Novel Field-Induced Quantum Phase Transitions in the Kagome-Lattice Antiferromagnet and Related Systems

Toru Sakai[A,B] and Hiroki Nakano[B]

[A]JAEA, SPring-8, [B]University of Hyogo

H. Nakano and TS: JPSJ 79 (2010) 053707 (arXiv:1004.2528)
TS and H. Nakano: PRB 83 (2011) 100405(R) (arXiv:1102.3486)
H. Nakano and TS: JPSJ 80 (2011) 053704 (arXiv: 1103.5829)
H. Nakan, T. Shimokawa, TS, JPSJ 80 (2011) 033709
M. Isoda, H. Nakano and TS: JPSJ 80 (2011) 084704
H. Nakano, M. Isoda and TS, JPSJ 83 (2014) 053702 (arXve: 1403.5008)
H. Nakano, TS and Y. Hasegawa, to appear JPSJ

Novel Field-Induced Quantum Critical Phenomena in Kagome-Lattice Antiferromagnet

Toru Sakai[A,B] and Hiroki Nakano[B]

[A]JAEA, SPring-8, [B]University of Hyogo

H. Nakano and TS: JPSJ 79 (2010) 053707 (arXiv:1004.2528)
TS and H. Nakano: PRB 83 (2011) 100405(R) (arXiv:1102.3486)
H. Nakano and TS: JPSJ 80 (2011) 053704 (arXiv: 1103.5829)
H. Nakan, T. Shimokawa, TS, JPSJ 80 (2011) 033709
M. Isoda, H. Nakano and TS: JPSJ 80 (2011) 084704
H. Nakano, M. Isoda and TS, JPSJ 83 (2014) 053702 (arXve: 1403.5008)
H. Nakano, TS and Y. Hasegawa, to appear JPSJ

Contents

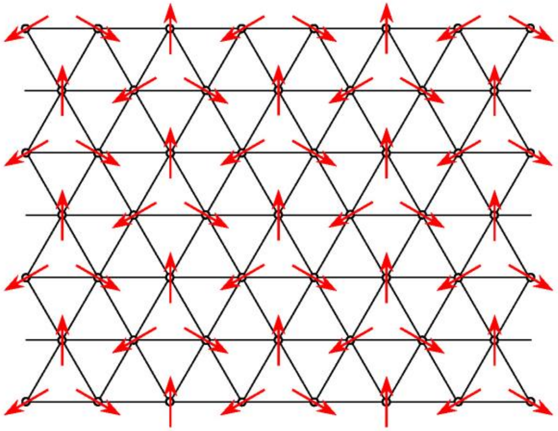
- Introduction
- Spin gap issue
- Magnetization process
- Related frustrated models

2D frustrated systems

- Heisenberg antiferromagnets

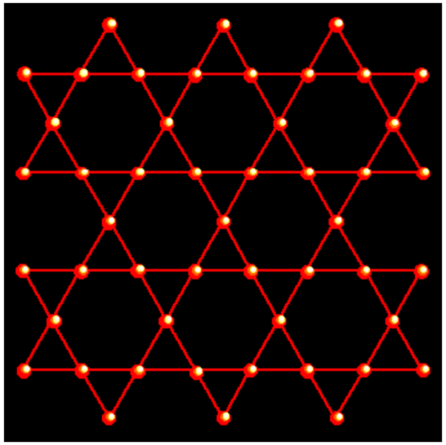
$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

Triangular lattice



Classical ground state
120 degree structure

Kagome lattice



Macroscopic degeneracy
(a global plane is not fixed)

S=1/2 Kagome Lattice AF

- Herbertsmithite $ZnCu_3(OH)_6Cl_2$ impurities

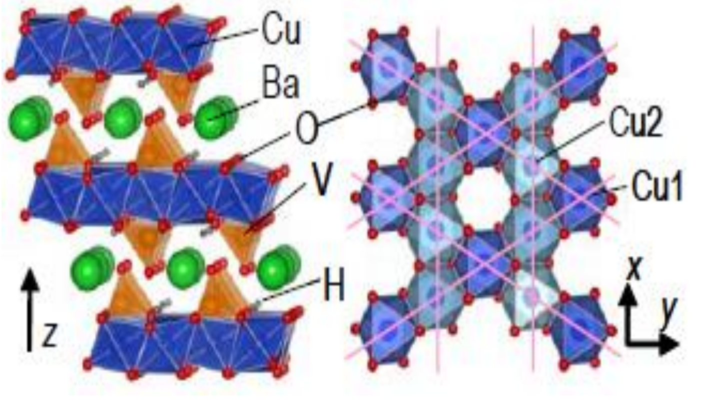
  Shores et al. J. Am. Chem. Soc. 127 (2005) 13426

- Volborthite $CuV_2O_7(OH)_2 \cdot 2H_2O$ lattice distortion

  Hiroi et al. J. Phys. Soc. Jpn. 70 (2001) 3377

- Vesignieite $BaCu_3V_2O_8(OH)_2$ ideal ?

  Okamoto et al. J. Phys. Soc. Jpn. 78 (2009) 033701



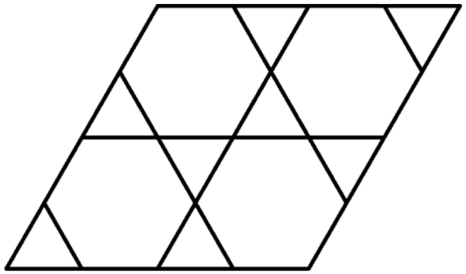
Methods

Frustration ⇨ Exotic phenomena

<u>Kagome lattice</u>

Triangular lattice

Pyrochlore lattice



Numerical approach

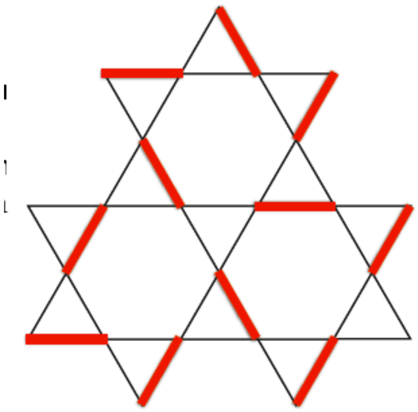
<u>Numerical diagonalization</u>

Quantum Monte Carlo (negative sign problem)

Density Matrix Renormalization Group

(not good for dimensions larger than one)

Spin gap issue of kagome-lattice AF



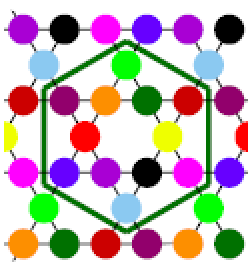
<u>Gapped</u>

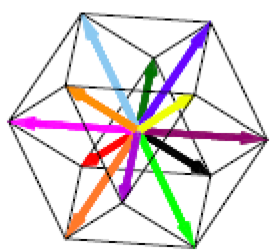
Valence Bond Crystal (VBC)[MERA]

Z_2 Spin Liquid [Sachdev, DMRG]

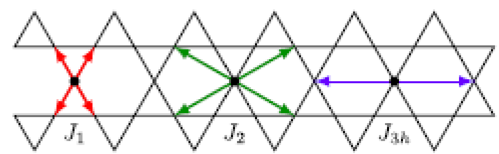
Chiral Liquid [Messio et al. PRL 108 (2012) 207204]

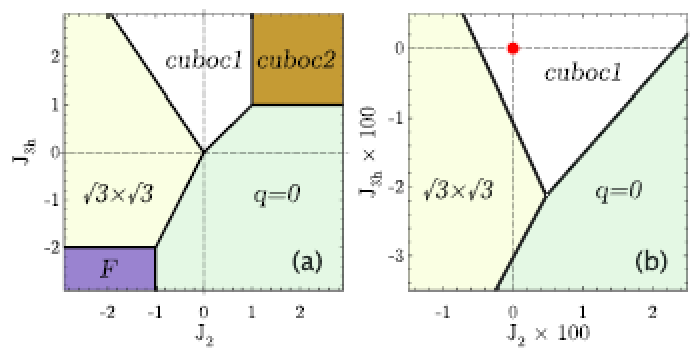
Cuboc 1





Chiral symmetry (Z_2) breaking





Classical S=1/2 Schwinger boson MF

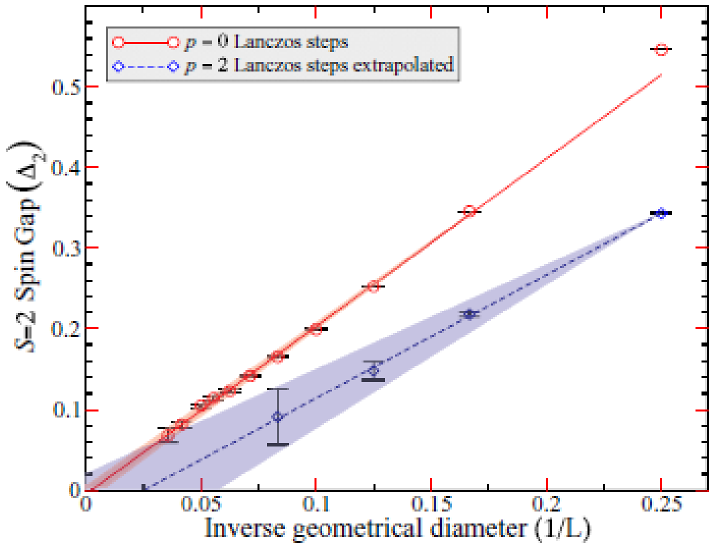
Gapless

U(1) Dirac Spin Liquid[Ran et al. PRL 98 (2007) 117205]

Variational function [Iqbal, Poilblanc, Becca, PRB 89 (2014) 020407]

S=2 gap : Δ_2= -0.04 ±0.06 (<0.02)

Spin gap : Δ_1 < 0.01 Gapless!



Computational costs

N=42, total Sz=0

Dimension of subspace d = 538,257,874,440

Δ= 0.14909214 cf. A. Laeuchli cond-mat/1103.1159

Memory cost

d * 8 Bytes * at least 3 vectors ～ 13TB

4 vectors ～ 20TB

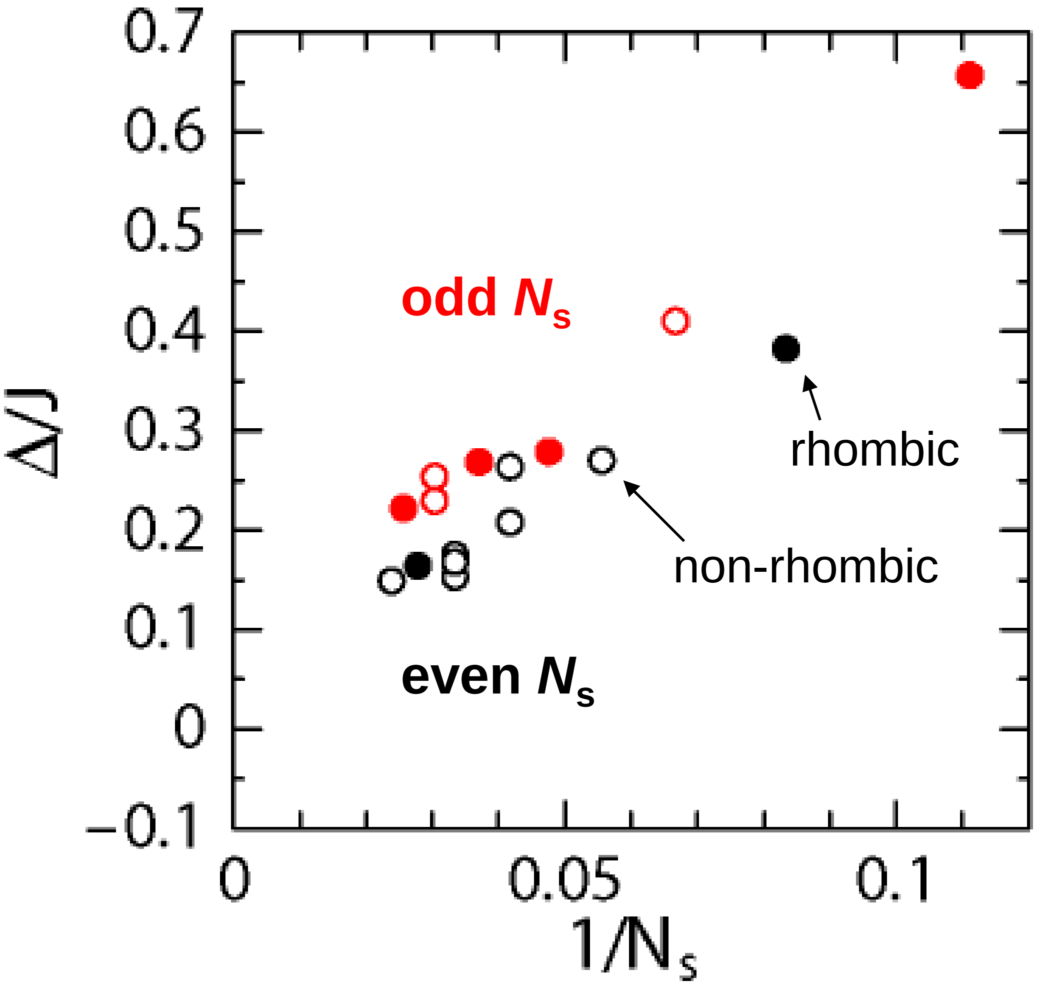
Time cost

d * # of bonds * # of iterations

d increases exponentially with respect to N.

