Matrix Renormalization Group(DMRG)

$J_r > 0$: Spin gap

$J_r/J_1 \rightarrow \infty$: $\Delta = 0.28J_1$

I. Affleck, Phys. Rev. B 37, 5186 (1988)

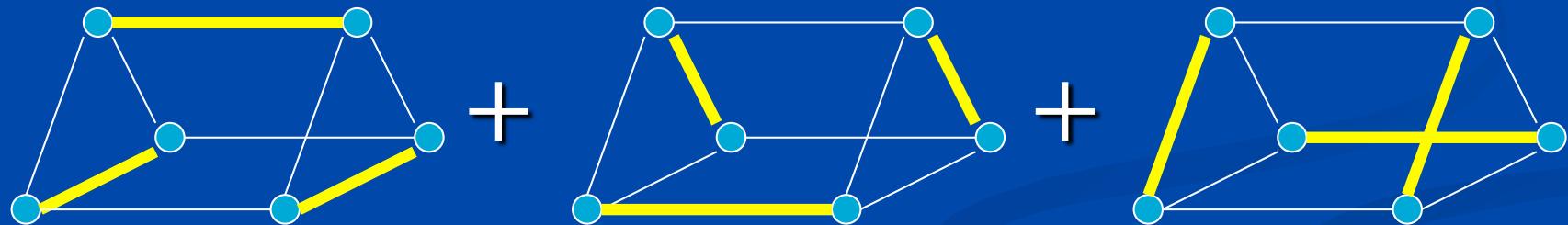
Lieb-Shultz-Mattis theorem

odd-leg ladders: gapless

or Ground state is degenerated.

Gap due to double periodicity

Singlet with double periodicity (Kawano-Takahashi)



⇒ Quantum phase transition
with respect to J_r/J_1

Analysis of Quantum Phase Transition

Numerical diagonalization: Low-lying excitation

$3 \times L$ spin systems: $L \leq 8$

Phenomenological renormalization

Scaled gap: $L\Delta$

$L\Delta$ is independent of size \Rightarrow Gapless

$L\Delta$ increasing with size : Gapped

$L\Delta$ decreasing with size : Degenerated with GS

(DMRG : Direct calculation of gap)

Spin Gap

$J_1=1$ fixed, varying J_r

Ground state : singlet

1st excited state: triplet $k=\pi$

$J_r=0$ three chains :gapless

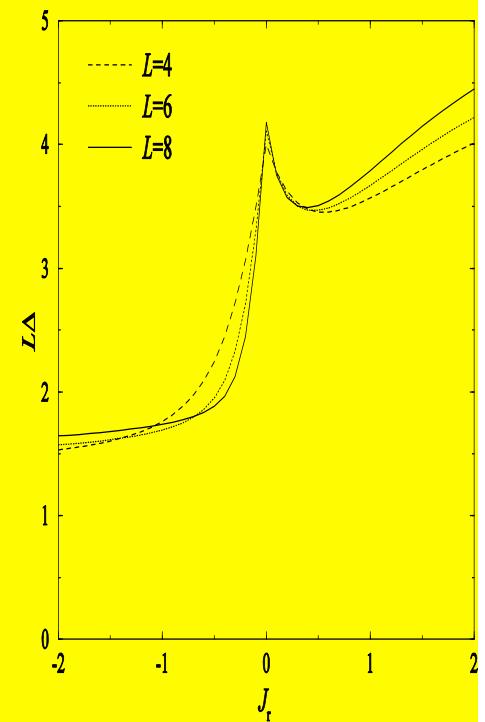
$J_r \rightarrow -\infty$ (S=3/2 chain) : gapless

Result:

$J_r > 0$: Spin gap is opening

with increasing J_r

$J_r < 0$: Always gapless



Doubly degenerated Ground State

Singlet excitations $k=\pi$

degenerated with GS



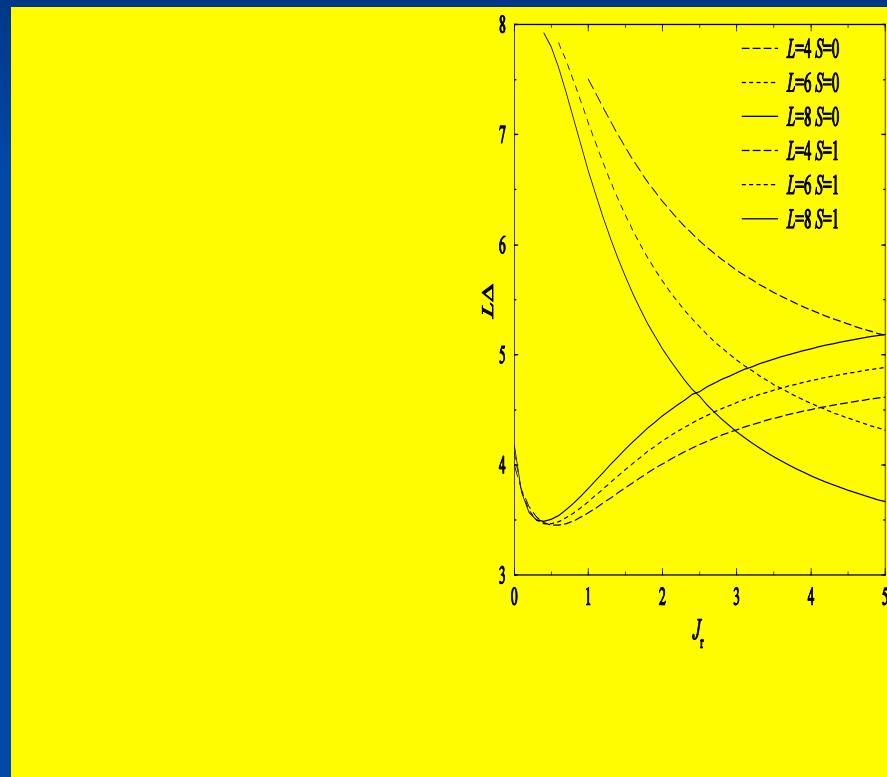
Double periodicity



Spin gap

Critical point J_{rc}

$J_{rc} = 0$ or finite ?



Quantum Phase Transition between 3-leg spin tube and ladder -Isosceles Triangle Tube-

Distortion from a regular triangle ($J_r > J_{rc}$)

$$\alpha = J_r' / J_r$$

$\alpha=0$: Three-leg ladder

gapless

$\alpha=1$: Spin gap

$\alpha \rightarrow \infty$: Dimer and monomer

gapless



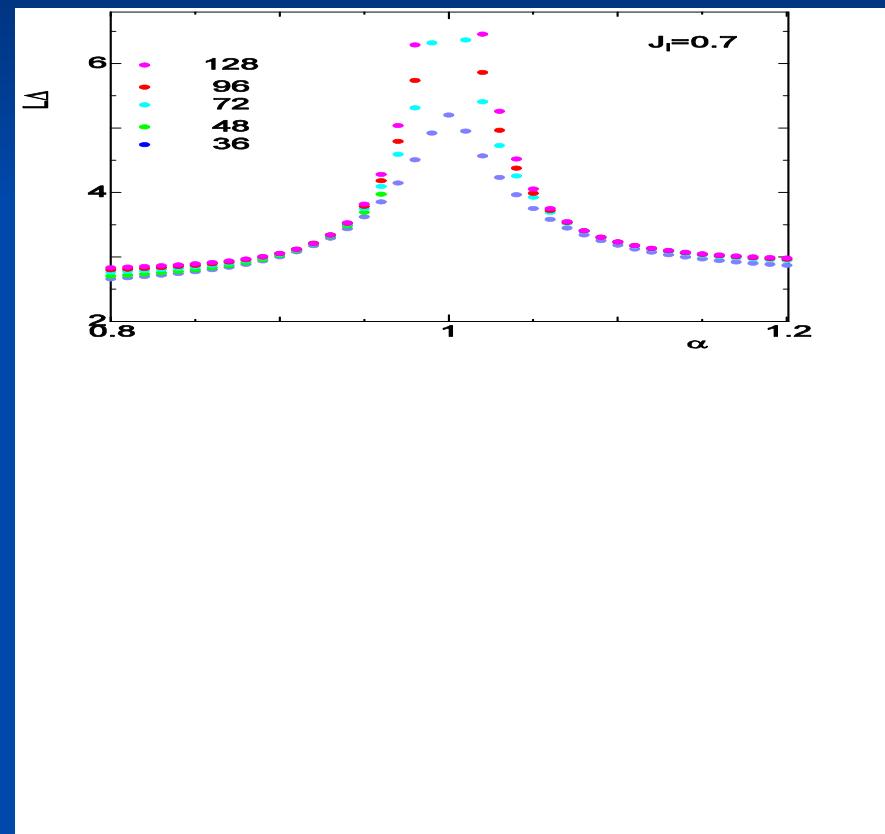
Quantum phase transition with respect to α

Spin Gap by DMRG

$J_1=0.7$ fixed

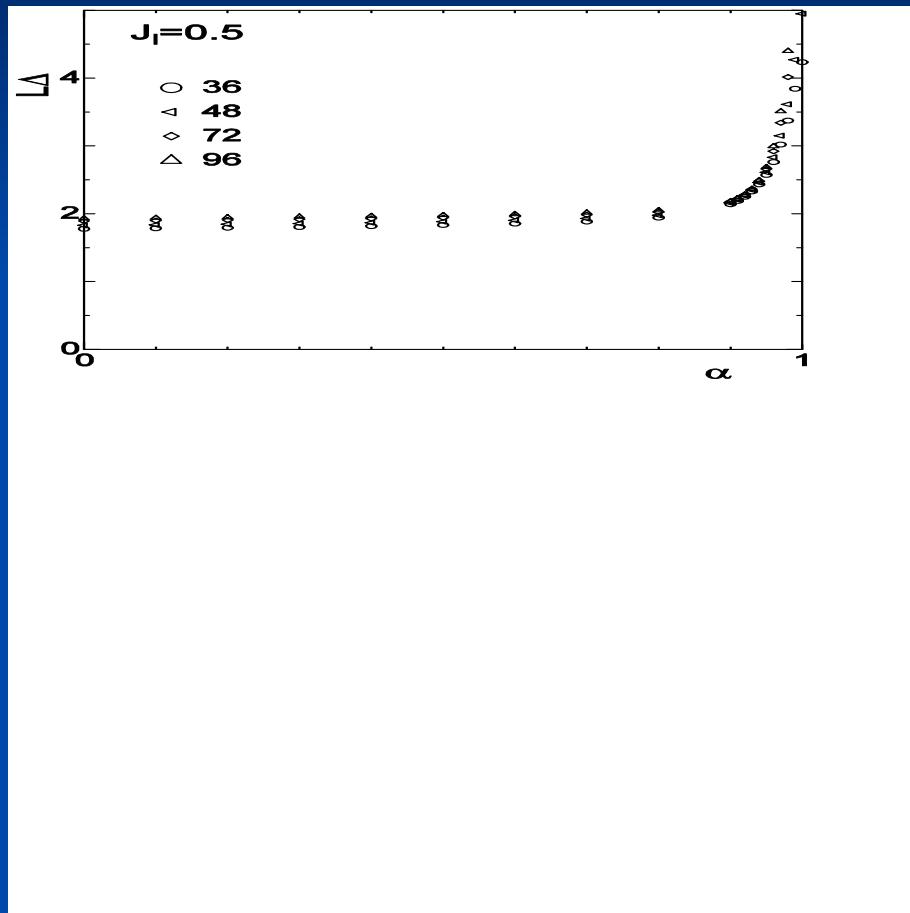
Spin gap is open
only in a very small region

$\alpha \sim 1$



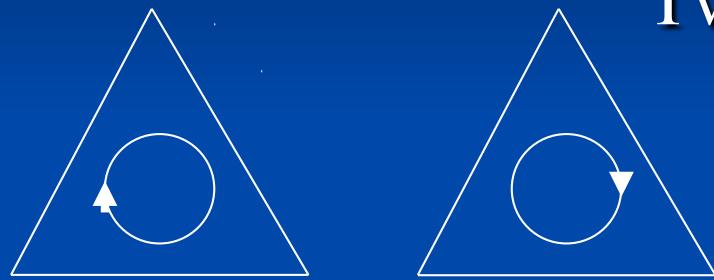
Large Size Corrections

- Logarithmic system size corrections
 $\sim 1/\log L$
- 3-leg ladder looks gapped !



Previous Effective Hamiltonian

Chiral symmetry: S=1/2 Regular triangle cluster
Two doublets are degenerated.



Chirality operators

$$\tau^+ |\cdot L\rangle = 0, \quad \tau^- |\cdot L\rangle = |\cdot R\rangle,$$
$$\tau^+ |\cdot R\rangle = |\cdot L\rangle, \quad \tau^- |\cdot R\rangle = 0.$$

$$|\uparrow L\rangle = \frac{1}{\sqrt{3}} (| \uparrow\uparrow\downarrow \rangle + \omega | \uparrow\downarrow\uparrow \rangle + \omega^{-1} | \downarrow\uparrow\uparrow \rangle),$$
$$|\downarrow L\rangle = \frac{1}{\sqrt{3}} (| \downarrow\downarrow\uparrow \rangle + \omega | \downarrow\uparrow\downarrow \rangle + \omega^{-1} | \uparrow\downarrow\downarrow \rangle),$$
$$|\uparrow R\rangle = \frac{1}{\sqrt{3}} (| \uparrow\uparrow\downarrow \rangle + \omega^{-1} | \uparrow\downarrow\uparrow \rangle + \omega | \downarrow\uparrow\uparrow \rangle),$$
$$|\downarrow R\rangle = \frac{1}{\sqrt{3}} (| \downarrow\downarrow\uparrow \rangle + \omega^{-1} | \downarrow\uparrow\downarrow \rangle + \omega | \uparrow\downarrow\downarrow \rangle), \quad \omega = \exp\left(\frac{2\pi i}{3}\right).$$

$$J_r/J_1 \rightarrow \infty$$

$$H = J_1/3 \sum_j \vec{S}_j \cdot \vec{S}_{j+1} [1 + \gamma (\tau_j^+ \tau_{j+1}^- + \tau_j^- \tau_{j+1}^+)]$$

SU(2) symmetry

New effective theory

■ Hubbard model on 3-leg tube

$$H = H_{\text{hop}} + H_{\text{int}},$$

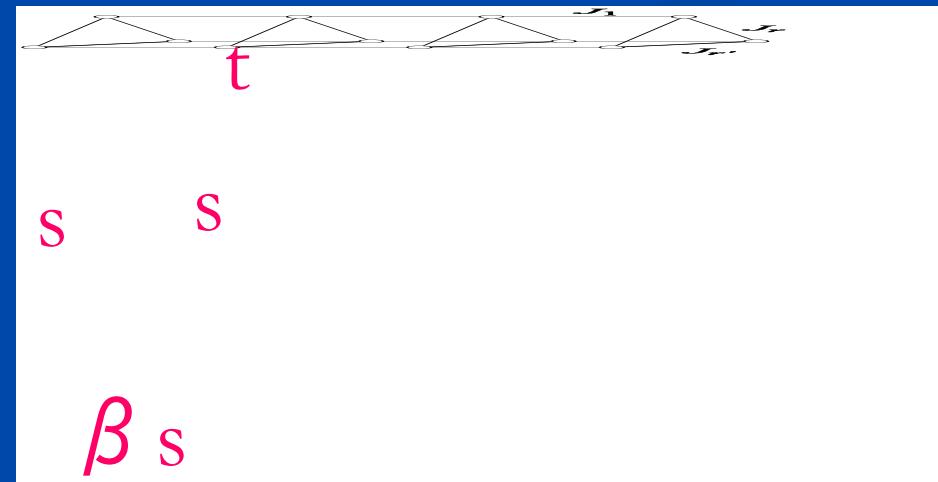
$$H_{\text{hop}} = \sum_{n=1}^L \sum_{i=1}^3 \sum_{\sigma=\uparrow,\downarrow} (t c_{n+1,i,\sigma}^\dagger c_{n,i,\sigma} + s_{i+1,i} c_{n,i+1,\sigma}^\dagger c_{n,i,\sigma} + h.c.),$$

$$H_{\text{int}} = U \sum_{n=1}^L \sum_{i=1}^3 n_{n,i,\uparrow} n_{n,i,\downarrow},$$

