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Quantum Spin Liquid in the Kagome-Lattice Antiferromagnet and Related Systems

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Abstract. The S=1/2 kagome-lattice antiferromagnet is investigated using the numerical diagonalization up to the 42-spin cluster. The analysis of the field derivative of the magnetization at the zero magnetization indicates that the magnetic excitation ot the system is gapless. It is consistent with our previous finite-scaling analysis of the spin gap.

1. Introduction

The $S = 1/2$ kagome-lattice antiferromagnet is one of interesting frustrated quantum spin systems. The system is supposed to exhibit the quantum spin liquid in the ground state[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12], which was proposed as an origin of the high-temperature superconductivity[13]. Experimental studies to observe a novel spin liquid phase have been accelerated, since discoveries of several candidate materials; the herbertsmithite[14, 15], the volborthite[16, 17] and the vesignieite[18] for the kagome lattice. The spin gap is an important physical quantity to characterize the spin liquid behavior. Whether the $S = 1/2$ kagome-lattice antiferromagnet is gapless or has a finite spin gap, is still an unsolved issue, because any recently developed numerical calculation methods are not enough to determine it in the thermodynamic limit. The quantum Monte Carlo (QMC) simulation has a so-called negative sign problem due to the frustration. The density matrix renormalization group (DMRG) method is not good because of the two-dimensionality of the system. Our large-scale numerical diagonalization up to the 42-spin cluster and a finite-size scaling analysis indicated that the $S = 1/2$ kagome-lattice antiferromagnet is gapless in the thermodynamic limit[19]. It is consistent with the U(1) Dirac spin liquid theory of the kagome-lattice antiferromagnet[8]. It was also supported by a variational method[20, 21]. On the other hand, some DMRG calculations[22, 23, 24] indicated a finite spin gap in the thermodynamic limit. Although the estimated magnitude of the spin gap is dependent on the method, they are qualitatively consistent with the gapped Z_2 topological spin liquid theory[1]. It was also supported by a numerical diagonalization study[25]. Although the recent neutron scattering experiment of the single crystal of the herbertsmithite[26, 27] suggested that the system is gapless, the spin gap issue of the kagome-lattice antiferromagnet is still theoretically controversial.

In this paper, we analyze the field derivative of the magnetization at the zero magnetization, using the numerical diagonalization up to the 42-spin cluster, to determine whether the kagome-lattice antiferromagnet is gapless or gapped.

2. Model and numerical exact diagonalization

Now we examine the spin gap issue of the $S = 1/2$ kagome lattice antiferromagnet. The Hamiltonian is given by

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

where $\langle i, j \rangle$ means all the nearest neighbor pairs on the kagome lattice. For an N-site system, the lowest energy of $\mathcal{H}$ in the subspace where $\sum_j S_j^z = M$ is denoted by $E(N, M)$. Using the numerical exact diagonalization, we have calculated all the values of $E(N, M)$ available for the clusters up to N =42 under the periodic boundary condition. The largest dimension of the $N = 42$ system is 538,257,874,440. To treat such huge matrices in computers, we have carried out parallel calculations using the MPI-parallelized code, which was originally developed in the study of the Haldane-gap issue[28]. Note especially that calculations for the N =42 cluster require the use of K computer, Kobe, Japan.

3. Field derivative of the magnetization

The effect of the applied external magnetic field h is discribed by the Zeeman energy term

$$\mathcal{H}_Z = -h \sum_j S_j^z \tag{2}$$

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

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

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

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

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.

In the next section, we confirm the validity of this condition for typical gapless and gapped spin systems.