Parallelization with respect to d

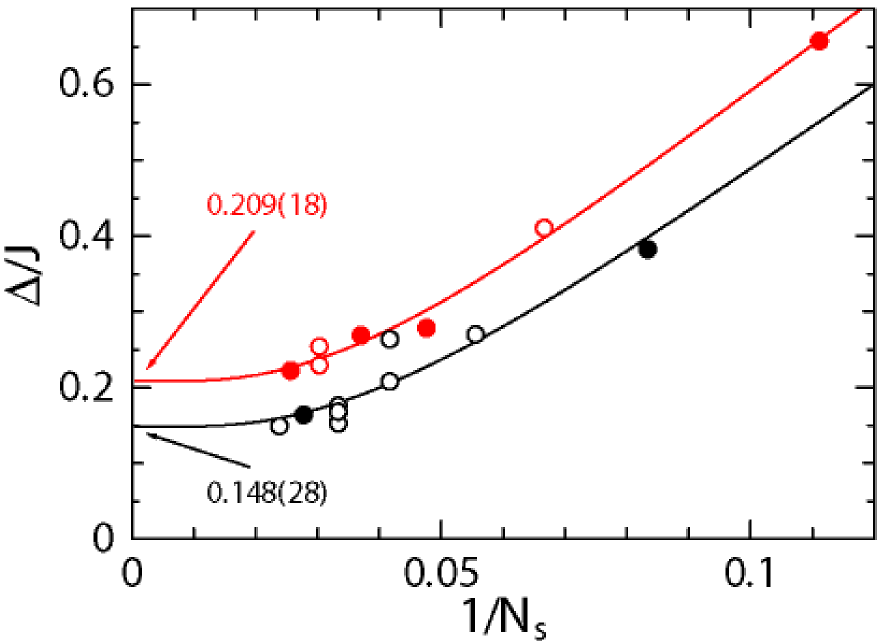
Classification of finite-size data

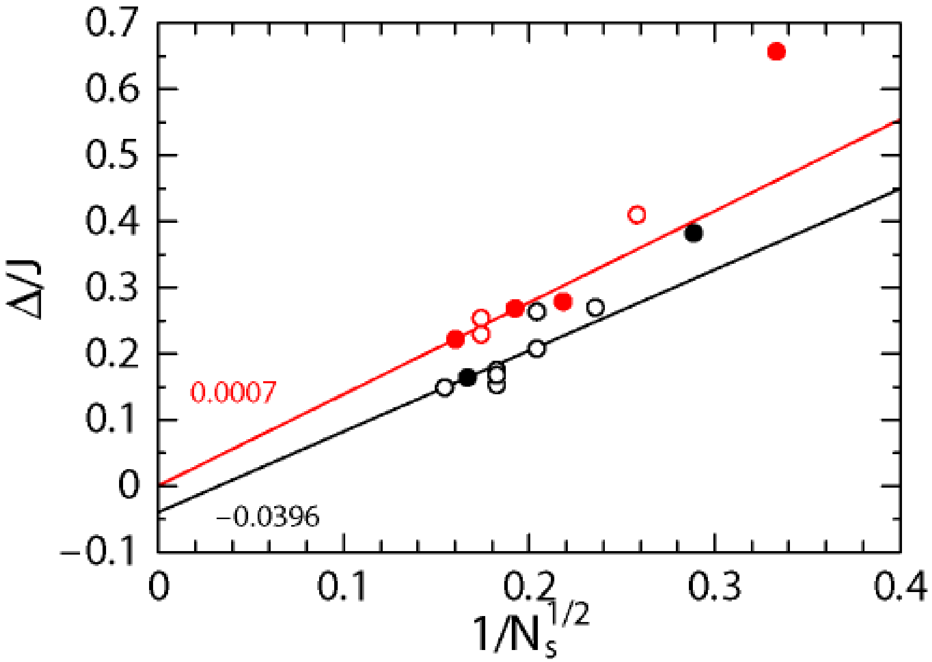


Important to divide data into two groups of even N_s and odd N_s.

Not good to treat all the data together.

Analysis of our finite-size gaps





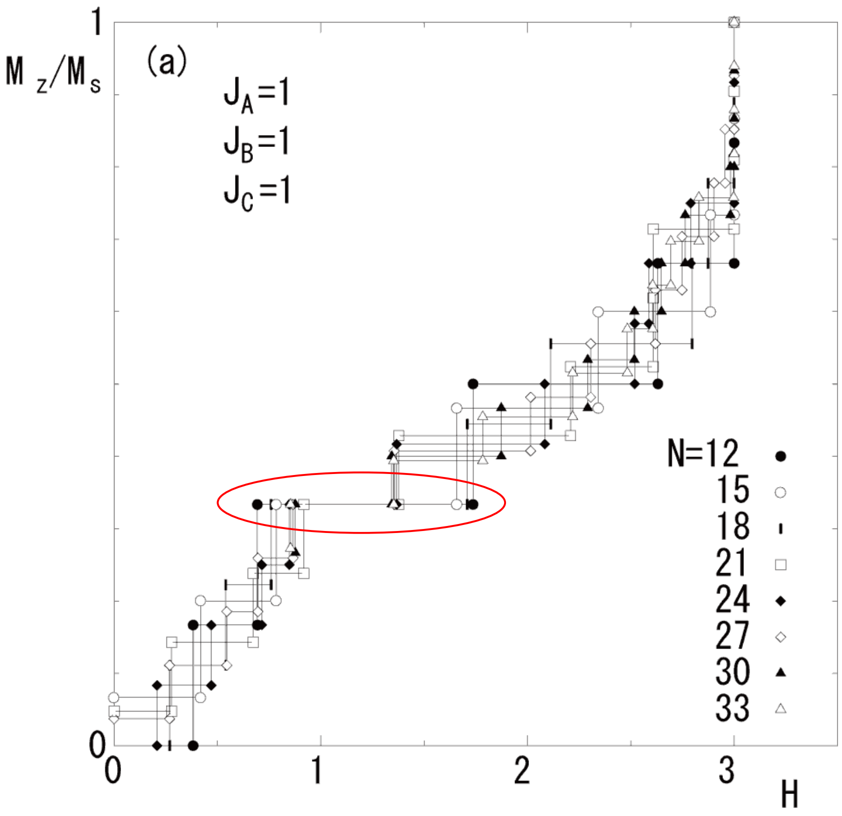
Two extrapolated results disagree from odd N_s and even N_s sequences.

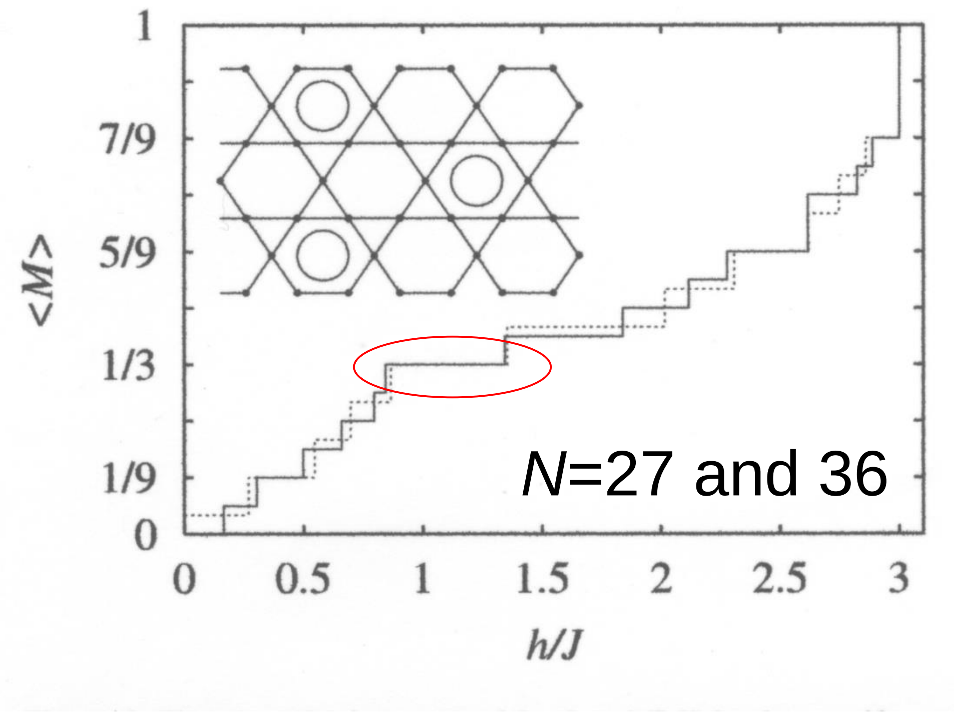
Feature of a gapless system

Magnetization process of S=1/2 kagome lattice AF

Hida: JPSJ **70** (2001) 3673

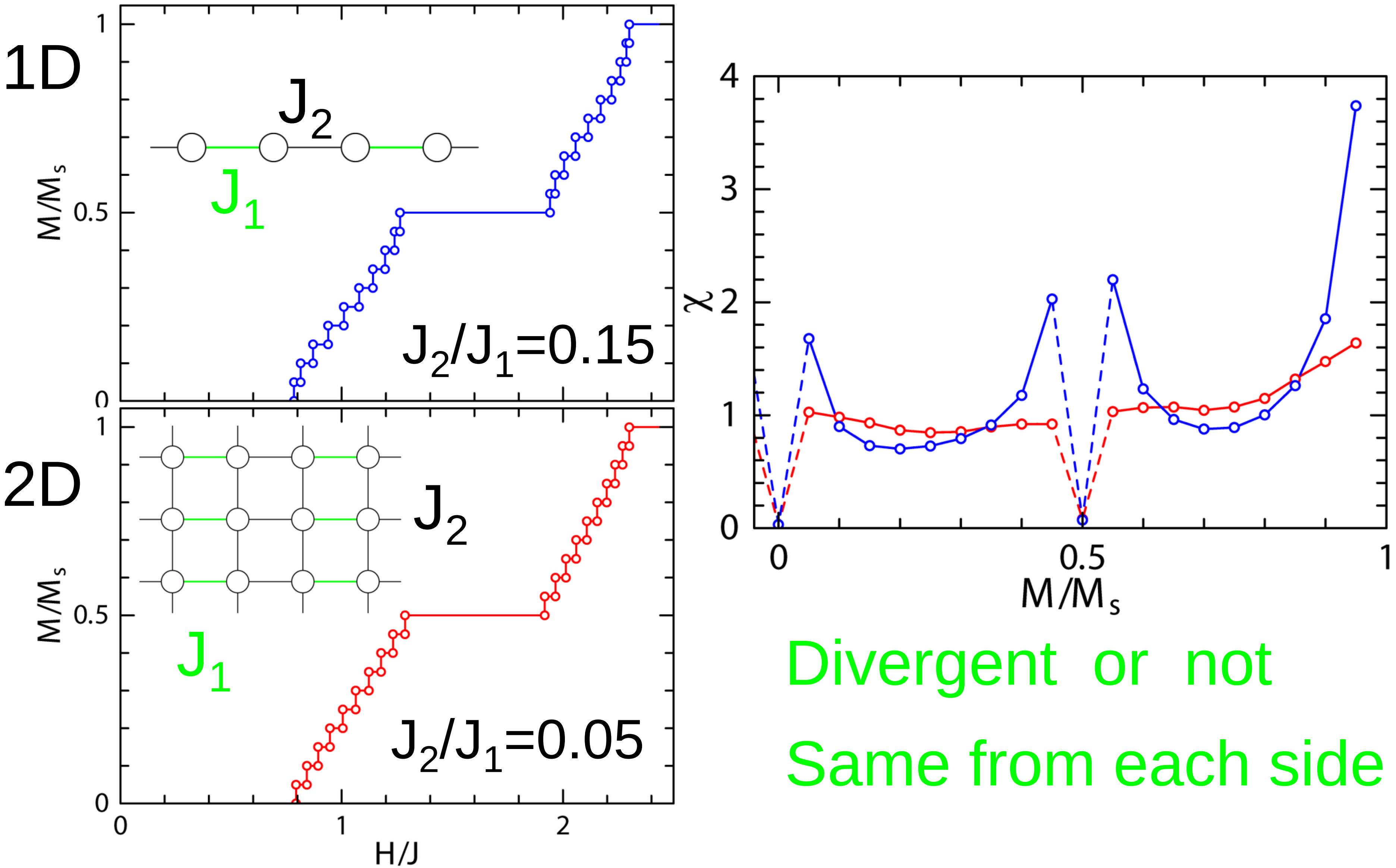
Honecker et al: JPCM **16**(2004)S749





1/3 plateau ?