Large $U \Rightarrow$ Heisenberg model

$$J_1 = t^2/U, \quad J_r = s^2/U,$$

$$\alpha = J_r'/J_r = \beta^2$$



Criterion of Spin Gap

- Hopping term: 3 bands

$$E_1(k) = -\beta s + 2t \cos k,$$

$$E_2(k) = \frac{1}{2}(\beta s - \sqrt{\beta^2 + 8} + 4t \cos k),$$

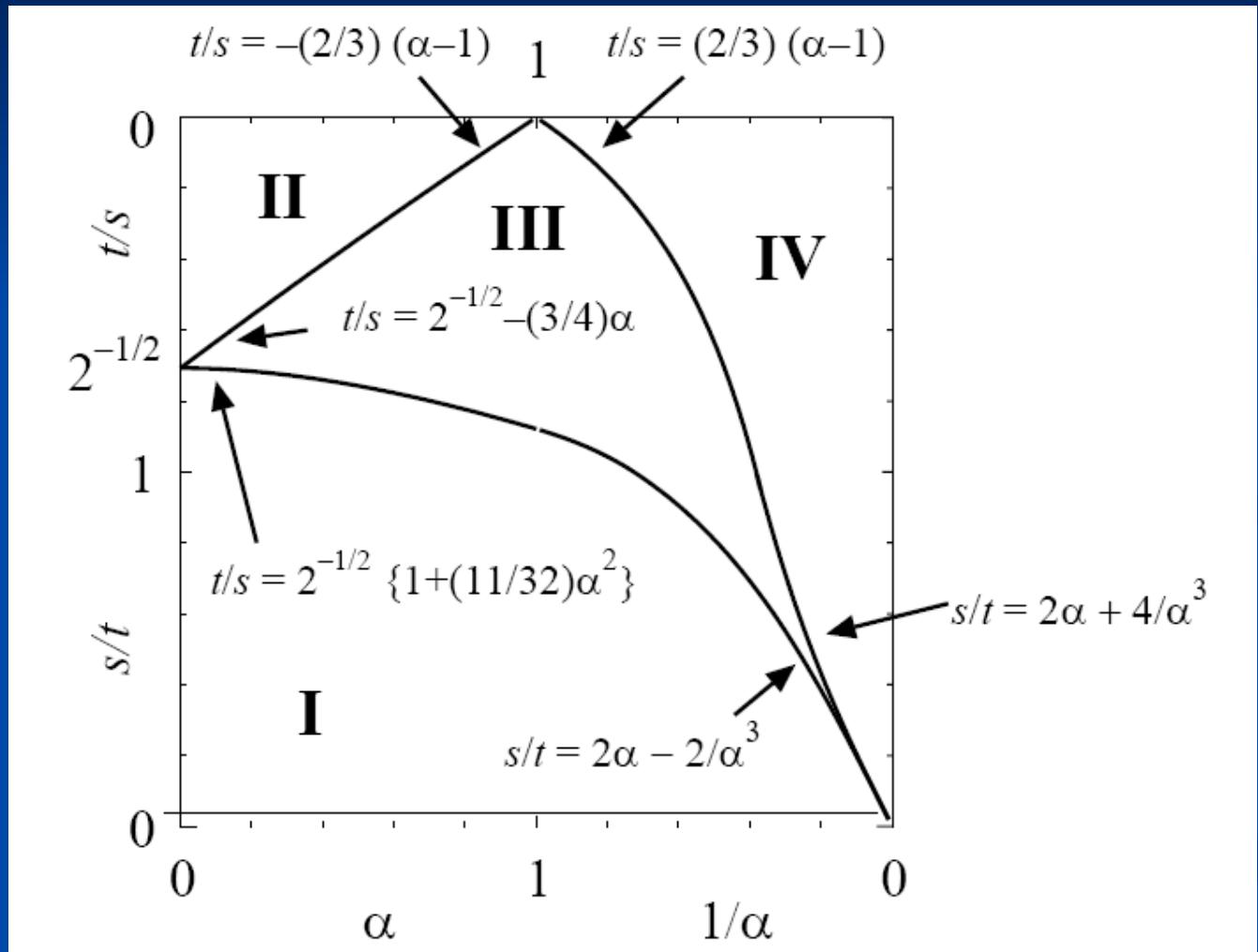
$$E_3(k) = \frac{1}{2}(\beta s + \sqrt{\beta^2 + 8} + 4t \cos k),$$

- Number of Fermi points
0 to 3 pairs of Fermi points
- Criterions
Even pairs: Gapped
Odd pairs: Gapless \Rightarrow phase boundary

Phase diagram by effective theory

Phase III:
Gapped

Phase I ?



Level spectroscopy

- KT phase boundary between gapped and gapless
Logarithmic size corrections (Okamoto-Nomura)
 J_1 - J_2 frustrated spin chain $(J_2/J_1)_c=0.2411\dots$

Triplet excitation gap $\Delta_t \sim 1/L (1 - C/\log L \dots)$

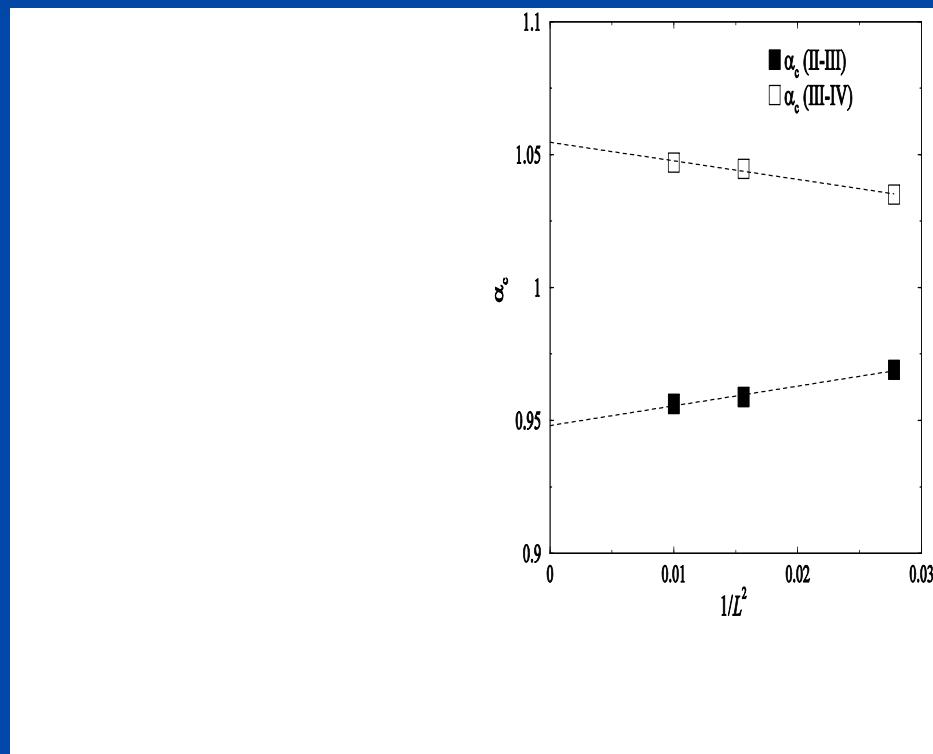
Singlet excitation gap $\Delta_s \sim 1/L (1 + 3C/\log L \dots)$

At the critical point $C=0$

$\Delta_t = \Delta_s \Rightarrow$ precise phase boundary

Phase boundary α_c

- By level spectroscopy with numerical diagonalization up to $L=10$
for $J_1=0.2$
($J_r=1$ fixed)



J_{1c} for symmetric case $\alpha=1$

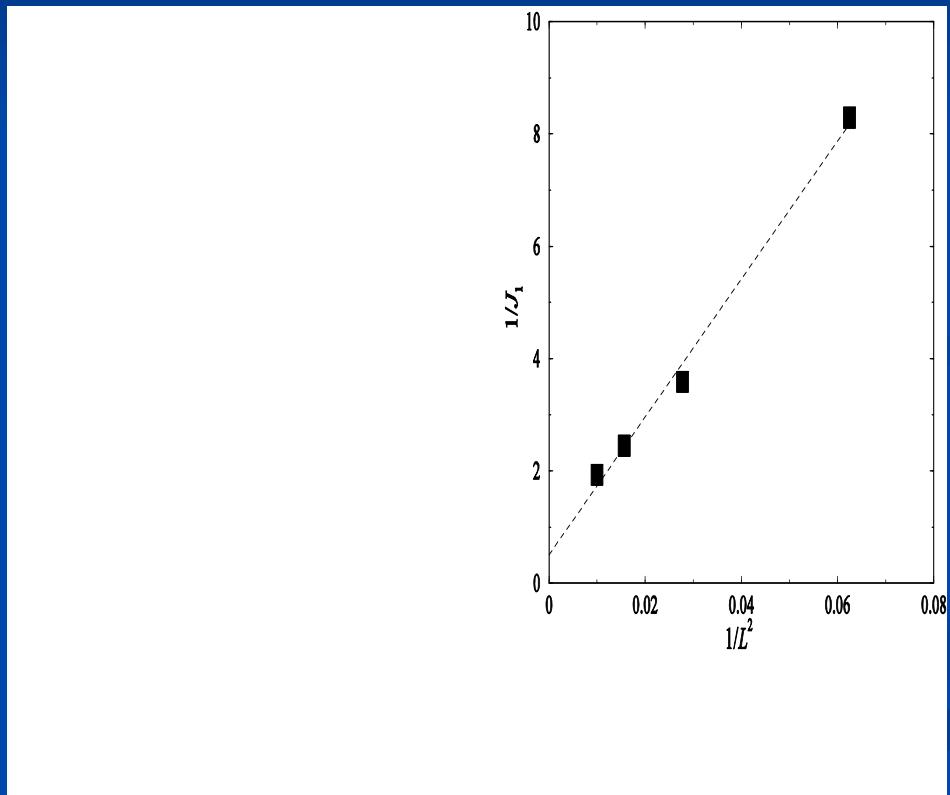
- Large size dependence

Critical point

$$1/J_1 = 0.51 \mp 0.4$$

It is difficult to
determine

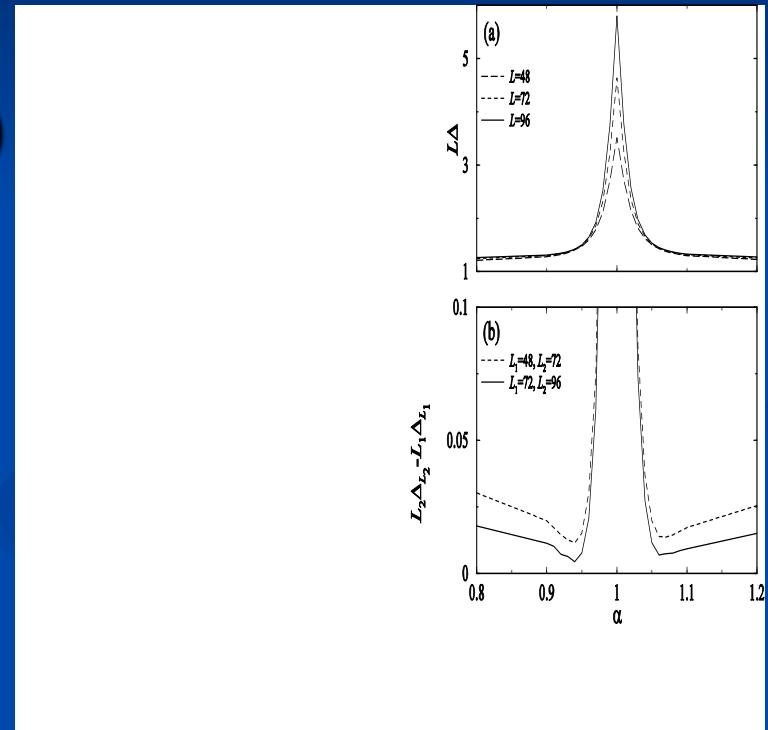
$J_{rc} = 0$ or not .



Phenomenological renormalization

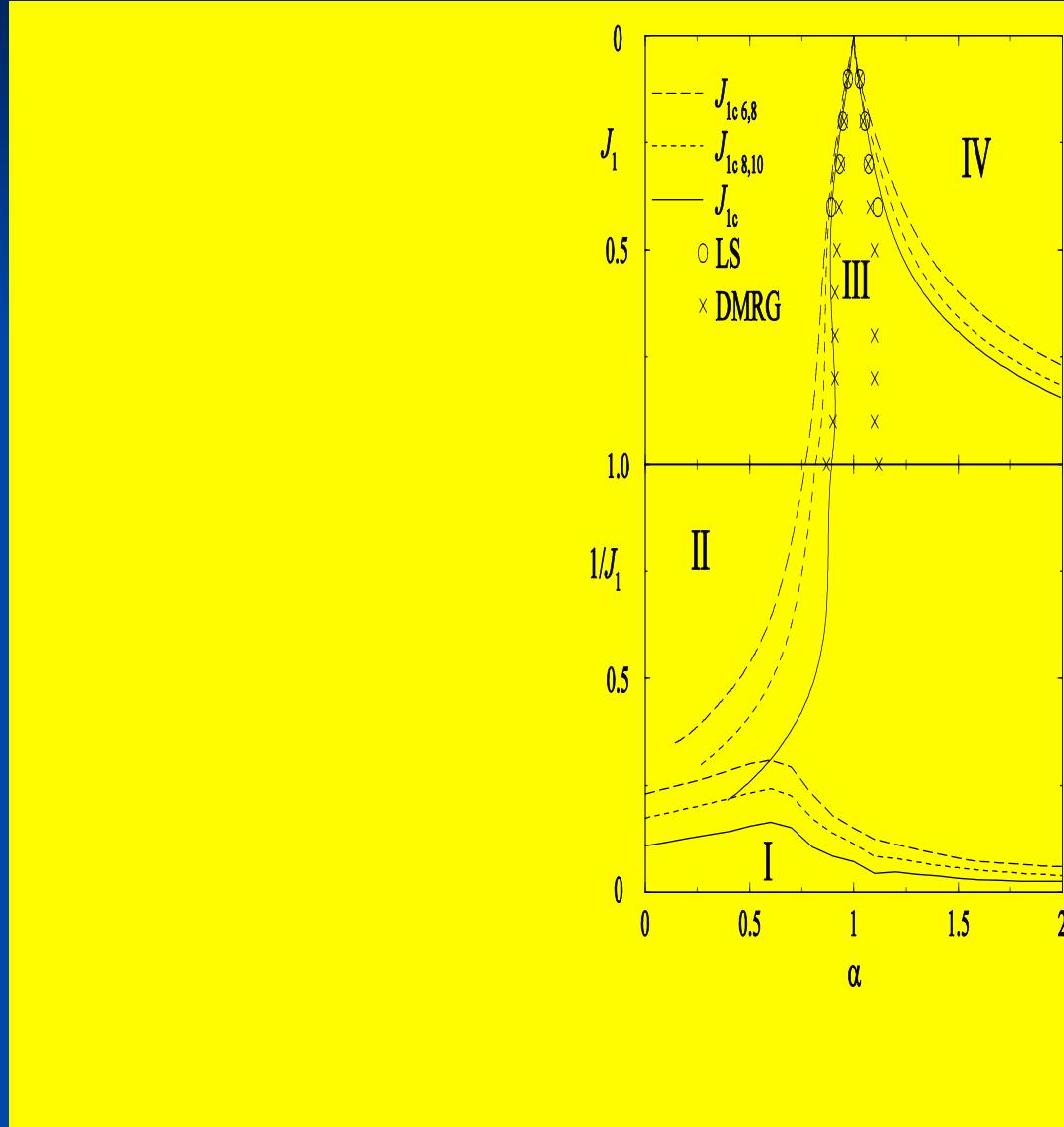
- DMRG up to $L=128$
- Diagonalization up to $L=10$
- No fixed points by
 $L_1\Delta_{L1} = L_2\Delta_{L2}$

