Magnetization ramp of the kagome lattice antiferromagnet

Hiroki Nakano and Toru Sakai

Univ of Hyogo, Hyogo, Japan

A SPring8, JAEA, Hyogo, Japan

E-mail: hnakano@sci.u-hyogo.ac.jp

Abstract. The magnetization process of the Heisenberg antiferromagnet on the kagome lattice is studied by numerical-diagonalization method. Though the magnetization plateau was considered to appear at the one-third of the magnetization saturation, recent reexamination of the magnetization process of the same model from another viewpoint of the field-derivative of the magnetization in finite-size data from the numerical-diagonalization calculation up to 36 sites suggests that the behavior at around one-third height of the saturation is clearly different from typical magnetization plateaux, which we should call the magnetization ramp. The present study reports our new numerical-diagonalization result up to 39 sites, which reveals well the characteristics of the magnetization ramp. The behavior of the kagome lattice antiferromagnet is compared with the typical magnetization plateaux of the Heisenberg antiferromagnet on the triangular lattice.

1. Introduction
Kagome lattice is one of the typical cases where frustrations play an important role to the properties of magnetic materials; the extensive studies have been carried out over 50 years. The kagome-lattice antiferromagnet has become a hot topic due to the discovery of new materials[1, 2, 3, 4, 5].

The magnetization process of the Heisenberg antiferromagnet on the kagome lattice was reported by numerical-diagonalization studies[6, 7]. These studies concluded that the magnetization plateau appears at the one-third of the magnetization saturation. Recently, reexamination from another viewpoint of the field-derivative of the magnetization in finite-size data from the numerical-diagonalization calculation up to 36 sites indicates that the behavior at around one-third height of the saturation is clearly different from typical magnetization plateaux[8]. The new phenomenon is called the magnetization ramp. In order to confirm that the behavior of the magnetization ramp is not a finite-size effect but an intrinsic phenomenon, the present study reports our new numerical-diagonalization result of the cluster including 39 sites. Our result of 39 sites reveals the characteristics of the magnetization ramp markedly. We also present the magnetization process of the Heisenberg antiferromagnet on the triangular lattice up to 39 sites and perform the same analysis of the field-derivative of the magnetization. It is clarified that the behavior of the kagome lattice antiferromagnet is quite different from the typical magnetization plateau of the Heisenberg antiferromagnet on the triangular lattice.

This paper is organized as follows. In the next section, the model Hamiltonian and the method of calculation will be explained. In §3, we present numerical results of the kagome
lattice antiferromagnet and the triangular lattice antiferromagnet. The final section is devoted to the summary of this study and some discussions.

2. Hamiltonian and method
In this study, we examine the model whose Hamiltonian is given by

$$H = \sum_{\langle i,j \rangle} J S_i \cdot S_j + h \sum_i S^z_i,$$

where $S_i$ is an $S = 1/2$ spin operator at site $i$. Spin sites are supposed to be on the kagome lattice or the triangular lattice. We consider the case when the interaction in the first term is isotropic. Energies are measured in units of $J$; thus we assume $J = 1$ hereafter. The second term in eq. (1) is the Zeemann term; $h$ is the external magnetic field. For a system with size $N$, we can obtain the lowest energy $E(N, M)$ in each of the subspace of a given value of $S^{\text{tot}}_z$ denoted by $M$ by the numerical diagonalization of the Lanczos algorithm and/or the householder one, where $S^{\text{tot}}_z$ represents the $z$-component of the total spin. The lowest energy $E(N, M)$ enable us to obtain magnetization process; at the field given by $h = E(N, M + 1) - E(N, M)$, the magnetization increases from $M$ to $M + 1$. The field-derivative of the magnetization is evaluated by the expression

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

where $M_{\text{sat}}$ denotes the saturation of the magnetization, namely $M_{\text{sat}} = N/2$.

It is known that numerical diagonalization method can treat only small clusters because the dimension of the matrix grows exponentially with respect to the number of spin sites. The maximum of available system sizes is determined by the quantity of resources in computers that one uses. The largest system sizes for the $S = 1/2$ spin model on the kagome lattice so far was $N = 36$[9, 10, 11, 12, 8]. In our numerical diagonalization, only the conservation of $S^{\text{tot}}_z$ is used for the division into subspaces. Thus, we can perform diagonalizations of the systems irrespective of the shapes of clusters. The shapes of $N = 39$ clusters for the kagome lattice and the triangular lattice are depicted in Fig.1 and Fig.2, respectively.

![Figure 1](image1.png)  
**Figure 1.** The shape of $N = 39$ cluster on the kagome lattice.

![Figure 2](image2.png)  
**Figure 2.** The shape of $N = 39$ cluster on the triangular lattice.
Figure 3. Magnetization process of the Heisenberg antiferromagnet on the kagome lattice. Results for \( N = 39 \) and 36 are represented by a black solid line and a red dotted line.

Figure 4. Field derivative of the magnetization of the Heisenberg antiferromagnet on the kagome lattice. Results for \( N = 39, 36, \) and 27 are denoted by black circles, red squares, and green triangles.

