

# Novel Field Induced Quantum Phase Transition of the Kagome Lattice Antiferromagnet

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**Abstract.** The  $S = 1/2$  kagome lattice antiferromagnet is investigated by the numerical diagonalization. We successfully obtained the ground-state full magnetization curve for the 42-spin cluster. Based on the finite-size scaling analysis including this new result, we consider the quantum critical magnetization behavior around the  $1/3$  of the saturation magnetization. As a result, some unconventional features of the  $1/3$  magnetization ramp, which was proposed by our previous work, are clarified.

## 1. Introduction

The  $S = 1/2$  Kagome-lattice antiferromagnet[1] is one of the most popular frustrated quantum spin systems. The previous theoretical studies indicated that the system is disordered in the ground state [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13]. In contrast to the triangular lattice antiferromagnet which has the  $120^\circ$  long-range order[14, 15, 16]. Experimental studies to observe a novel spin liquid phase in the Kagome-lattice antiferromagnet have been accelerated since discoveries of several realistic materials; the herbertsmithite[17, 18], the volborthite[19, 20] and the vesignieite[21, 22]. Since the quantum Monte Carlo simulation is useless for the system, the numerical exact diagonalization is one of the best numerical method for it, as well as the density matrix renormalization group (DMRG) calculation. The numerical diagonalization studies suggested a magnetization plateau-like behavior at  $1/3$  of the saturation magnetization [23, 24, 25, 26, 27], although the classical spin systems have no plateau in the ground state[28]. In our recent numerical diagonalization study on the  $S = 1/2$  Kagome-lattice antiferromagnet up to  $N = 36$ , the calculated field derivatives revealed an anomalous behavior at  $1/3$  of the saturation magnetization[29]. Namely, the field derivative is divergent at the low-field side of the critical field  $H_c$ , while almost zero at the high-field side. This critical behavior is quite different from conventional magnetization plateaux in two-dimensional systems where the field derivative is finite at both sides of  $H_c$ . To distinguish such an anomalous property at the  $1/3$  magnetization of the Kagome-lattice from conventional plateaux, we called it a “magnetization ramp”. Our recent finite-size scaling analyses up to  $N=39$  revealed some characteristic features of the magnetization ramp quantitatively[30, 31]. In these works the critical exponent defined by

$$|m - \frac{1}{3}| \sim |H - H_c|^{\frac{1}{\delta}}, \quad (1)$$



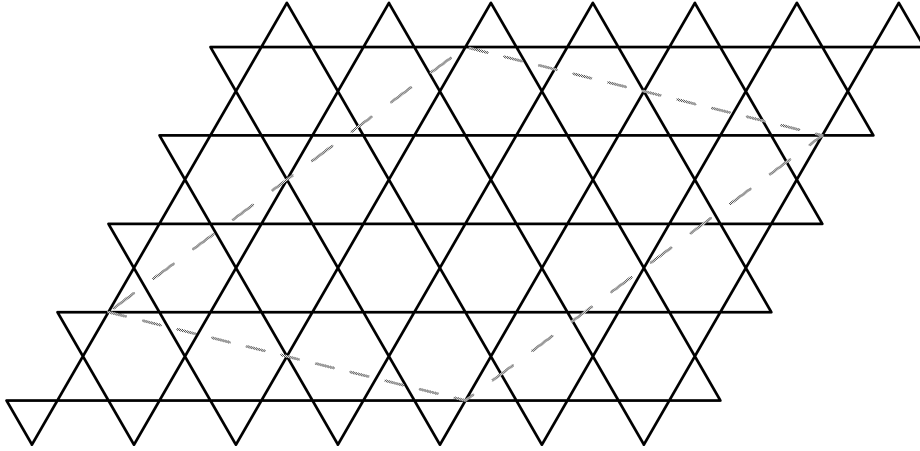


**Figure 1.** Shape of the kagome-lattice cluster for  $N=42$  under the periodic boundary condition.

was revealed to be larger than one at the lower-field side, while smaller than one at the higher-field side. Namely, the divergent(zero) field derivative at the lower(higher)-field side was confirmed. However, whether a finite plateau width (flat region) appears or not at the  $1/3$  magnetization was not conclusive, within the finite-size scaling analysis up to  $N=39$ , because finite-size effects are still quite large.

