YIPQS long-term and Nishinomiya-Yukawa memorial workshop
Novel Quantum States in Condensed Matter 2017 at Kyoto on Oct. 23- Nov. 24., 2017

Quantum Spin Liquid of the Kagome- and Triangular-Lattice Antiferromagnets and Related Materials

- Spin gap issue -

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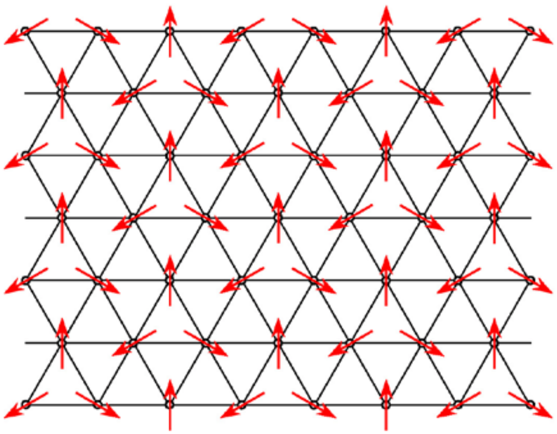
TS and H. Nakano: PRB 83 (2011) 100405(R) (arXiv:1102.3486)
H. Nakano and TS: JPSJ 80 (2011) 053704 (arXiv: 1103.5829)
H. Nakano, Y.Hasegawa, and TS, JPSJ **84,** 114703 (2015)
H. Nakano and TS: J. Phys.: Conf. Series 868 (2017) 012006
TS and H. Nakano: in preparation

SPring-8

Candidates of Quantum Spin Fluid 2D frustrated systems

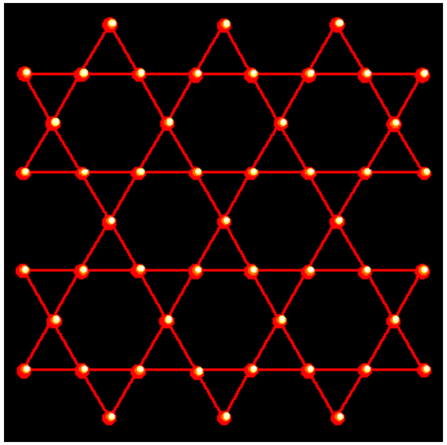
- S=1/2 Heisenberg antiferromagnets $H = J\sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j$

Triangular lattice



120 degree LRO

Kagome lattice

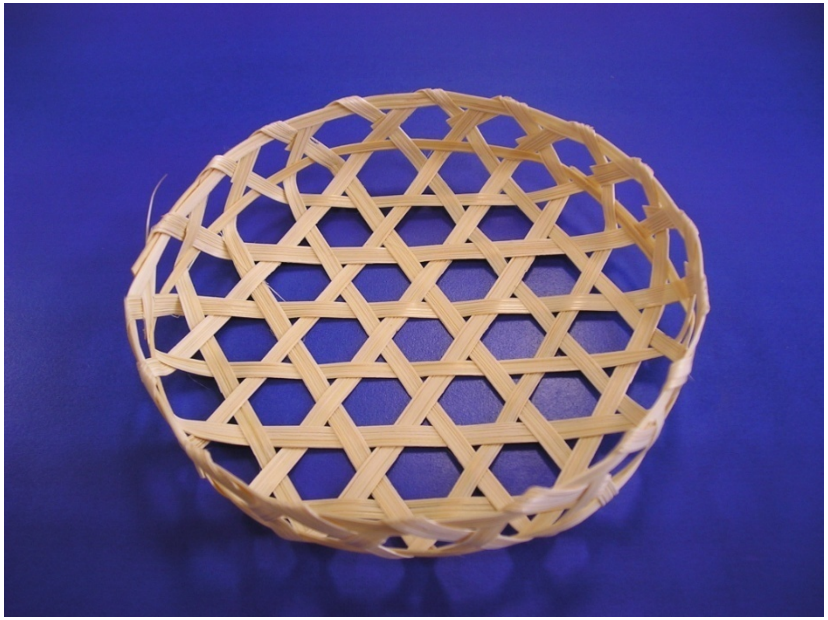


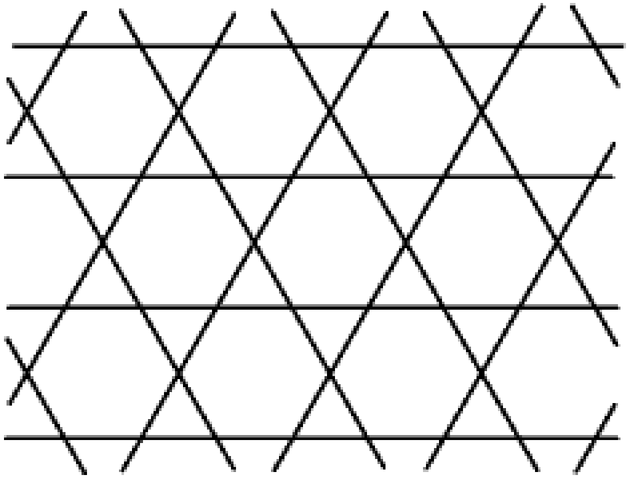
No (conventional) LRO

Kagome lattice

Itiro Syôzi: Statistics of Kagomé Lattice, PTP **6** (1951)306

kagome





Corner sharing triangles

S=1/2 Kagome Lattice AF

- Herbertsmithite $ZnCu_3(OH)_6Cl_2$ impurities

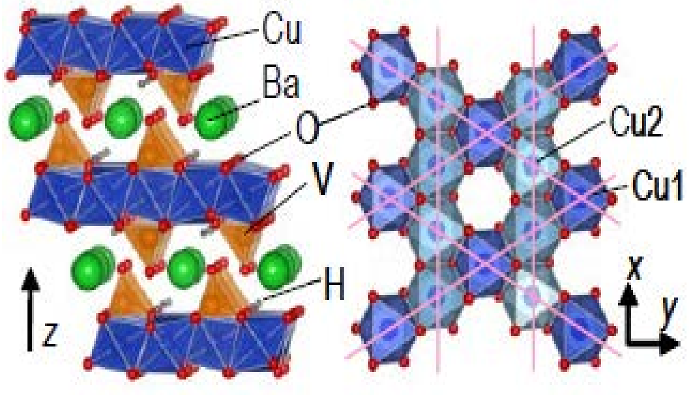
  Shores et al. J. Am. Chem. Soc. 127 (2005) 13426

- 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



Spin gap issue of kagome-lattice AF

Gapped theories

Valence Bond Crystal (VBC)

MERA[Vidal]

Z_2 Topological Spin Liquid [Sachdev (1992)]

DMRG [White (2011)]

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

Gapless theories

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

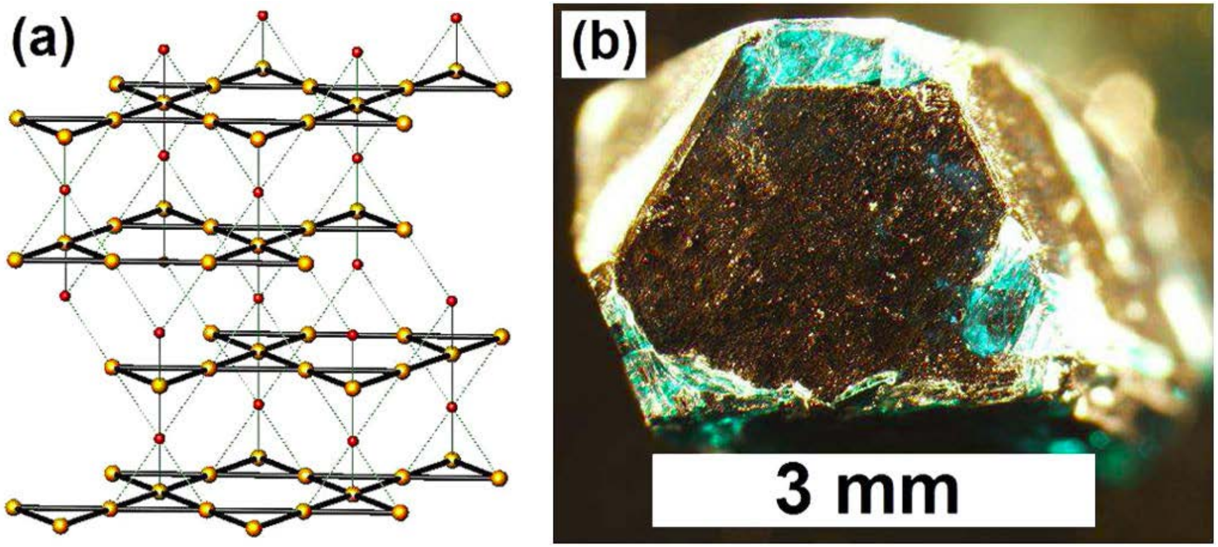
Variational method [Iqbal, Poilblanc, Becca, PRB 89 (2014) 020407]

