Quantum Spin Fluid Behaviors of the Kagome- and Triangular-Lattice Antiferromagnets

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Abstract. The $S=1/2$ kagome-lattice antiferromagnet is investigated using the numerical diagonalization of finite-size clusters. The analysis of the susceptibility at the zero magnetization indicates that the magnetic excitation of the system is gapless. It is consistent with our previous finite-scaling analysis of the spin gap. The application of the method for the triangular-lattice antiferromagnet confirms the validity of the analysis.

1. Introduction

The $S = 1/2$ kagome-lattice antiferromagnet has attracted a lot of interests in the field of the highly frustrated magnetism. Particularly since discoveries of several candidate materials; the herbertsmithite\cite{1, 2}, the volborthite\cite{3, 4} and the vesignieite\cite{5} for the kagome lattice, the study on the system has been accelerated. The quantum spin fluid behaviour of the system was predicted by many theoretical studies\cite{6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18}. The $U(1)$ Dirac spin liquid theory\cite{13} indicated a gapless spin excitation in the thermodynamic limit, which has been supported by the recent variational approach\cite{19, 20}. Our recent numerical diagonalization study\cite{21} also concluded that the system is gapless. On the other hand, the recent density matrix renormalization group (DMRG) analyses\cite{22, 23, 24} suggested that the system has a finite spin gap even in the thermodynamic limit and supported the $Z_2$ topological spin liquid picture\cite{6}. Thus whether the $S=1/2$ kagome-lattice antiferromagnet has a spin gap or not is still theoretically controversial, although the recent neutron scattering experiment of the single crystal of the herbertsmithite\cite{25, 26} suggested that the system is gapless.

In this paper, using the recently developed susceptibility analysis based on the numerical diagonalization of finite-size clusters\cite{27}, we try to approach the spin-gap issue of the $S = 1/2$ kagome-lattice antiferromagnet. Particularly, we examine the gapless-feature result of the susceptibility analysis of the $S = 1/2$ kagome-lattice antiferromagnet by comparing the result with the result of the $S = 1/2$ triangular-lattice one, which is widely believed to be gapless. These two cases are typical among frustrated antiferromagnets. Although a randomness effect in these systems was additionally examined\cite{28, 29}, in the present study, properties of ideal systems without randomness are investigated as a fundamental issue.
2. Numerical diagonalization
Using the numerical exact diagonalization of finite-size clusters under periodic boundary condition, we investigate the $S = 1/2$ kagome-lattice antiferromagnet defined by the Hamiltonian
\[ \mathcal{H} = \sum_{\langle i, j \rangle} S_i \cdot S_j, \tag{1} \]
where $\langle i, j \rangle$ means all the nearest neighbor pairs on the kagome lattice. For an $N$-site system, we consider subspaces characterized by $M = \sum_j S^z_j$; we obtain the lowest energy denoted by $E(N, M)$ of the Hamiltonian matrix in each subspace. We calculate all the values of $E(N, M)$ available for the clusters up to $N = 42$ by the numerical diagonalization.

3. Susceptibility analysis
In order to investigate the spin gap issue, we apply the susceptibility analysis which was developed in our previous work [27]. The argument of the analysis is briefly reviewed as follows: the effect of the applied external magnetic field $h$ is described by the Zeeman energy term
\[ \mathcal{H}_Z = -h \sum_j S^z_j \tag{2} \]
The energy of $\mathcal{H}$ per site in the thermodynamic limit is defined as
\[ \frac{E(N, M)}{N} \sim \epsilon(m) \quad (N \to \infty) \tag{3} \]
where $m = M/(SN)$ is the magnetization normalized by the saturated magnetization $SN$. If we assume $\epsilon(m)$ is an analytic function of $m$, the spin excitation energy would become
\[ E(N, M + 1) - E(N, M) \sim \frac{1}{S} \left( \epsilon'(m) + \frac{1}{2} \epsilon''(m) \frac{1}{NS} + \cdots \right) \tag{4} \]
Thus, this equation gives the quantity corresponding to the width of the magnetization plateau at $m$ as follows,
\[ (E(N, M + 1) - E(N, M)) - (E(N, M) - E(N, M - 1)) \sim \epsilon''(m) \frac{1}{NS^2} \tag{5} \]
Minimizing the energy of the total Hamiltonian $\mathcal{H} + \mathcal{H}_Z$, the ground state magnetization curve is derived by
\[ h = \epsilon'(m)/S \tag{6} \]
The field derivative of the magnetization is defined as
\[ \chi = \frac{dm}{dh} = \frac{S}{\epsilon''(m)} \tag{7} \]
If we assume $\chi \neq 0$, namely $\epsilon''(m)$ is finite, the magnetization plateau at $m$ would vanish in the thermodynamic limit, because of (5). Thus a necessary condition for the existence of a magnetization plateau at $m$ is $\chi = 0$ in the thermodynamic limit. Now we apply this argument for the spin gap. We should examine the case of $m = 0$. In this case, the equation (5) can be rewritten as
\[ 2\Delta_N \sim \epsilon''(0) \frac{1}{NS^2} \tag{8} \]
where $\Delta_N = E(N, 1) - E(N, 0)$ is the spin gap for an $N$-spin cluster. Thus a necessary condition of the finite spin gap would be $\chi = 0$ at $m = 0$ in the thermodynamic limit.
Figure 1. Magnetization curves of the kagome-lattice antiferromagnet for \( N = 36, 39 \) and 42. The results for \( N = 36 \) and 39 are denoted by green and black lines, respectively; that for \( N = 42 \) is denoted by red lines with squares.