Note here that both the clusters of \( N = 39 \) are rhombic. Since the clusters show a high symmetry in their shapes, it is reasonable to consider that two-dimensionality is included in our calculations for \( N = 39 \). All the results in our present study are based on the calculations for the case of the rhombic clusters. The dimension of the subspace divided by \( S_z^{\text{tot}} \) is the largest when \( S_z^{\text{tot}} = 0 \) (\( S_z^{\text{tot}} = 1/2 \)) for a system of even (odd) \( N \). The largest dimension of the \( N = 39 \) system is 68 923 264 410. In order to treat such huge matrices in computers, we have carried out parallel calculations using the MPI-parallelized code that we developed[13]. We have succeeded
in calculations of \( N = 39 \) in Hitachi SR16000 at National Institute for Fusion Science. Note here that 8192 logical cores have been used in the largest case of our calculations.

3. Numerical results

3.1. Kagome lattice antiferromagnet

First, we present our new result of the magnetization process of the kagome lattice antiferromagnet for \( N = 39 \) depicted in Figure 3; for comparison, the magnetization process for \( N = 36 \) \cite{7, 8} are accompanied. One observes that the two magnetization processes for \( N = 36 \) and \( N = 39 \) in Figure 3 seem to agree with each other. Near the 1/3 magnetization that is the primary interest, a flat part of the processes certainly exists in both the cases. However, the width of \( N = 39 \) is getting slightly narrower than that of \( N = 36 \). It is not so clear whether the width survives or not in the thermodynamic limit. Every finite-size step of the magnetization process of \( N = 39 \) appears from \( M = 0 \) to the saturation whereas a jump at \( M/M_{\text{sat}} = 11/18 \) appears for \( N = 36 \). This suggests two possibilities. One is that the jump is a finite-size effect that is absent in the thermodynamic limit. The other is that the anomalous behavior occurs at the value of \( M/M_{\text{sat}} \) that is not included in the system of \( N = 39 \).

In order to observe carefully the behavior near the 1/3 magnetization, we evaluate the gradient \( \chi \) depicted in Figure 4. One finds that the characteristics of magnetization ramp appear more clearly in our new result of \( N = 39 \). In the smaller-\( M \) side of 1/3 magnetization, the divergent behavior occurs more remarkably. In the larger-\( M \) side of 1/3 magnetization, on the other hand, no discontinuous behavior exists. These two characteristics will be compared with the case in the triangular lattice antiferromagnet which reveals the behavior of a typical magnetization plateau in a two-dimensional magnet.

3.2. Triangle lattice antiferromagnet

Numerical-diagonalization studies were done from the results up to \( N = 36 \)\cite{7, 14}. Reference 15 reported that diagonalization calculations of \( N = 39 \) were carried out; unfortunately we were not able to find printed research papers.

We here present the magnetization process of the triangular lattice; our results are depicted in Figure 5. One observes that the behavior of a plateau appears at 1/3 magnetization irrespective to \( N \). No significant change can be seen in the width at 1/3 magnetization with increasing \( N \). No anomalous behavior seems present in other parts of \( M/M_{\text{sat}} \) than \( M/M_{\text{sat}} = 1/3 \).

Next, let us examine the behavior of the magnetization process by evaluating the gradient \( \chi \). One cannot find a significant system-size dependence in the region of \( M/M_{\text{sat}} \lesssim 0.5 \) although a small oscillating behavior appears in the region of \( M/M_{\text{sat}} \gtrsim 0.5 \). One observes clearly that \( \lim_{M/M_{\text{sat}} \rightarrow 1/3} \chi \) does not meet \( \chi \) just at \( M/M_{\text{sat}} = 1/3 \) and that \( \lim_{M/M_{\text{sat}} \rightarrow 1/3} \chi \) does not meet \( \chi \) just at \( M/M_{\text{sat}} = 1/3 \); the finite-size gradient \( \chi \) just at \( M/M_{\text{sat}} = 1/3 \) takes a small value that is getting smaller with increasing \( N \). Note that no diverging behavior is observed in the smaller-\( M \) side of \( M/M_{\text{sat}} = 1/3 \) although \( \chi \) gradually increases when \( M/M_{\text{sat}} \) is increases. This behavior of \( \chi \) is the one of a typical magnetization plateau in a two-dimensional magnet.

4. Summary and discussions

We have studied the magnetization process of the kagome lattice Heisenberg antiferromagnet by numerical diagonalization of finite-size clusters. We have presented new results of the system size \( N = 39 \). The magnetization process of the kagome lattice model for \( N = 39 \) shows the characteristics of the magnetization ramp more clearly, which are different from the behavior of the typical magnetization plateau observed in the triangular lattice antiferromagnet. The diverging behavior in the smaller-\( M \) side of \( M/M_{\text{sat}} = 1/3 \) suggests that a one-dimensional spin structure forms in the two-dimensional lattice structure, which is an interesting issue in
Figure 5. Magnetization process of the Heisenberg antiferromagnet on the triangular lattice. Results for $N = 39$ and 36 are represented by a black solid line and a red dotted line.

Figure 6. Field derivative of the magnetization of the Heisenberg antiferromagnet on the triangular lattice. Results for $N = 39$, 36, and 27 are denoted by black circles, red squares, and green triangles.

future studies. The critical behavior around the magnetization ramp of the kagome lattice antiferromagnet is discussed based on the results up to $N = 39$ in Reference 16.

It was pointed out that the ground state at $M/M_{sat} = 1/3$ in the magnetic field in the isotropic case is related to the state of the system of the XXZ-type anisotropic interactions[17]. Our study is now in progress concerning with the relationship between the magnetization ramp of the isotropic case and the magnetization process of the anisotropic case; results will be published
elsewhere.

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