DMRG [He et al. PRX 7 (2017) 031020]

Single crystal of herbertsmithite

T. Han, S. Chu, Y. S. Lee: PRL 108 (2012) 157202

$ZnCu_3(OH)_6Cl_2$



Inelastic neutron scattering: Spin gap < J/70

Gapless

M. Fu, T. Imai, T.-H. Han, Y. S. Lee: Science 350 (2015) 655

NMR : Gapped

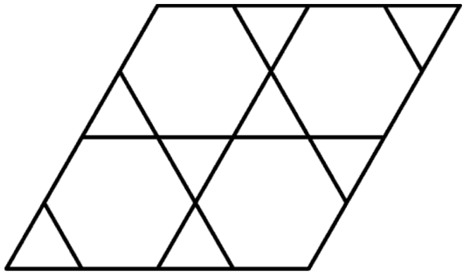
Methods

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)

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

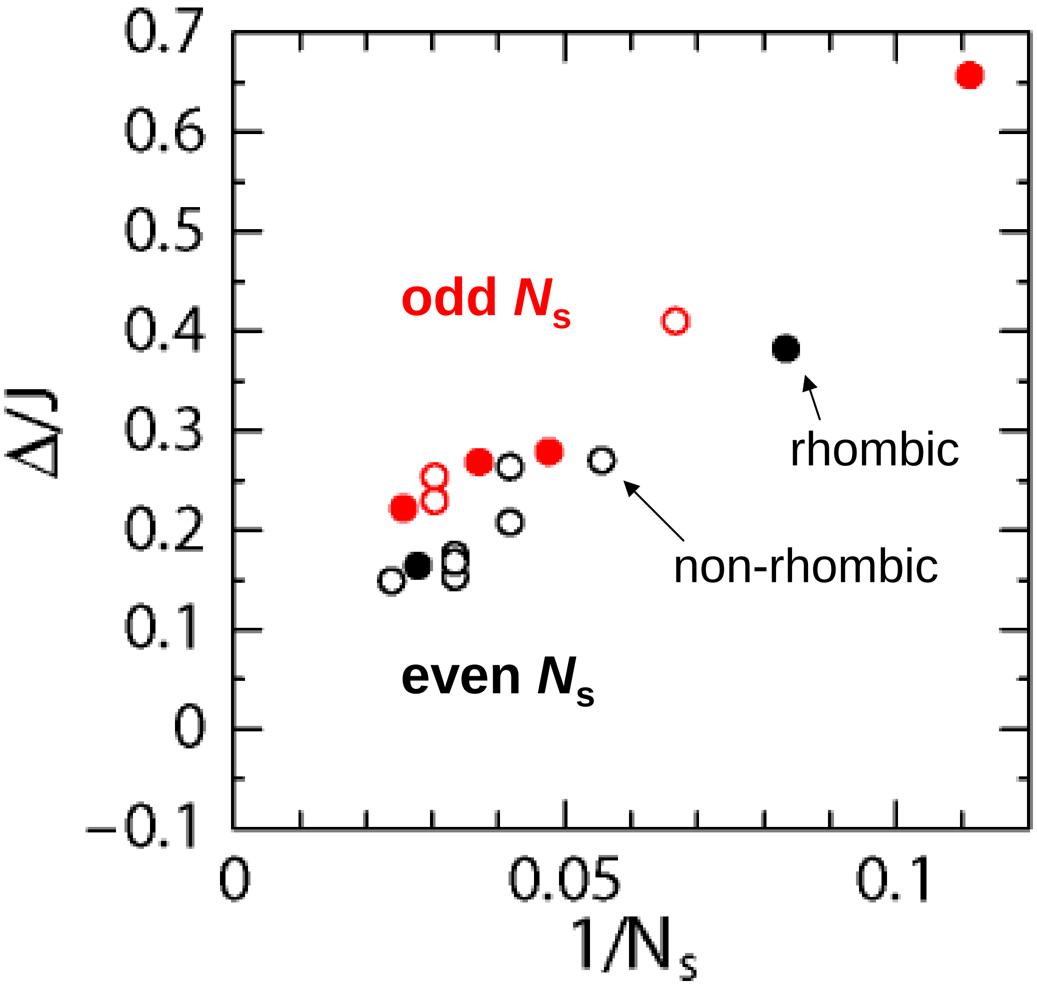
Time cost

d * # of bonds * # of iterations

d increases exponentially with respect to *N*.

⇒ Parallelization with respect to *d*

Numerical diagonalizations of finite-size clusters up to N_s=42

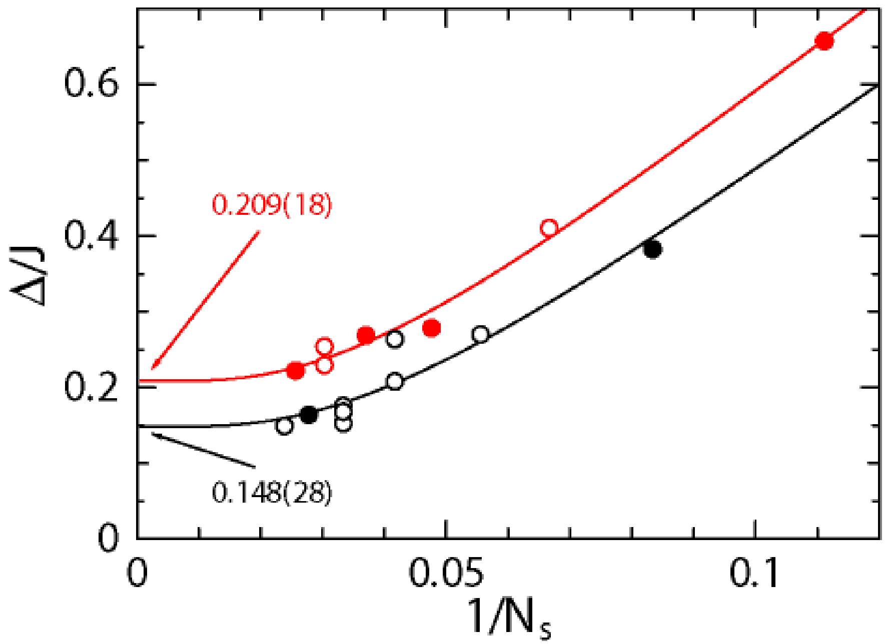


Important to divide data into two groups of even N_s and odd N_s.

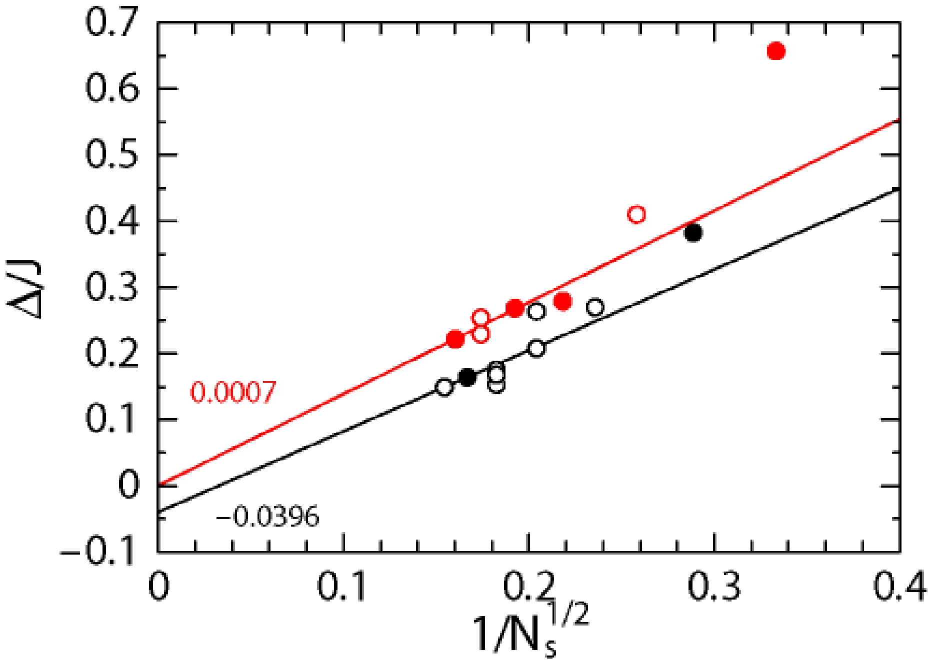
Not good to treat all the data together.

Analysis of our finite-size gaps

H. Nakano and TS: JPSJ 80 (2011) 053704 (arXiv: 1103.5829)



$\Delta/J=A+B\exp(-CN_s^{1/2})$



$\Delta/J=A+B/(N_s^{1/2})$

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

gapless is better !

