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Gapless spin excitations in the $S = 1/2$ Kagome- and triangular-lattice Heisenberg antiferromagnets

Tôru Sakai[a,b,*], Hiroki Nakano[a]

[a] Graduate School of Material Science, University of Hyogo, Hyogo 678-1297, Japan
[b] National Institutes for Quantum and Radiological Science and Technology (QST) SPring-8, Hyogo 679-5148, Japan

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A B S T R A C T

The $S = 1/2$ kagome- and triangular-lattice Heisenberg antiferromagnets are investigated using the numerical exact diagonalization and the finite-size scaling analysis. The behaviour of the field derivative at zero magnetization is examined for both systems. The present result indicates that the spin excitation is gapless for each system.

1. Introduction

Frustration in magnets is one of important topics in the field of the strongly correlated electron systems. Among such magnets, the kagome- and triangular-lattice antiferromagnets attract a lot of interests. Since discoveries of several candidate materials of the kagome-lattice antiferromanget; the herbertsmithite [1,2], the volborthite [3,4] and the vesignieite [5], particularly, the study on this system has been accelerated. The quantum spin-fluid behaviour of the system was predicted by many theoretical studies [6–18]. The $U(1)$ Dirac spin-liquid theory [13] indicated a gapless spin excitation in the thermodynamic limit, which has been supported by the recent variational approach [19,20]. Our recent numerical diagonalization study [21] also concluded that the system is gapless. On the other hand, the recent density matrix renormalization group (DMRG) analyses [22–24] suggested that the system has a finite spin gap even in the thermodynamic limit and supported the Z_2 topological spin-liquid picture [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 [25,26] suggested that the system is gapless.

On the other hand, the triangular-lattice antiferromagnet is widely believed to be gapless, based on the previous precise numerical analysis [27]. Thus it would be interesting to compare the low-lying spin excitation of the kagome-lattice antiferromagnet with the one of the triangular lattice. In this paper, using the recently developed field-derivative analysis based on the numerical diagonalization of finite-size clusters [28], we try to approach the spin-gap issue of the $S = 1/2$ kagome-lattice antiferromagnet, as well as the triangular-lattice one. When one examines field-derivatives of the magnetization within the numerical data for finite-size systems, it is difficult to eliminate finite-size effects completely. It is therefore required to reduce such effects by means of a feasible way. Under these circumstances, the purpose of this study is to present such a field-derivative analysis based on numerical data whose finite-size deviations are presumably reduced. The kagome- and triangular-lattice antiferromagnets have wide diversity of further studies in various aspects. Under large magnetic fields, nontrivial anomalous behaviours are observed in their magnetization curves; however, the behaviours are different between the kagome- and triangular-lattice antiferromagnets [29–31]. Such behaviours were also examined in various frustrated magnets [32–36]. A randomness effect in these systems was additionally examined [37,38]. Under such circumstances, the present study tackles a fundamental issue concerning properties of systems without effects owing to significantly large fields and randomness are investigated.

2. Model and calculation

Using the numerical exact diagonalization of finite-size clusters under periodic boundary condition, we investigate the $S = 1/2$ kagome- and triangular-lattice Heisenberg antiferromagnets defined by the Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where site i is assumed to be the vertices of the kagome or triangular

* Corresponding author at: Graduate School of Material Science, University of Hyogo, Hyogo 678-1297, Japan.
E-mail address: sakai@spring8.or.jp (T. Sakai).
URL: http://cmt.spring8.or.jp/ (T. Sakai).

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lattice. Here, $\langle i, j \rangle$ runs over all the nearest-neighbor pairs on each lattice. For an N-site system, we consider subspaces characterized by $M = \sum_j S_j^z$; 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 $N = 36$ by the numerical diagonalization. The diagonalization is carried out based on the Lanczos algorithm and/or the Householder algorithm. Part of the Lanczos diagonalizations were carried out using an MPI-parallelized code which was originally developed in the study of Haldane gaps [39]. The usefulness of our program was confirmed in large-scale parallelized calculations [21,31,40–42].

3. Field-derivative analysis

In order to investigate the low-lying spin excitation, we apply the field-derivative analysis which was developed in our previous work [28]. 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

$$\mathcal{H}_Z = -h \sum_j S_j^z. \quad (2)$$

The energy of $\mathcal{H}$ per site in the thermodynamic limit is defined as

$$\frac{E(N, M)}{N} \sim \epsilon(m) \quad (N \to \infty), \quad (3)$$

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

$$E(N, M+1) - E(N, M) \sim \frac{1}{S}\left(\epsilon'(m) + \frac{1}{2}\epsilon''(m)\frac{1}{NS} + \cdots\right). \quad (4)$$

Thus, this equation gives the quantity corresponding to the width of the magnetization plateau at m as follows,

$$(E(N, M+1) - E(N, M)) - (E(N, M) - E(N, M-1)) \sim \epsilon''(m)\frac{1}{NS^2}. \quad (5)$$

Minimizing the energy of the total Hamiltonian $\mathcal{H} + \mathcal{H}_Z$, the ground state magnetization curve is derived by

$$h = \epsilon'(m)/S. \quad (6)$$

The field derivative of the magnetization is defined as

$$\chi \equiv \frac{dm}{dh} = \frac{S}{\epsilon''(m)}. \quad (7)$$

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 $h \to 0$ corresponding to $m = 0$. In this case, the equation (5) can be rewritten as

$$2\Delta_N \sim \epsilon''(0)\frac{1}{NS^2}, \quad (8)$$

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.