- Gapless points determined by the minimum of
 $L_1\Delta_{L1} - L_2\Delta_{L2}$

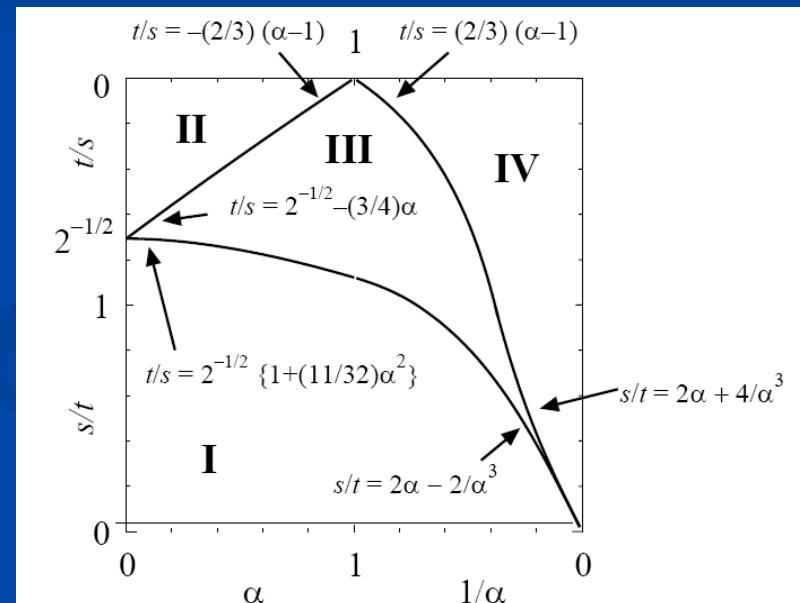


DMRG for $J_1=0.3$

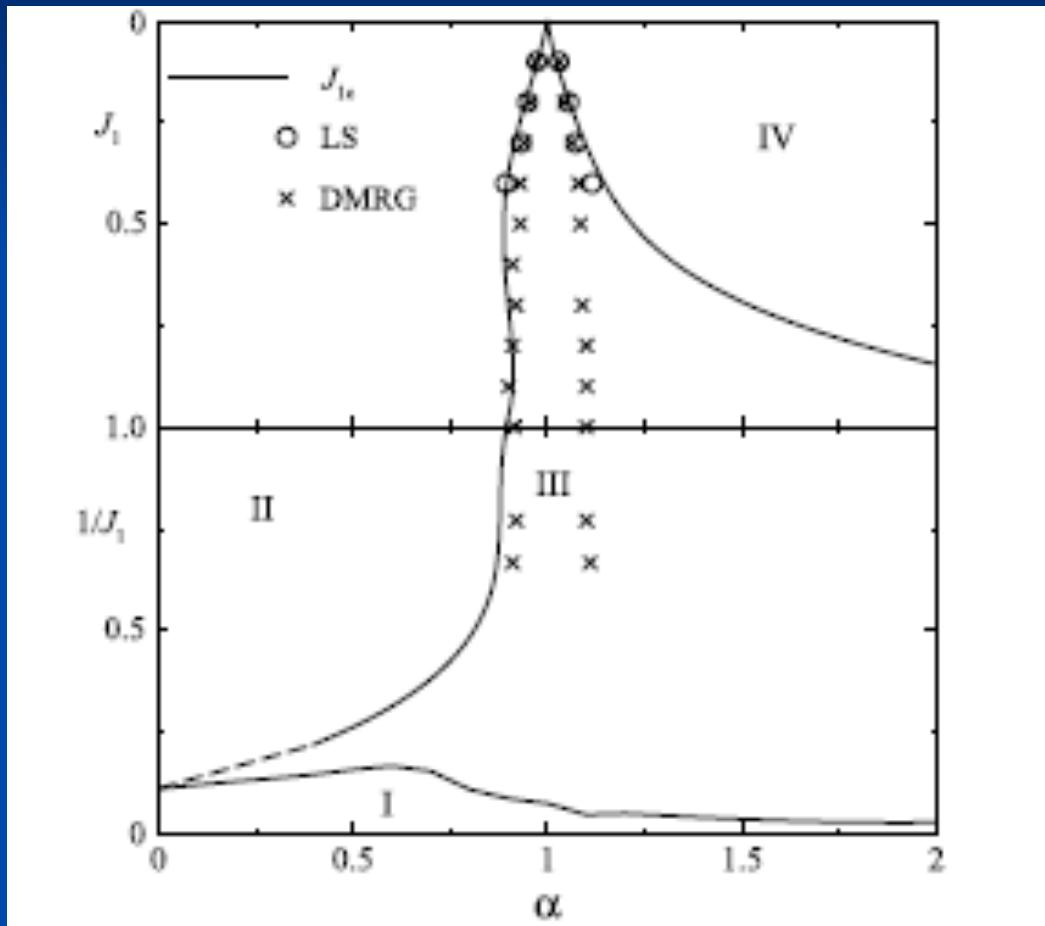
Numerical Phase Diagram



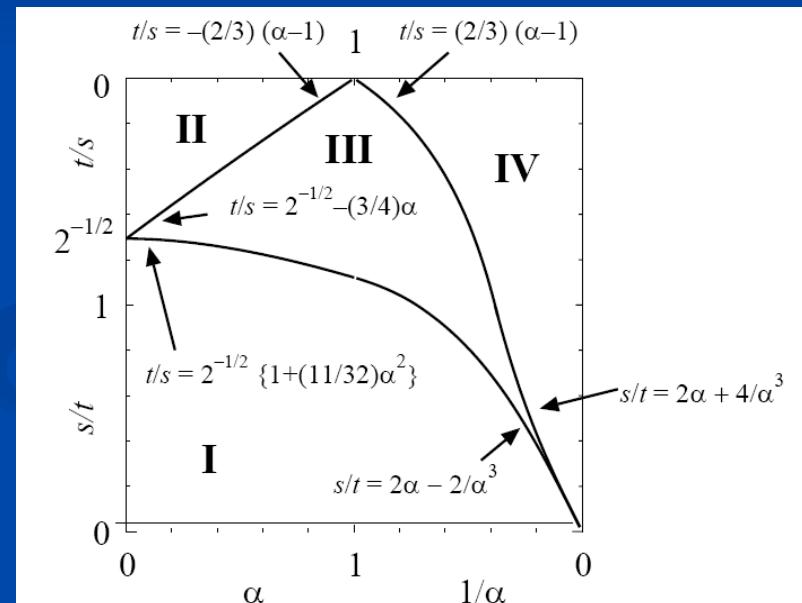
Effective theory



Numerical Phase Diagram



Effective theory



BKT transition

Conformal field theory analysis

$$\langle S_0^z S_r^z \rangle \sim (-1)^r r^{-\eta}$$

$$\Delta \sim \pi v s \eta / L \rightarrow \eta$$

Central charge : c

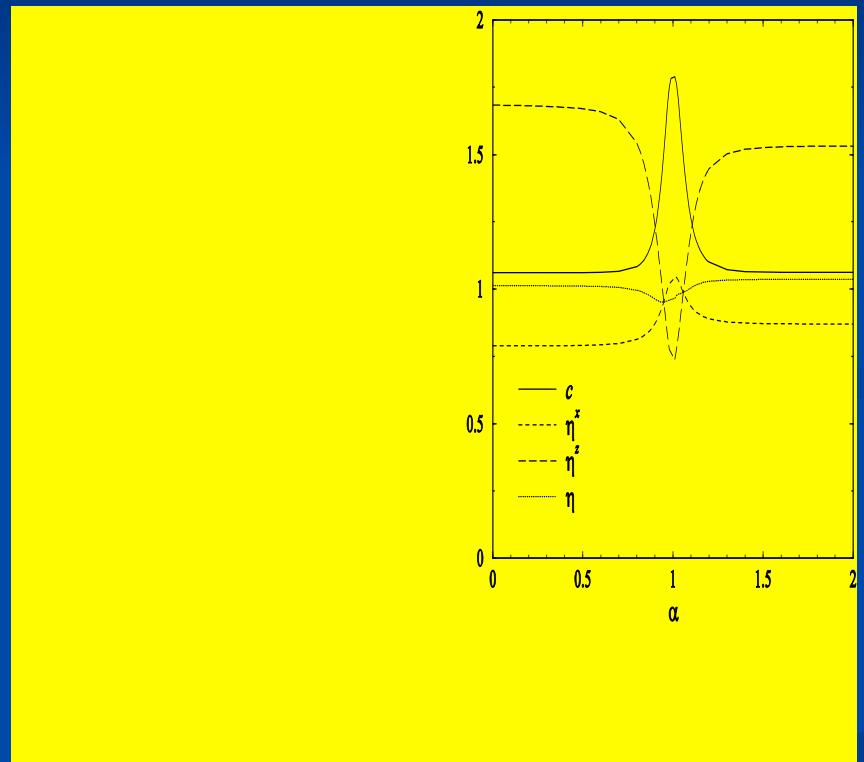
Numerical diagonalization:

$\eta=1$ $c=1$ for gapless phases

\Rightarrow BKT transition

Berezinskii-Kosterlitz-Thouless

$J_1=0.3$

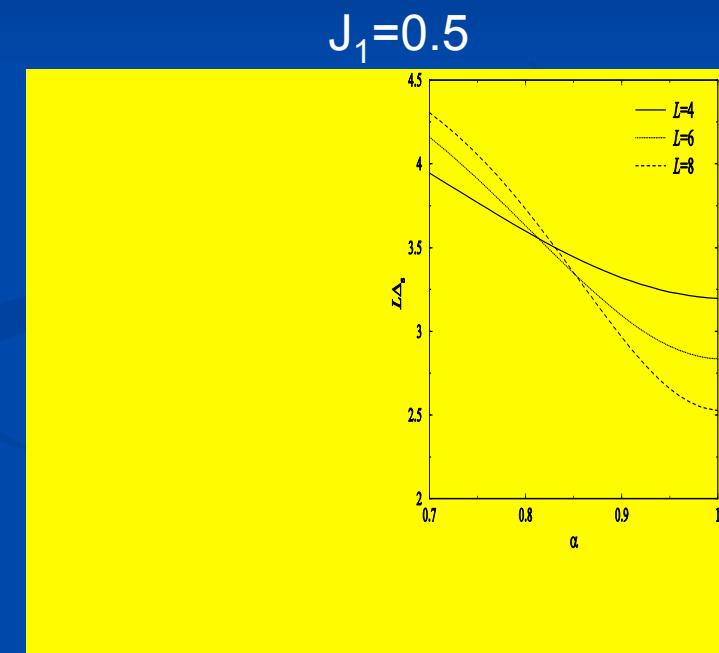


Phenomenological Renormalization -Singlet gap-

- Spin gap (singlet-triplet) : large size correction
- Singlet-singlet gap
Degenerated in gapped phase

Size-dependent fixed point
 $(L+2) \Delta(L+2, \alpha_c) = L \Delta(L, \alpha_c)$

Extrapolate $\alpha_c(L) \Rightarrow \alpha_c(\infty)$



Quantized Berry phase

Y.Hatsugai, JPSJ (2006)

"Local characterization of quantum liquids"

For spin systems (without magnetic field),

- make a local $SU(2)$ twist θ only at one link as,

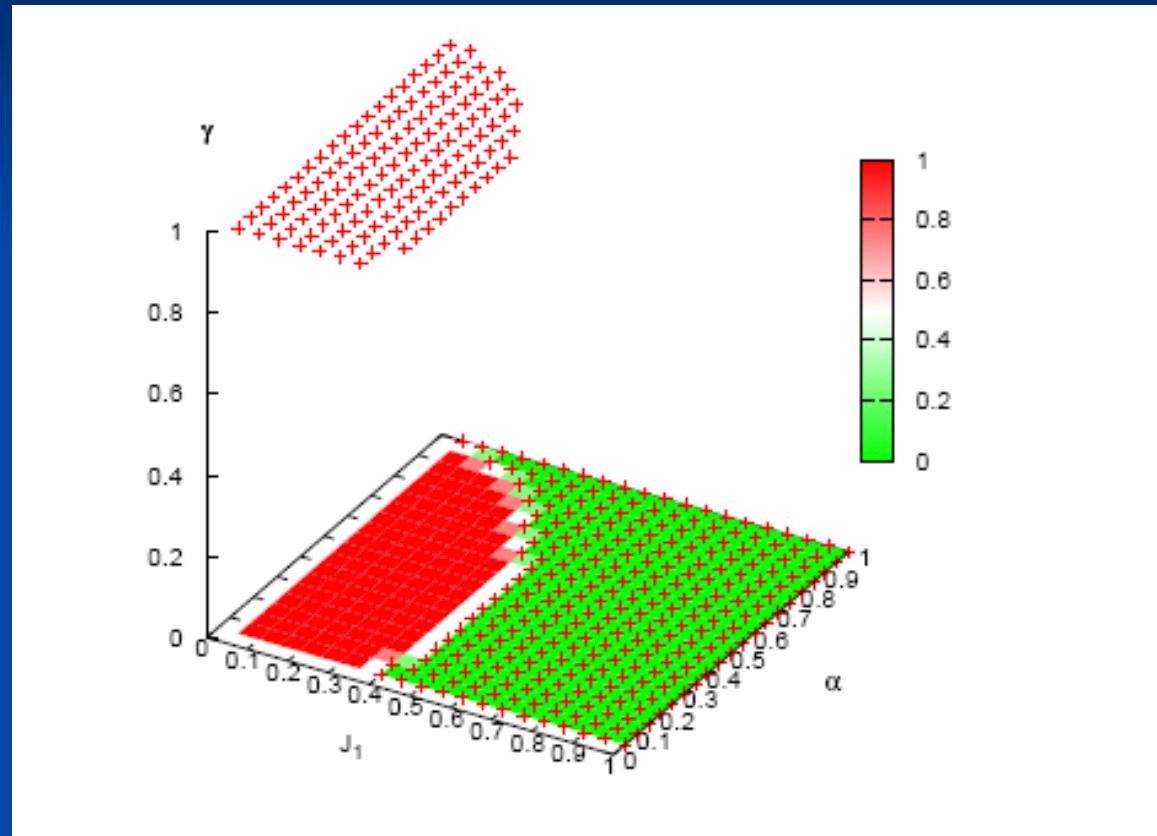
$$J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \rightarrow J_{ij}/2 \left(e^{-i\theta} S_i^+ S_j^- + e^{i\theta} S_i^- S_j^+ + 2 S_i^z S_j^z \right)$$

- sum up the (lattice) Berry connection,

$$\gamma = \text{Arg} \prod_C \langle \psi_{\theta_j}^U | \psi_{\theta_{j+1}}^U \rangle, \quad |\psi_{\theta_j}^U\rangle = |\psi_{\theta_j}\rangle \langle \psi_{\theta_j}|\phi\rangle$$

$|\phi\rangle$: (arbitrary) reference state to fix the gauge

Calculation of quantized Berry phase for L=4 (Otsuka-TS 2012)

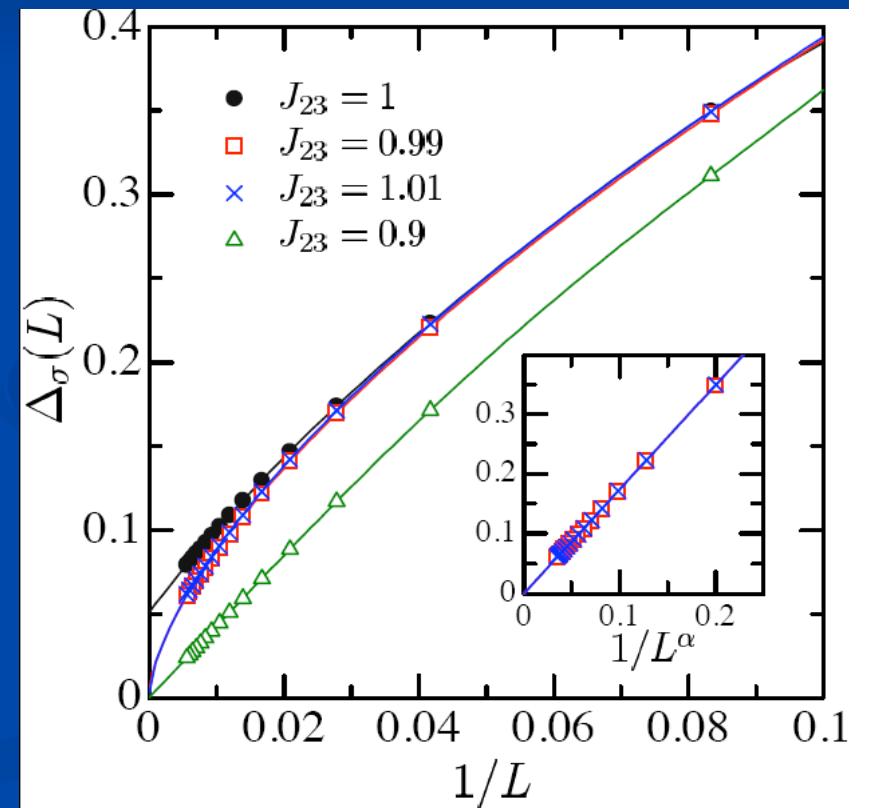


It supports the mechanism of spin gap.

Another work

- DNRG by Nishimoto and Arikawa :
PRB 2008

Spin gap is open just for
the symmetric tube($\alpha=1$),
otherwise gapless,
assuming the size correction
has a power law.