In the present study, in order to clarify whether a finite plateau exists or not at the  $1/3$  magnetization of the  $S=1/2$  kagome-lattice antiferromagnet, we extended the same finite-size scaling analysis up to the larger system size  $N = 42$ , using the numerical diagonalization at K Computer Center in Kobe, Japan. The result based on the analysis up to  $N = 42$  is reported. The magnetization curve for  $N = 42$ , which is the largest system size in present in the world obtained by the numerical diagonalization, is also presented.

## 2. Model

The magnetization processes of the  $S = 1/2$  Kagome- and triangular-lattice antiferromagnets are described by the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_Z, \quad \mathcal{H}_0 = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad \mathcal{H}_Z = -H \sum_j^N S_j^z, \quad (2)$$

where  $\langle i, j \rangle$  means all the nearest neighbor pairs on each lattice. Throughout we use the unit such that  $g\mu_B = 1$ . For  $N$ -site systems, the lowest energy of  $\mathcal{H}_0$  in the subspace where  $\sum_j S_j^z = M$  is denoted as  $E(N, M)$ . The macroscopic magnetization  $m$  is defined by  $m \equiv M/M_s = 2M/N$ , where  $M_s = N/2$  is the saturation magnetization. In our previous work[30] we restrict us to the rhombic cluster under the periodic boundary condition to investigate the  $1/3$  magnetization. The used system sizes are  $N=9, 12, 21, 27, 36$  and  $39$ . Using the numerical exact diagonalization, we can calculate all the values of  $E(N, M)$  for these clusters.

In the present work, we treat the larger system size,  $N = 42$ , although it is not rhombic. The shape of the 42-spin cluster used here is shown in Fig. 1.

## 3. Results

Using the numerical diagonalization based on the Lanczos method, we successfully obtained the full ground-state magnetization curve for  $N = 42$ , which is shown in Fig. 2. At least as the

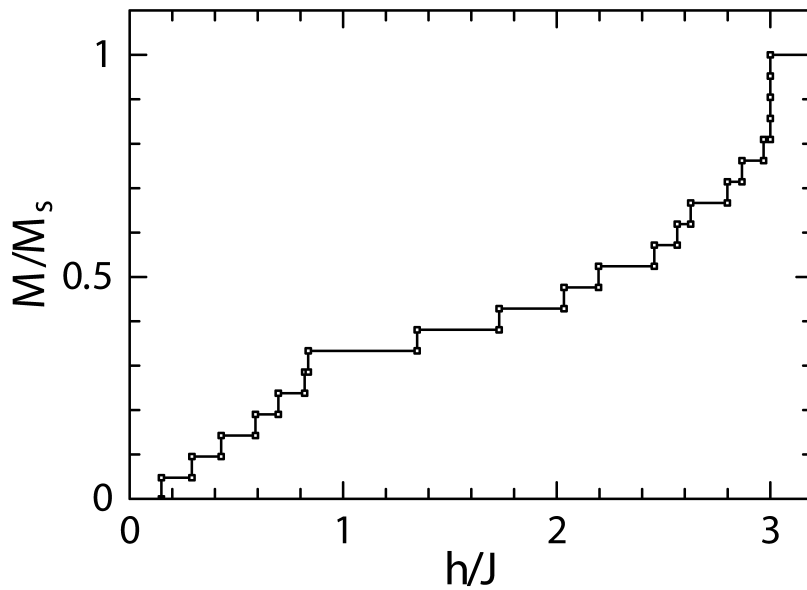


**Figure 2.** Ground-state magnetization curve of the  $S=1/2$  kagome-lattice antiferromagnet calculated by the numerical diagonalization for the 42-spin cluster.

magnetization curve of the  $S=1/2$  kagome-lattice antiferromagnet obtained by the numerical diagonalization, this system size is the present world record.