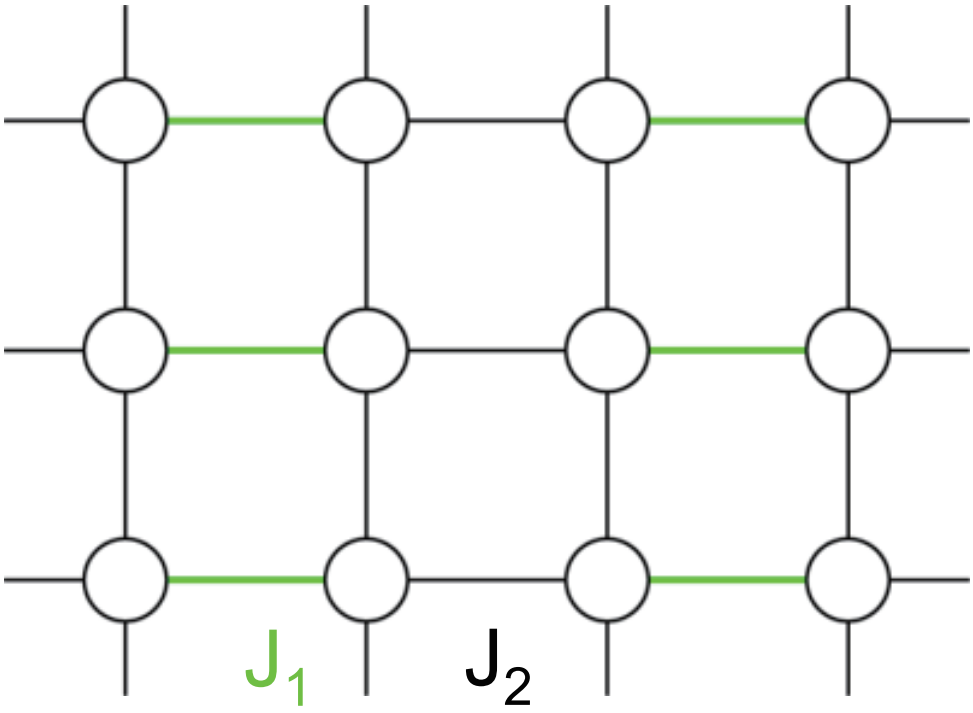

Figure 1. Square-lattice antiferromagnet with the dimerization. The green and black lines denote bonds of interactions J_1 and J_2, respectively. The case of $J_2/J_1 = 1$ corresponds to the square-lattice antiferromagnet without the dimerization.

4. Square-lattice Heisenberg antiferromagnet with and without dimerization

As typical gapless and gapped spin systems, we consider the $S = 1/2$ square-lattice Heisenberg antiferromagnet, and the one with the dimerization, respectively. These models are shown in Figure 1. The ratio of the two antiferromagnetic exchange interactions is defined as $\alpha = J_2/J_1$. The previous QMC simulation study[29] revealed that the critical ratio is $\alpha_c = 0.52337(3)$ and the system is gapless for $\alpha > \alpha_c$, while gapped for $\alpha < \alpha_c$. Using the numerical diagonalization, we investigate the two typical cases; $J_2/J_1 = 1$ (gapless) and $J_2/J_1 = 0.2$ (gapped). The ground state magnetization curves for $J_2/J_1 = 1$ and $J_2/J_1 = 0.2$ are shown in Figures 2 and 3, respectively. The former seems gapless, while the latter clearly looks gapped at $m = 0$. The field derivatives of the magnetization χ for $J_2/J_1 = 1$ and $J_2/J_1 = 0.2$ are shown in Figures 4 and 5, respectively. In both cases the system size dependence of χ at $m = 0$ looks small. We can easily expect that χ is finite for $J_2/J_1 = 1$, while $\chi = 0$ for $J_2/J_1 = 0.2$ in the thermodynamic limit. χ at $m = 0$ plotted versus $1/N$ in Figure 6 for $J_2/J_1 = 1$ and Figure 7 for $J_2/J_1 = 0.2$ clearly confirms these features. The result justifies the argument in the previous section that χ is finite for the gapless system, while $\chi = 0$ for the gapped one in the thermodynamic limit.

5. Kagome lattice antiferromagnet

In this section, we investigate the field derivative of the magnetization χ for the $S = 1/2$ kagome-lattice antiferromagnet. The ground state magnetization curves for N=36, 39 and 42 are shown in Figure 8; 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 χ for N=42, 39 and 36 in Figure 9. The behaviors around $m = 0$ are magnified in Figure 10. At least for N=36 and 42,