Summary1

$S=1/2$ Three-leg spin tube

Regular triangle tube Chiral symmetry

$J_r > 0 \Rightarrow$ Spin gap

Isosceles triangle tube No chiral symmetry

Spin gap in a small region $\alpha = J_r' / J_r \sim 1$

Quantum phase transition (BKT transition)

$\alpha = 1$

Spin tube

\leftrightarrow

$\alpha = 0$

Spin ladder

Spin gap

Gapless

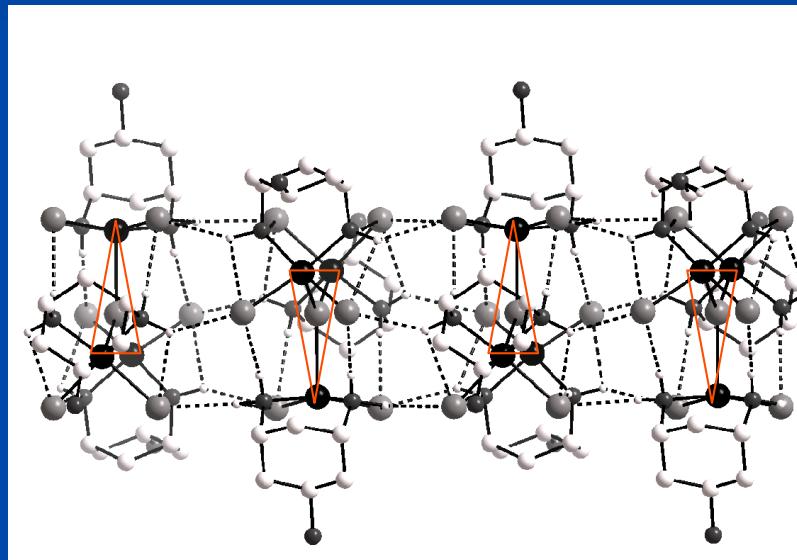
Distortion from regular triangle \Rightarrow Gap vanishes rapidly

J_{rc} =finite or 0 ? still an open question

2. A real spin tube $[(\text{CuCl}_2\text{tachH})_3\text{Cl}]\text{Cl}_2$

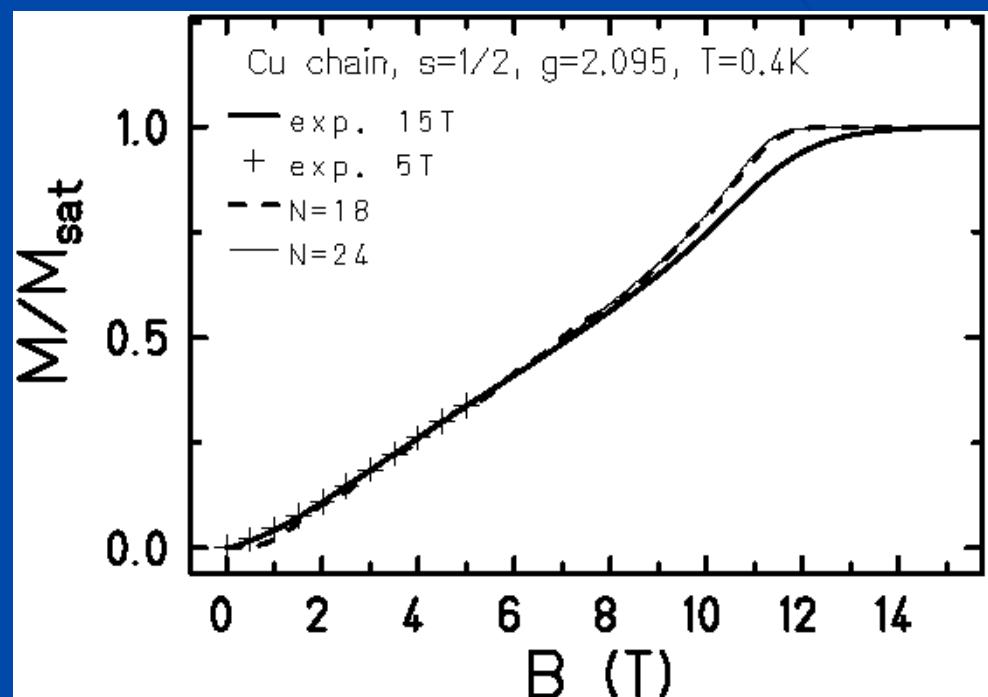
J. Schnack, H. Nojiri, P. Kögerler, G.J. T. Cooper and L. Cronin
Phys. Rev. B **70**, 174420 (2004)

Assembly of triangular clusters



Phys. Rev. B **70**, 174420 (2004)

MH-curve



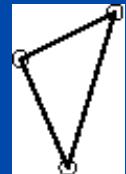
The model parameter is about $J'/J=2$

What is the triangular lattice quantum spin tube? ¹

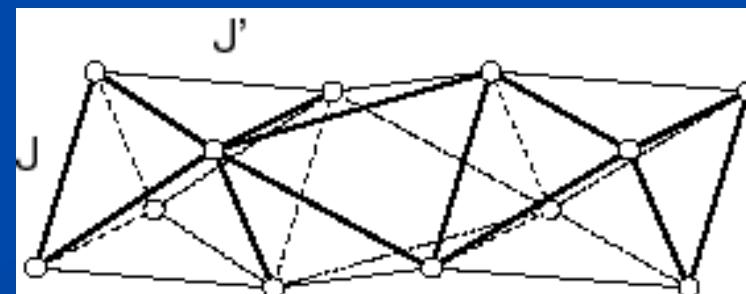
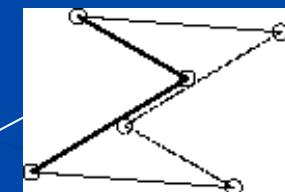
Hamiltonian:

$$H = J \sum_i \sum_{j=1}^3 S_{i,j} \cdot S_{i,j+1} + J' \sum_i \sum_{j=1}^3 [S_{i,j} \cdot S_{i+1,j} + S_{i,j} \cdot S_{i+1,j+1}]$$

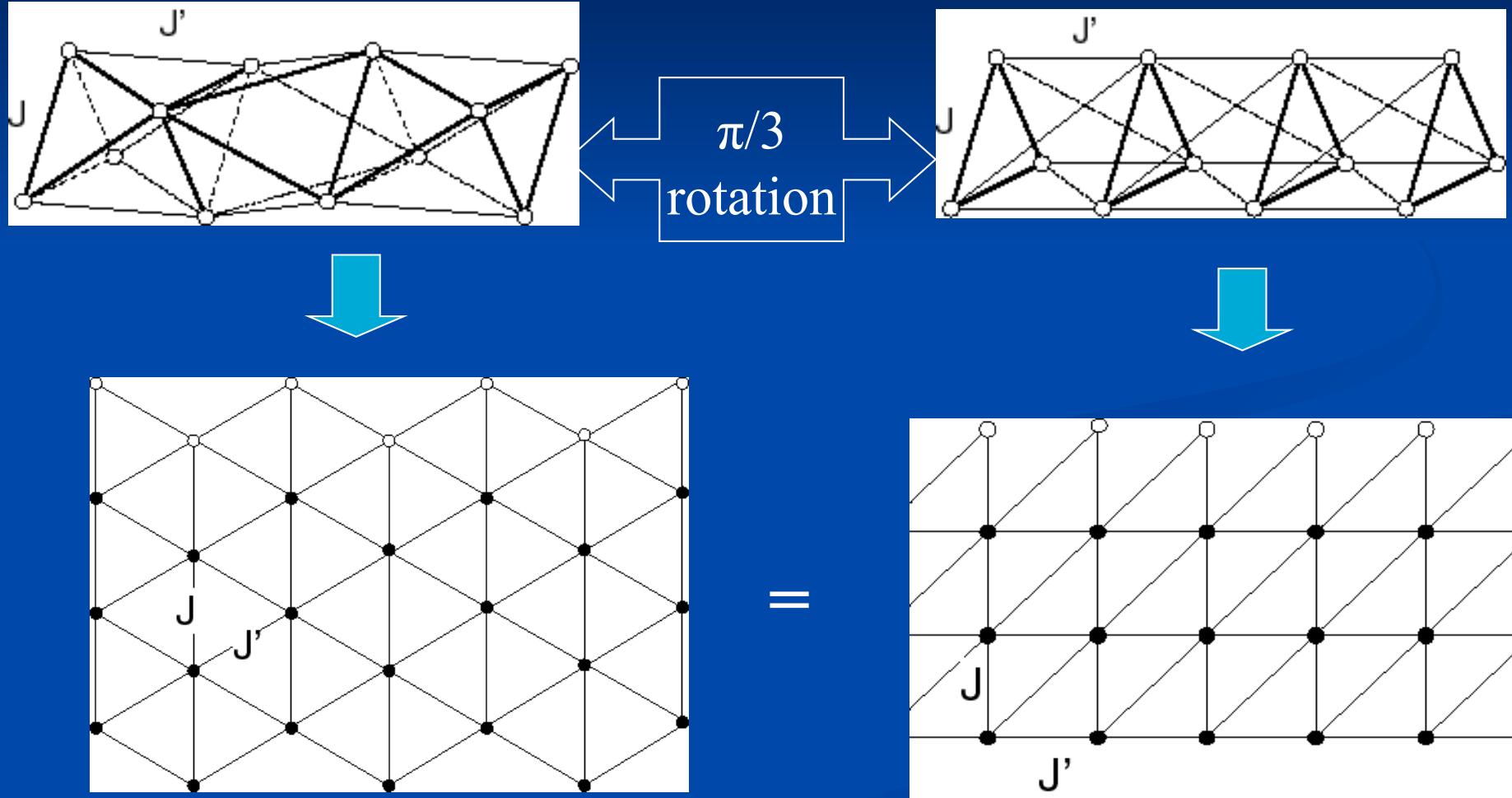
intra triangle
coupling



inter triangle
coupling



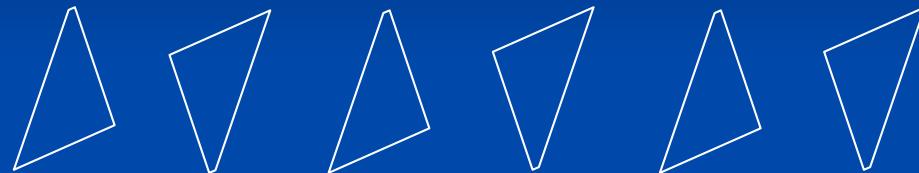
Expand the tube



Triangular lattice structure

We can expect two phases

(A) $J \gg J'$ weakly coupled triangles



quantum phase transition

(B) $J \ll J'$ rhombic lattice(modulated square lattice)
If $J=0$, no frustration!



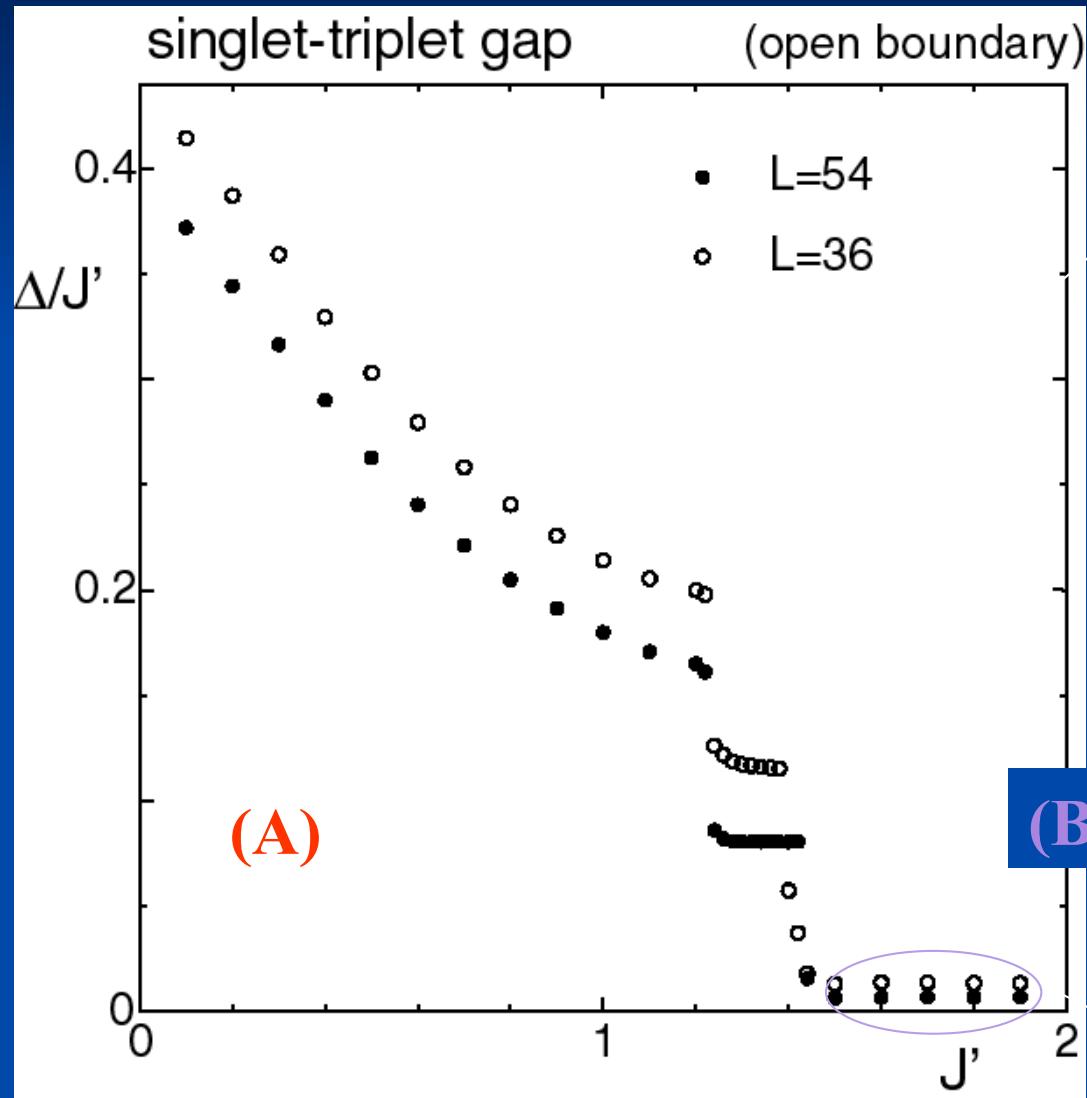
Numerical calculation

DMRG, finite size method

MH-curve : 36×3 spins, $m=80$

Spin gap : up to 144×3 spins,
up to $m=220$ with m extrapolation
(empirical)

Spin gap (Okunishi et al. 2005, Fouet et al. 2006)



(C) intermediate phase??

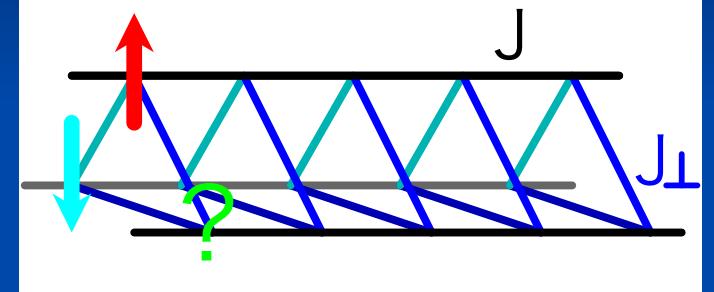
First order transition
is expected, since the
gap exhibits discontinuities

1/3 magnetization plateau

Three-leg spin tube

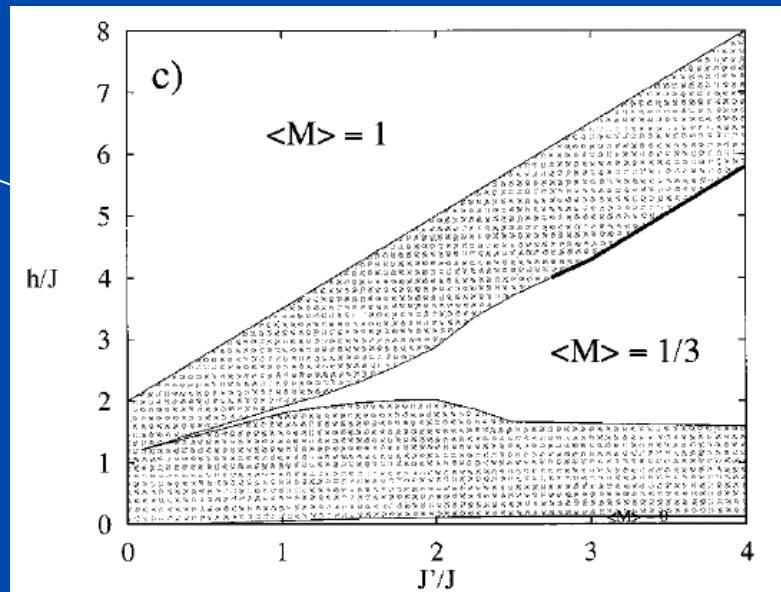
$$\mathcal{H} = \sum_{l,j} \left[J \vec{S}_{l,j} \cdot \vec{S}_{l,j+1} + J_{\perp} \vec{S}_{l,j} \cdot \vec{S}_{l+1,j} - H S_{l,j}^z \right].$$

One of the simplest 1D magnets
with geometrical **frustration**



Phase diagram of the $S=1/2$ tube (Exact Diagonalization)

critical



$M=1/6$ plateau

*Cabra, Honecker and Pujol,
PRL79, 5126 (1997);
PRB58, 6241 (1998).*

$S = 1/2$ Three-Leg Spin Nanotube

- Isosceles case

all the spin-couplings are of $\vec{S} \cdot \vec{S}$ type (isotropic)

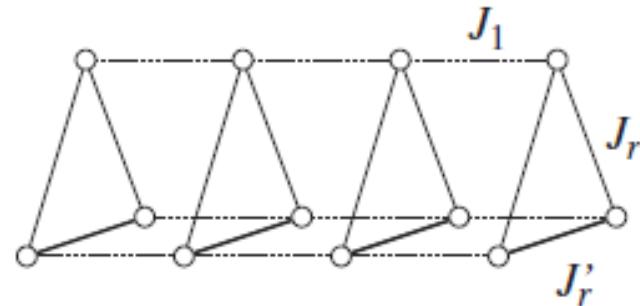
$$J'_r / J_r \equiv \alpha$$

$J_r = 1$, unit energy

$\alpha = 0$: 3-leg ladder

$\alpha = 1$: regular triangle tube

$\alpha \rightarrow \infty$: 2-leg ladder + single chain

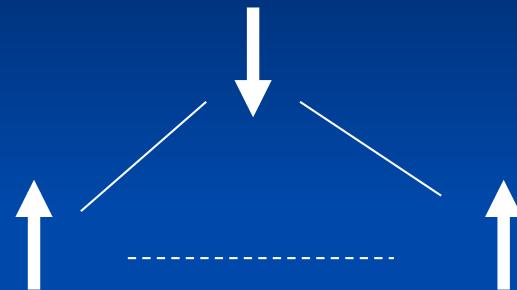


- $M = M_s/3$ state (M_s : saturation magnetization)