Gapless or Gapped ？

Susceptibility analysis

Field derivative of magnetization

$$\chi \propto \frac{\partial M}{\partial H}$$ at M=0

as a function of $m = \frac{M}{M_s}$

$$\hat{H} = J\sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j - g\mu_B H \sum_j S_j^z \qquad (g\mu_B=1)$$

$$\begin{array}{ccc} \downarrow & & \downarrow \\ E(M) & & -HM \end{array} \qquad M=\Sigma_j S_j^z$$

$E(M)/N \sim \varepsilon(m)$ $(N\rightarrow\infty)$ $\qquad m=M/N$

$E(M+1)-E(M) \sim \varepsilon'(m) + \varepsilon''(m)/2N + \cdots$

$(E(M+1)-E(M))-(E(M)-E(M-1)) \sim \varepsilon''(m)/N$

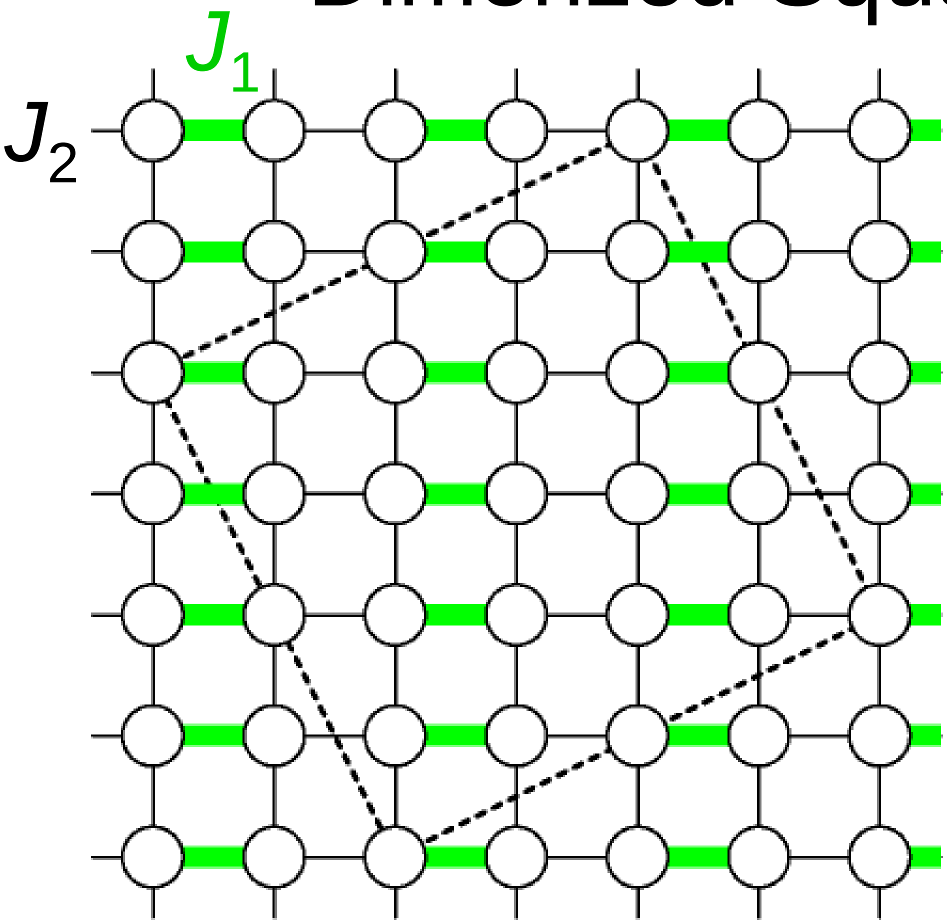
$m=0$ $\downarrow$

$2\Delta \sim \varepsilon''(m)/N$

$\chi = dm/dh = 1/\varepsilon''(m) \rightarrow 0$ for $\Delta\neq 0$ $N\rightarrow\infty$

Demonstration of analysis

Dimerized Square Lattice



$\alpha = J_2/J_1$

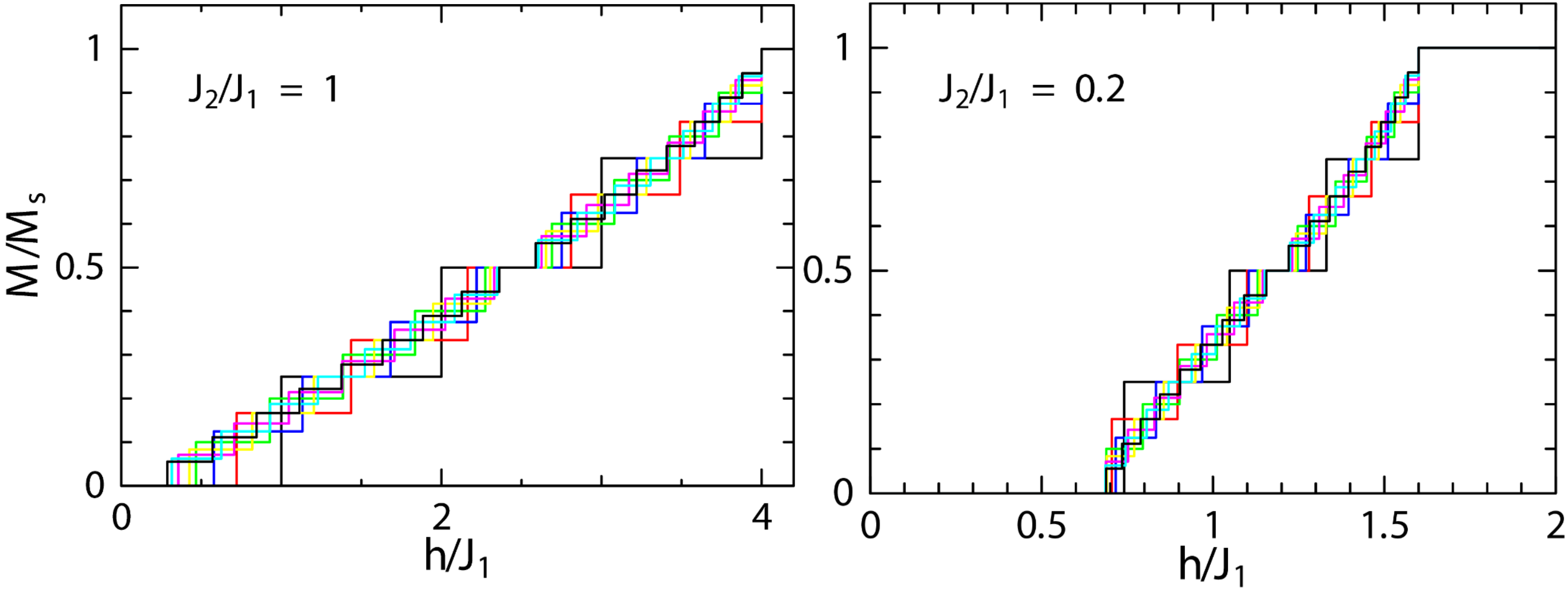
$\alpha=1$: square lattice,
LRO, gapless