Figure 2. Magnetization dependence of \( \chi \) of the kagome-lattice antiferromagnet for \( N = 36, 39 \) and 42. The results for \( N = 36, 39, \) and 42 are denoted by green diamonds, black circles, and red squares, respectively.

4. Result of the kagome-lattice antiferromagnet
We investigate the field derivative of the magnetization \( \chi \) for the \( S = 1/2 \) kagome-lattice antiferromagnet. The ground state magnetization curves for \( N = 36, 39 \) and 42 are shown in Figure 1; the results for \( N = 39 \) and 42 were originally presented in [30] and [31], respectively. From the magnetization curves, it is difficult to determine whether the system is gapless or gapped. Next we show the magnetization dependence of the calculated \( \chi \) for \( N = 42, 39 \) and 36 in Figure 2. The behaviors around \( m = 0 \) are magnified in Figure 3. At least for \( N = 36 \) and 42, the size dependence of \( \chi \) at \( m = 0 \) is very small. \( \chi \) at \( m = 0 \) is plotted versus \( 1/N \) and \( 1/\sqrt{N} \) for \( N = 42, 36, 30, 24, 18, 12 \) in Figures 4(a) and (b), respectively. Although the system size dependence exhibits a slight oscillation, both plots clearly indicate that \( \chi \) at \( m = 0 \) is still finite in the thermodynamic limit. Thus the system does not meet the condition for the finite spin gap. It should be one of strong evidences to justify that the \( S = 1/2 \) kagome-lattice antiferromagnet is gapless.

5. Triangular-lattice antiferromagnet
In order to test the validity of the present method, we apply it for the \( S = 1/2 \) triangular-lattice antiferromagnet, for which the triplet excitation is gapless. The ground-state magnetization curves calculated by the numerical exact diagonalization for \( N = 33, 36, \) and 39 are shown in Figure 5. The magnetization dependence of the susceptibility is shown in Figure 6. The behaviors around \( m = 0 \) are magnified in Figure 7. \( \chi \) at \( m = 0 \) is plotted versus \( 1/N \) and \( 1/\sqrt{N} \) for \( N = 36, 30, 24, 18, 12 \) in Figures 8(a) and (b), respectively. Both plots indicate that the extrapolated value in the thermodynamic limit seems to be finite (\( \chi \neq 0 \)). It is consistent...
Figure 3. Magnetization dependence of $\chi$ of the kagome-lattice antiferromagnet for $N = 36, 39$ and 42 around $m = 0$. Symbols are the same as in Fig. 2.

Figure 4. $\chi$ plotted versus $1/N$ (a) and $1/\sqrt{N}$ (b) for the kagome-lattice antiferromagnet. Closed symbols denote the results for the cases when the shape of the finite-size clusters are the rhombus with an interior angle $\pi/3$. When a finite-size cluster for a given $N$ cannot form the same rhombus even if the rhombus is tilted, on the other hand, the cluster forms a parallelogram; the results are given by open symbols. Both of (a) and (b) suggest that the extrapolated value in the thermodynamic limit seems to be finite ($\chi \neq 0$).

Figure 5. Magnetization curves of the triangular-lattice antiferromagnet for $N = 33, 36$ and 39. The results for $N = 33$ and 36 are denoted by green and black lines, respectively; that for $N = 39$ is denoted by red lines with squares.
Figure 6. Magnetization dependence of $\chi$ of the triangular-lattice antiferromagnet for $N=33$, 36 and 39. The results for $N=33$, 36, and 39 are denoted by green diamonds, black circles, and red squares, respectively.

Figure 7. Magnetization dependence of $\chi$ of the kagome-lattice antiferromagnet for $N=33$, 36 and 39 around $m=0$. Symbols are the same as in Fig. 6.

Figure 8. $\chi$ plotted versus $1/N$ (a) and $1/\sqrt{N}$ (b) for the triangular-lattice antiferromagnet. Both plots indicate that the extrapolated value in the thermodynamic limit seems to be finite ($\chi \neq 0$).

with the gapless feature of the triangular-lattice antiferromagnet. Thus it confirms the validity of the present method.

6. Summary
The spin gap issue of the kagome-lattice antiferromagnet is investigated using the numerical diagonalization up to $N=42$. The analysis of the field derivative of the magnetization $\chi$ is successfully applied to the triangular-lattice antiferromagnet that is gapless in its spin excitation. The behavior of $\chi$ for the kagome-lattice antiferromagnet shares with that of triangular-lattice antiferromagnet. The agreement strongly suggests that the gapless spin excitation in the kagome-
lattice antiferromagnet.

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