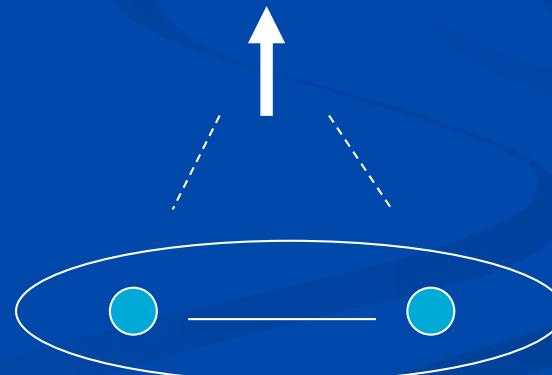
we are interested in the $M = M_s/3$ state when $J_1 \ll 1$ (maybe plateau)

Two mechanisms of 1/3 plateau

- 3-leg ladder
uud plateau

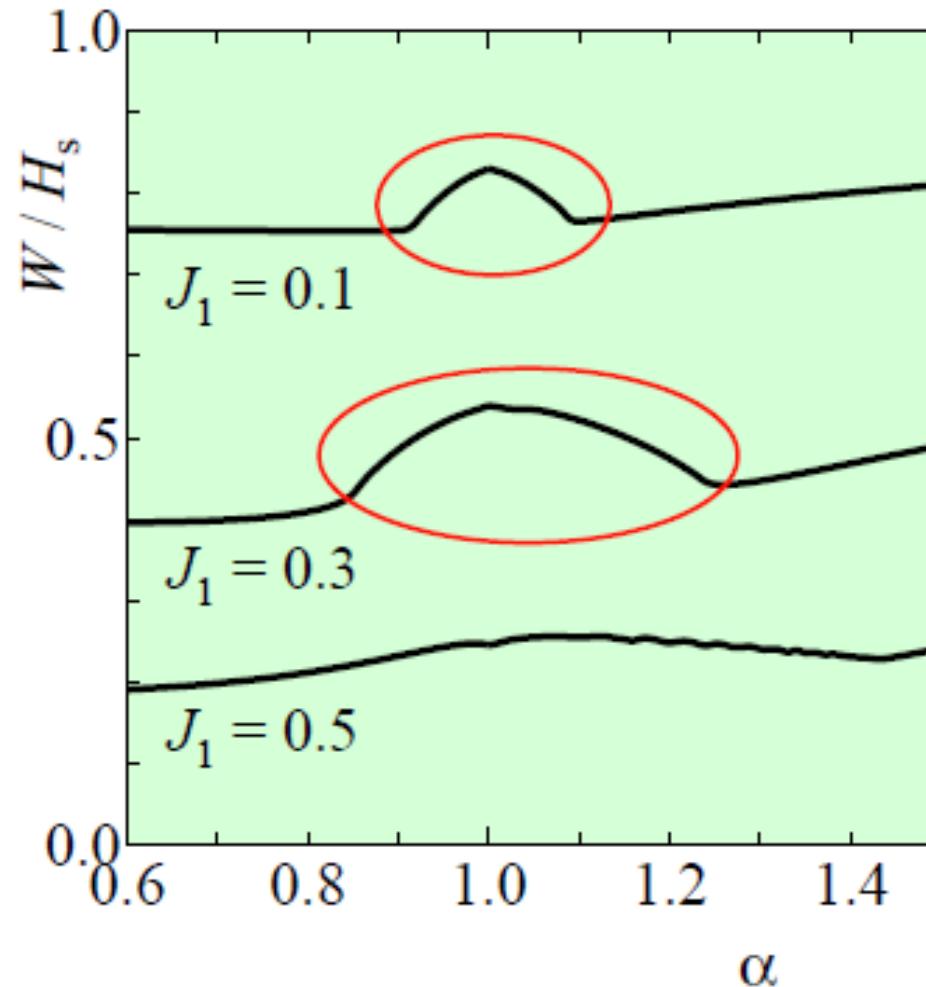


- Dimer-monomer
plateau



- Plateau width W near $\alpha = 1$ and $J_1 \ll 1$ (by DMRG)

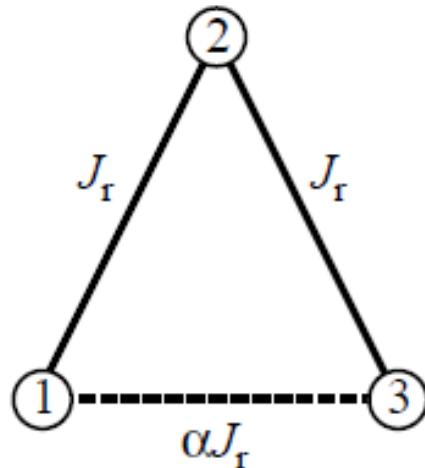
normalized by the saturation field H_s



anomalous behavior of the plateau width near $\alpha = 1$
new and exotic!!

Spin States of Isosceles Triangles

- Eigenstates of isosceles triangles at $S_{\text{tot}}^z = 1/2$

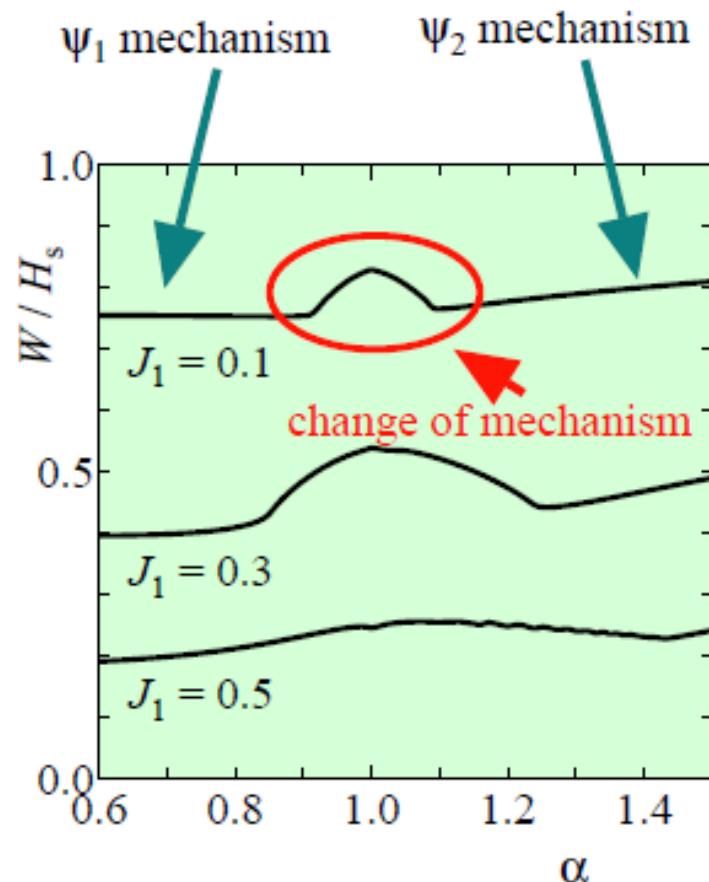


state	energy	S_{tot}	P
$\psi_1 = \frac{1}{\sqrt{6}} (\uparrow\uparrow\downarrow \rangle - 2 \uparrow\downarrow\uparrow \rangle + \downarrow\uparrow\uparrow \rangle)$	$-1 + \alpha/4, (\alpha < 1, \text{GS})$	$1/2$	$+1$
$\psi_2 = \frac{1}{\sqrt{2}} (\uparrow\uparrow\downarrow \rangle - \downarrow\uparrow\uparrow \rangle) = \uparrow\rangle_2[1, 3]$	$-3\alpha/4, (\alpha > 1, \text{GS})$	$1/2$	-1
$\psi_3 = \frac{1}{\sqrt{3}} (\uparrow\uparrow\downarrow \rangle + \uparrow\downarrow\uparrow \rangle + \downarrow\uparrow\uparrow \rangle)$	$1/2 + \alpha/4$	$3/2$	$+1$

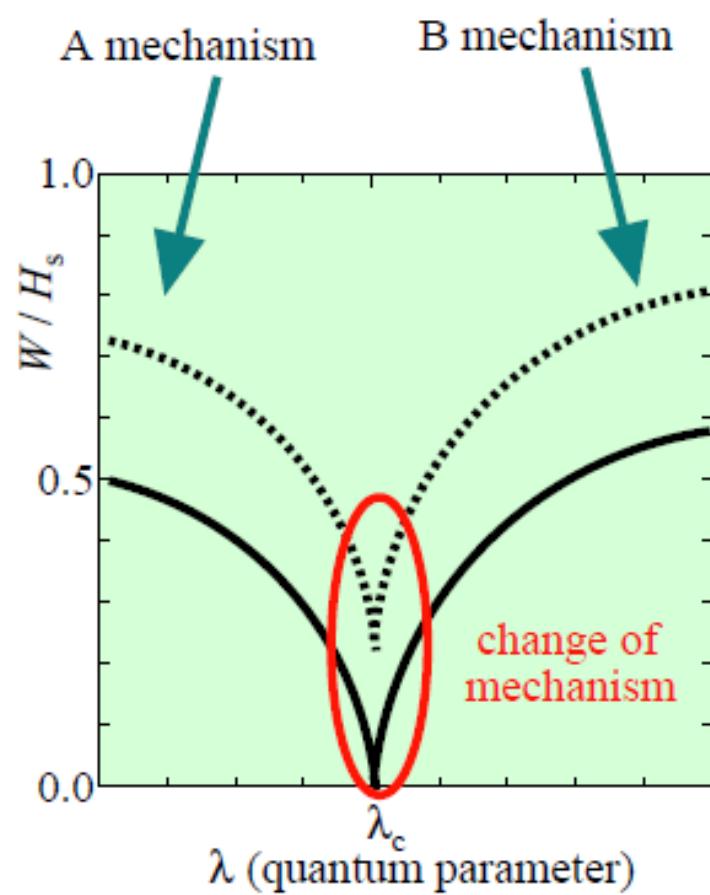
$P : 1 \Leftrightarrow 3$ parity

wave functions do not depend on α

- Behavior of plateau width near the mechanism-changing point



present case



usual cases

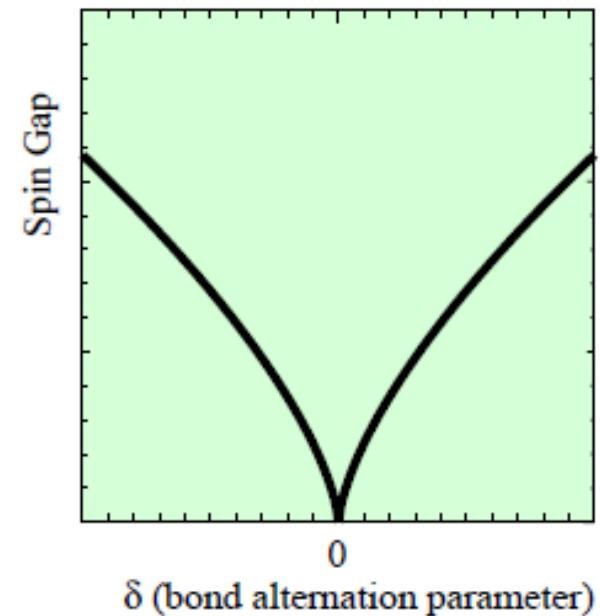
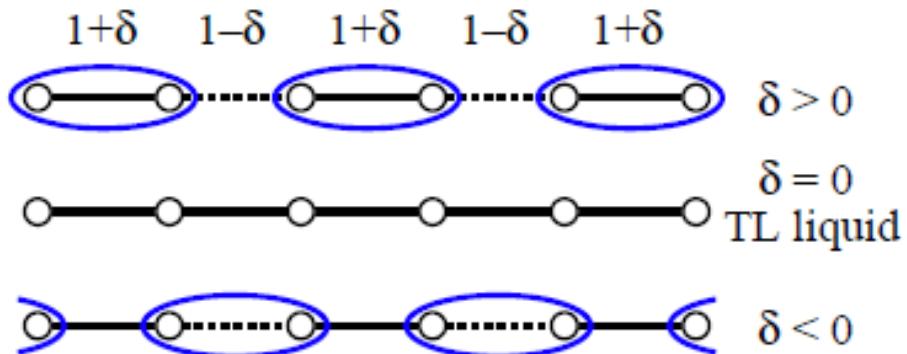
● Usual cases

W decreases near λ_c

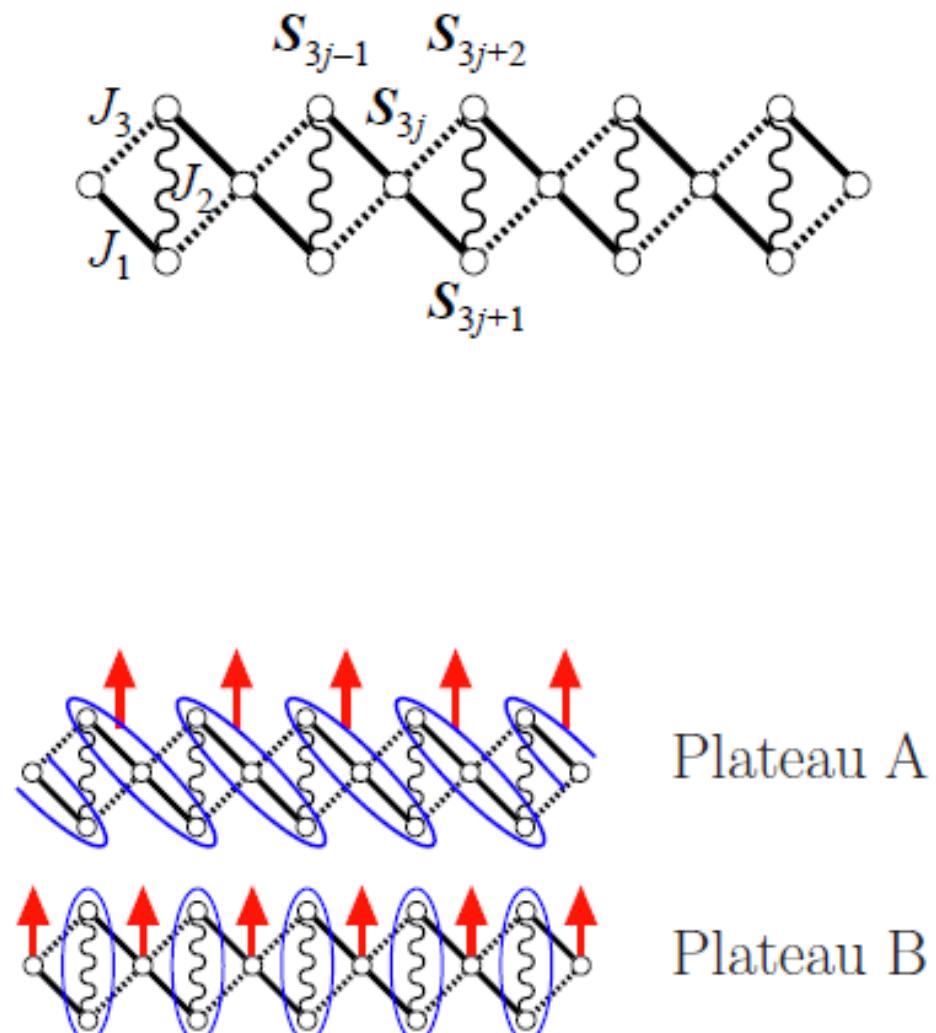
reconstruction of the unit cell occurs at λ_c