The field derivative  $\chi$  estimated by the form

$$\chi^{-1} = \frac{E(N, M+1) - 2E(N, M) - E(N, M-1)}{1/M_{\text{sat}}}, \quad (3)$$

is more useful to clarify characters of the magnetization ramp, than the simple magnetization curve. The magnetization dependence of  $\chi$  for  $N=27, 36, 39$  and  $42$  is shown in Fig. 3. The present result for  $N=42$  qualitatively confirms the properties of the magnetization ramp;  $\chi \rightarrow \infty$  at lower-field side, while  $\chi = 0$  at higher-field side in the thermodynamic limit.

Finally, using the present result for  $N=42$ , we try to clarify whether the  $1/3$  magnetization plateau exists or not. The plateau widths  $H_{c+} - H_{c-}$  of the finite size systems for  $N=9, 12, 15, 18, 21, 24, 27, 30, 36, 39$  and  $42$  are plotted versus  $1/N^{1/2}$  in Fig. 4. If we use all the points to extrapolate them to the thermodynamic limit, the result is  $H_{c+} - H_{c-} = -0.3 \pm 0.4$ . It can still suggest the absence of the plateau. However, the plot in Fig. 4 obviously indicates a drastic change between  $N=18$  and  $N=21$ . If we neglect smaller-size data than the change, the extrapolation leads to the result  $H_{c+} - H_{c-} = 0.5 \pm 0.3$ . It possibly suggests a finite plateau, which is consistent with the recent numerical diagonalization[36] and density matrix renormalization group (DMRG)[37] studies. Even in such a case, the divergent  $\chi$  before the plateau and the zero  $\chi$  after the plateau are still unconventional and interesting phenomena.

#### 4. Summary

The magnetization process of the  $S=1/2$  kagome-lattice antiferromagnet is investigated using the numerical diagonalization up to  $N=42$ . The present results support the characters of the  $1/3$  magnetization ramp;  $\chi \rightarrow \infty$  at the lower field side and  $\chi = 0$  at the higher field side of it. On the other hand, it would be difficult to exclude the existence of the  $1/3$  plateau with the present result up to  $N=42$ .

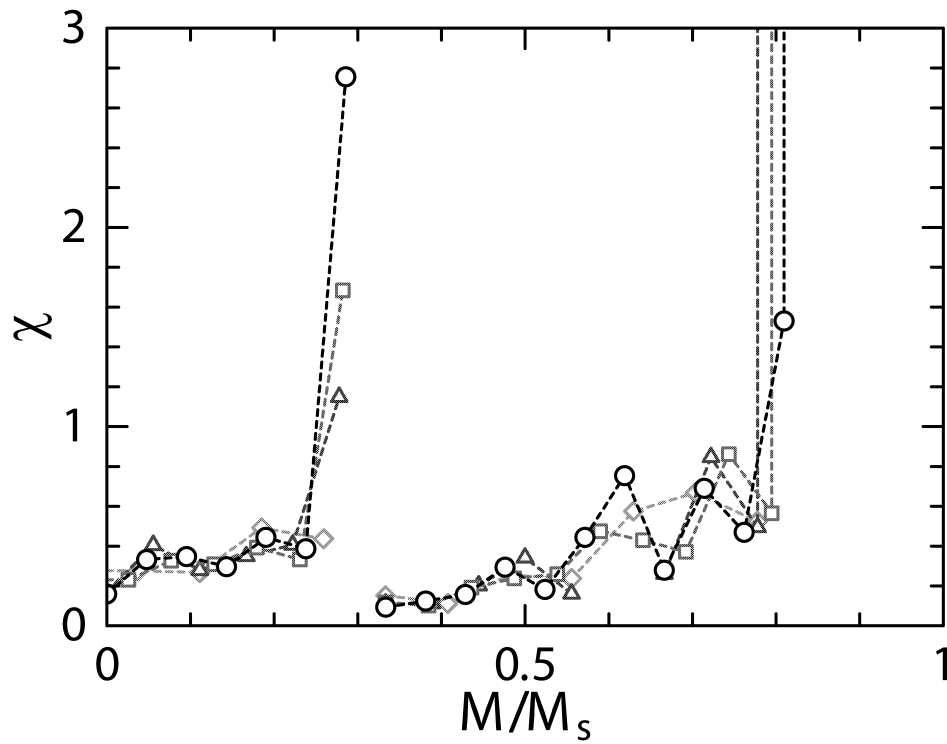


**Figure 3.** Magnetization dependence of the field derivative  $\chi = dM/dH$  calculated by the numerical diagonalization for  $N=27$ (diamonds),  $36$ (triangles),  $39$ (squares) and  $42$ (circles).

