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

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Abstract.

The magnetization process of the $S = 1/2$ kagome-lattice quantum antiferromagnet is investigated using the numerical exact diagonalization up to 39-site clusters. The finite-size scaling analysis with the rohmbic clusters indicated the “magnetization ramp” as a novel field-induced quantum phase transition at 1/3 of the saturation magnetization. The magnetization ramp is characterized by the following properties; (i) the field derivative $dm/dH$ is divergent at the lower-field side, (ii) $dm/dH$ is vanishing at the higher-field side, and (iii) there is a single critical field $H_c$ (no plateau). Applying the critical exponent analysis for the non-rohmbic clusters, as well as the rohmbic ones, we confirmed the above properties of the magnetization at 1/3 of the saturation for the kagome lattice antiferromagnet.

The $S = 1/2$ Kagome\textsuperscript{[1]} lattice antiferromagnets is one of the most popular frustrated quantum spin systems. The previous theoretical studies indicated that the system is disordered in the ground state \textsuperscript{[2, 3, 4, 5, 6, 7]}. 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\textsuperscript{[8, 9]}, the volborthite\textsuperscript{[10, 11]} and the vesignieite\textsuperscript{[12]}. Since the quantum Monte Carlo simulation and the DMRG calculation are useless for the system, the numerical exact diagonalization is one of the best numerical method for it. The numerical diagonalization studies suggested a magnetization plateau-like behavior at 1/3 of the saturation magnetization \textsuperscript{[13, 14, 15, 16, 17]}, although the classical spin systems have no plateau in the ground state\textsuperscript{[18]}. 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\textsuperscript{[19]}. 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 restricting us to rohmbic clusters revealed some characteristic features of the magnetization ramp quantitatively\textsuperscript{[20]}. However, these features are possibly some artificial ones due to some specified symmetries of small-size clusters. Thus more general clusters should be included to the size scaling analyses.

In this paper, applying the same finite-size scaling analyses for some non-rohmbic clusters as well as rohmbic ones, the properties of the magnetization ramp are confirmed more definitely.
The magnetization processes of the $S = 1/2$ kagome lattice antiferromagnet is described by the Hamiltonian

$$
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_Z, \quad \mathcal{H}_0 = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad \mathcal{H}_Z = -H \sum_j S_j^z, \quad (1)
$$

where $(i, j)$ means all the nearest neighbor pairs. 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 $\sum_j S_j^z = M$ (the macroscopic magnetization is $m = M/N$) is denoted as $E(N, M)$. In our previous work[20] we restrict us to the rhombic cluster under the periodic boundary condition. The available system sizes of rhombic clusters are $N =$9, 12, 21, 27, 36 and 39. In order to treat more general clusters, we also calculated for $N = 15, 18, 24, 30, 33$ this time. Using the numerical exact diagonalization, we can calculate all the values of $E(N, M)$ for $N = 9, 12, 15, \cdots, 33, 36$ and 39.

In order to characterize the unconventional magnetization behavior at $m = 1/3$ of the Kagome lattice antiferromagnet in a quantitative way, we introduce the critical exponent $\delta$. It is defined by the form

$$
|m - m_c| \sim |H - H_c|^{1/\delta}, \quad (2)
$$

is an important index to specify the universality class of the field induced quantum phase transition. The previous theoretical works indicated $\delta = 2$ for some typical one-dimensional gapped systems[21, 22], while $\delta = 1$ for two-dimensional systems[23]. In order to clarify the anomalous critical behavior at $m = 1/3$ of the Kagome lattice antiferromagnet, we estimate $\delta$ by the finite-size scaling developed by the previous work[24], and compare it with the triangular lattice antiferromagnet. Although the method was proposed for one-dimensional systems, it can be easily generalized for two dimensions. We assume the asymptotic form of the size dependence of the energy as

$$
\frac{1}{N} E(N, M) \sim \epsilon(m) + C(m) \frac{1}{N^\theta} \quad (N \to \infty), \quad (3)
$$

where $\epsilon(m)$ is the bulk energy and the second term describes the leading size correction. We also assume that $C(m)$ is an analytic function of $m$. The lowest and highest magnetic field corresponding to $m = 1/3$ in the thermodynamic limit are defined as $H_{c1}$ and $H_{c2}$, respectively, as the form

$$
E(N, \frac{N}{3}) - E(N, \frac{N}{3} - 1) \to H_{c1} \quad (N \to \infty), \quad (4)
$$

$$
E(N, \frac{N}{3} + 1) - E(N, \frac{N}{3}) \to H_{c2} \quad (N \to \infty). \quad (5)
$$