Interacting S=1 Dimer Systems



Divergent or not

Same from each side

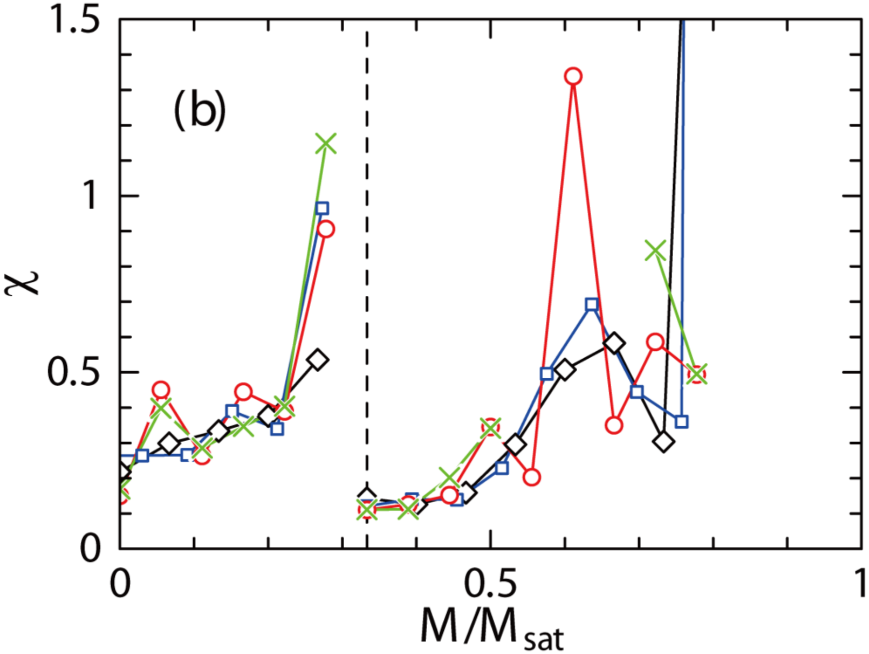
Not a plateau

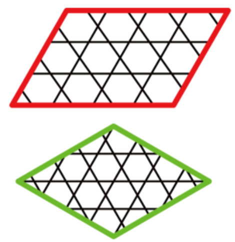
H. Nakano and TS: JPSJ **79** (2010) 053707

Reexamination from the viewpoint of

Field derivative of magnetization

$$\chi \propto \frac{\partial M}{\partial H} \quad \text{as a function of} \quad m = \frac{M}{M_s}$$





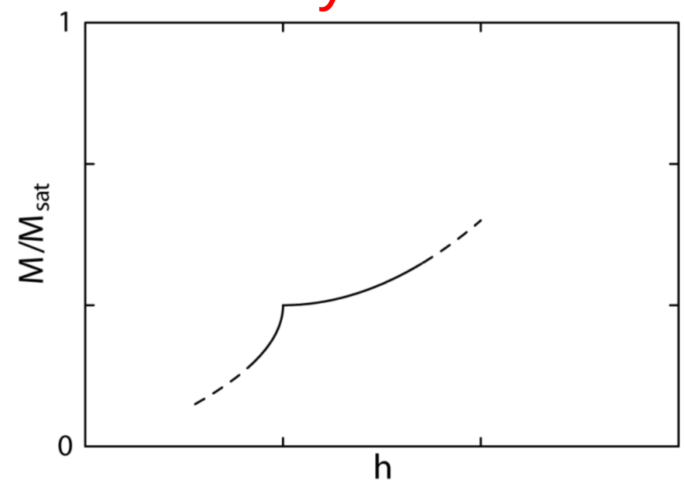
N=36

N=36

N=33

N=30

Anomaly at m=1/3

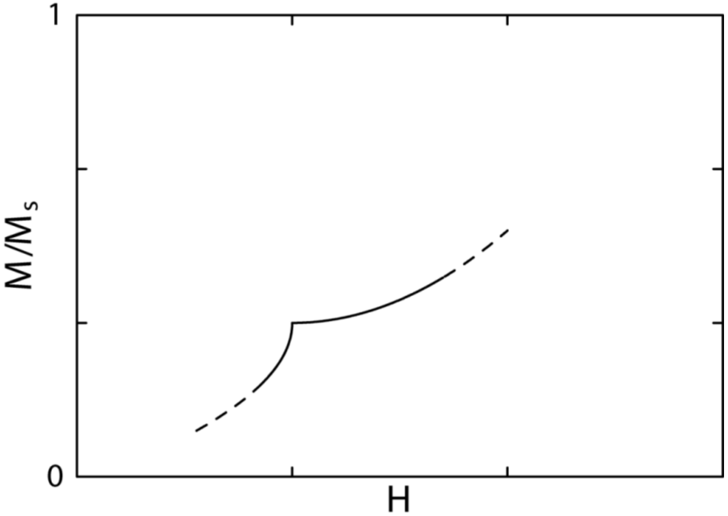


Magnetization ramp

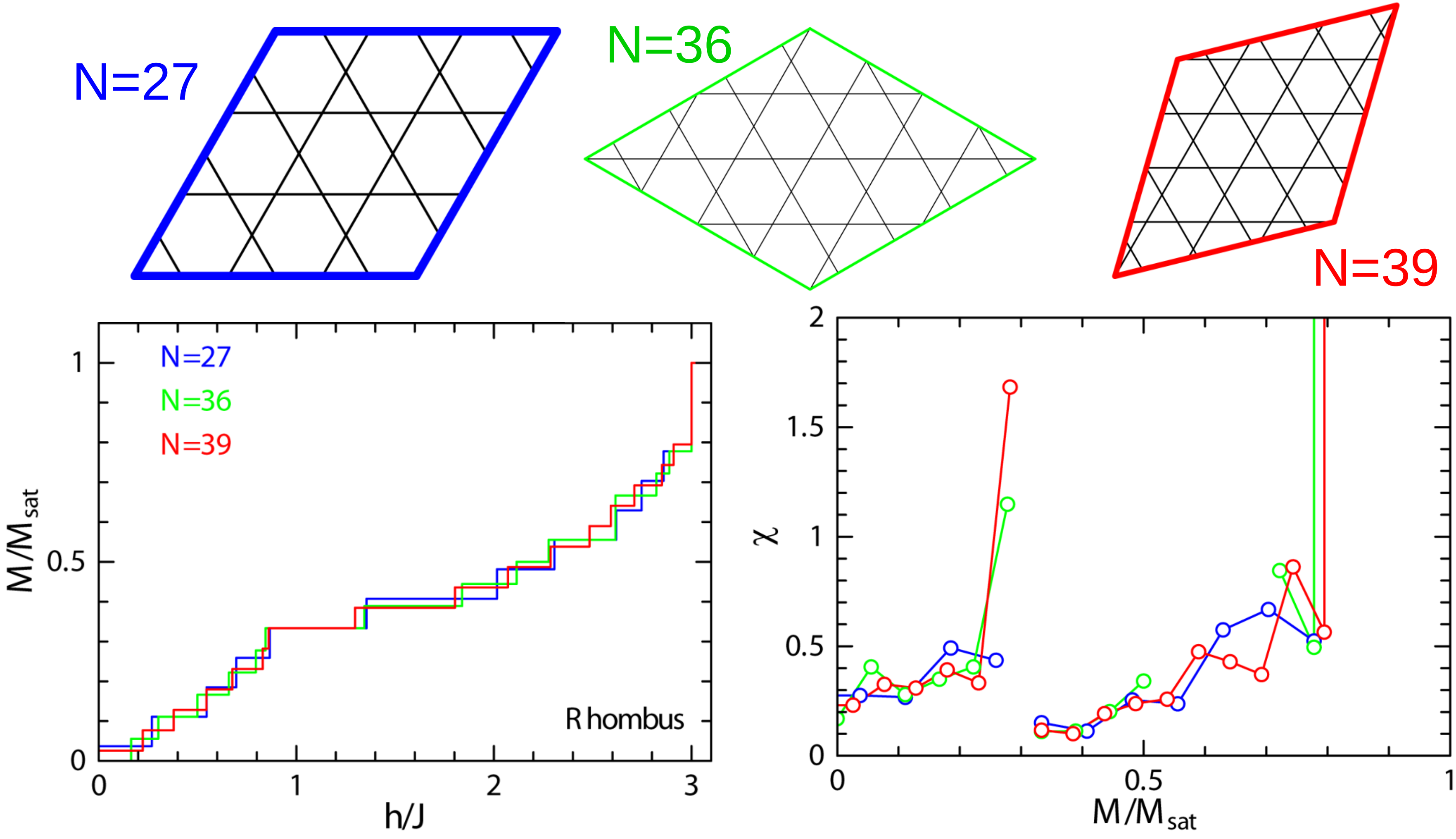
Ski jump

Jump ramp

Magnetization curve of Kagome lattice AF



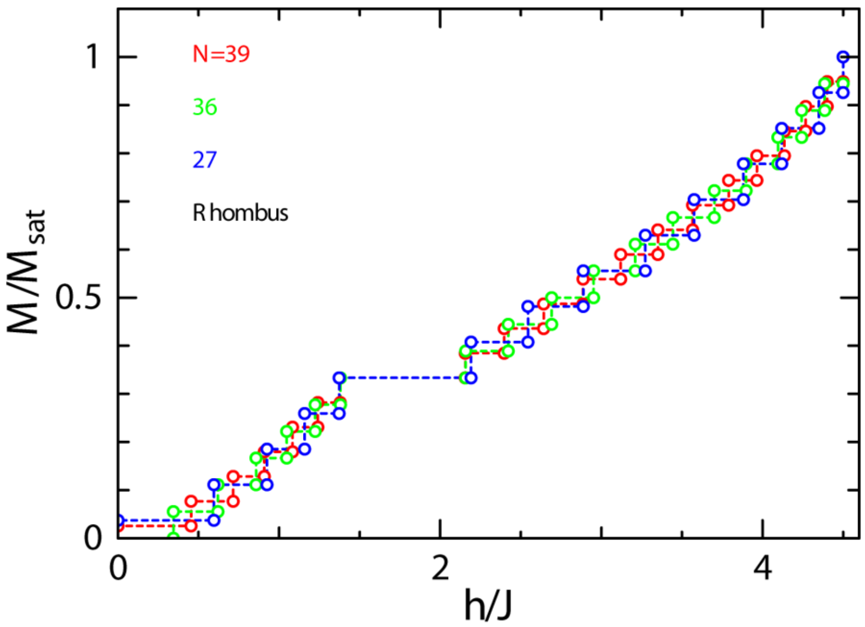
Results for Rhombic Clusters

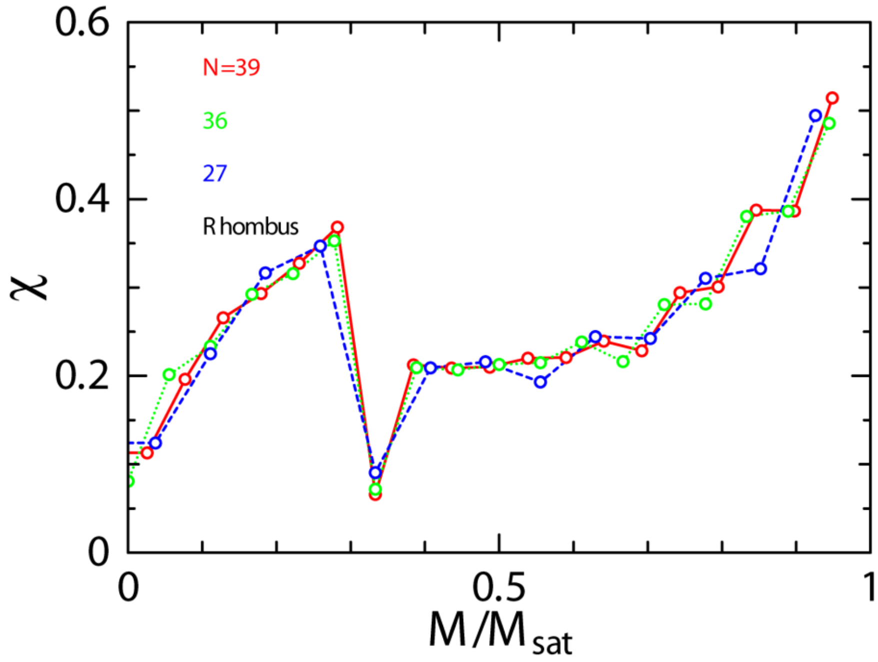


Characteristics of the ramp appear clearly for N=39.

