Ferrimagnetism of the Heisenberg model on the Kagome strip lattice

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Abstract. We study ground-state properties of the $S = 1/2$ Heisenberg model on the Kagome strip lattice by using exact-diagonalization and density matrix renormalization group methods. When the strength of magnetic frustration is tuned, we find from our numerical calculations that there exists an intermediate phase between the non-magnetic phase and the ferrimagnetic phase of the well-known Lieb-Mattis type and that the local magnetization shows an incommensurate modulation with long-distance periodicity in the intermediate phase. Since the present model shares the same lattice structure in its inner part with the spatially anisotropic two-dimensional Kagome lattice in which an intermediate phase with a similar behavior is certainly observed, the intermediate phases of these models are the ferrimagnetic one of the unconventional non-Lieb-Mattis type.

1. Introduction
Ferrimagnetism is one of the most important phenomena in the field of magnetism. From studies on ferrimagnetism in recent years, a new type of ferrimagnetism was reported in several one-dimensional models with frustration\[1, 2, 3, 4, 5, 6, 7, 8\], which is different from the conventional ferrimagnetic state of the Lieb-Mattis (LM) type; the nontrivial ferrimagnetism of the new type is called the non-Lieb-Mattis (NLM) type.

The occurrence of the LM ferrimagnetism is understood from a viewpoint of the Marshall-Lieb-Mattis theorem\[9, 10\]. This theorem indicates that the spontaneous magnetization in the LM ferrimagnetic state is fixed to a simple fraction of the saturated magnetization. In the ferrimagnetism of the NLM type, on the other hand, the spontaneous magnetization changes continuously when the strength of the frustration is changed. The incommensurate modulation with long-distance periodicity of the local magnetization in the ground state is a characteristic behavior of the NLM ferrimagnetism. However, the mechanism of the occurrence of the NLM ferrimagnetism is still unclear.

Quite recently, it was found that the Heisenberg model on the spatially anisotropic Kagome lattice depicted in Fig.1(a) shows an intermediate-magnetization state between the LM ferrimagnetism and the non-magnetic state of the isotropic Kagome lattice as the first candidate of the NLM among the two-dimensional systems\[11\]. In this intermediate-magnetization state, it was confirmed that the spontaneous magnetization changes continuously when the strength of the frustration is changed and also that the local magnetization shows large dependence on the position of a site. However, it is difficult to judge certainly whether this behavior of the local
Figure 1. (a) Structure of spatially anisotropic Kagome lattice. (b) Structure of Kagome strip lattice with antiferromagnetic bonds $J_1$ (bold line) and $J_2$ (dotted line), and ferromagnetic bond $J_F$ (thin line). An $S = 1/2$ spin is located at each site denoted by a circle. Sublattices are represented by A, A’, B and C in each unit cell.

magnetization corresponds to the incommensurate modulation of the NLM ferrimagnetism or not because available system sizes are not sufficiently large in such a two-dimensional system.

In this study, we examine the ground-state properties of Heisenberg model on the Kagome strip lattice depicted in Fig.1(b) instead of the two-dimensional lattice of Fig.1(a), where the inner part of the strip lattice of Fig.1(b) is common to a part of the two-dimensional lattice of Fig.1(a). We show that the model on the strip lattice of Fig.1(b) reveals the NLM ferrimagnetism in the ground state. We also present our result of the local magnetization in the NLM ferromagnetic ground state, which clearly shows the incommensurate modulation with long-distance periodicity.

This paper is organized as follows. In the next section, we present the model Hamiltonian on the strip lattice depicted in Fig.1(b) and the methods of our numerical calculations. After we examine the ground-state properties in the classical model of the same Hamiltonian in §3, we present results of those of the quantum Hamiltonian in §4. The final section is devoted to summary and some remarks.

2. Model and Method

The Hamiltonian of the $S = 1/2$ Heisenberg model on the Kagome strip lattice depicted in Fig.1(b) is given by

$$
\mathcal{H} = J_1 \sum_i [S_{i,A} \cdot S_{i,B} + S_{i,B} \cdot S_{i,A'} + S_{i,B} \cdot S_{i,C} + S_{i,B} \cdot S_{i-1,C}] + J_2 \sum_i [S_{i,A} \cdot S_{i+1,A'} + S_{i,A'} \cdot S_{i+1,A'}] + J_F \sum_i [S_{i,A} \cdot S_{i+1,A} + S_{i,A'} \cdot S_{i+1,A'}].
$$

Here $S_{i,\xi}$ is an $S = 1/2$ spin operator at $\xi$ sublattice in the unit cell $i$, where sublattices A, A’, B and C are depicted in Fig.1(b). The number of spin sites is denoted by $N$; we consider $N/4$ is an integer. Energies are measured in units of $J_1$; we take $J_1 = 1$ hereafter. Here we examine the region of $0 < J_2/J_1 < \infty$ and limit $J_F/J_1 = -1$.