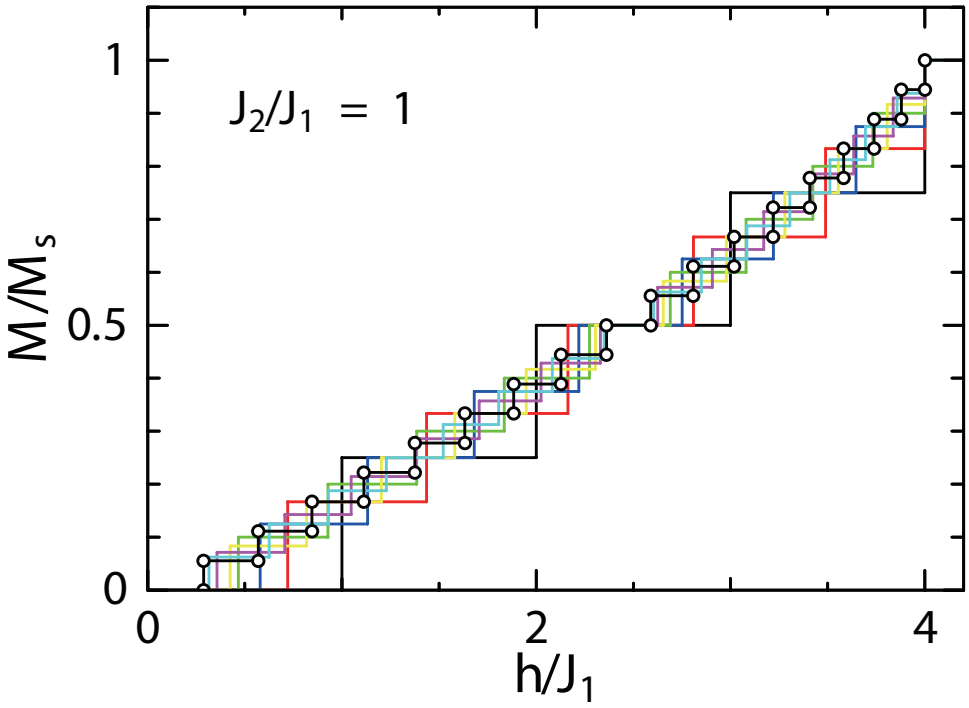

Figure 2. Magnetization curves of the square-lattice antiferromagnet for several system sizes up to $N = 36$. The results for $N = 8$, 12, 16, 20, 24, 28, and 32 are denoted by black, red, dark-blue, green, yellow, violet, light-blue lines without symbols, respectively; the result for $N = 36$ is denoted by black lines with circles.