Triangular lattice

N=39, 36, and 27 Rhombus

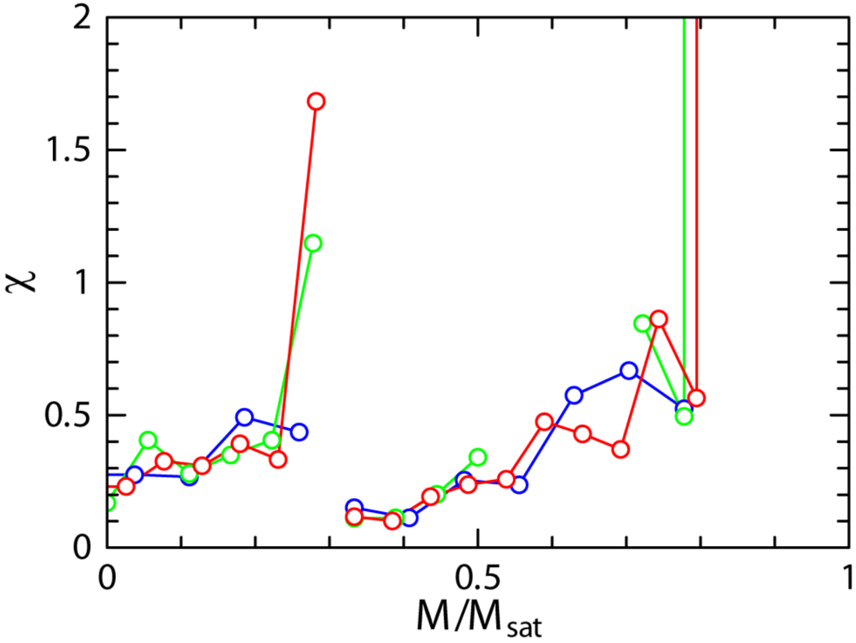




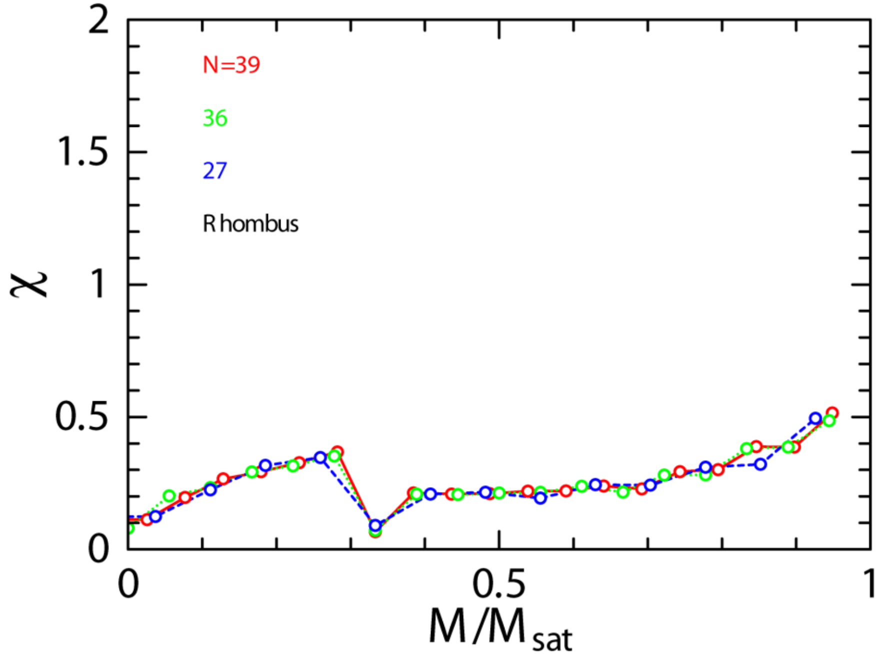
Typical magnetization plateau at M/M_{sat}=1/3

Comparison of χ

Kagome



Triangular



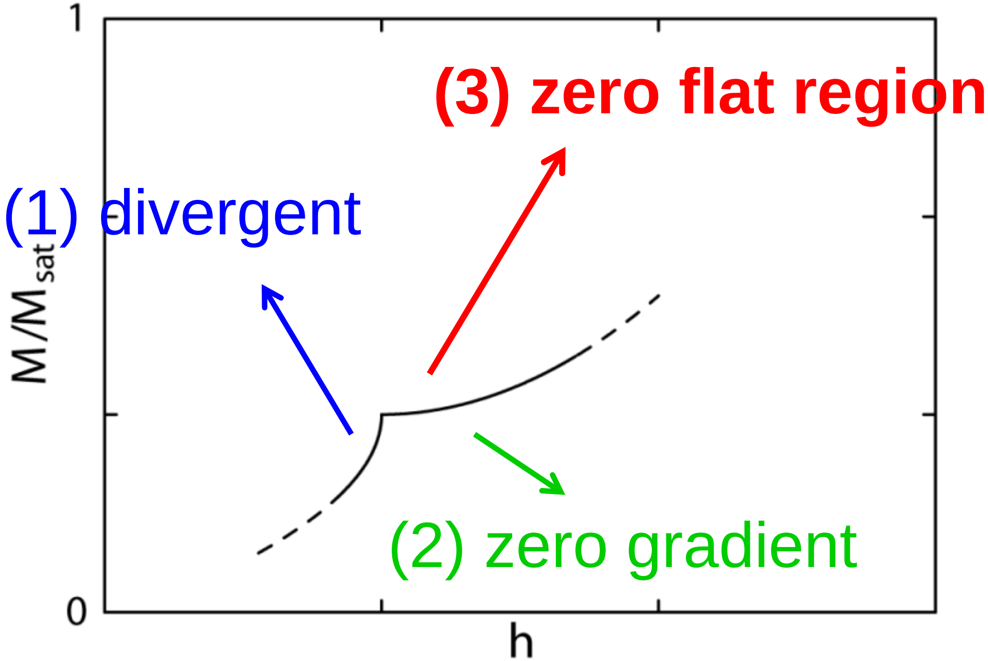
Clear difference at M/M_{sat}=1/3

Ramp

Plateau

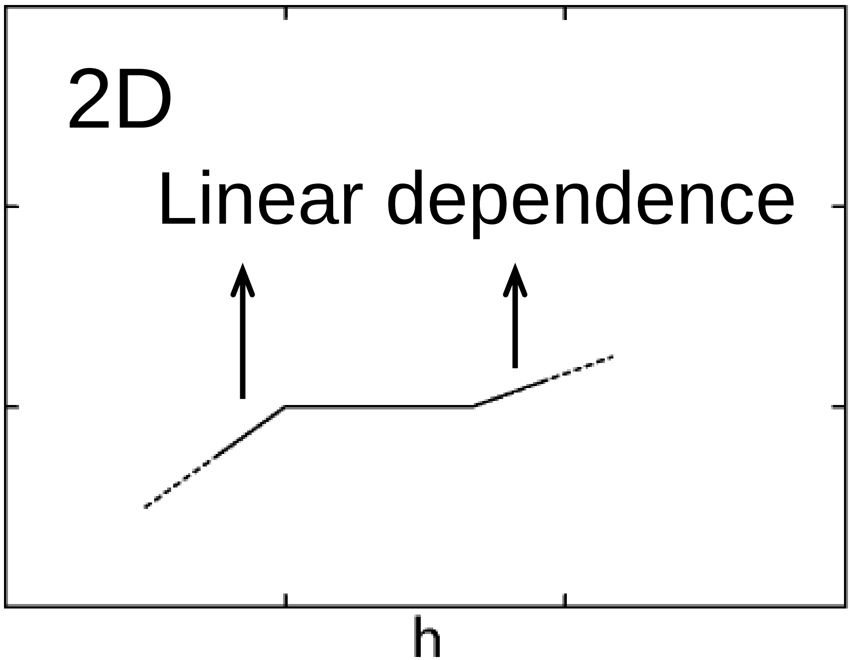
Features of Magnetization Ramp

Magnetization ramp



Kagome lattice

Magnetization plateau



Triangular lattice

Critical exponent

$|m\text{-}mc| = |H\text{-}Hc|^{1/\delta}$

$\delta=2$ *1D*

Affleck 1990, Tsvelik 1990, TS-Takahashi 1991

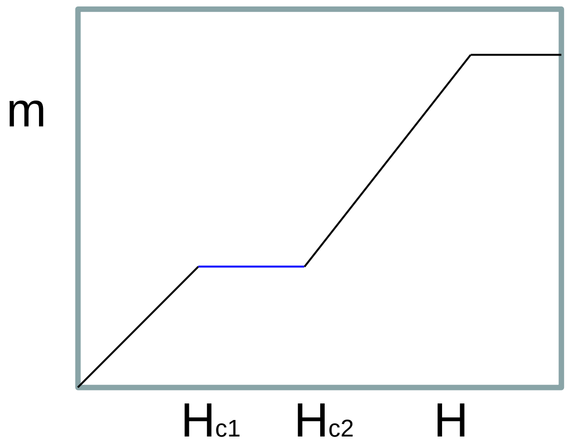
$\delta=1$ *2D*

Katoh-Imada 1994

1/3 magnetization plateau

$$m - \frac{1}{3} \sim (H - H_{c2})^{1/\delta_+},$$
$$\frac{1}{3} - m \sim (H_{c1} - H)^{1/\delta_-}.$$

$H_{c1}=H_{c2}$?



Estimation of δ

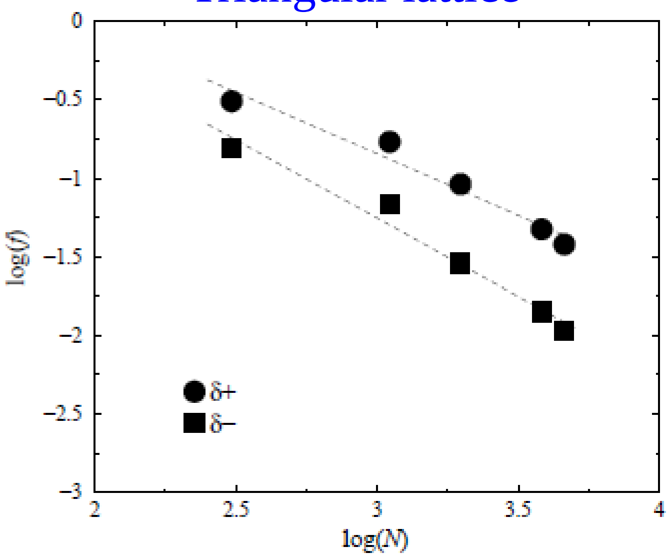
cf. TS and M. Takahashi: PRB 57 (1998) R8091

$$f_\pm(N) \equiv \pm[E(N, \frac{N}{3} \pm 2) + E(N, \frac{N}{3}) - 2E(N, \frac{N}{3} \pm 1)],$$

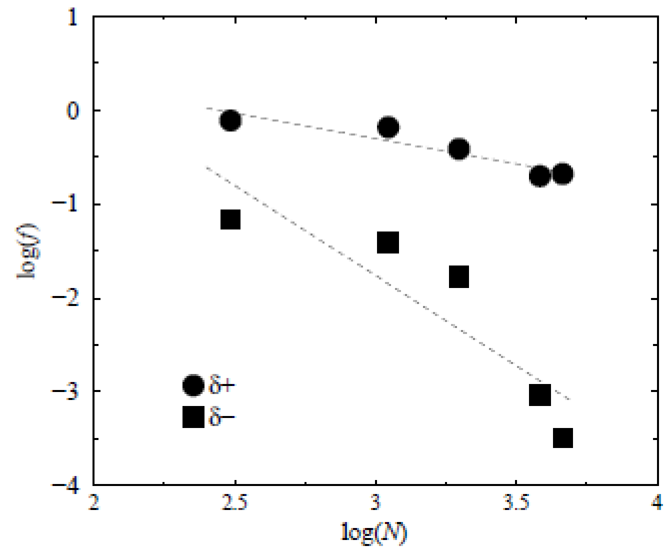
$$f_\pm(N) \sim \frac{1}{N^{\delta_\pm}}$$

Numerical diagonalization of rhombic clusters for N=12, 21, 27, 36, 39

Triangular lattice



Kagome lattice



$\delta_- = 1.0 \pm 0.2, \qquad \delta_+ = 0.8 \pm 0.2,$

$\delta_- = 1.9 \pm 1.0, \qquad \delta_+ = 0.5 \pm 0.2,$

$\delta_- = \delta_+ = 1$ Conventional (2D)

$\delta_- = 2$ $\chi \to \infty$ (1D like)

$\delta_+ = 1/2$ $\chi = 0$

$H_{c1}=H_{c2}$? (Plateau vs Ramp)