$\alpha=0.52337(3)$: critical

Matsumoto et al:
PRB**65**(2001) 014407

$\alpha=0$: isolated dimers
gapped

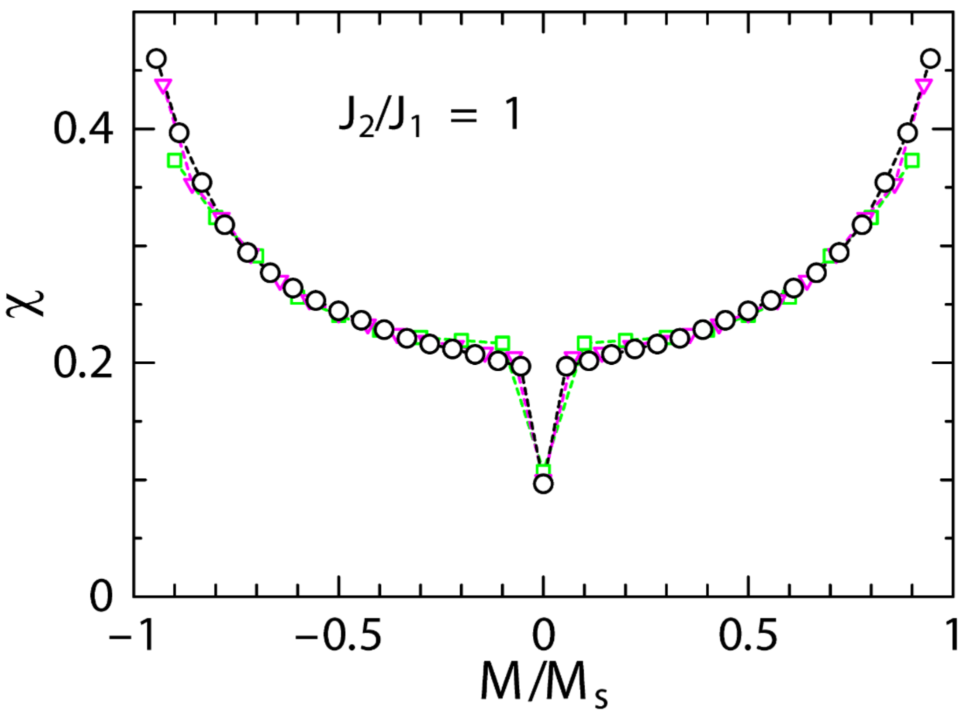
Magnetization processes

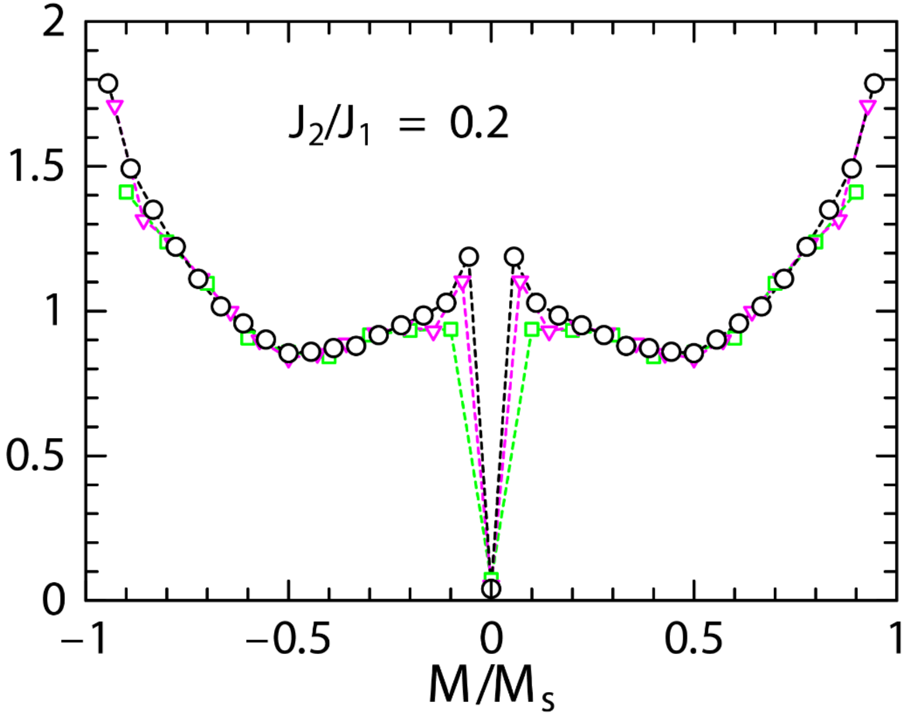


Gapless

Gapped

Differential susceptibility vs. M

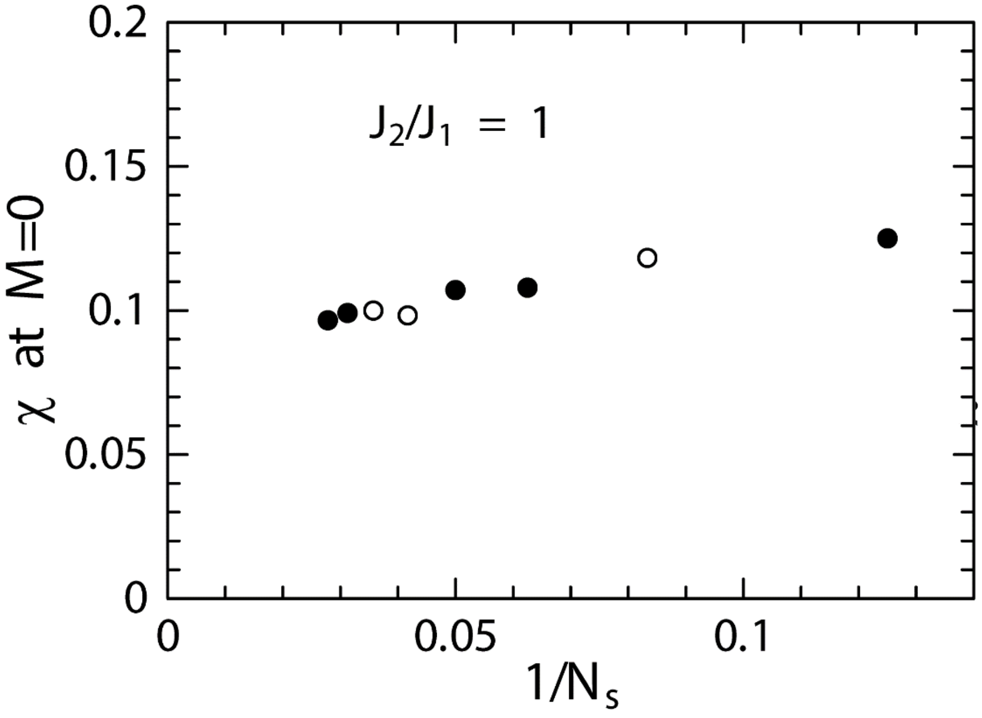


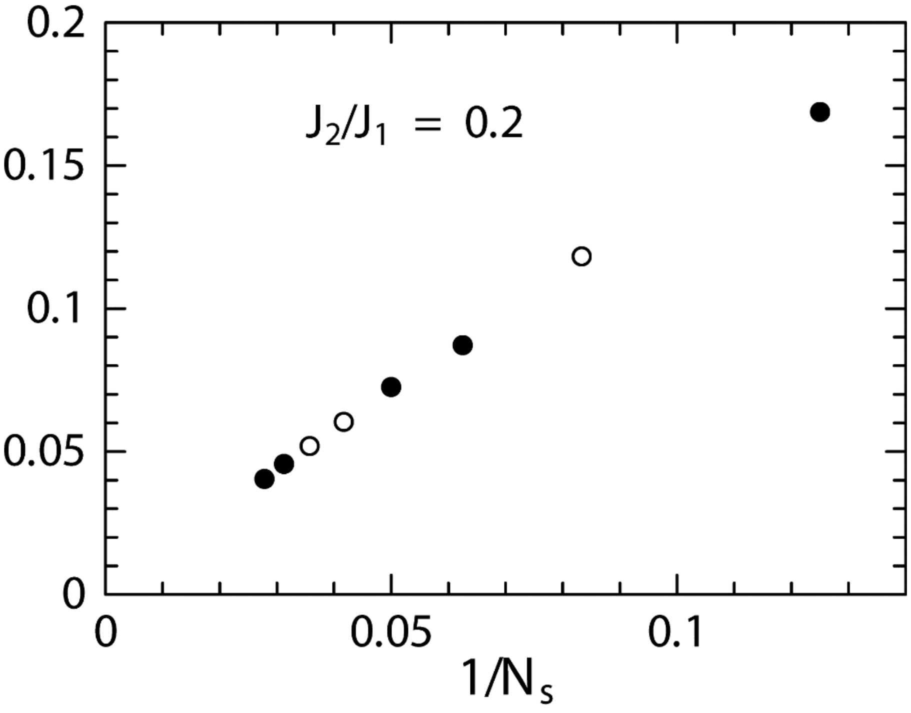


Gapless

Gapped

Size dependence of χ at M=0

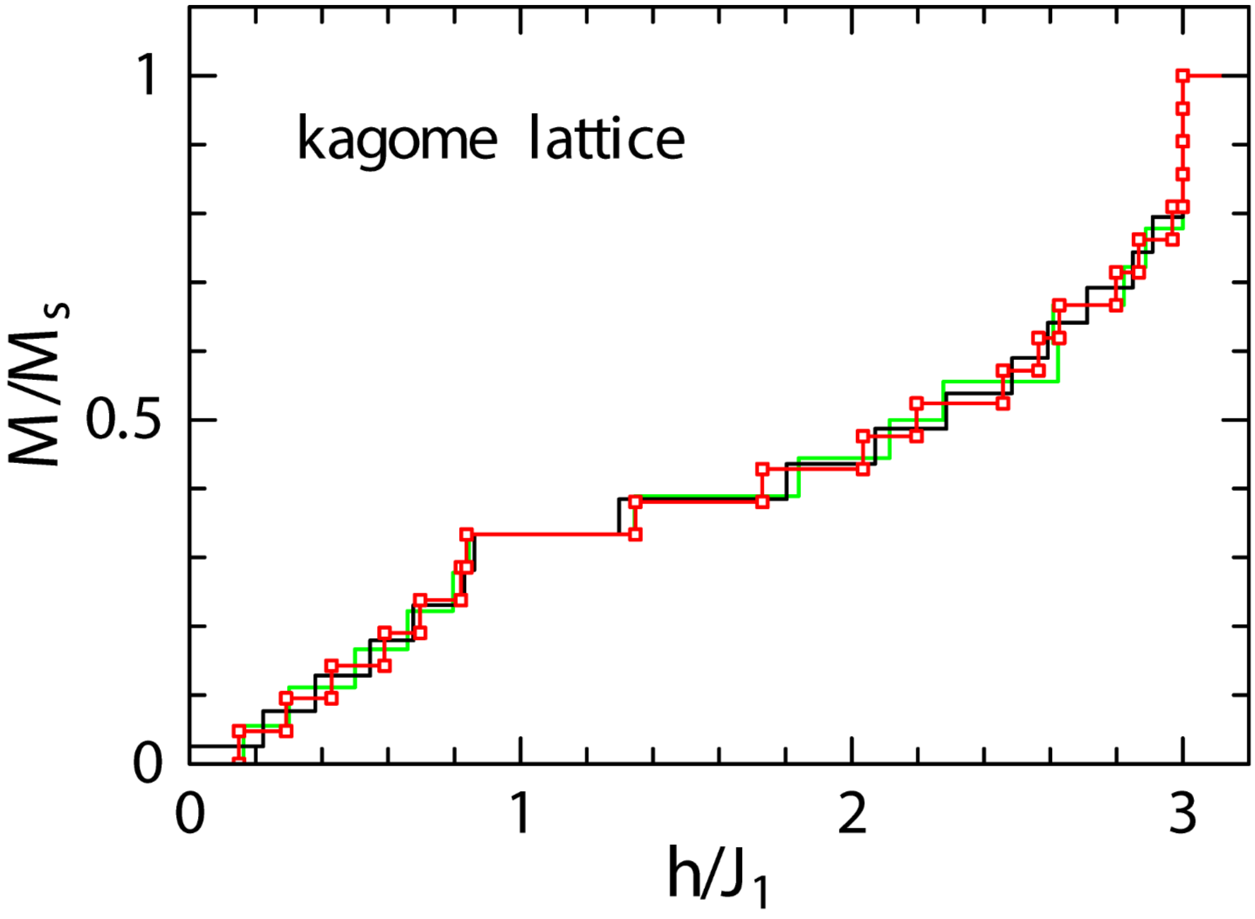