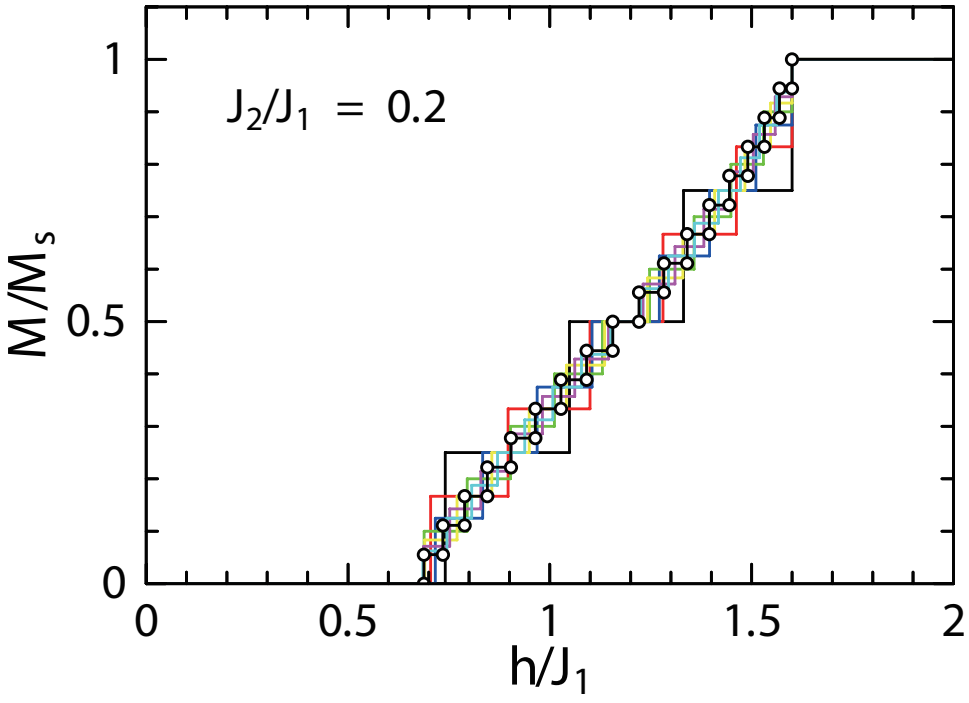

Figure 3. Magnetization curves of the square-lattice antiferromagnet with the dimerization of $J_2/J_1 = 0.2$ for several system sizes up to $N = 36$. Lines and symbles are the same as in Fig. 2.

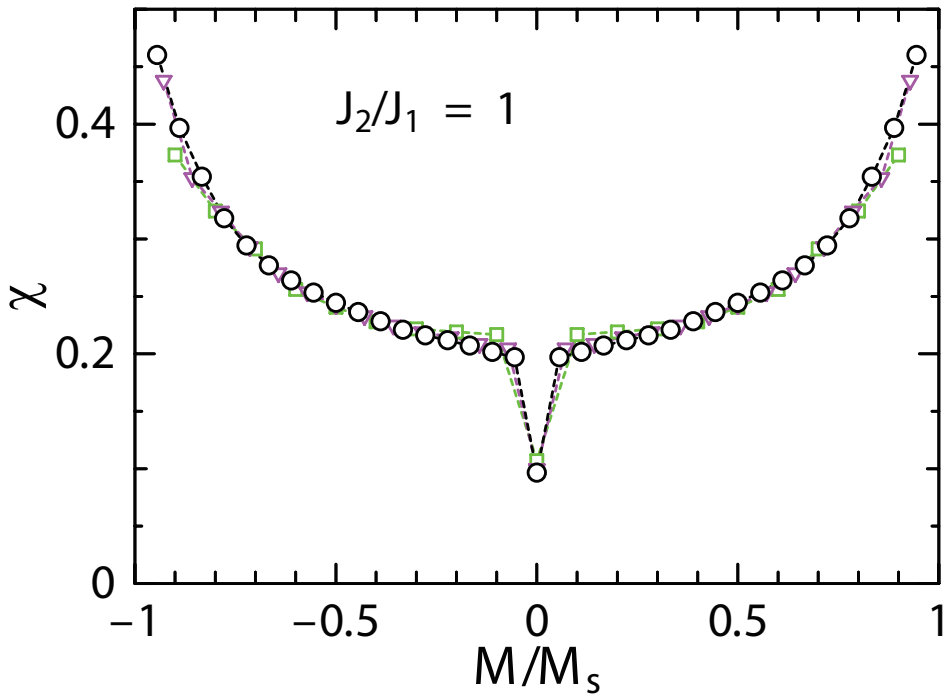

Figure 4. Magnetization dependence of χ of the square-lattice antiferromagnet for several system sizes. The results for N =36, 28, 20 are denoted by black circles, violet inversed triangles, and green squares, respectively.