Triangular lattice

$$H_{c2}-H_{c1}=0.3\pm0.2$$

$H_{c1}\neq H_{c2}$

1/3 plateau

Kagome lattice

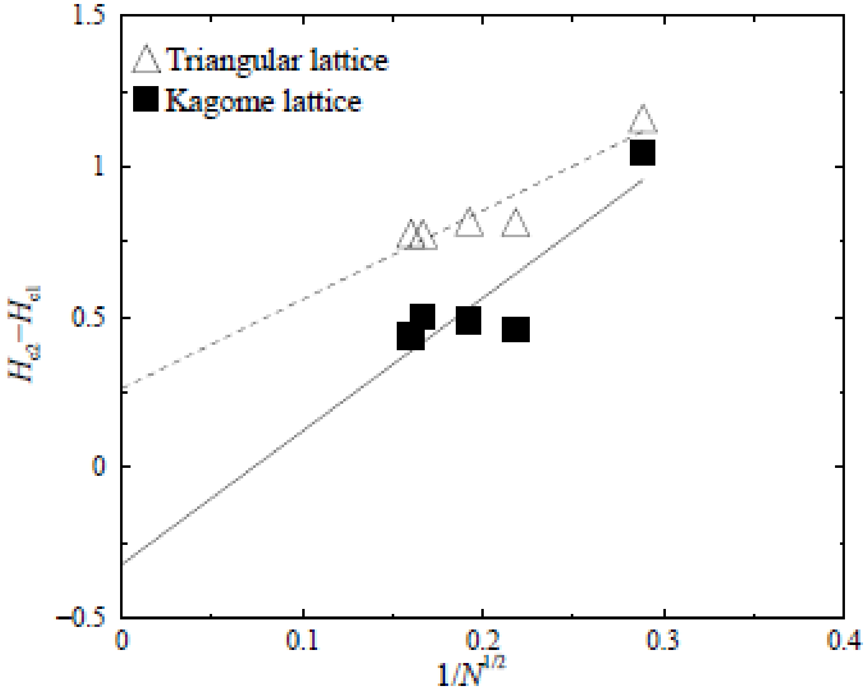
$$H_{c2}-H_{c1}=-0.3\pm0.5$$

$H_{c1}=H_{c2}$

No plateau

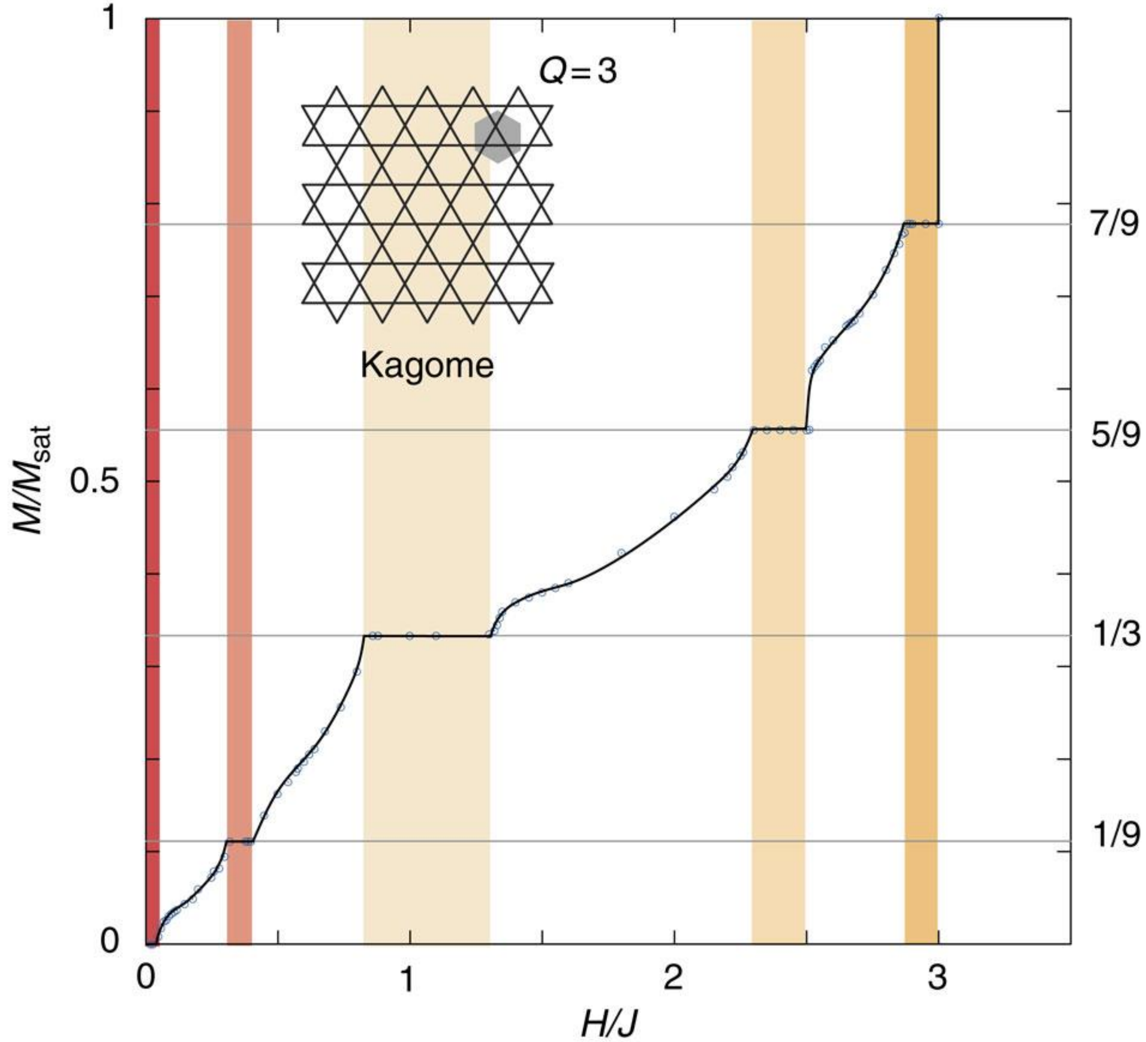
$\Delta \sim k \Rightarrow \Delta \rightarrow 1/N^{1/2}$ $(N\rightarrow\infty)$