example 1 : $S = 1/2$ bond-alteranting model at $M = 0$,

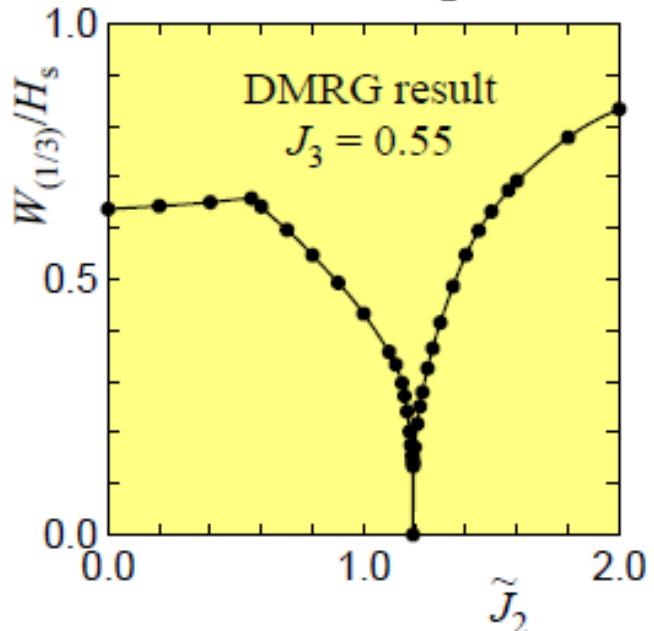
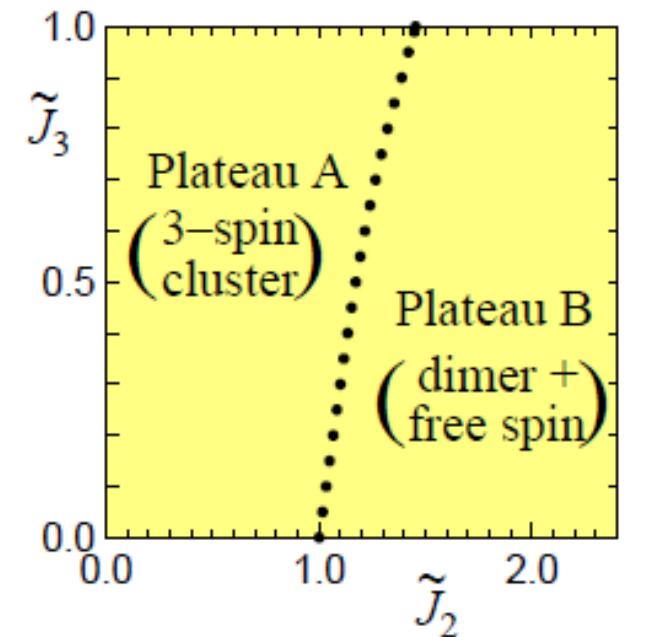
$$\text{spingap} \propto |\delta|^{2/3} / \sqrt{|\log |\delta||}$$



example 2 : $S = 1/2$ distorted diamond chain model at $M = M_s/3$



also, reconstruction of the unit cell



present case (note that $J_r \gg J_1$)

reconstruction of the unit cell **does not** occur at $\alpha = 1$

unit cell is always a triangle for $\alpha \leq 1$

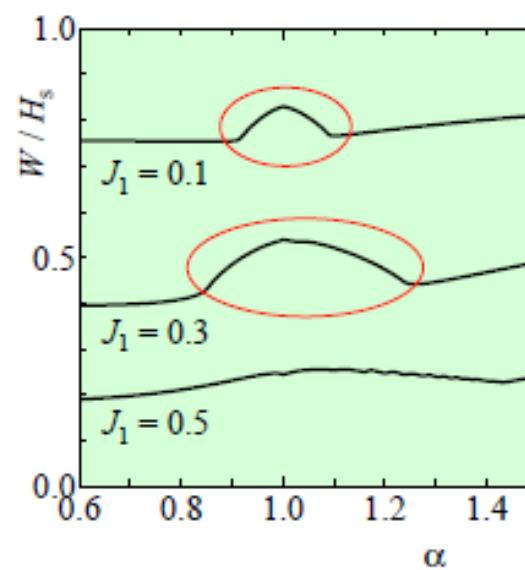
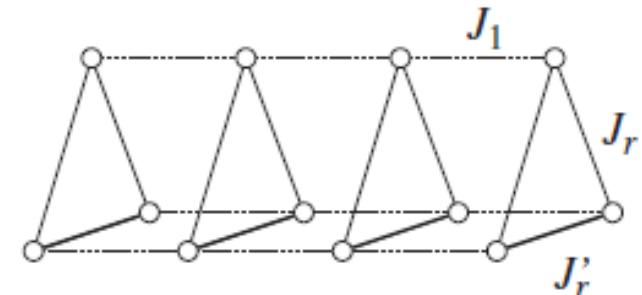
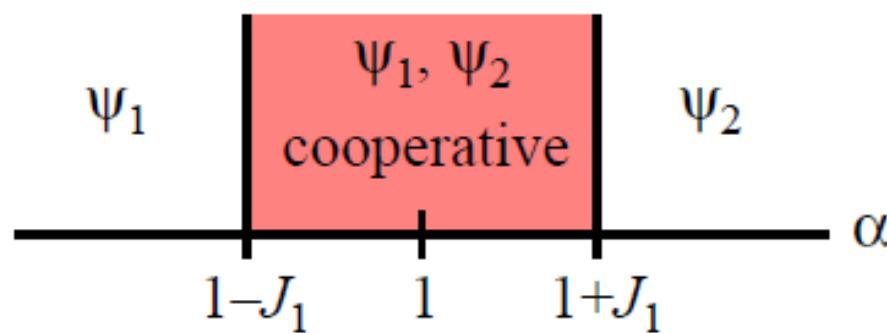
GS of a triangle is changed at $\alpha = 1$

energy difference between ψ_1 and ψ_2 states, $E_2 - E_1 = 1 - \alpha$

perturbation by J_1 , both of ψ_1 and ψ_2 states are relevant when $J_1 \gtrsim |1 - \alpha|$

thus, in the $1 - J_1 \lesssim \alpha \lesssim 1 + J_1$ region, interesting phenomena will occur

in fact, the increase of W is observed in this region



Perturbation Theory from the $J_1 \ll 1$ Limit

- Eigenstates of isosceles triangles at $S_{\text{tot}}^z = 1/2$

state	energy	S_{tot}	P
$\psi_1 = \frac{1}{\sqrt{6}} (\uparrow\uparrow\downarrow\rangle - 2 \uparrow\downarrow\uparrow\rangle + \downarrow\uparrow\uparrow\rangle)$	$-1 + \alpha/4$, ($\alpha < 1$, GS)	$1/2$	$+1$
$\psi_2 = \frac{1}{\sqrt{2}} (\uparrow\uparrow\downarrow\rangle - \downarrow\uparrow\uparrow\rangle) = \uparrow\rangle_2[1, 3]$	$-3\alpha/4$, ($\alpha > 1$, GS)	$1/2$	-1
$\psi_3 = \frac{1}{\sqrt{3}} (\uparrow\uparrow\downarrow\rangle + \uparrow\downarrow\uparrow\rangle + \downarrow\uparrow\uparrow\rangle)$	$1/2 + \alpha/4$	$3/2$	$+1$

- Perturbation theory by use of pseudospin representation

pseudospin \vec{T} ($T = 1/2$), $\psi_2 \Leftrightarrow |\uparrow\rangle$, $\psi_1 \Leftrightarrow |\downarrow\rangle$

note that $S_{\text{tot}}^z = 1/2$ for both of $|\uparrow\rangle$ and $|\downarrow\rangle$

lowest order in J_1

$$\mathcal{H}_{\text{eff}} = J_1 \sum_j (T_j^x T_{j+1}^x + T_j^z T_{j+1}^z) - (\alpha - 1) \sum_j T_j^z$$

transverse field XZ (or equivalently, XY) model

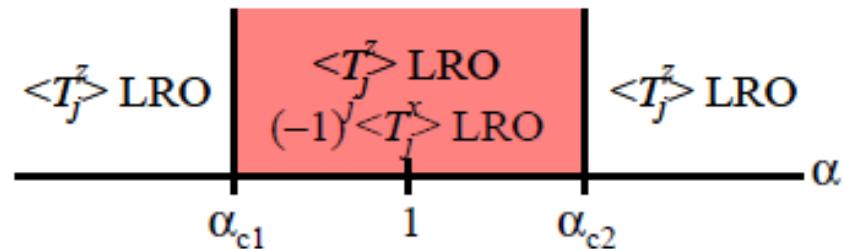
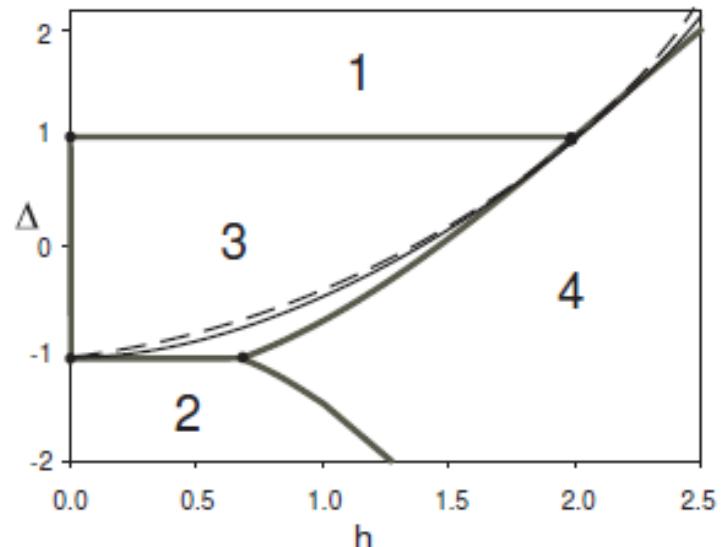
● Transverse field XZ model

transverse field XXZ model ($\Delta \equiv J_z/J_{xy}$)

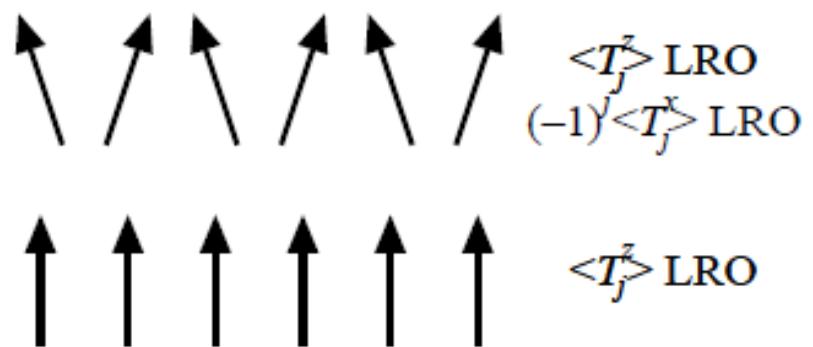
field h along the x -direction

(Dmitriev et al, PRB **65**, 172409 (2002);
JETP **95**, 538 (2002))

- 1: z -Néel, $(-1)^j \langle S_j^z \rangle$ LRO, (of course $\langle S_j^x \rangle$ LRO)
- 2: z -Ferro, $\langle S_j^z \rangle$ LRO, (of course $\langle S_j^x \rangle$ LRO)
- 3: y -Néel, $(-1)^j \langle S_j^y \rangle$ LRO, (of course $\langle S_j^x \rangle$ LRO)
- 4: No LRO, (of course $\langle S_j^x \rangle$ LRO)



their results read for our case



semiclassical picture

suppose the pseudo spin \vec{T} turn to the $+x$ direction

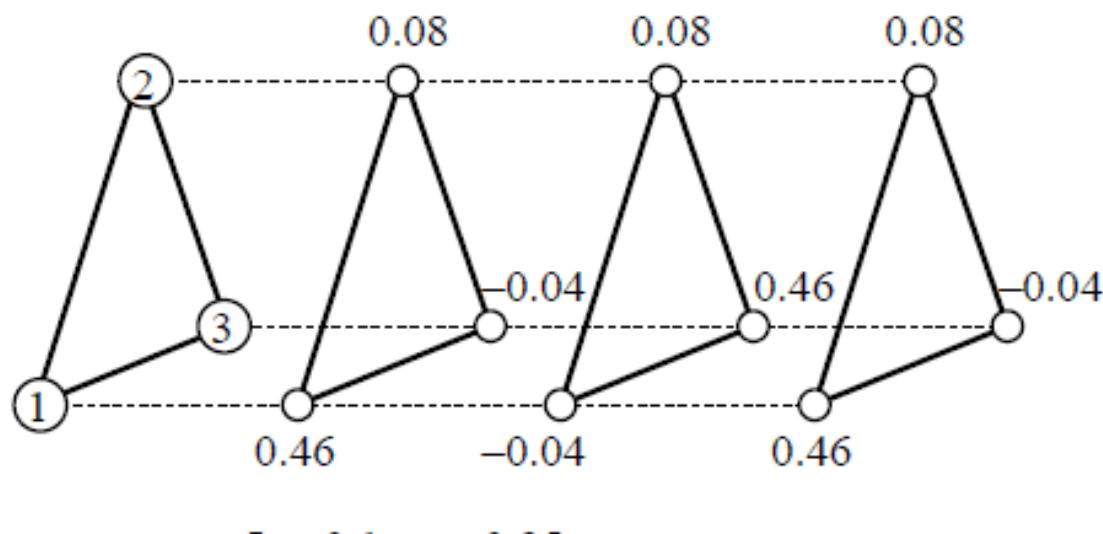
$$|T_{+x}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) = \left(\frac{1}{2} + \frac{1}{4\sqrt{3}}\right)|\uparrow\uparrow\downarrow\rangle - \frac{1}{\sqrt{3}}|\uparrow\downarrow\uparrow\rangle + \left(\frac{1}{2} - \frac{1}{4\sqrt{3}}\right)|\downarrow\uparrow\uparrow\rangle$$

$$\langle S_1^z \rangle \equiv \langle T_{+x}|S_1^z|T_{+x}\rangle = \frac{1}{2\sqrt{3}} + \frac{1}{6} = 0.455$$

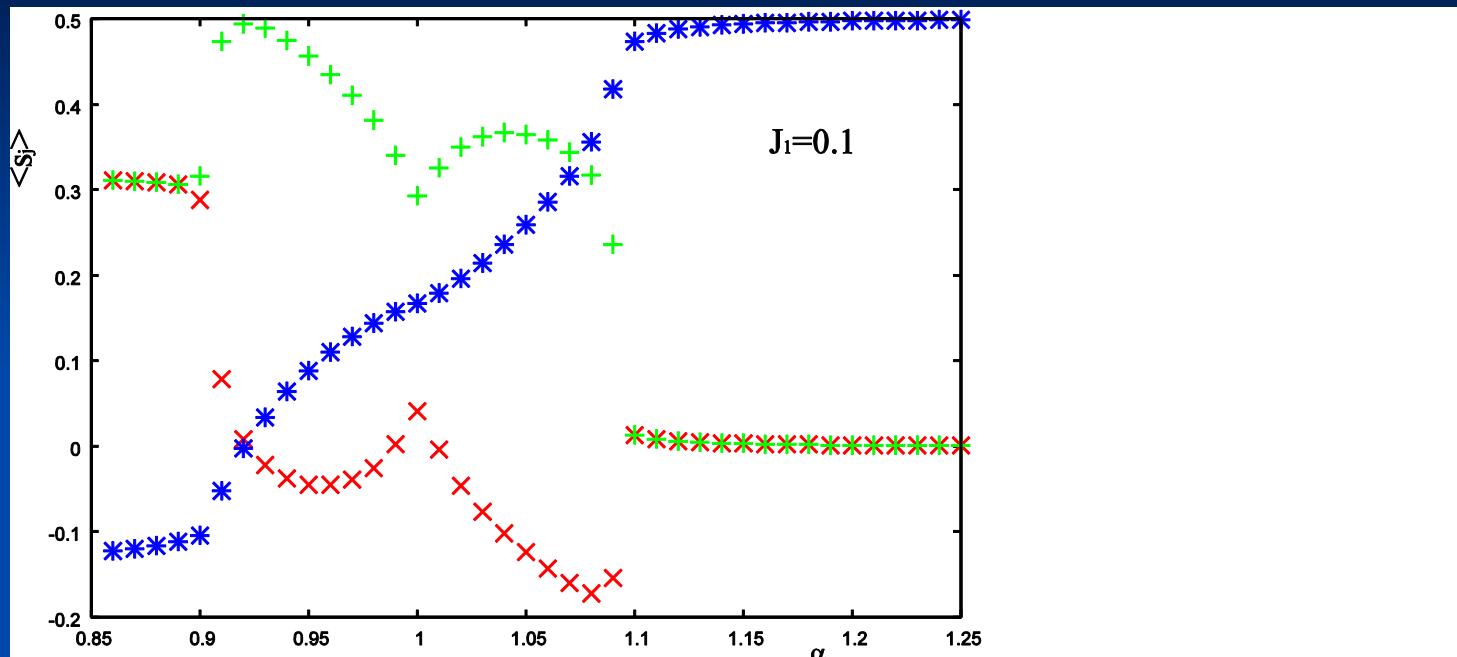
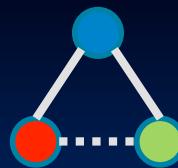
$$\langle S_2^z \rangle \equiv \langle T_{+x}|S_2^z|T_{+x}\rangle = \frac{1}{6} = 0.167$$

$$\langle S_3^z \rangle \equiv \langle T_{+x}|S_3^z|T_{+x}\rangle = \frac{1}{2\sqrt{3}} - \frac{1}{6} = -0.122$$