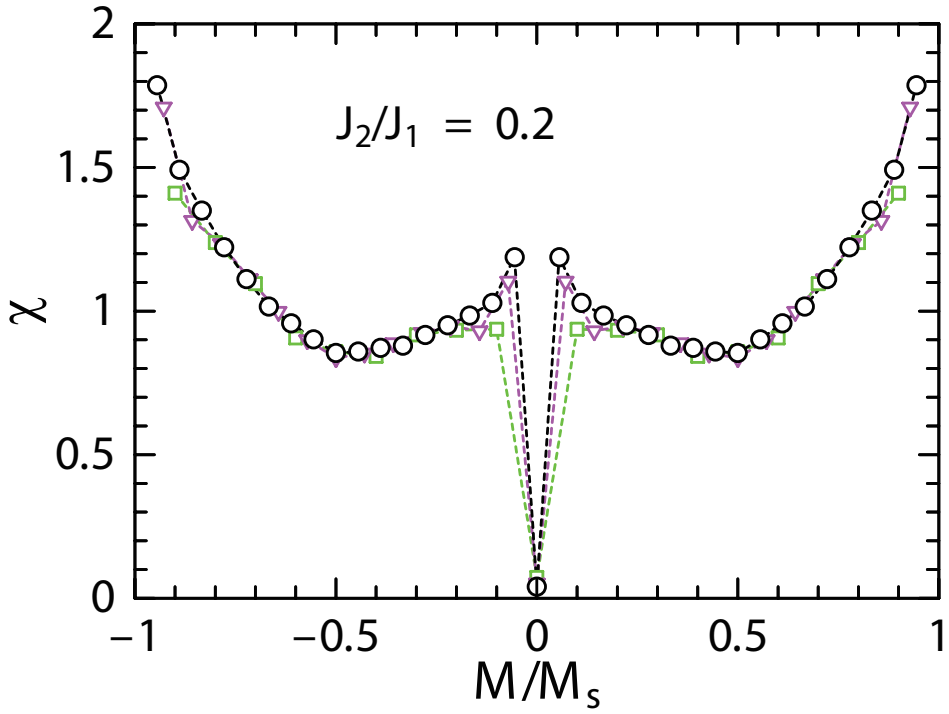

Figure 5. Magnetization dependence of χ of the square-lattice antiferromagnet with the dimerization of $J_2/J_1 = 0.2$ for several system sizes. Lines and symbles are the same as in Fig. 4.

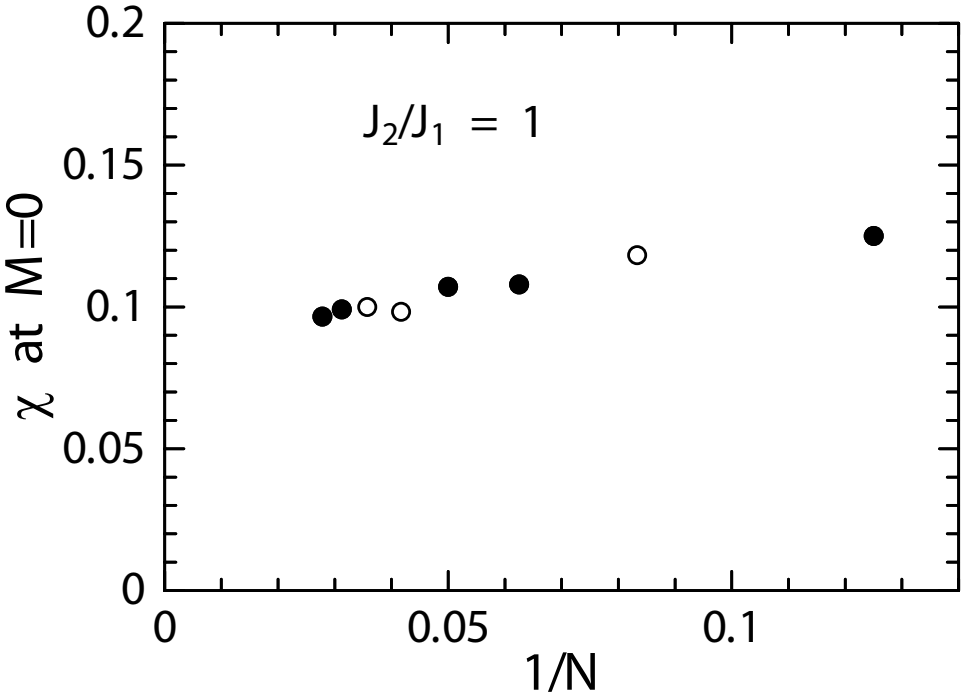

Figure 6. χ plotted versus $1/N$ for the square-lattice antiferromagnet ($J_2/J_1 = 1$). The results are presented for the cases up to $N = 36$. Closed symbols denote the results for the cases when the shape of the finite-size clusters are squares. When a finite-size cluster for a given N cannot form a square even if the square is tilted, on the other hand, the cluster forms a parallelogram; the results are given by open symbols. The extrapolated value in the thermodynamic limit seems to be finite ($\chi \neq 0$).

the size dependence of χ at $m = 0$ is very small. χ at $m = 0$ is plotted versus $1/N$ for N=42, 36, 30, 24, 18, 12 in Figure 11. Although the system size dependence exhibits a slight oscillation, it clearly indicates that χ 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.

6. Conclusion

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 χ gives one of strong evidences of the gapless feature.