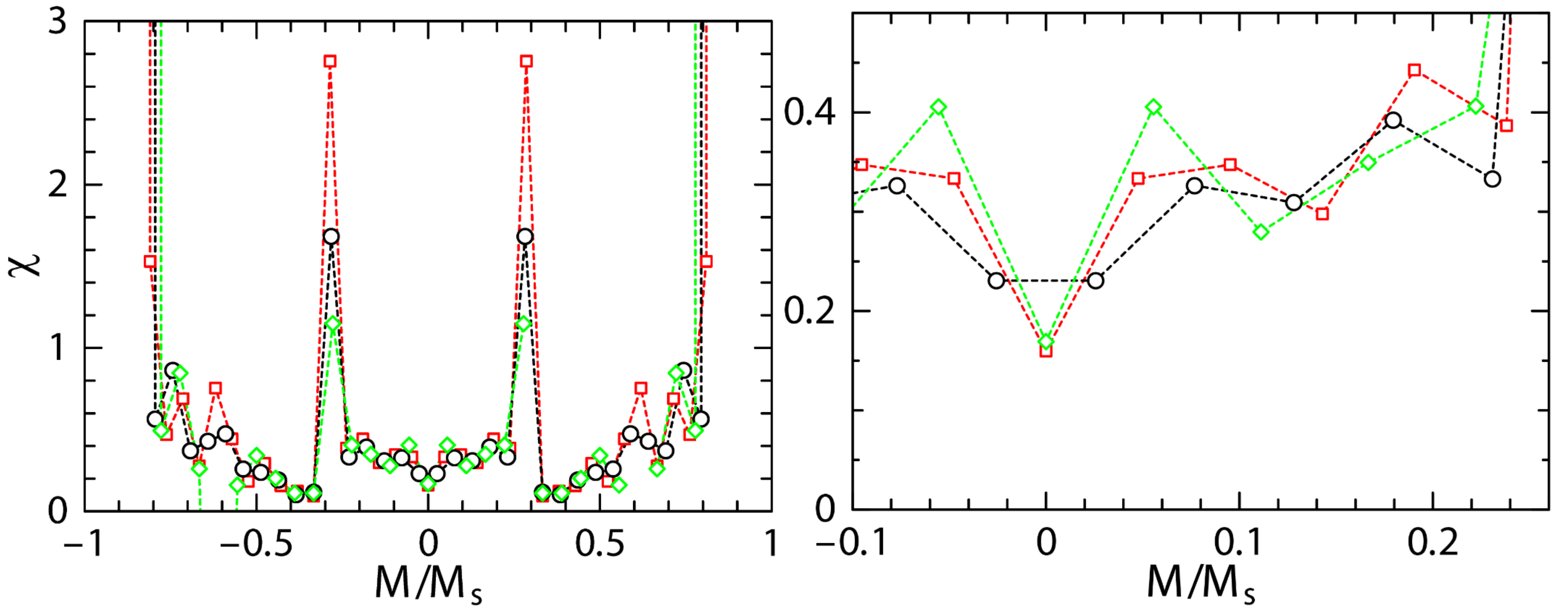
Gapless

Gapped

Kagome-lattice Heisenberg AF



Kagome lattice AF
Differential susceptibility vs. M

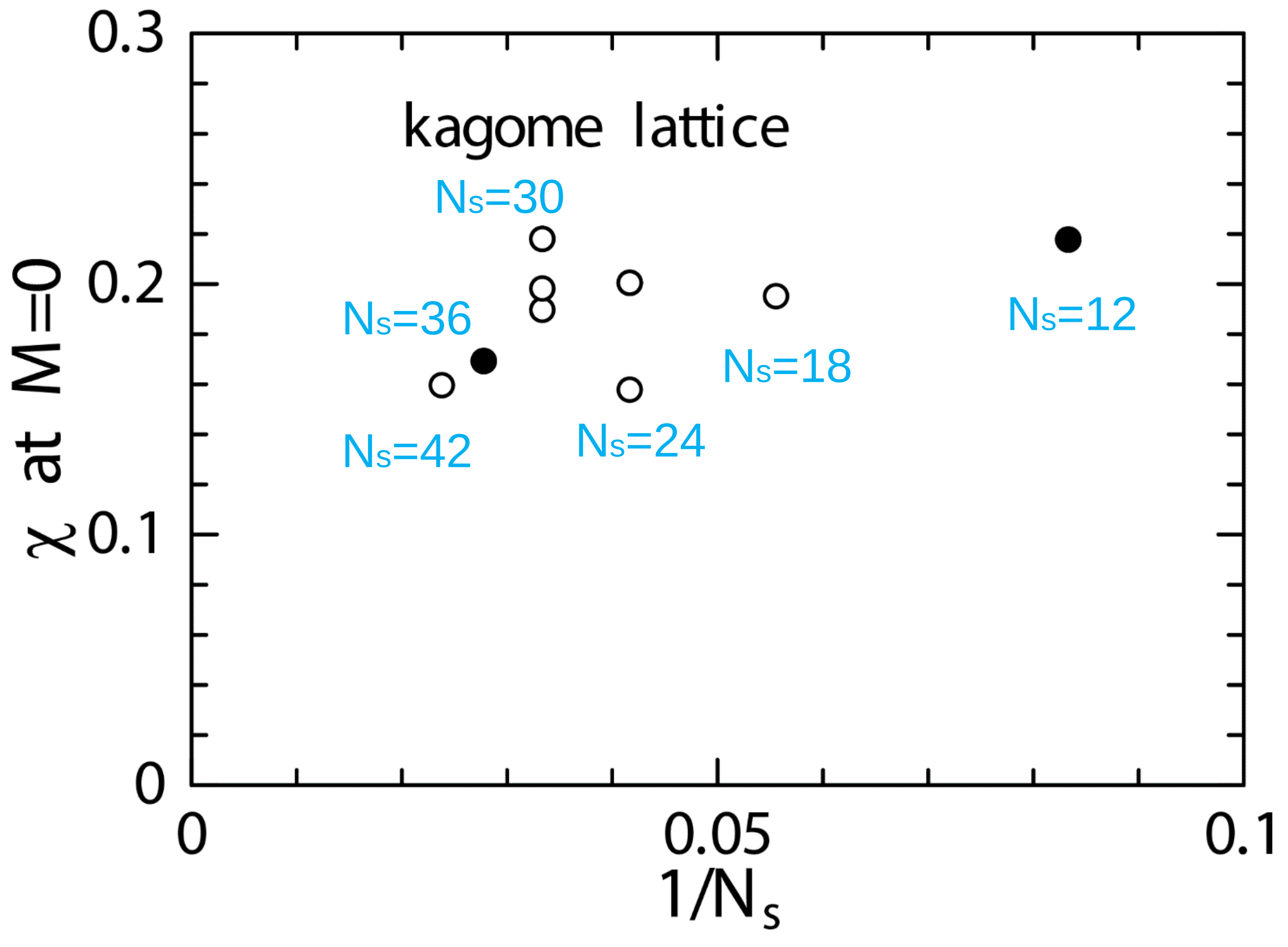


Ns=39

Ns=36

Ns=42

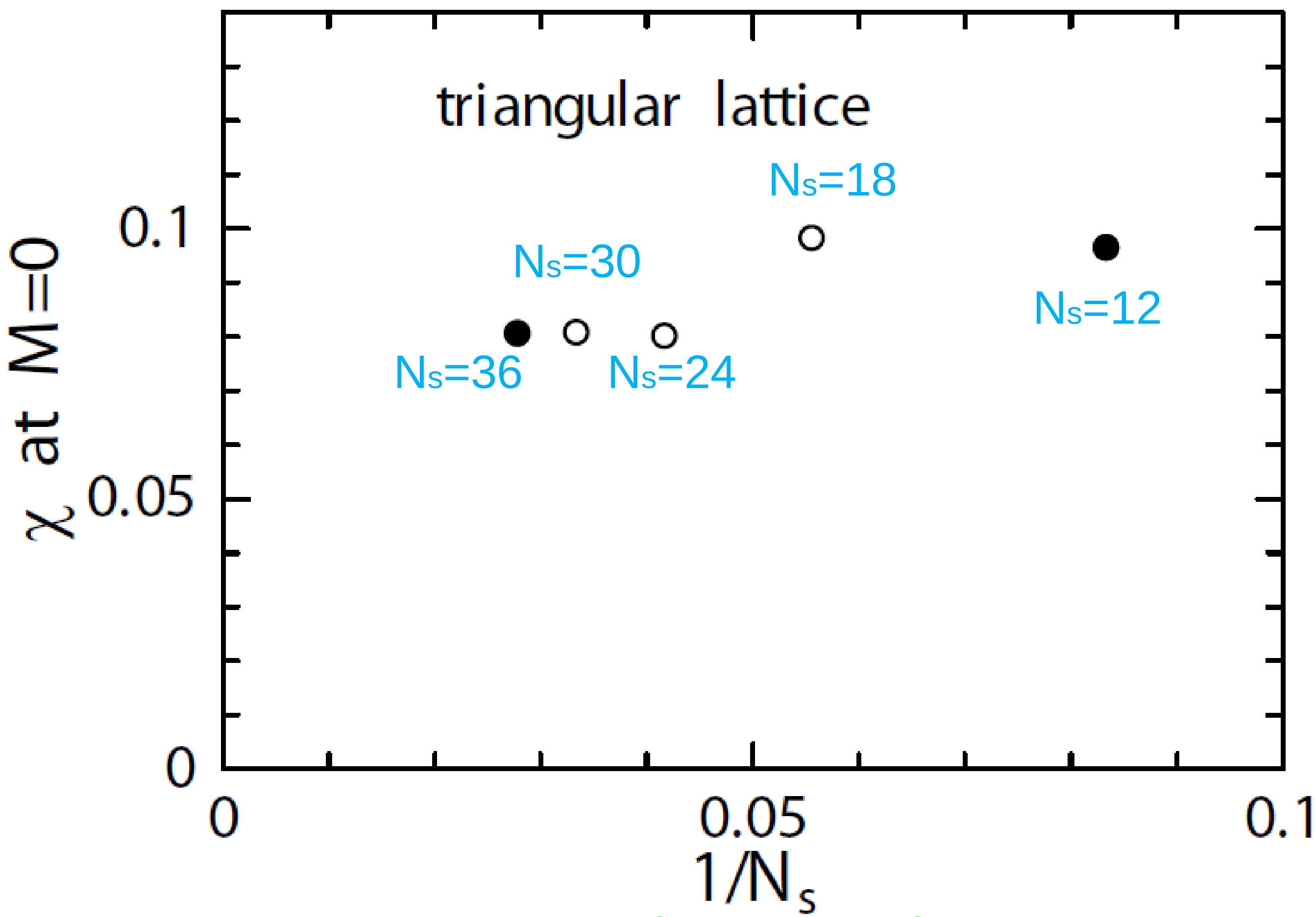
Size dependence of χ at M=0



$\chi \rightarrow$ finite ($N_s \rightarrow \infty$) $\Rightarrow$ Gapless

Triangular lattice AF

Size dependence of χ



Consistent with gapless feature of triangular lattice AF