if gapless



DMRG on cylinder kagome lattice

Nishimoto et al. Nature Communications 4 (2013) 2287

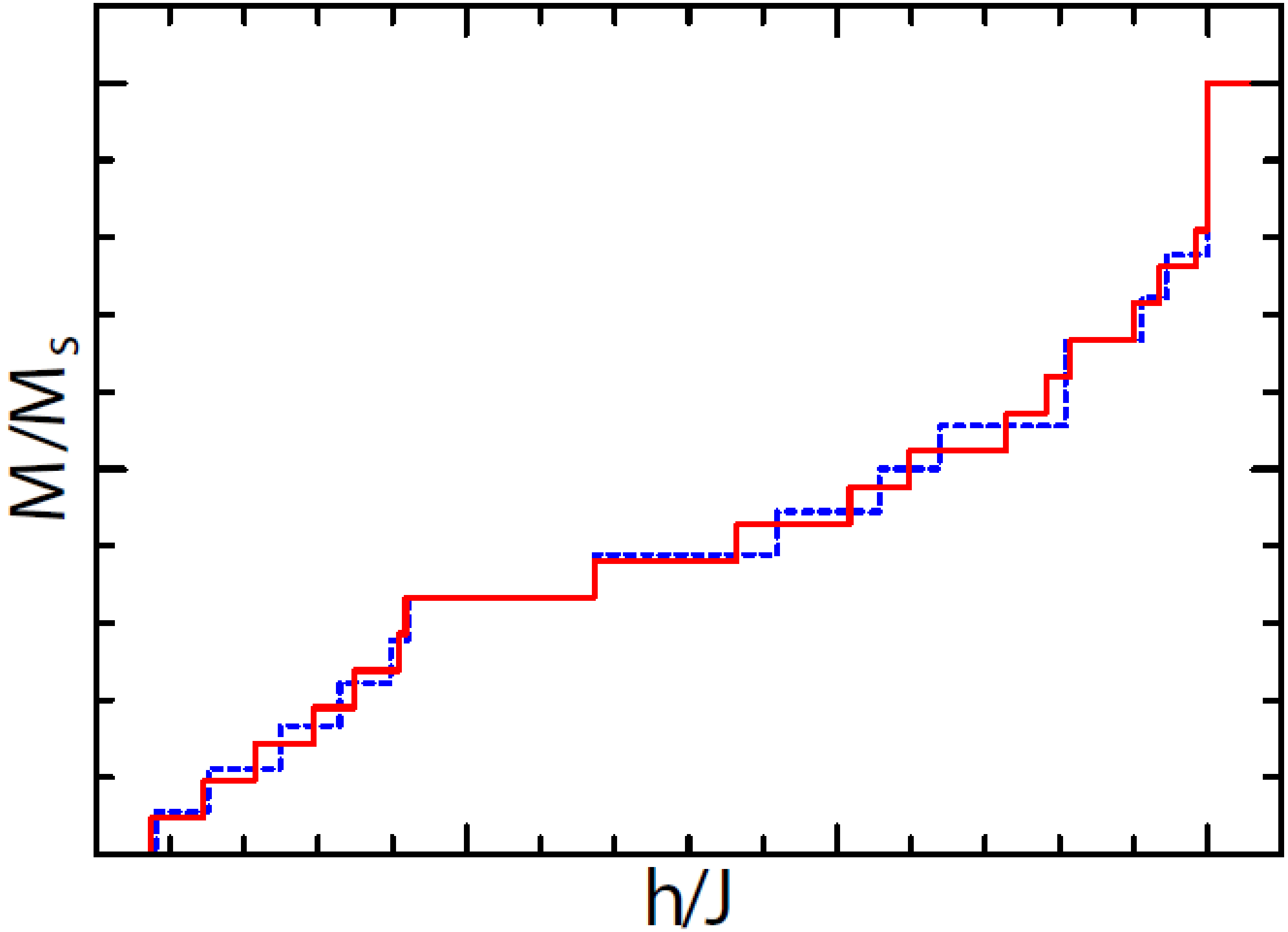


Diagonalization up to 63 spins

Capponi et al. PRB 88 (2013) 144416

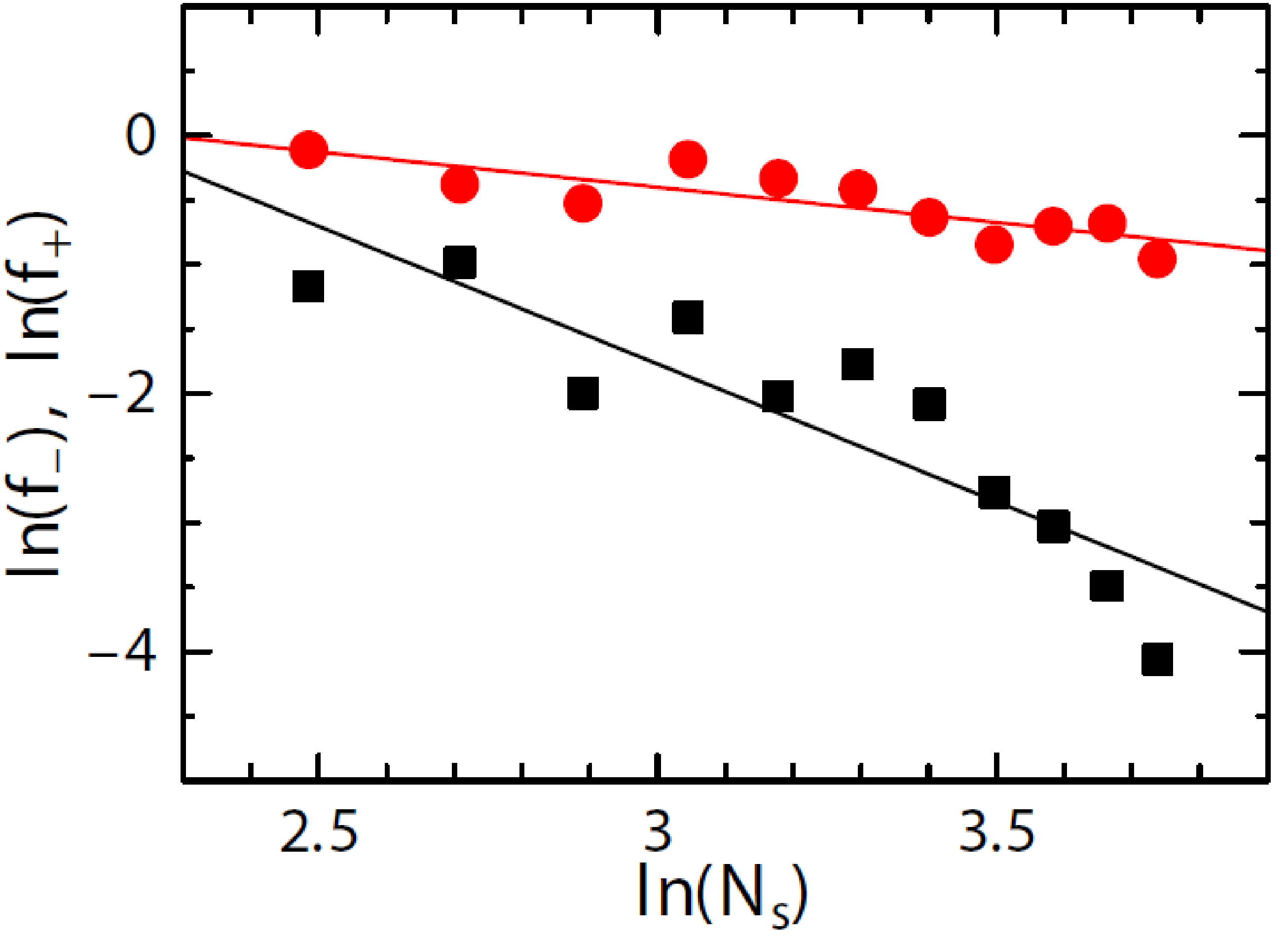
Plateaux at 1/3, 5/9, 7/9

N=36 and 42



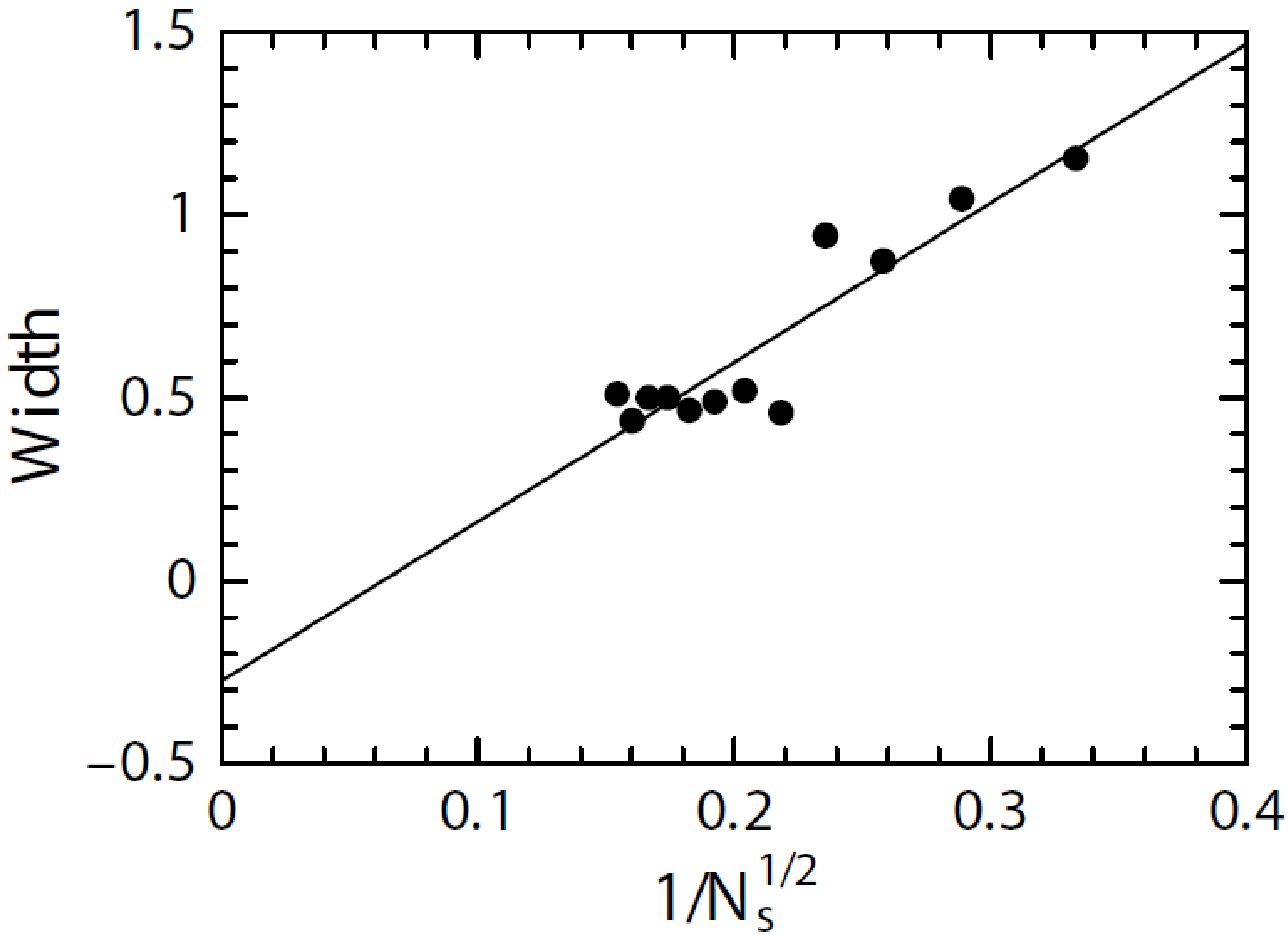
by 京コンピューター

12 ~ 42-spin clusters



$\delta_- = 1.83$ $\delta_+ = 0.47$

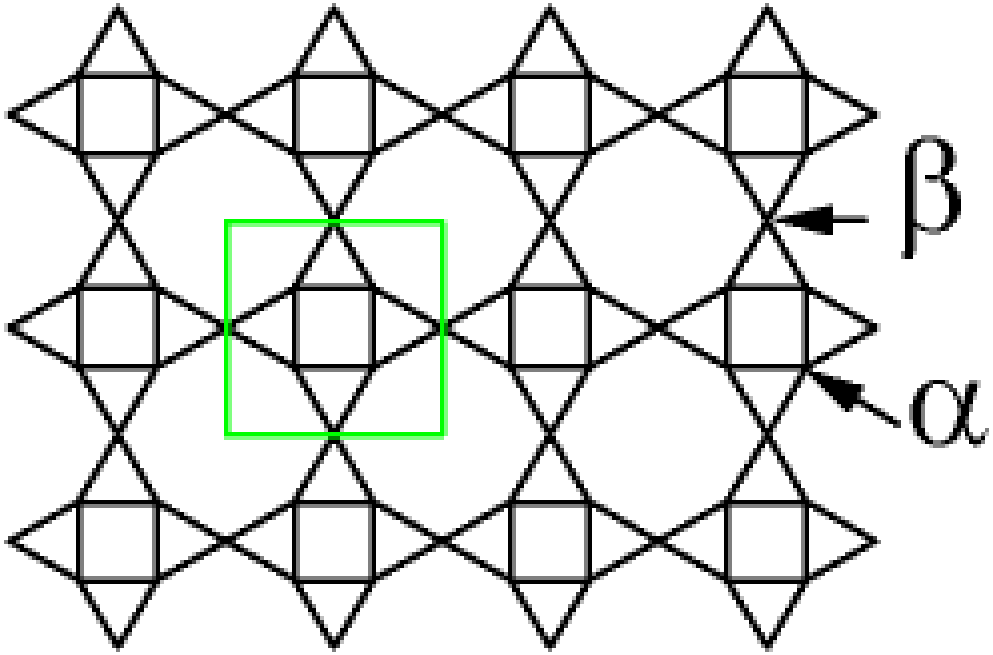
Plateau width
9~42-spin clusters



Square-Kagome (SK) Lattice

Corner-sharing

***z*=4**

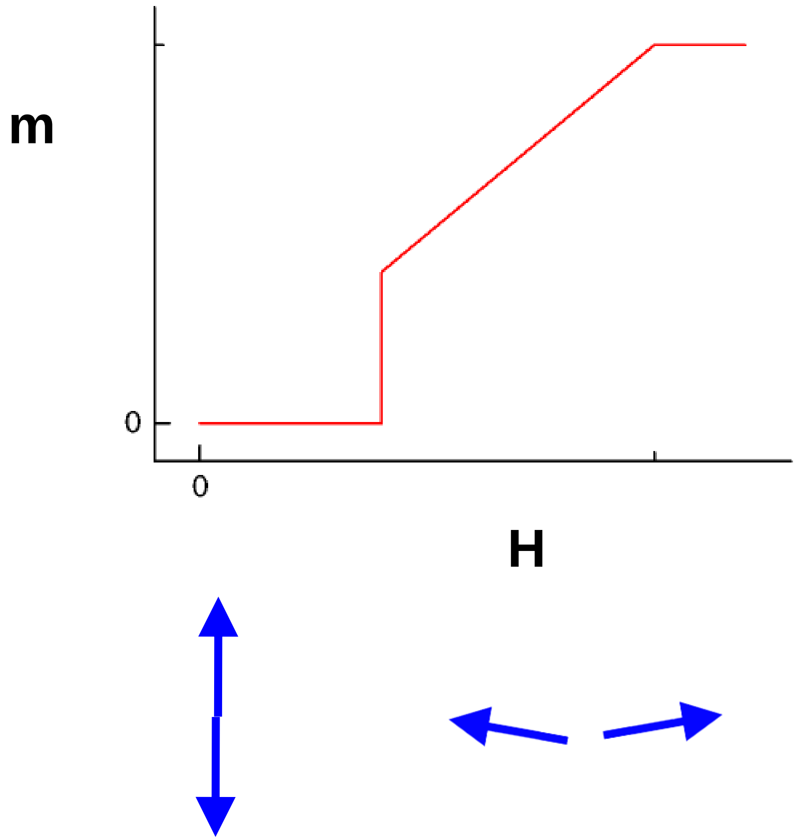


Siddharthan and Georges: PRB 65 (2001) 014417

Shuriken lattice

HN and T. Sakai: JPSJ 82 (2013) 083709 (Le

Spin Flop



Method

Unbiased methods beyond approximations

<u>Numerical diagonalization</u>

(Lanczos algorithm) **Large dimension of matrix**

⇒Huge-scale parallelization

MPI/OpenMP

Data transfer between nodes

cf.)