In this study, we use mainly two numerical methods: the numerical exact diagonalization (ED) method based on the Lanczos algorithm and the density matrix renormalization group (DMRG) method[12, 13]. We choose these two methods because it is well known that they are
reliable when one investigates low-energy properties of one-dimensional quantum systems with frustration. Note that we use the "finite-system" DMRG method in the present research. We carefully choose a maximum retained states number \((MS)\) and a sweep number \((SW)\) in the DMRG calculations; \(MS\) and \(SW\) are given in the caption of Fig.3.

3. Classical system

Before we present our results of the quantum system, we examine ground-state properties of the Hamiltonian \((1)\) within a classical picture with a characteristic angle \(\theta\) depicted in Fig.2, in which arrows denote classical spin vectors in a unit cell. Each classical vector has its length \(S\). Note that the state of \(\theta = 0\) shows the LM ferrimagnetism with \(M/M_s = 1/2\), where \(M_s\) represents the saturated magnetization. For \(J_2/J_1 = -1\), one can obtain the classical energy under the periodic boundary condition to be

\[
E(J_2, \theta) = J_1 N S^2 [- \cos(\theta) + (J_2/2J_1) \cos(2\theta) - 1/2].
\]

Minimizing \(E(J_2, \theta)\) enable us to obtain the magnetization of the selected state. One finds that the LM ferrimagnetism of \(\theta = 0\) with \(M/M_s = 1/2\) is realized for \(J_2/J_1 \leq 1/2\). When \(J_2/J_1\) is larger than \(1/2\), the lowest energy is given by \(J_1/J_2 = 2 \cos(\theta)\). Therefore, the normalized magnetization is given by

\[
M/M_s = (3 J_1/2 J_2 - 1)/4.
\]

Finally, the ground state becomes non-magnetic at \(J_1/J_2 = 2/3\). This result of the magnetization is depicted in Fig.3(b) and will be compared the results of the quantum system from our numerical calculations in the next section.

4. Quantum system

First, let us explain the way to obtain the spontaneous magnetization \(M\) in the ground state of the quantum system with isotropic Heisenberg interactions. Calculations by ED or DMRG methods provide us with the lowest energy \(E(N, S_{\text{tot}}^z, J_2/J_1)\) in each subspace of Hilbert space divided by \(S_{\text{tot}}^z\), where \(S_{\text{tot}}^z\) is the \(z\)-component of the total spin. For example, we present our results of the \(N = 96\) system from our DMRG calculations in Fig.3(a), in which energies of each value of \(S_{\text{tot}}^z\) are depicted for \(J_2/J_1 = 0.5\) and \(J_2/J_1 = 0.58\). The spontaneous magnetization \(M\) is determined by the following procedure. One finds the lowest energy among \(E(N, S_{\text{tot}}^z, J_2/J_1)\) for all the case of \(S_{\text{tot}}^z\). Among states having the lowest-energy level, the highest value of \(S_{\text{tot}}^z\) is the spontaneous magnetization. (See arrows displayed in Fig.3(a).)

Let us now present results of the \(J_1/J_2\)-dependence of \(M/M_s\) in Fig.3(b). The magnetization of the classical argument discussed in the above section is accompanied. We successfully find the existence of the intermediate region between the region of \(M/M_s = 1/2\) and the region...
of \( M/M_s = 0 \). Since the present model for \( J_2/J_1 = 0 \) meets conditions of the Marshall-Lieb-Mattis theorem, the LM ferrimagnetism is realized; thus the consequence of the theorem gives us \( M/M_s = 1/2 \). The region of \( J_1/J_2 \gtrsim 2 \) with \( M/M_s = 1/2 \) is directly connected to the LM ferrimagnetic state. Therefore, the region of \( M/M_s = 1/2 \) is regarded as the one of the LM ferrimagnetism. In the limit of \( J_2/J_1 \to \infty \), on the other hand, three spins of \( S_{i,A}, S_{i,C} \) and \( S_{i+1,A'} \) form a single \( S = 1/2 \) spin in the low-energy state; the system totally forms the \( S = 1/2 \) \( \Delta \) chain in one dimension and has the non-magnetic ground state. The properties of the system for finite but large \( J_2/J_1 \) are nontrivial at least now. The present results in Fig.3(b) indicate that the system undergoes a phase transition between the magnetically ordered state and the magnetically disordered state at around \( J_1/J_2 \sim 0.8 \).