In order to consider the critical magnetization behaviors for $m < 1/3$ and $m > 1/3$ independently, we define the critical exponents $\delta_1$ and $\delta_2$ by the forms

$$
\frac{1}{3} - m \sim (H - H_{c2})^{1/\delta_2}, \quad (6)
$$

$$
\frac{1}{3} - m \sim (H_{c1} - H)^{1/\delta_1}. \quad (7)
$$

If we define the quantities $f_2(N)$ and $f_1(N)$ by the forms

$$
f_1(N) = [E(N, \frac{N}{3} - 2) + E(N, \frac{N}{3}) - 2E(N, \frac{N}{3} - 1)], \quad (8)
$$

$$
f_2(N) = [E(N, \frac{N}{3} + 2) + E(N, \frac{N}{3}) - 2E(N, \frac{N}{3} + 1)], \quad (9)
$$
the asymptotic forms of them are expected to be

\[ f_1(N) \sim \frac{1}{N^{\delta_1}} + O\left( \frac{1}{N^{\theta+1}} \right) \quad (N \to \infty), \]

\[ f_2(N) \sim \frac{1}{N^{\delta_2}} + O\left( \frac{1}{N^{\theta+1}} \right) \quad (N \to \infty), \]

as far as we assume the form (4). Thus the exponents \( \delta_1 \) and \( \delta_2 \) can be estimated from the slope of the log \( f_1 \)-log \( N \) and log \( f_2 \)-log \( N \) plots, respectively, under the condition \( \theta > \delta_1 - 1 \) and \( \theta > \delta_2 - 1 \). The plots of log \( f_1 \) and log \( f_2 \) versus log \( N \) for the triangular and Kagome lattice antiferromagnets are shown in Figures. 1 (a) and (b), respectively. Applying the standard least square fitting of lines to the points for \( N = 9, 12, \cdots, 36, 39 \), we estimate the exponents as \( \delta_1 = 2.56 \pm 1.19 \) and \( \delta_2 = 0.55 \pm 0.30 \). Our previous estimations by the same method applied for only rhombic clusters indicated \( \delta_1 = 1.92 \pm 0.99 \) and \( \delta_2 = 0.56 \pm 0.15 \). \( \delta_2 \) well coincides between the two analyses. The new estimation of \( \delta_1 \) confirms \( \delta_1 > 1 \) more definitely than the previous one. In any case, the new results strongly justify the two important features of the magnetization ramp; (i) the field derivative \( dm/dH \) is divergent at the lower-field side, and (ii) \( dm/dH \) is vanishing at the higher-field side.

We consider whether a flat part of the magnetization curve at \( m = 1/3 \) exists or not for the triangular and Kagome lattice antiferromagnets. Namely, we examine whether each system has no plateau \( (H_{c1} = H_{c2}) \) or a finite plateau \( (H_{c1} \neq H_{c2}) \) at \( m = 1/3 \) in the thermodynamic limit. We evaluate the length of the flat part \( H_{c2} - H_{c1} \) corresponding to the plateau width of the finite-size clusters with \( N = 9, 12, \cdots, 36 \) and 39. If the system has a gapless excitation like a spin wave from some ordered states, the low-lying energy spectrum is expected to be proportional to the wave vector \( k \) in the long wave length limit. Thus the excitation energy gap of the finite-size systems should have the asymptotic form \( \sim 1/N^{1/2} \) in two-dimensional gapless systems. On the other hand, in gapped systems the gap is expected to converge to the thermodynamic limit with exponentially decaying (faster than \( 1/N^{1/2} \)) finite-size correction, as the system size increases. Thus if the extrapolation by fitting the gap versus \( 1/N^{1/2} \) leads to a finite gap in the thermodynamic limit, it would be a strong evidence to confirm the gapped ground state. The length of a flat part \( W \equiv H_{c2} - H_{c1} \) is plotted versus \( 1/N^{1/2} \) in Figure 2. The least square fitting to a line leads to the following results: \( W = -0.34 \pm 0.42 \). The previous analysis for the rhombic clusters indicated \( W = -0.32 \pm 0.35 \). Thus both results are consistent with each other and suggest no plateau \( (W = 0) \) within the errors.

In summary, we have investigated critical magnetization behaviors at \( m = 1/3 \) for the \( S = 1/2 \) Kagome lattice quantum antiferromagnet, using the numerical exact diagonalization of general clusters up to \( N = 39 \). The system is revealed to exhibit unconventional critical properties;
$\delta_- < 1 < \delta_+$, namely the field derivative $\chi$ is diverging at the lower field side, while zero at the higher one of a single critical field $H_c = H_{c1} = H_{c2}$. The conclusion supports the magnetization ramp behavior at $m = 1/3$ of the Kagome lattice antiferromagnet.

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