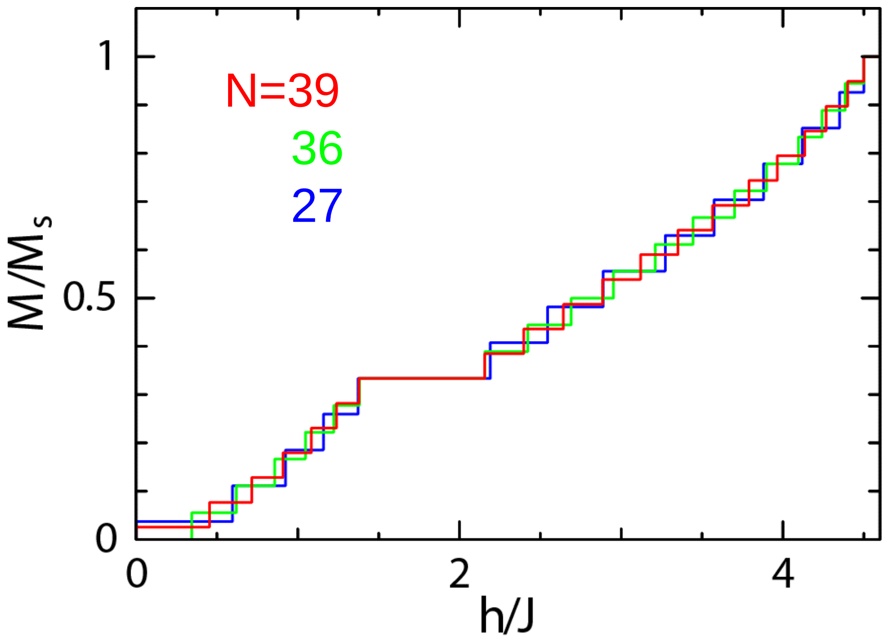
Conclusion

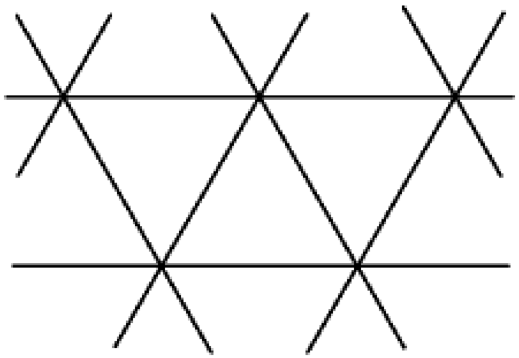
- "Susceptibility analysis" confirmed that <u>S=1/2 kagome-lattice AF is gapless</u>, as well as S=1/2 triangular-lattice AF.
- In order to confirm it, we should do the numerical diagonalization of larger-size clusters than 42 spins.

K-Computer

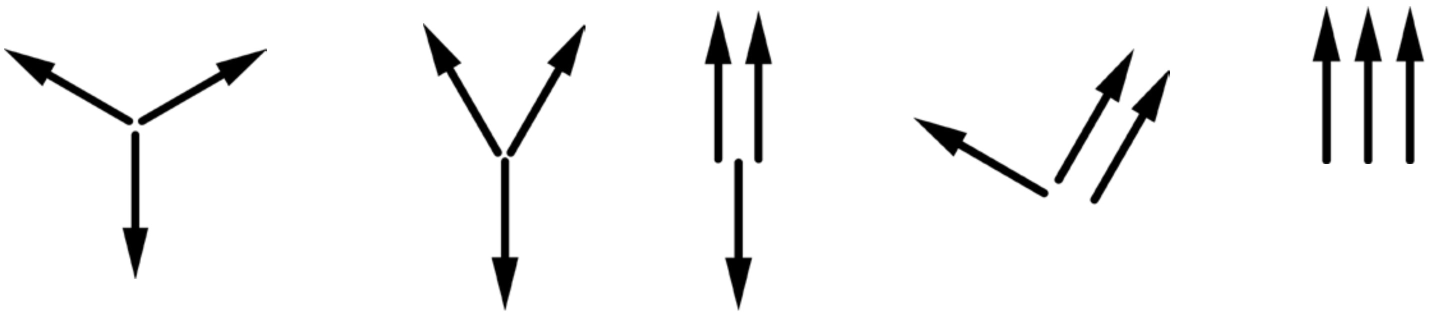
1/3 magnetization plateau of triangular lattice AF