Next, we study \( N \) dependences of the following two phase boundaries: the boundary between the phases of \( M/M_s = 1/2 \) and \( 0 < M/M_s < 1/2 \) denoted by the ratio \( r_1 = J_2/J_1 \) and the boundary between the phases of \( 0 < M/M_s < 1/2 \) and \( M/M_s = 0 \) denoted by the ratio of \( J_2/J_1 \) as \( r_2 \). We present results of \( N = 16, 20 \) and 24 from ED calculations under the periodic and the open boundary conditions and those of \( N = 48 \) and 96 from DMRG calculations under the open boundary condition. Results of \( r_1 \) from ED and DMRG calculations are consistent with each other irrespective of the difference of boundary conditions. One finds that the ratio \( r_1 \) converges to \( r_1 \sim 0.55 \) in the limit of \( N \to \infty \). Although the size dependence of \( r_2 \) is relatively larger than \( r_1 \), \( r_2 \) seems to go to the common value of \( r_2 \sim 1.18 \) in the thermodynamic limit. These results suggest that the presence of the region of intermediate-magnetization state with \( 0 < M/M_s < 1/2 \) is evident in the thermodynamic limit.

Let us study local magnetization \( \langle S_{i,\xi}^z \rangle \) within the subspace of the highest \( S_{tot}^z \) corresponding to the spontaneous magnetization \( M_0 \), where \( \langle Q \rangle \) denotes the expectation value of a physical quantity \( Q \). We investigate \( \langle S_{i,\xi}^z \rangle \) in the two phases of \( 0 < M/M_s < 1/2 \) and \( M/M_s = 1/2 \).
Figure 4. Size dependence of the phase boundary. The boundary between the phase of $M/M_s = 1/2$ and $0 < M/M_s < 1/2$ is denoted by $r_1$. The boundary between the phase of $M/M_s = 0$ and $0 < M/M_s < 1/2$ is represented by $r_2$. Triangles (Squares) denote the results under the periodic (open) boundary condition. Results for $N = 16, 20$ and $24$ are obtained from our ED calculations and those for $N = 48$ and $96$ are obtained from our DMRG calculations. The ratios $r_1$ and $r_2$ seem to be converged to $\sim 0.55$ and $\sim 1.18$ in the thermodynamic limit, respectively. The dotted lines are drawn as guides for eyes between the ED and DMRG data.

Results of $\langle S^z_{i, \xi} \rangle$ of the system of $N = 96$, namely $i = 1, 2, \cdots, 24$, at each sublattice A, A', B and C are depicted in Fig.5(a) and Fig.5(b) for $J_2/J_1 = 0.5$ and 0.58 respectively. In Fig.5(a), one can observe the uniform behavior of upward directions at sublattice A, A', and C and a downward direction at sublattice B although small boundary effects appear near the edges of the system. In Fig.5(b), on the other hand, we find an incommensurate modulation with long-distance periodicity clearly. This characteristic behavior of the local magnetization is a common phenomenon of the NLM ferrimagnetism in some one-dimensional quantum frustrated spin systems[4, 5]. Therefore we conclude that the phase of $0 < M/M_s < 1/2$ is the NLM

Figure 5. Local magnetization $\langle S^z_{i, \xi} \rangle$ at each sublattice, A (cross), A' (triangle), B (square) and C (pentagon). Panels (a) and (b) are results for $J_2/J_1 = 0.5$ and 0.58 respectively. These results are obtained from our DMRG calculations for $N = 96$ ($i = 1, 2, \cdots, 24$).
ferrimagnetism.

We briefly comment the case of $-1 < J_F \leq 0$. We confirm that the width of the intermediate-magnetization region is getting narrower when $|J_F|$ is decreased and that the region disappears before $J_F$ reaches $J_F = 0$. (not shown in this paper). This suggests that the interaction of $J_F$ stabilizes the intermediate phase as a substitute of a part which we cut off from the two-dimensional Kagome lattice depicted in Fig.1(a).

5. Summary and remarks

We have studied the ground state properties of $S = 1/2$ Heisenberg model on the Kagome strip lattice by using ED and DMRG methods. We have found the intermediate-magnetization phase between the non-magnetic phase and LM ferrimagnetic phase. In the intermediate-magnetization state, local magnetization is found to show an incommensurate modulation with long-distance periodicity. This characteristic behavior indicates that the intermediate-magnetization state is the ferrimagnetic state of the NLM type. If we remind that a symptom of the NLM ferrimagnetism is observed in the two-dimensional system on the spatially anisotropic Kagome lattice[11] although the reported results are not direct evidences, the phenomenon observed in the two-dimensional case is also the NLM ferrimagnetism presumably.

Finally, we mention the case of three-leg ladder with diagonal interactions which is a part of the spatially anisotropic triangular lattice[15]. In this case, intermediate phase is found between the ferrimagnetic and the non-magnetic Luttinger-liquid phases; but the intermediate phase is not NLM ferrimagnetic. This is different from the NLM ferrimagnetic intermediate phase in the present study.

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