Quantum Monte Carlo

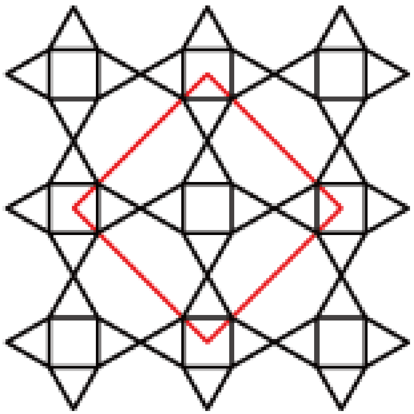
(Negative sign problem) Frustration

Density Matrix Renormalization Group

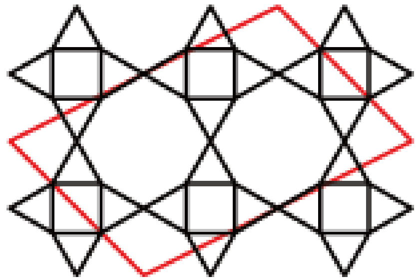
(powerful to 1D systems) 2D systems

Finite-Size Clusters

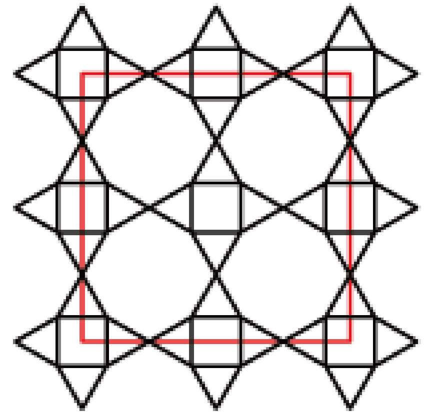
$N_s=12$

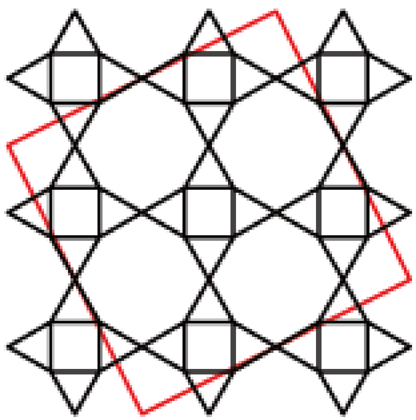


$N_s=18$

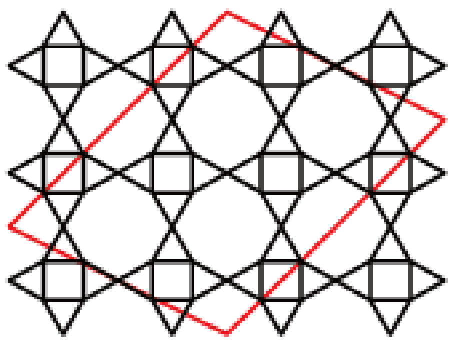


$N_s=24$

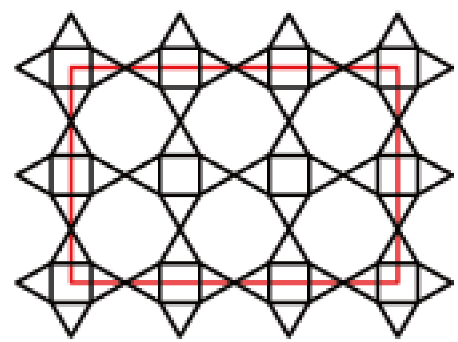




$N_s=30$

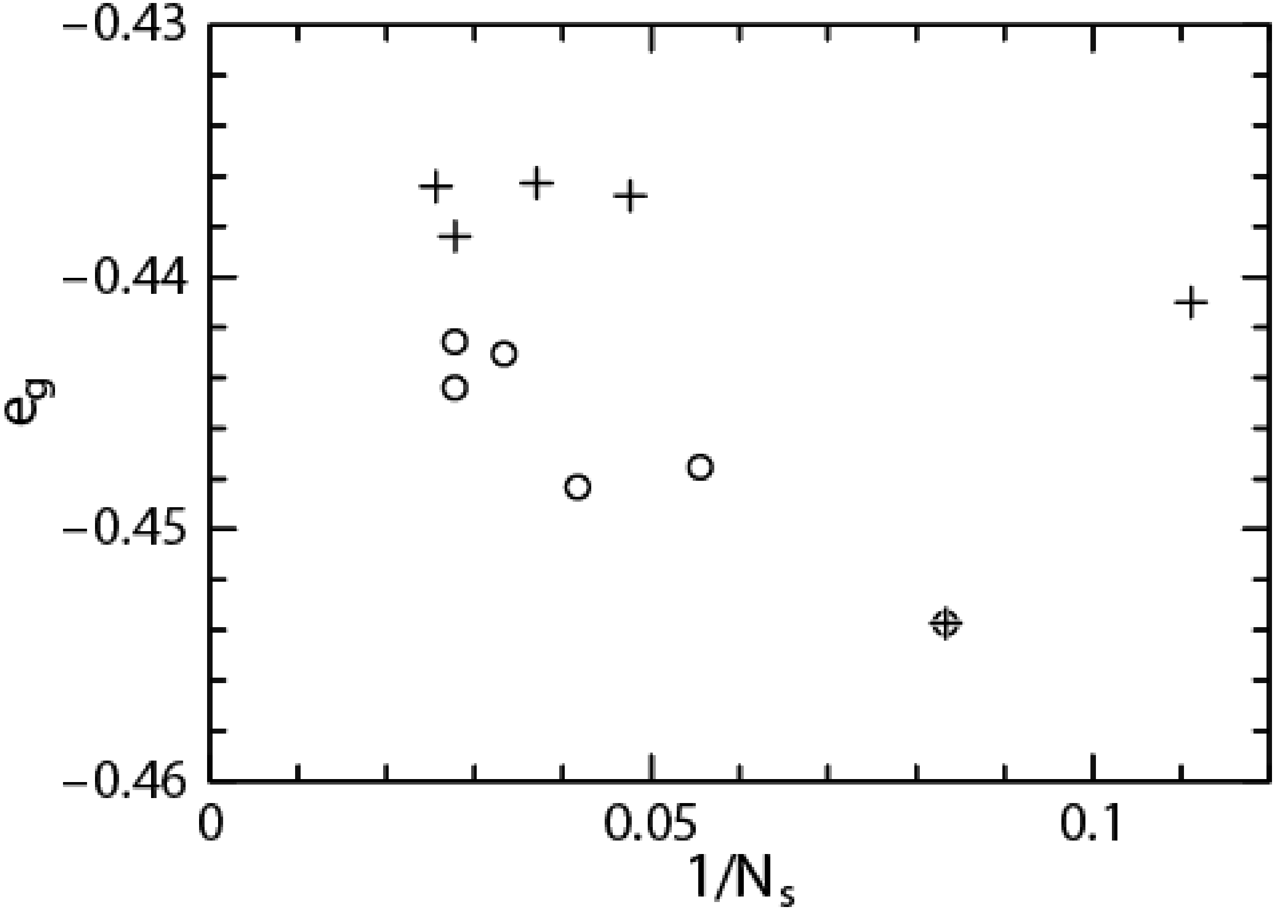


$N_s=36$



$N_s=36$

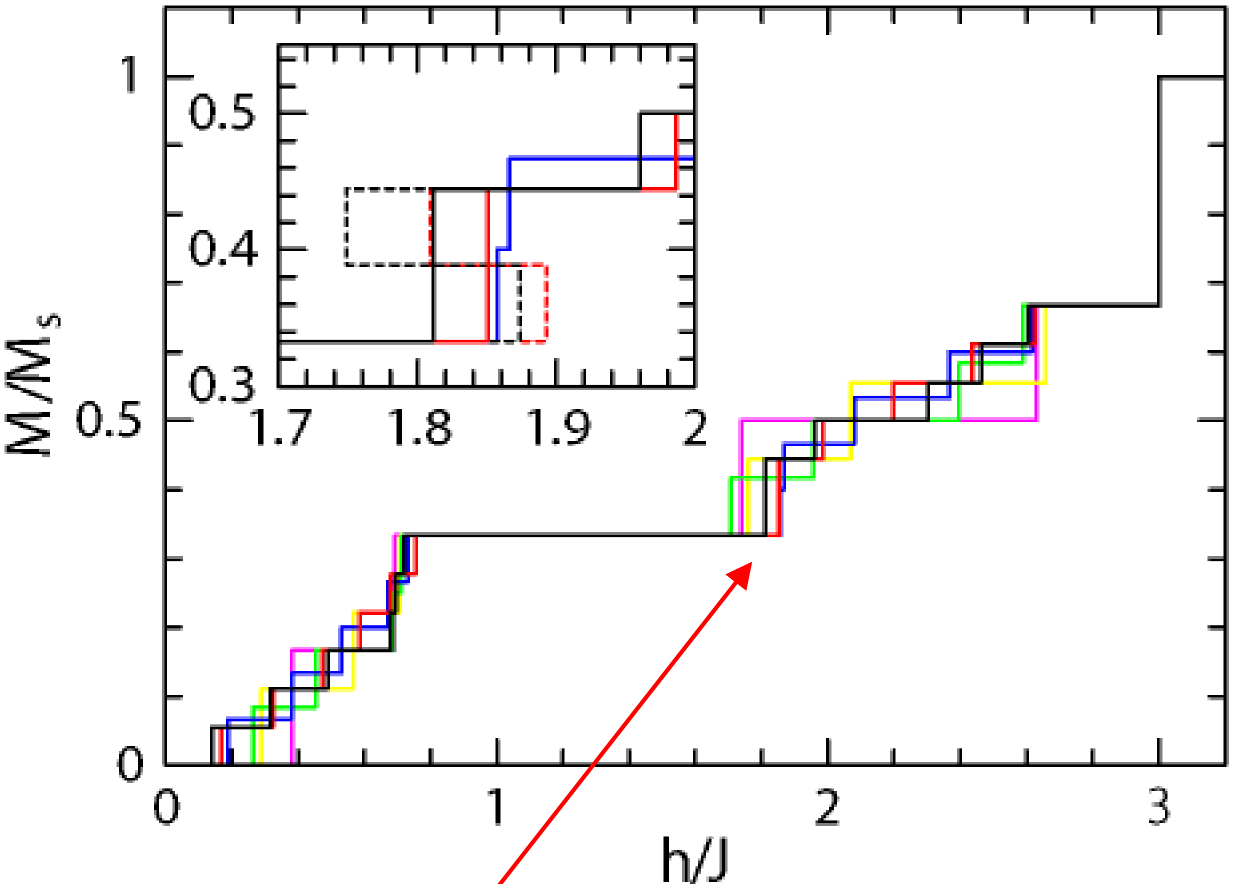
Ground-State Energy



kagome

SK lattice

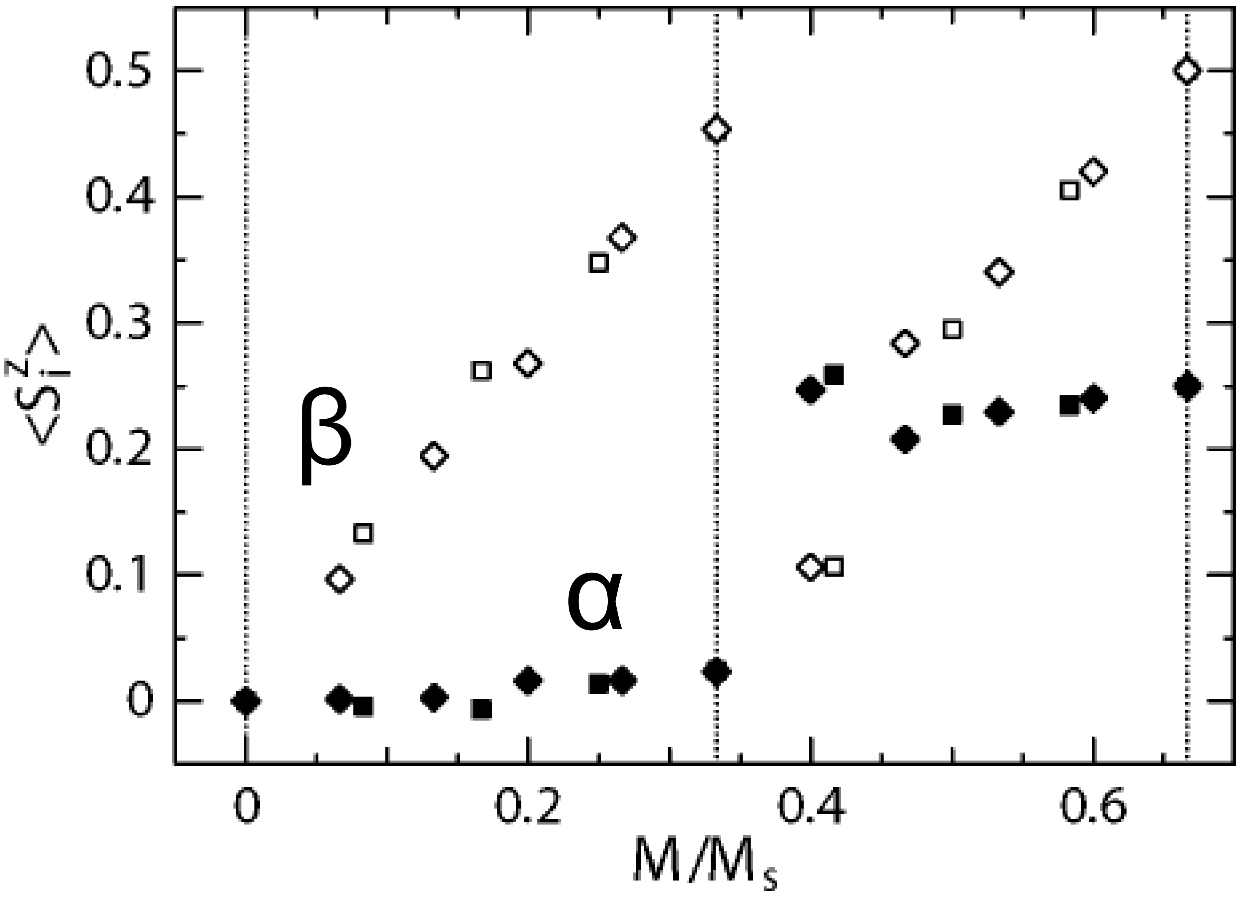
Magnetization Process



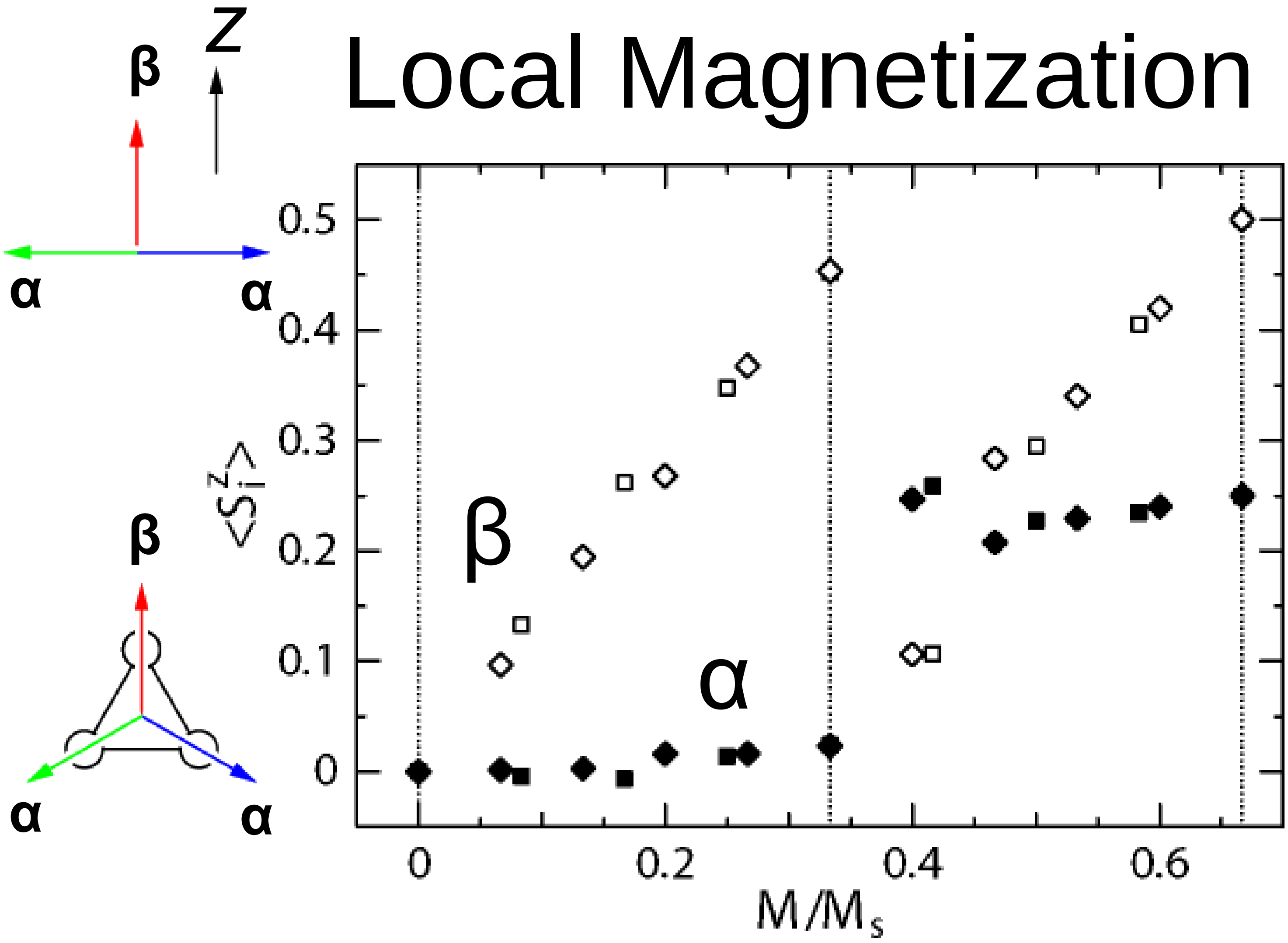
Plateau & jump

A jump of *M* during its increase

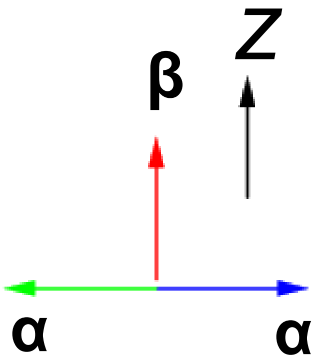
Local Magnetization

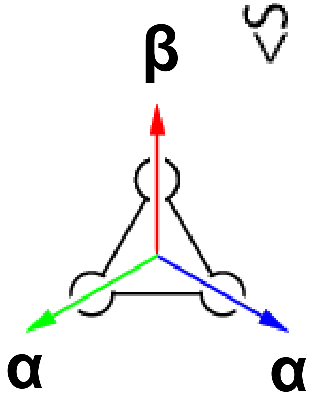


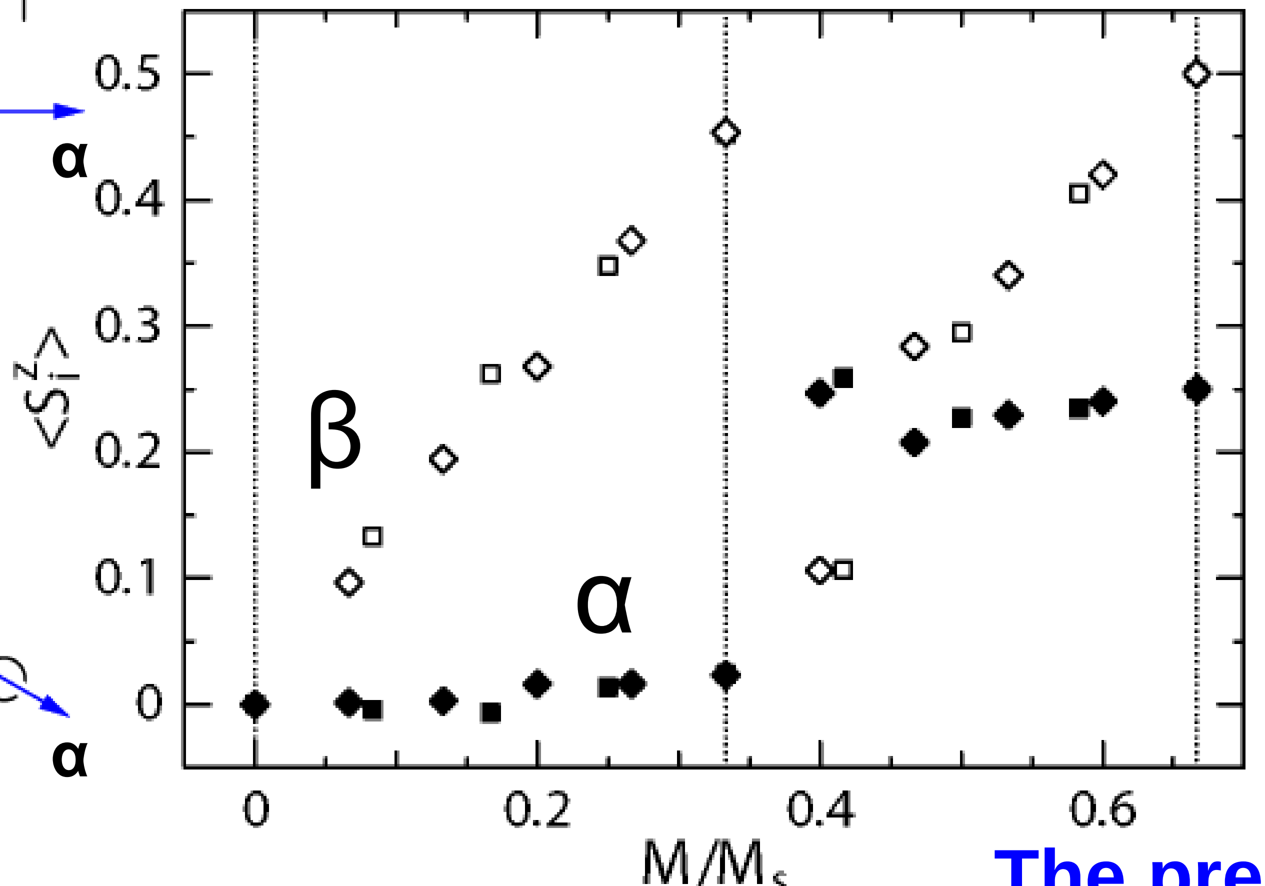
Local Magnetization

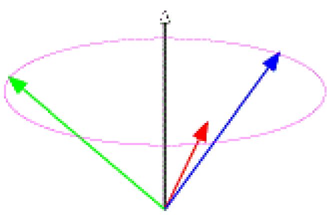


Local Magnetization





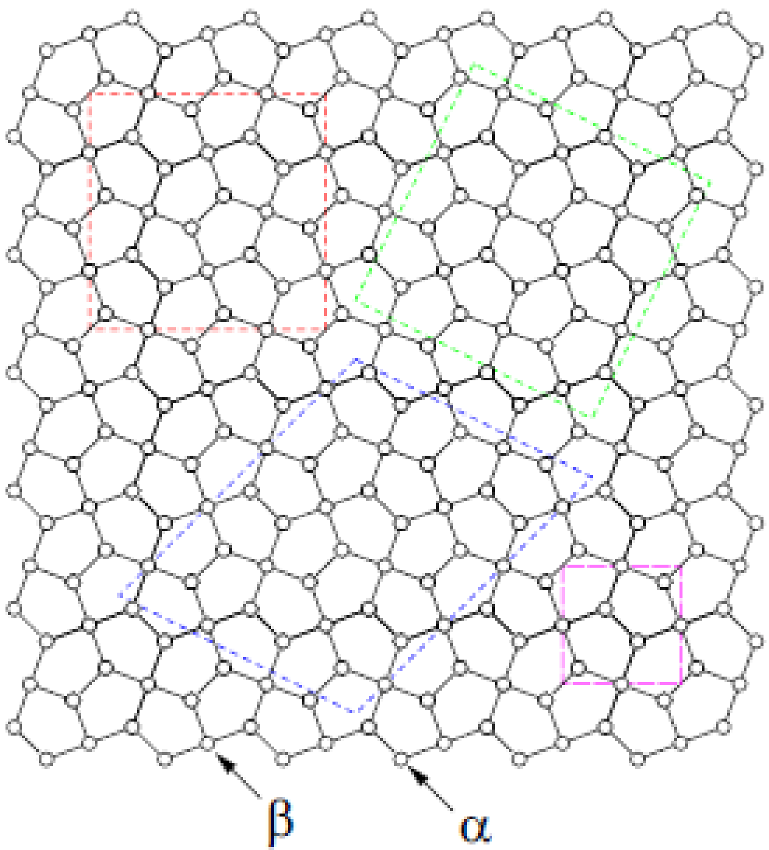




An abrupt change in spin orientation between two states