S=1/2 Heisenberg AF

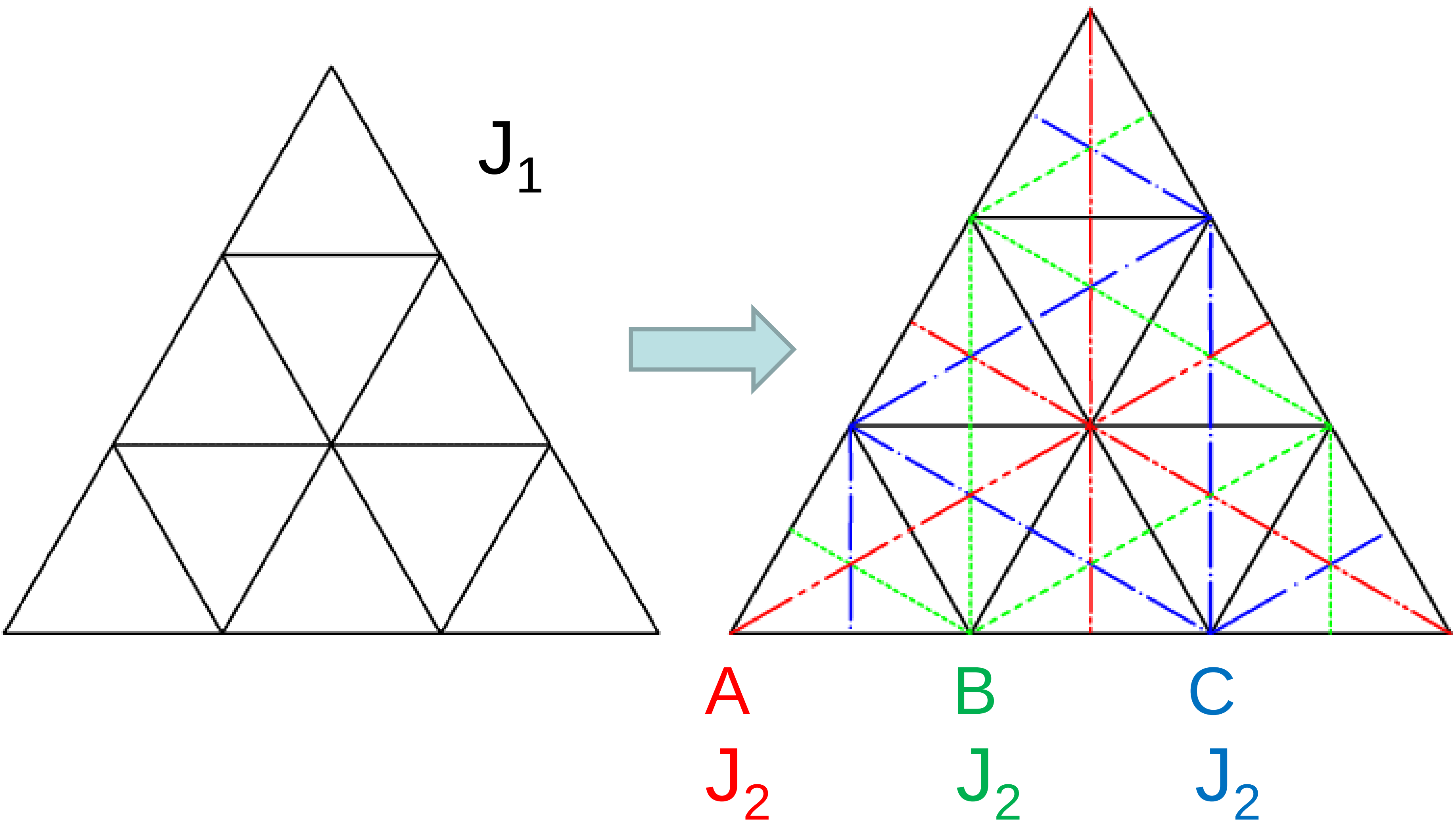




Order from disorder



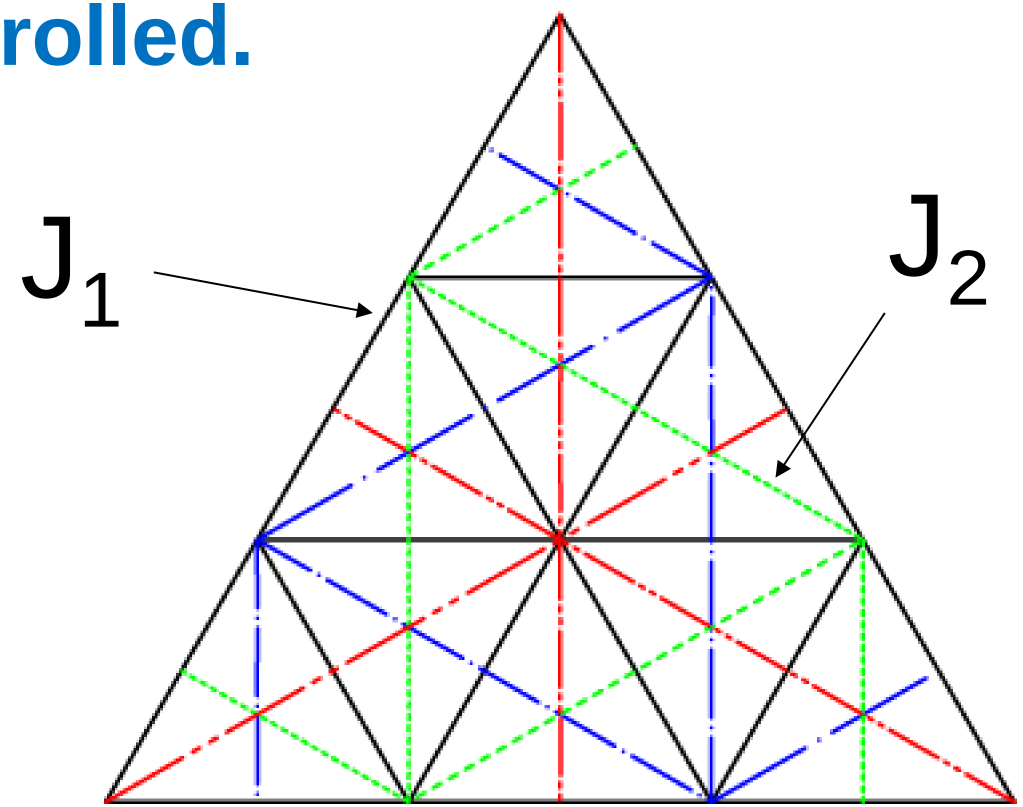
Next-nearest-neighbor interactions



Purpose of this study

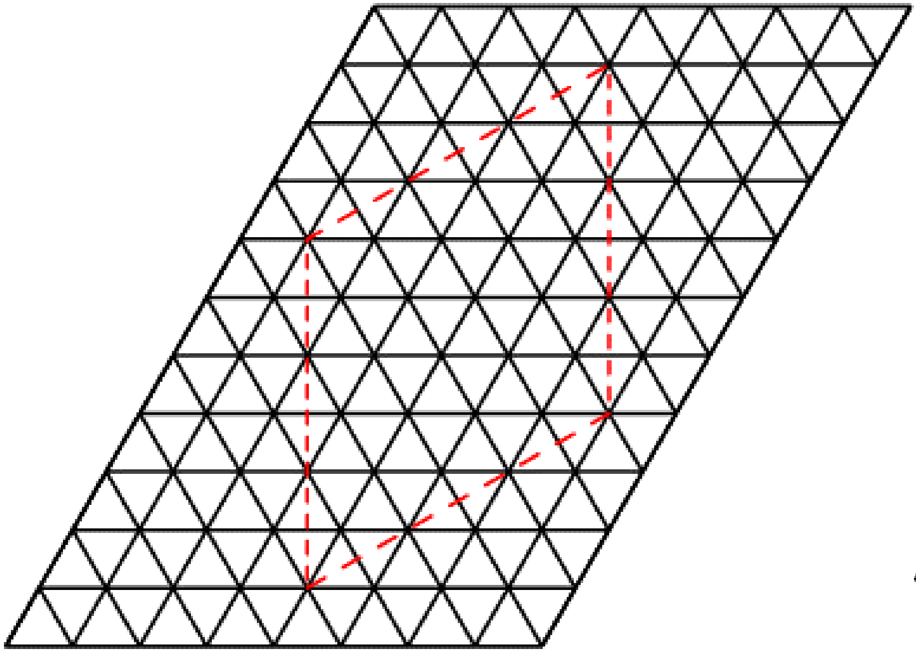
is to study how the m=1/3 state behaves when the next-nearest-neighbor interaction is controlled.