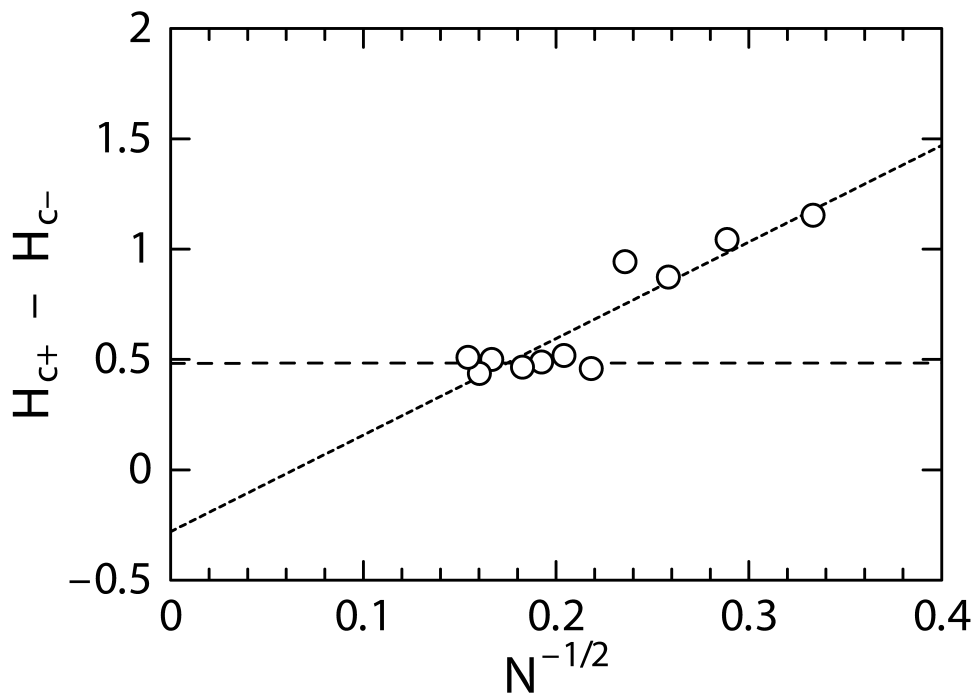


**Figure 4.** Magnetization plateau width  $H_{c+} - H_{c-}$  plotted versus  $1/N^{1/2}$ .

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#### References

- [1] A brief history of the study on the Kagome-lattice magnetism was given in M. Mekata, Phys. Today Feb., 12 (2003).
- [2] P. Lecheminant, B. Bernu, C. Lhuillier, L. Pierre, and P. Sindzingre, Phys. Rev. B **56**, 2521 (1997).
- [3] Ch. Waldtmann, H.-U. Everts, B. Bernu, C. Lhuillier, P. Sindzingre, P. Lecheminant and L. Pierre, Eur. Phys. J. B **2**, 501 (1998).
- [4] F. Mila, Phys. Rev. Lett. **81**, 2356 (1998).
- [5] Y. Ran, M. Hermele, P. A. Lee and X. -G. Wen, Phys. Rev. Lett. **98**, 117205 (2007).
- [6] H. C. Jiang, Z. Y. Weng and D. N. Sheng, Phys. Rev. Lett. **98**, 117203 (2008).
- [7] P. Sindzingre and C. Lhuillier, Europhys. Lett. **88**, 27009 (2009).
- [8] O. Cepas, C. M. Fong, P. W. Leung, and C. Lhuillier, Phys. Rev. B **78**, 140405(R) (2008).
- [9] G. Evenbly and G. Vidal, Phys. Rev. Lett. **104**, 187203 (2010).
- [10] A. M. Läuchli, J. Sudan and E. S. Sorensen, Phys. Rev. B **83**, 21241 (2011).
- [11] Y. Iqbal, F. Becca and D. Poilblanc, Phys. Rev. B **83**, 100404 (2011); *ibid* **84**, 020407 (2011).
- [12] S. Yan, D. A. Huse and S. R. White, Science **332**, 1173 (2011).
- [13] H. Nakano and T. Sakai: J. Phys. Soc. Jpn. **80**, 053704 (2011).
- [14] D. A. Huse and V. Elser, Phys. Rev. Lett. **60**, 2531 (1988).
- [15] B. Bernu, P. Lecheminant, C. Lhuillier and L. Pierre, Phys. Rev. B **50**, 10048 (1994).
- [16] L. Capriotti, A. E. Trumper and S. Sorella, Phys. Rev. Lett. **82**, 3899 (1999).
- [17] M. P. Shores, E. A. Nytko, B. M. Barlett, and D. G. Nocera, J. Am. Chem. Soc. **127**, 13462 (2005).