The present model on SK-lattice AF without anisotropy

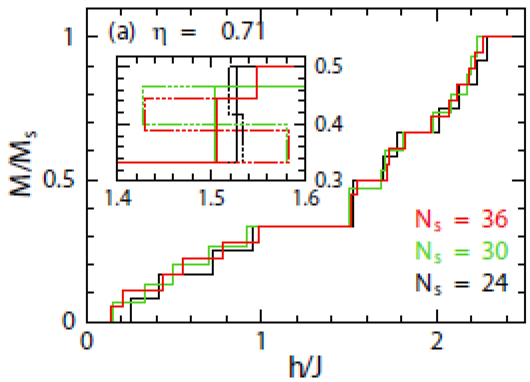
Cairo pentagon lattice



J : α-α bond
J’: α-β bond

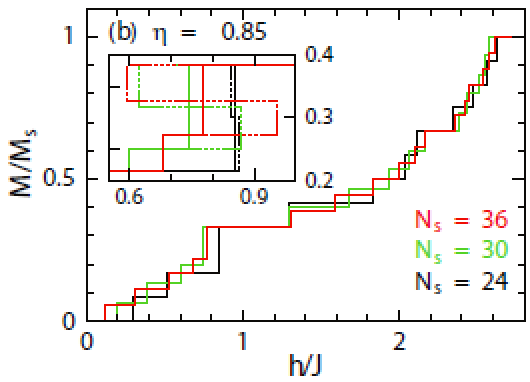
η= J’/J

Magnetization jump



Higher side of 1/3 plateau

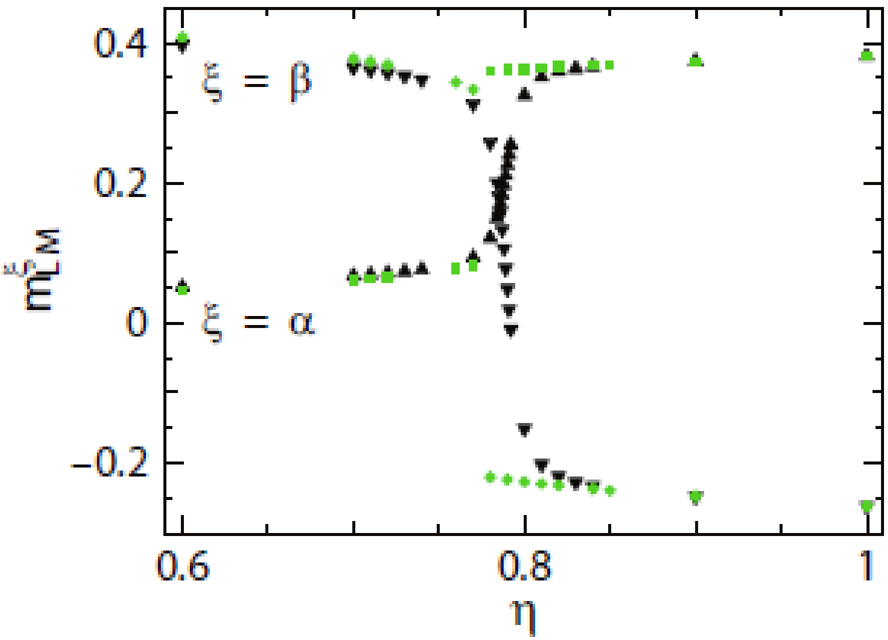
Critical point η ~ 0.8



lower side of 1/3 plateau

Jump ⇔ Classical long-range order

Quantum phase transition



Cairo pentagon lattice AF

Critical ration J'/J ~ 0.8 quantum phase transition

Spin flop after 1/3 plateau for J'/J < 0.8

Spin flop before 1/3 plateau for J'/J >0.8

- **Square-kagome lattice AF**
- **Cairo pentagon lattice AF**

Spin-flop phenomenon in the case when the system is isotropic in spin space.

Cairo pentagon lattice AF

Critical ration J'/J ~ 0.8 quantum phase transition

Spin flop after 1/3 plateau for J'/J < 0.8

Spin flop before 1/3 plateau for J'/J >0.8

Publication

H. Nakano and TS: JPSJ 82 (2013) 083709 (Letter)

H. Nakano, M. Isoda and TS JPSJ to appear (arXve:1403.5008)

H. Nakano, TS and Y. Hasegawa in preparation.