Acknowledgments

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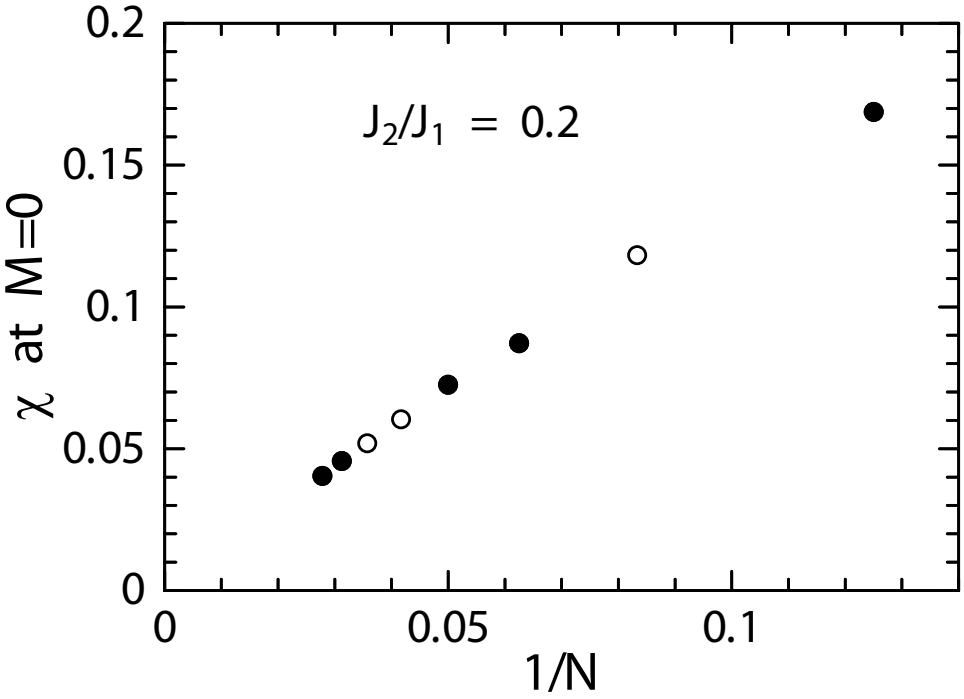

Figure 7. χ plotted versus $1/N$ for the dimerized square-lattice antiferromagnet ($J_2/J_1 = 0.2$). The extrapolated value in the thermodynamic limit seems to be zero. Symbols are the same as in Fig. 6.