- [18] P. Mendels and F. Bert, J. Phys. Soc. Jpn. **79**, 011001 (2010).
- [19] H. Yoshida, Y. Okamoto, T. Tayama, T. Sakakibara, M. Tokunaga, A. Matsuo, Y. Narumi, K. Kindo, M. Yoshida, M. Takigawa, and Z. Hiroi, J. Phys. Soc. Jpn. **78**, 043704 (2009).
- [20] M. Yoshida, M. Takigawa, H. Yoshida, Y. Okamoto, and Z. Hiroi, Phys. Phys. Lett. **103**, 077207 (2009).
- [21] Y. Okamoto, H. Yoshida, and Z. Hiroi, J. Phys. Soc. Jpn. **78**, 033701 (2009).
- [22] Y. Okamoto, M. Tokunaga, H. Yoshida, A. Matsuo, K. Kindo and Z. Hiroi, Phys. Rev. B **83**, 180407 (2011).
- [23] K. Hida, J. Phys. Soc. Jpn. **70**, 3673 (2001).
- [24] D. C. Cabra, M. D. Grynberg, P. C. W. Holdsworth, and P. Pujol, Phys. Rev. B **65**, 094418 (2002).
- [25] J. Schulenberg, A. Honecker, J. Schnack, J. Richter, and H.-J. Schmidt, Phys. Rev. Lett. **88**, 016207 (2002).
- [26] A. Honecker, J. Schulenberg, and J. Richter, J. Phys.: Condens. Matter **16**, S749 (2004).
- [27] D. C. Cabra, M. D. Grynberg, P. C. W. Holsworth, A. Honecker, P. Pujol, J. Schmalfus and J. Schulenburg, Phys. Rev. B **71**, 144420 (2005).
- [28] M. E. Zhitomirsky, Phys. Rev. Lett. **88**, 057204 (2002).
- [29] H. Nakano and T. Sakai, J. Phys. Soc. Jpn. **79**, 053707 (2010).
- [30] T. Sakai and H. Nakano, Phys. Rev. B **83**, 100405(R) (2011).
- [31] H. Nakano, T. Shimokawa and T. Sakai, J. Phys. Soc. Jpn. **80**, 033709 (2011).
- [32] I. Affleck, Phys. Rev. B **43**, 3215 (1991).
- [33] T. Sakai and M. Takahashi, Phys. Rev. B **43**, 13383 (1991); J. Phys. Soc. Jpn. **60**, 3615 (1991).
- [34] N. Katoh and M. Imada, J. Phys. Soc. Jpn. **63**, 4529 (1994).

- [35] T. Sakai and M. Takahashi, Phys. Rev. B **57**, R8091 (1998).
- [36] S. Capponi et al., Phys. Rev. B **88**, 144416 (2013).
- [37] S. Nishimoto et al., Nature Comm. **4**, 2287 (2013).