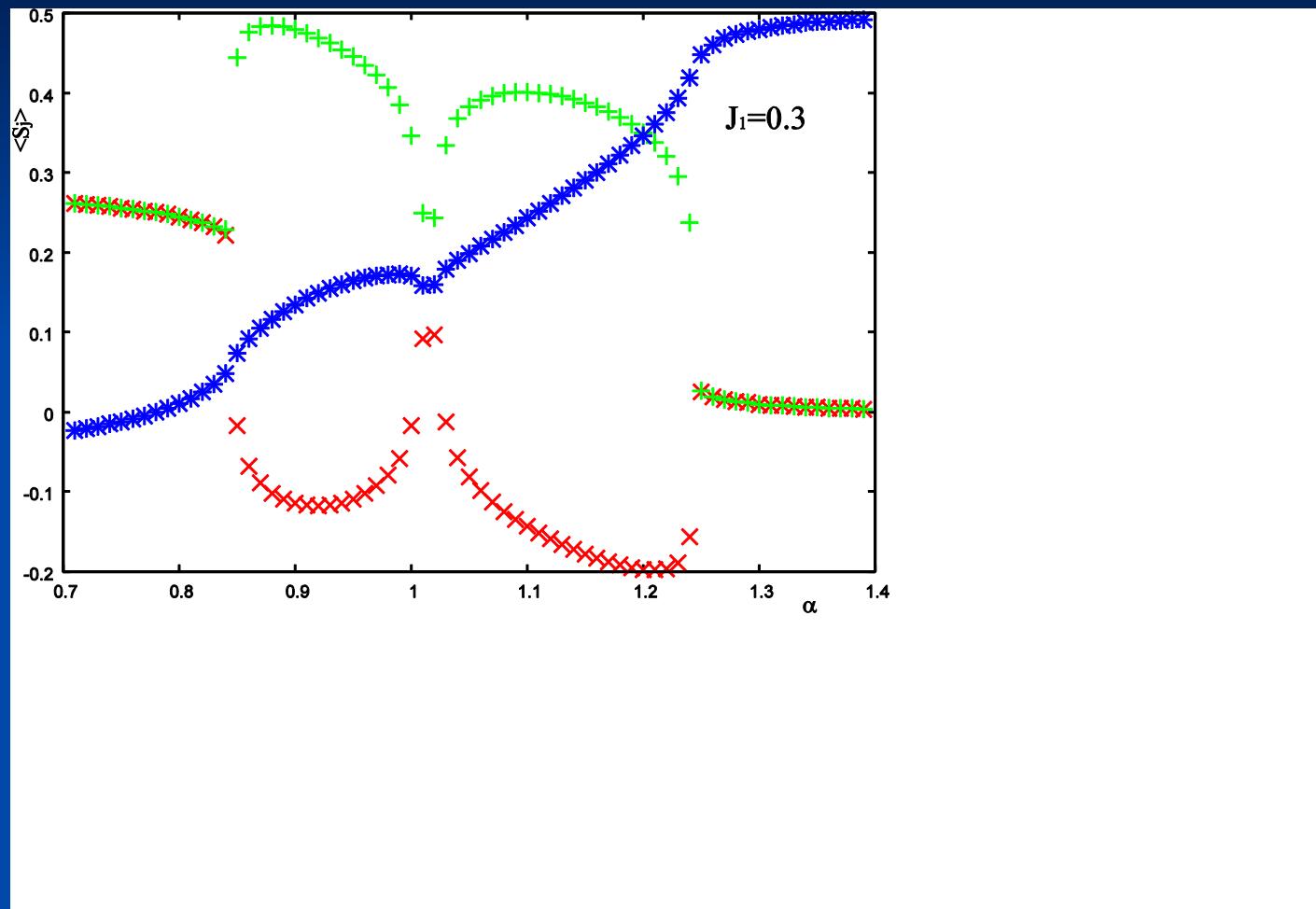
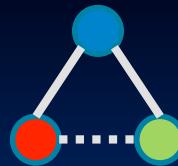
these expectation values well explain the DMRG results



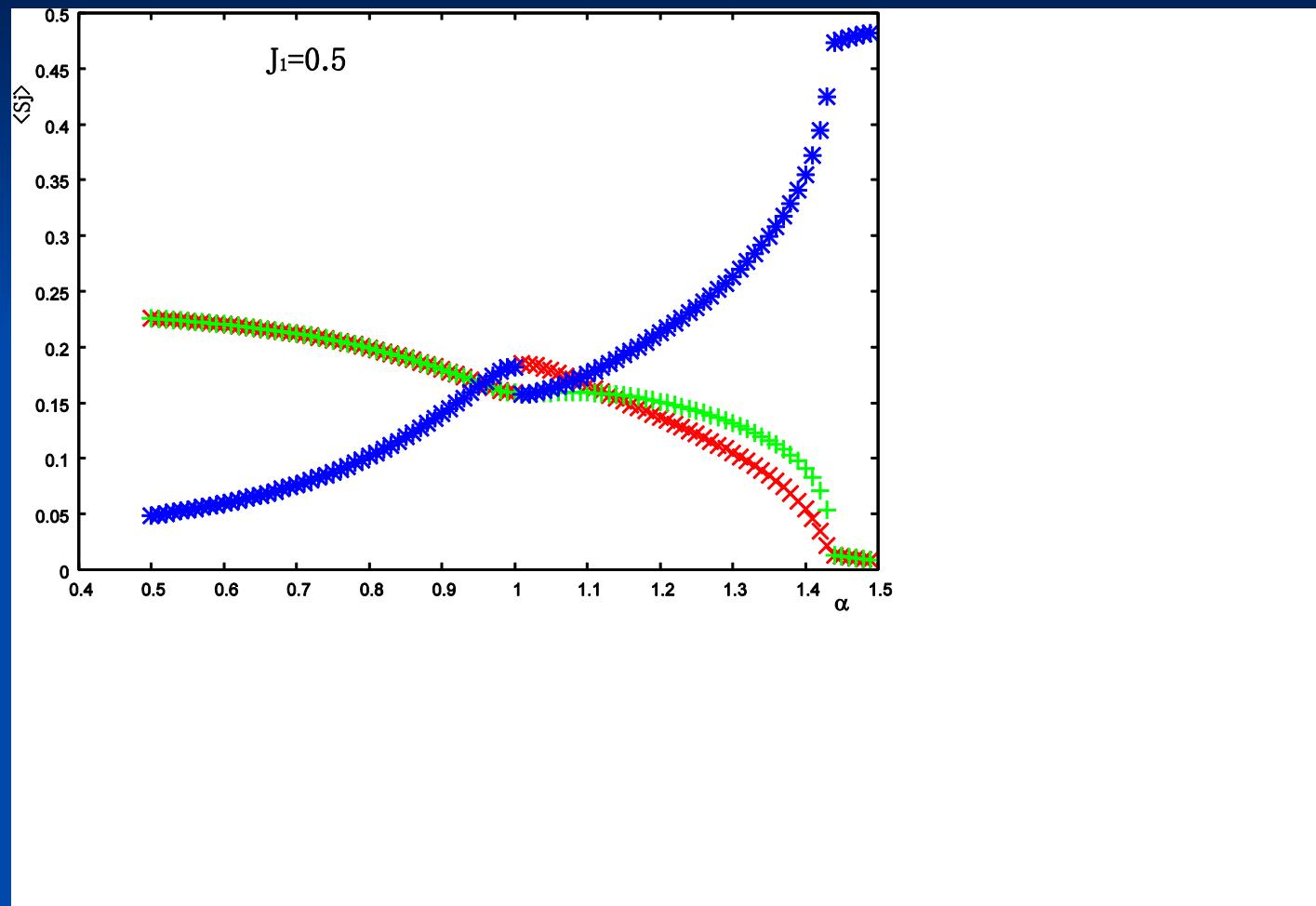
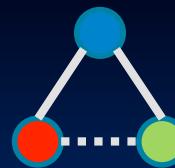
Expectation value of each spin by DMRG for small J_1



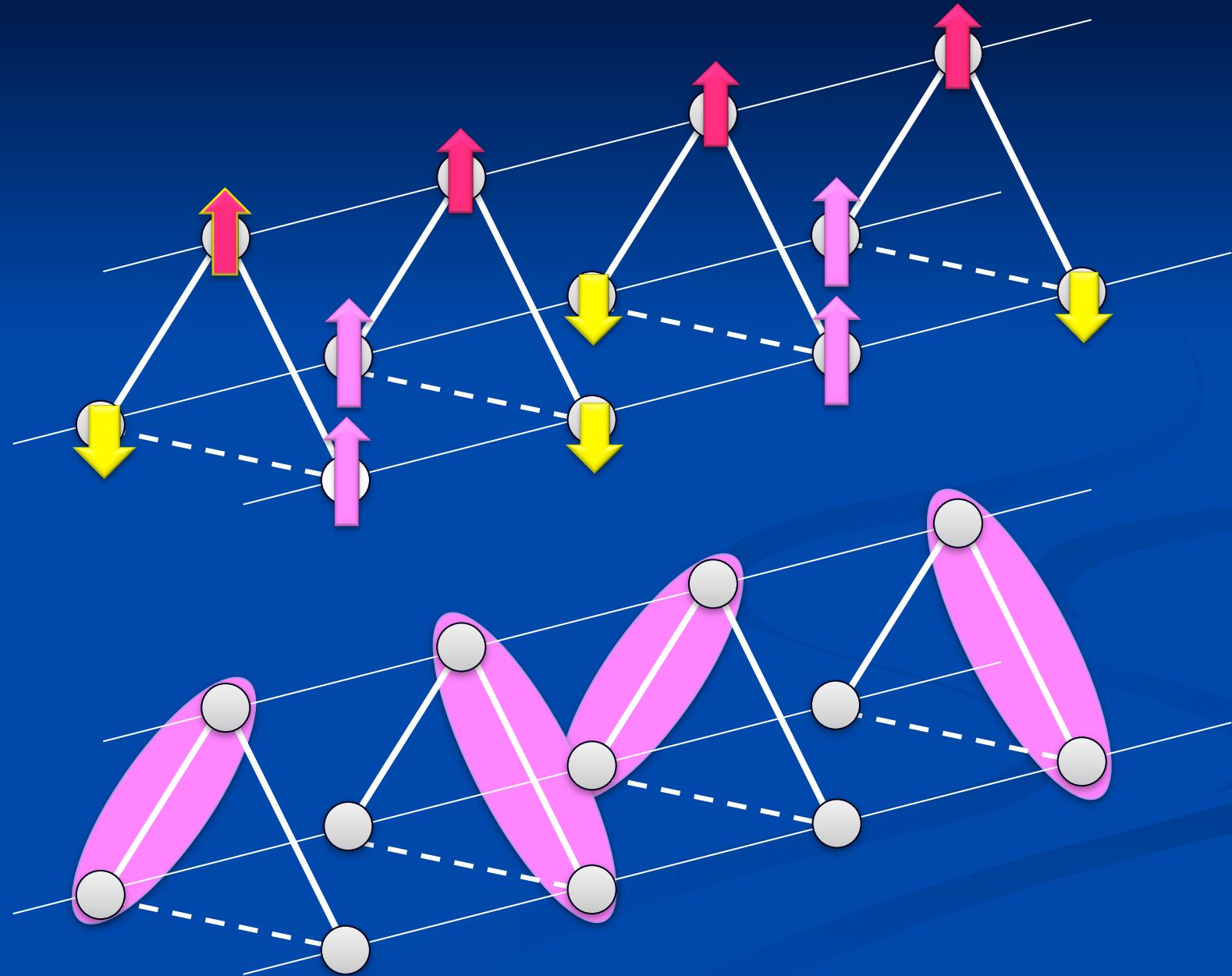
Expectation value of each spin by DMRG
for intermediate J_1

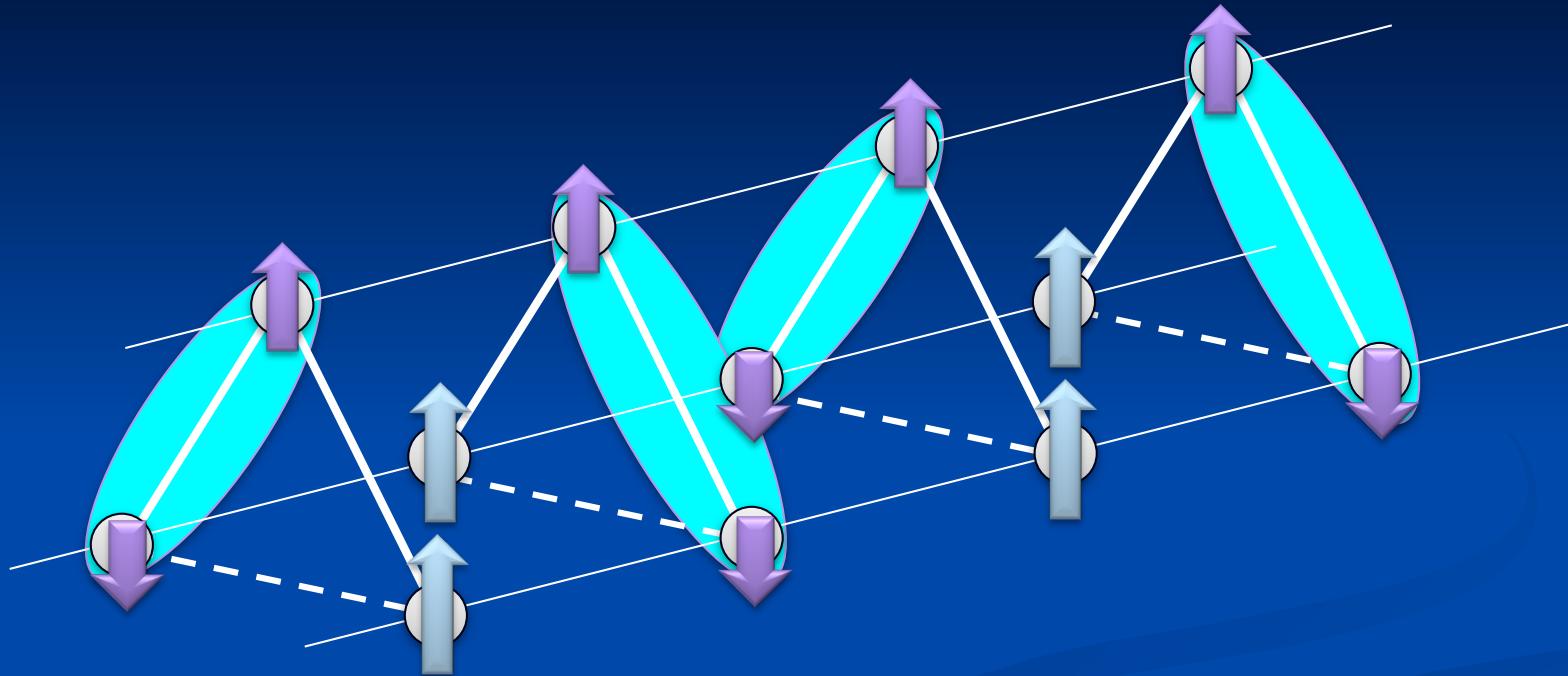


Expectation value of each spin by DMRG
for large J_1



Z_2 -symmetry breaking state
in the $1/3$ plateau of asymmetric spin tube





\approx triplet dimer

Phenomenological renormalization

- New phase

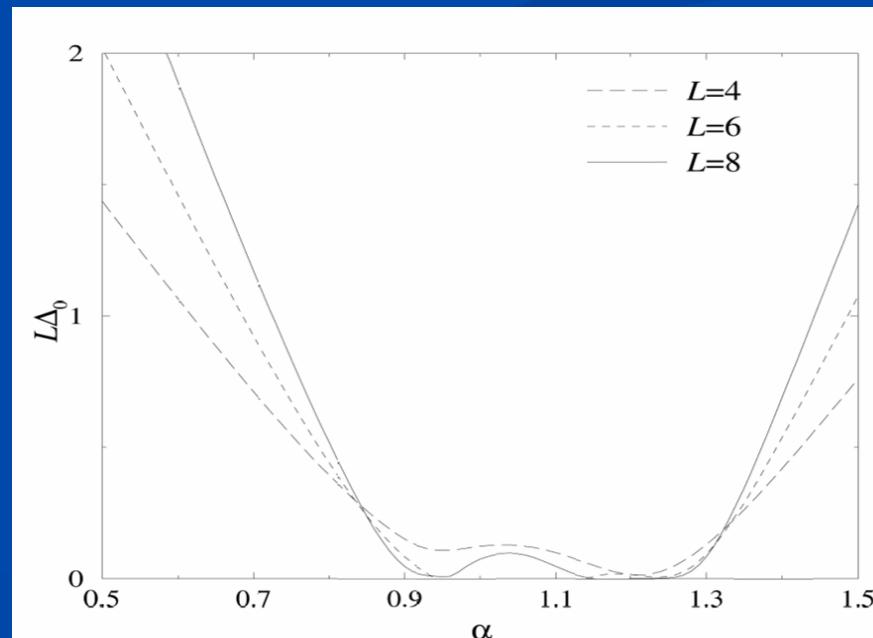
 - Excitation Δ_0 with $k=\pi$, Parity=odd