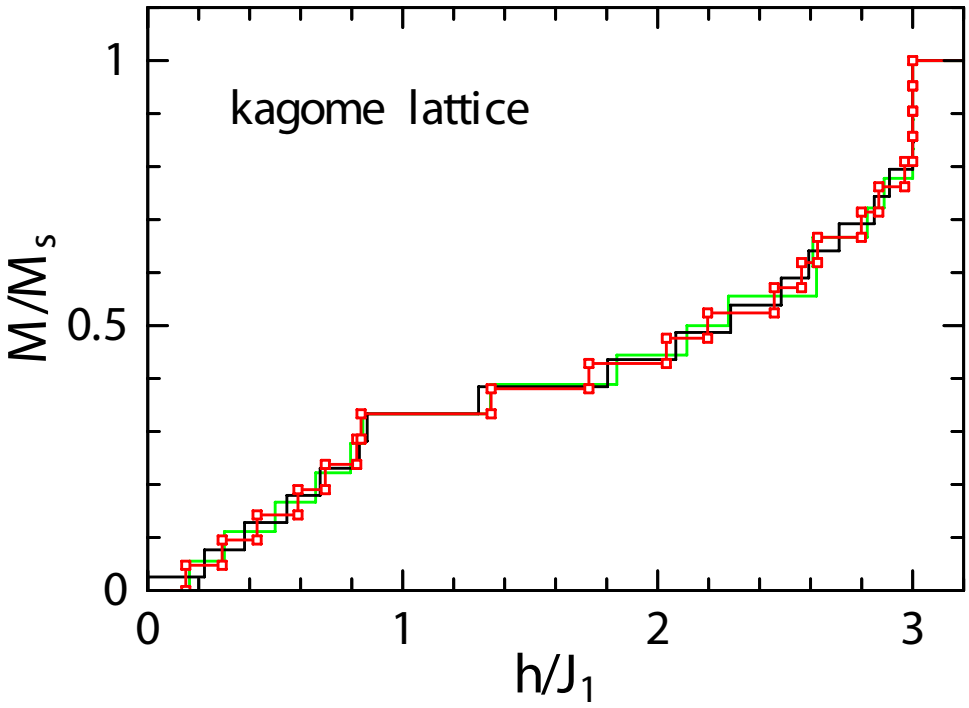

Figure 8. Magnetization curves of the kagome-lattice antiferromagnet for N =36, 39 and 42. The results for N =36 and 39 are denoted by green and black lines, respectively; that for N =42 is denoted by red lines with squares.

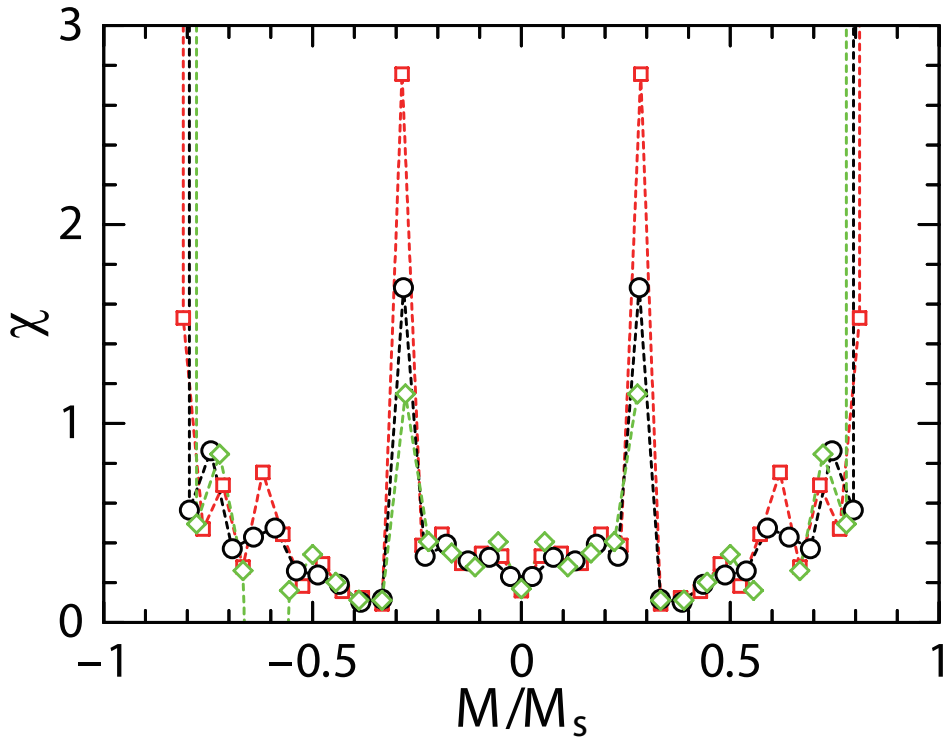

Figure 9. Magnetization dependence of χ of the kagome-lattice antiferromagnet for N =36, 39 and 42. The results for N =36, 39, and 42 are denoted by green diamonds, black circles, and red squares, respectively.