$r = J_2/J_1$

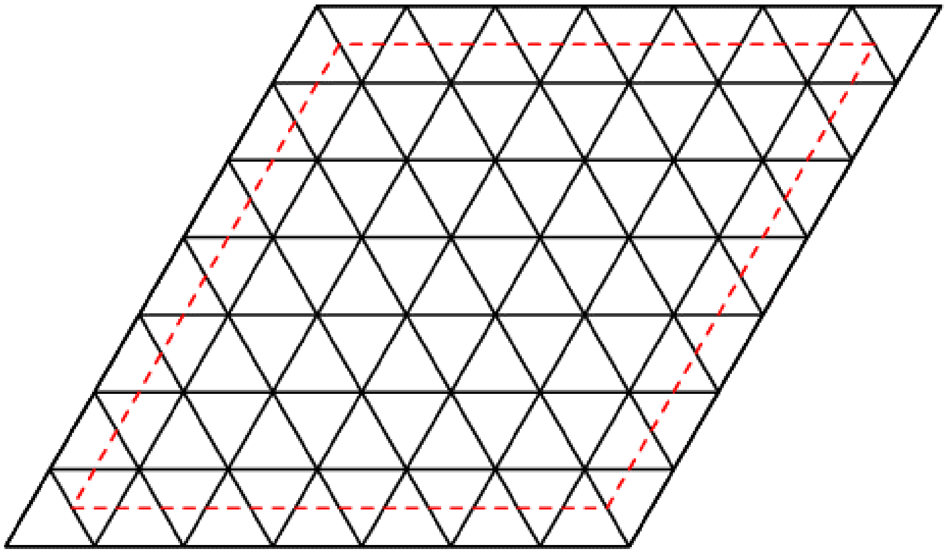


Possible finite-size clusters

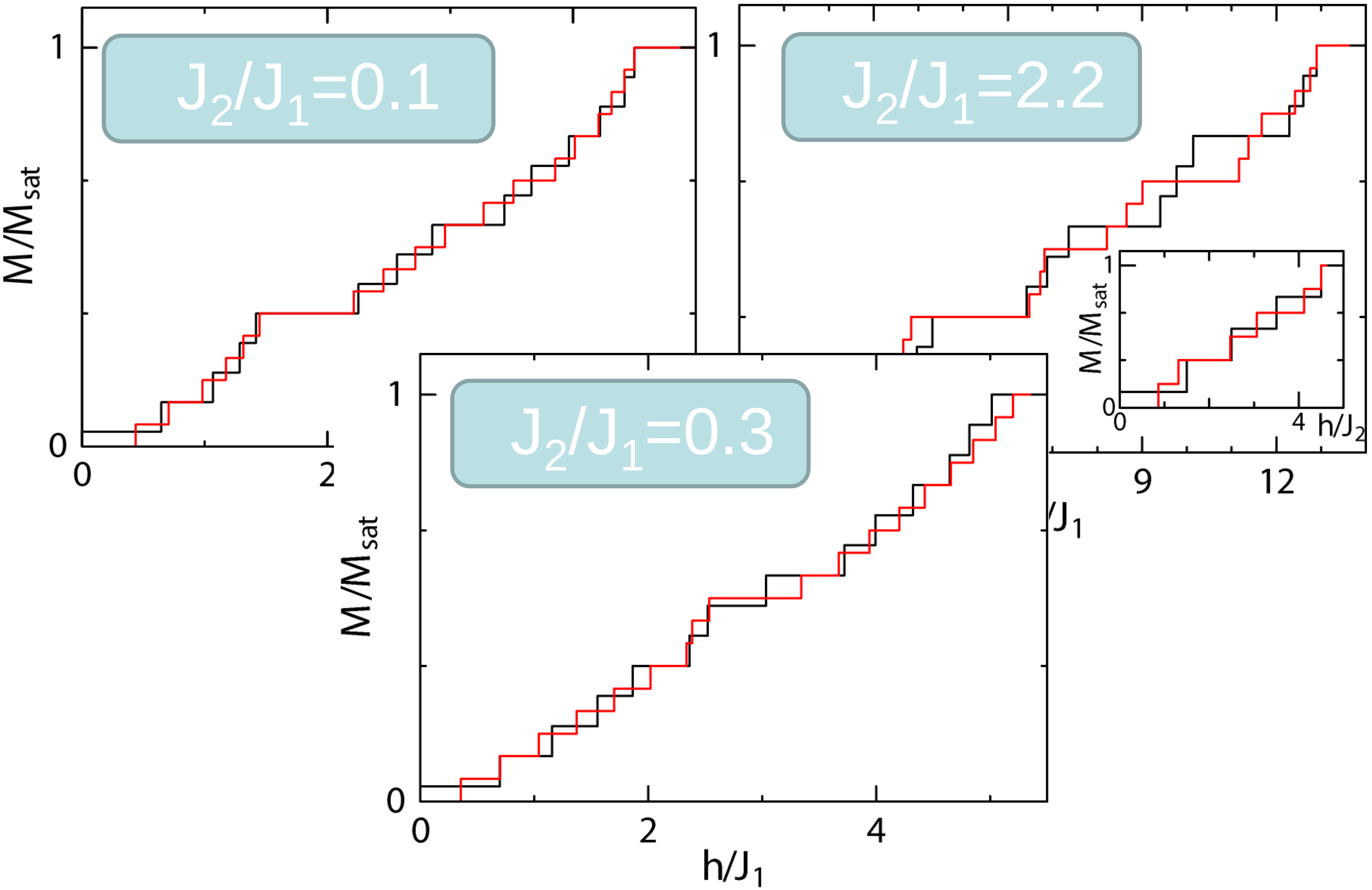
N=27(=3*9)



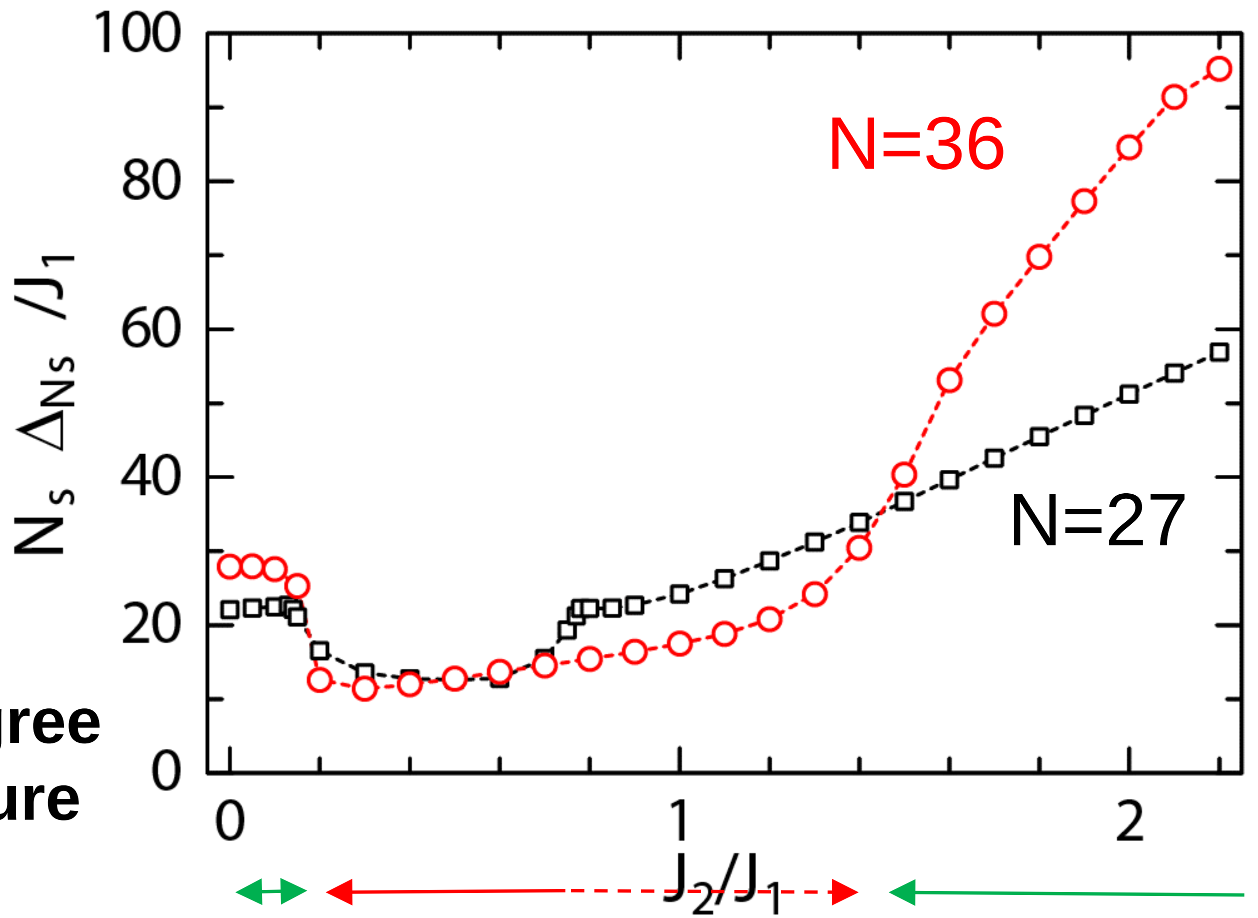
N=36(=3*12)



Magnetization curves



Analysis of plateau width



120-degree structure

120-degree structure
+
120-degree structure
+
120-degree structure

gapped **gapless** **gapped**

Summary

S=1/2 Heisenberg antiferromagnet
on the triangular lattice
with next-nearest-neighbor interactions

Numerical-diagonalization method

The m=1/3 plateau disappears
between weak-J_2 and strong-J_2 regions.

H. Nakano and TS, J. Phys. Soc. Jpn. 86 (2017) 114705 (arXiv: 1708.07248)