In order to estimate χ at $m = 0$ from discrete data for finite-size systems, it is the most simple way to use neighboring three data in the form χ_3 defined as

$$\chi_3^{-1} = NS[-2E(N, M) + E(N, M+1) + E(N, M-1)]. \quad (9)$$

Actually, Eq. (9) was used in our previous examination [28]. However, a significant possibility cannot be denied that there remain deviations from the ideal quantity owing to the discreteness. It is expected to

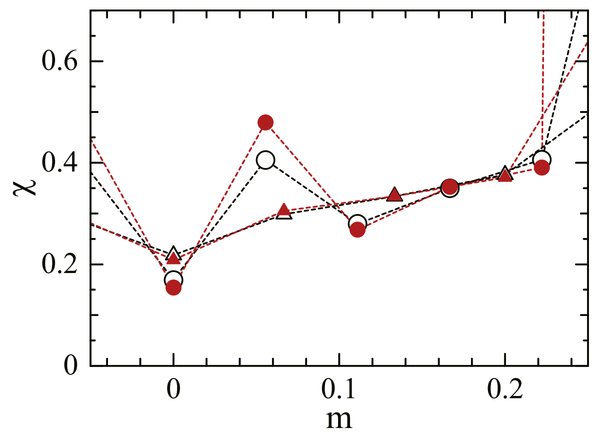

Fig. 1. Field-derivative of the magnetization as a function of m for $N = 36$ and 30 in the kagome-lattice antiferromagnet. Circles and triangles denote results for $N = 36$ and 30, respectively. Black open and red closed symbols represent results of χ_3 obtained from Eq. (9) and χ_5 obtained from Eq. (10), respectively.

reduce the deviations if one uses neighboring five data instead of the above three under the assumption that $\epsilon(m)$ is analytic. In the method employing neighboring five data, we use χ_5 defined as

$$\chi_5^{-1} = NS\left[-\frac{5}{2}E(N, M) + \frac{4}{3}(E(N, M+1) + E(N, M-1)) - \frac{1}{12}(E(N, M+2) + E(N, M-2))\right]. \quad (10)$$

In the thermodynamic limit, χ_3 should agree with χ_5. We show the estimated χ_3 and χ_5 for the kagome- and triangular-lattice antiferromagnets in the following sections.

4. Kagome-lattice antiferromagnet

We investigate the field derivative of the magnetization χ for the $S = 1/2$ kagome-lattice antiferromagnet.

Let us, first, show differences between χ_3 obtained from Eq. (9) and χ_5 obtained from Eq. (10); results are depicted in Fig. 1. One can confirm that the differences are small irrespective of the values of m. The smallness is also observed irrespective of N. It is expected that we can obtain better estimates of χ by the small deviations from χ_3 to χ_5.

Let us, next, focus our attention on the system-size dependence of the field derivative of the magnetization at $m = 0$. We plot χ_5 at $m = 0$ calculated by the form (10) as a function of $1/N$ for $N = 36$, 30, 24, 18, and 12 in Fig. 2. Although the system-size dependence exhibits a slight

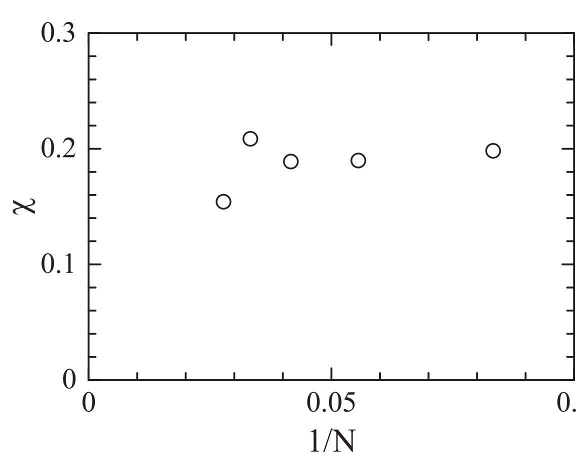

Fig. 2. The system-size dependence of the field derivative of the magnetization at $m = 0$ estimated by the form (10) in the case of the kagome-lattice antiferromagnet. Numerical data are plotted as a function of $1/N$ for $N = 36$, 30, 24, 18, and 12.