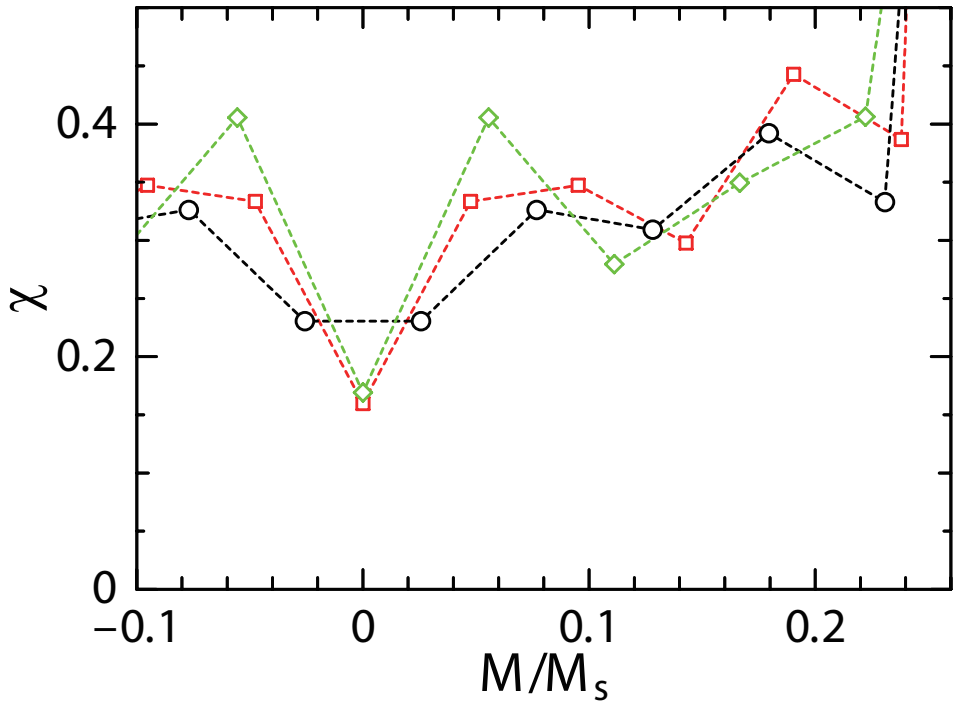

Figure 10. Magnetization dependence of χ of the kagome-lattice antiferromagnet for N =36, 39 and 42 around $m = 0$. Symbols are the same as in Fig. 9.

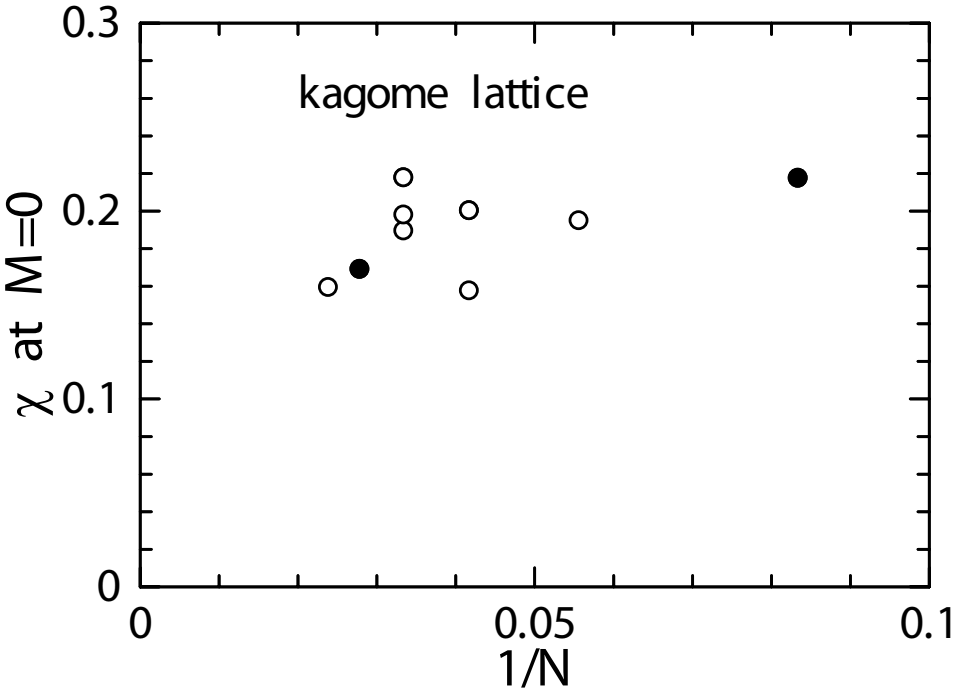

Figure 11. χ plotted versus $1/N$ for the kagome-lattice antiferromagnet. Closed symbols denote the results for the cases when the shape of the finite-size clusters are the rhombus with an interior angle $\pi/3$. When a finite-size cluster for a given N cannot form the same rhombus even if the rhombus is tilted, on the other hand, the cluster forms a parallelogram; the results are given by open symbols. The extrapolated value in the thermodynamic limit seems to be finite ($\chi \neq 0$).

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