 - is degenerated with the ground state at $m/ms=1/3$

- Scaled gap $L\Delta_0$

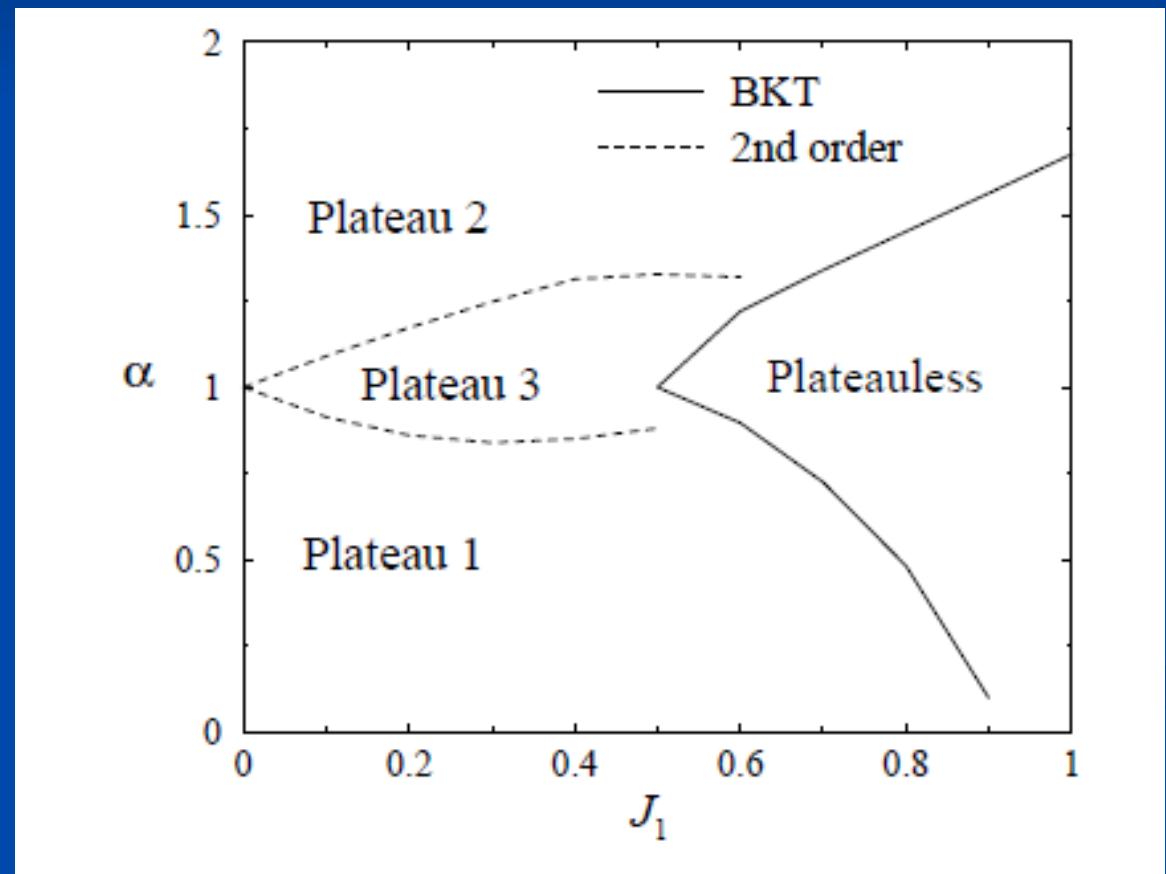
 - should be decreasing fn. of L at the new phase.

$J_1=0.3$

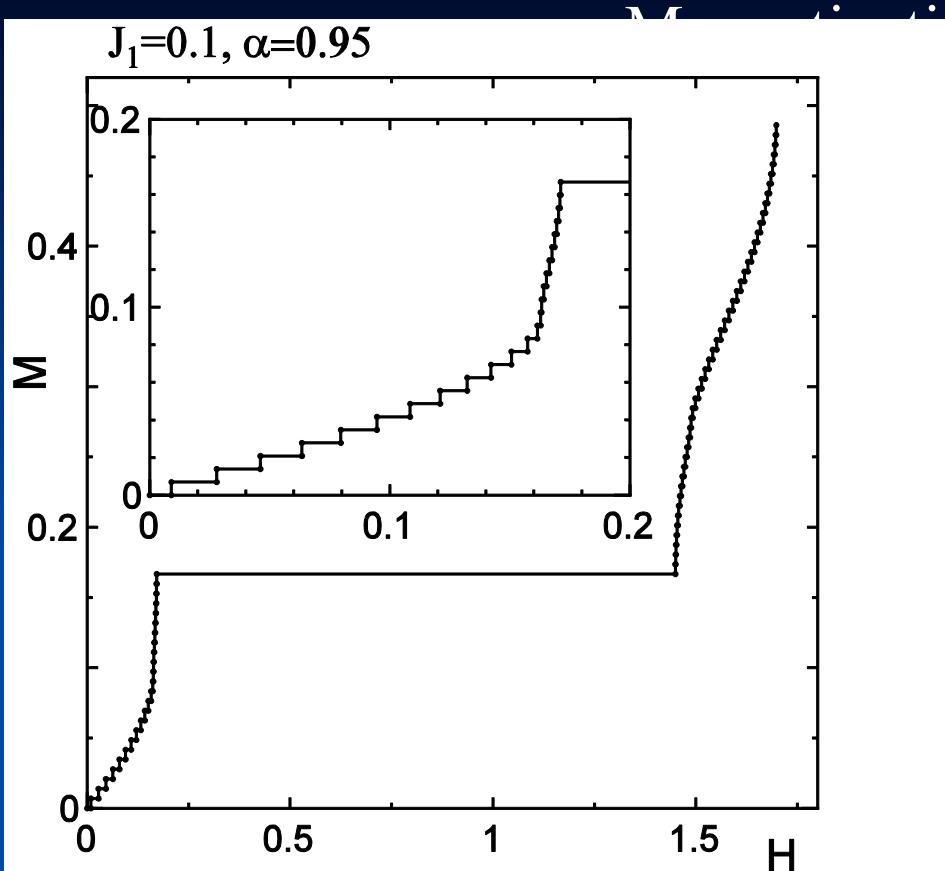


Phase diagram for $m/m_s=1/3$

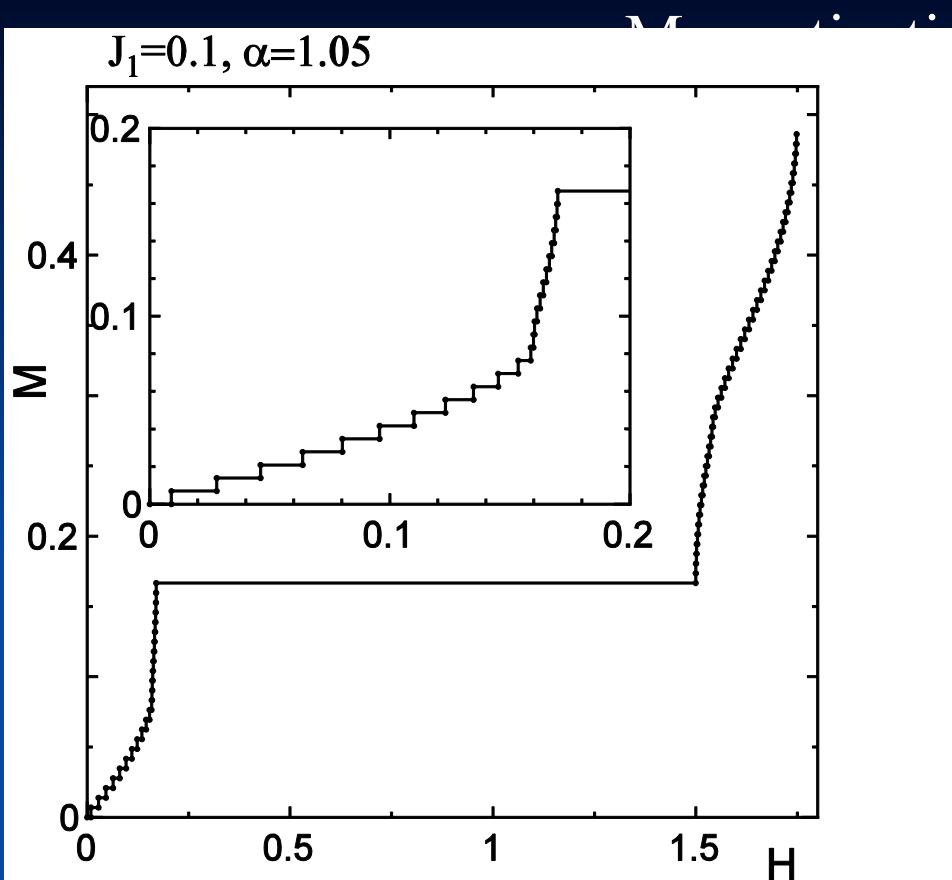
- Dimer-monomer plateau
- New phase Staggered order
- uud plateau



M vs H DMRG



$J_1=0.1$, $\alpha=1.05$



M

H

$J_1=0.1, \alpha=1.05$

1 by DMRG

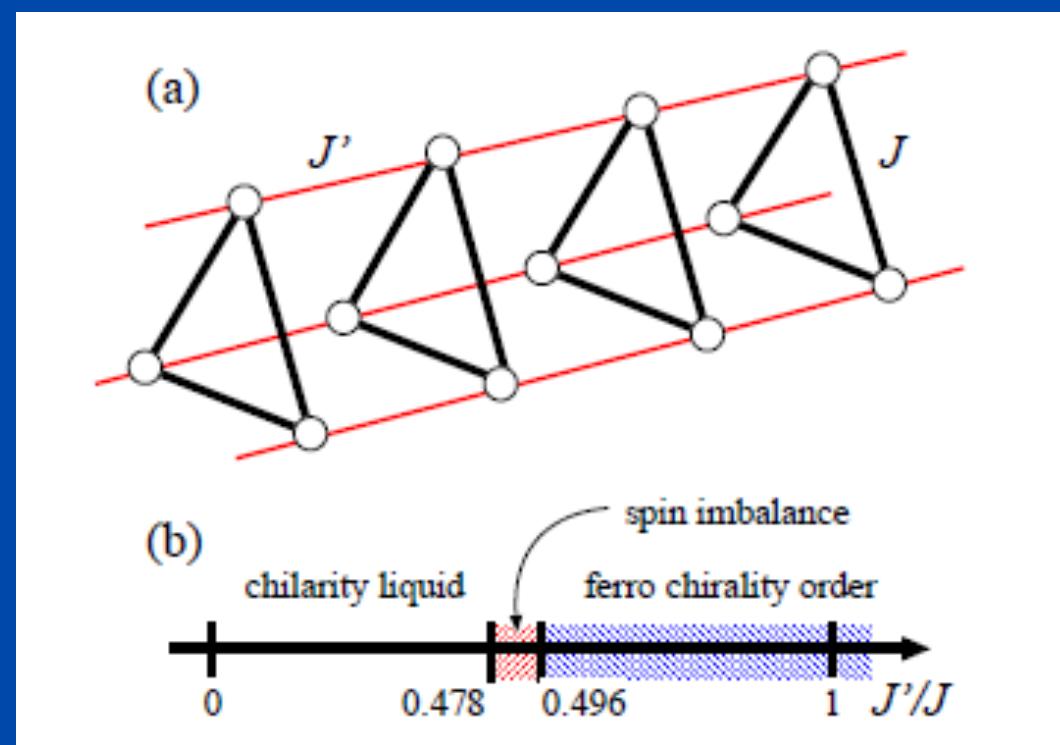
Summary

- 1/3 magnetization plateau of S=1/2 three-leg spin tube
- New exotic phase between two conventional plateau phases
- New phase:
translational symmetry breaking,
staggered magnetization, dimer, chial order

$$\left\langle \vec{S}_1 \times \vec{S}_2 \times \vec{S}_3 \right\rangle$$

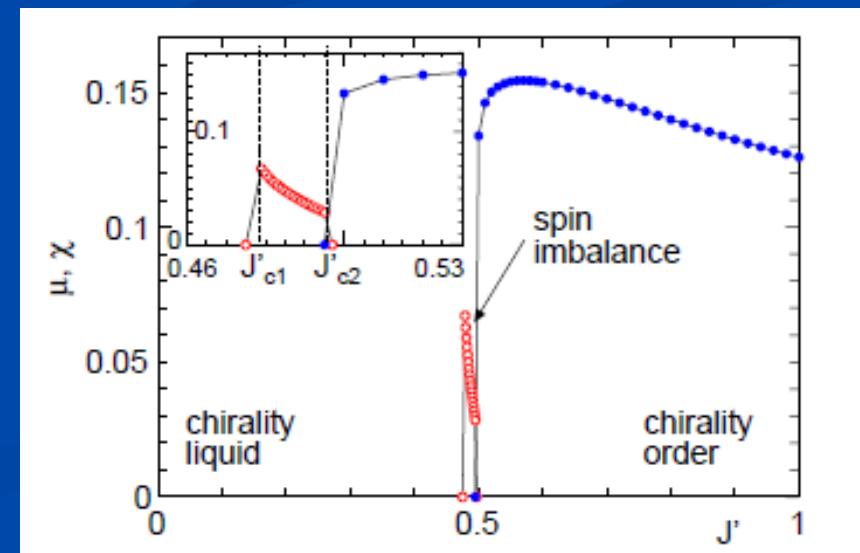
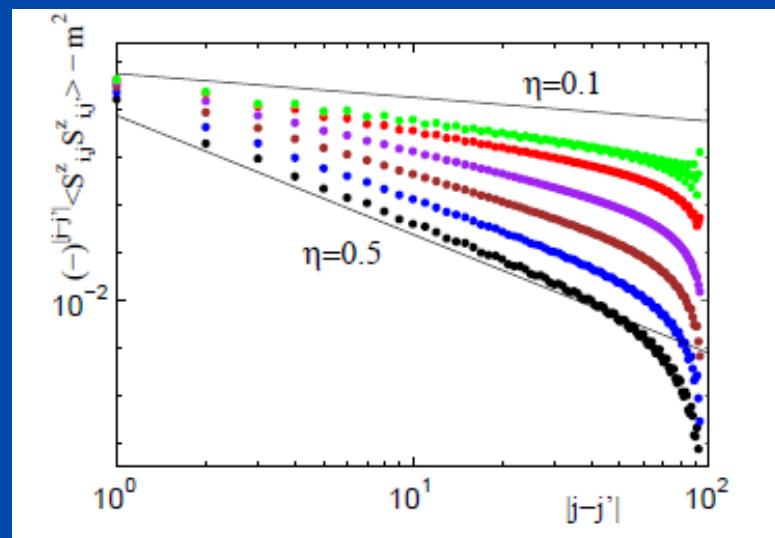
Chirality at $m=1/3$

K. Okunishi et al. PRB 2012

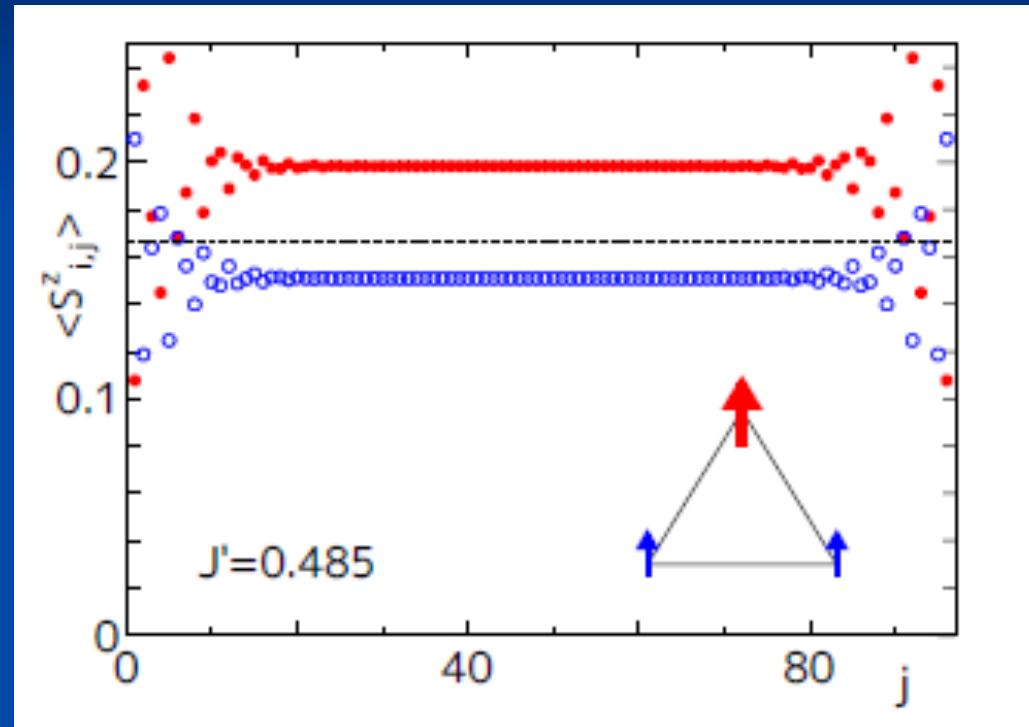


DMRG calculation (L=144)

$$\chi_j = \sum_{i=1}^3 (S_{i,j} \times S_{i+1,j})^z / 3,$$
$$\mu_j = S_{1,j}^z - (S_{2,j}^z + S_{3,j}^z) / 2,$$



Spin imbalance phase



Phase diagram

