Frustration-Induced Ferrimagnetism in Heisenberg Spin Chains

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We study ground-state properties of the Heisenberg frustrated spin chain with interactions up to fourth nearest neighbors by the exact-diagonalization method and the density matrix renormalization group method. We find that ferrimagnetism is realized not only in the case of $S = 1/2$ but also $S = 1$ despite that there is only a single spin site in each unit cell determined from the shape of the Hamiltonian. Our numerical results suggest that a “multi-sublattice structure” is not required for the occurrence of ferrimagnetism in quantum spin systems with isotropic interactions.

KEYWORDS: quantum spin chain, frustration, ferrimagnetism, DMRG, exact diagonalization

Ferrimagnetism is a fundamental phenomenon in the field of magnetism. One of the most typical examples of ferrimagnetism is the $(S, s) = (1, 1/2)$ mixed spin chain with a nearest-neighbor antiferromagnetic (AF) interaction.\(^1\) In this system, the so-called Lieb-Mattis-type ferrimagnetism\(^2,3\) is realized in the ground state because two different spins are arranged alternately in a line owing to the AF interaction. This system includes two spins in a unit cell of the system. In other known ferrimagnetic cases of quantum spin systems except the $S = 1/2$ Heisenberg frustrated spin chain studied in ref. 4, the situation that the system has more spins than one in each unit cell has been the same. Until our recent study\(^4\) demonstrated the occurrence of ferrimagnetism in the ground state of the $S = 1/2$ Heisenberg frustrated spin chain despite the fact that a unit cell of the chain includes only a single spin, namely, it has no sublattice structure, it had been unclear whether the “multi-sublattice structure” is required for the occurrence of the ferrimagnetism in a quantum spin system composed of isotropic interactions. The Hamiltonian examined in ref. 4 is given by

$$\mathcal{H} = J \sum_i [S_i \cdot S_{i+1} + \frac{1}{2} S_i \cdot S_{i+2}]$$

$$-J' \sum_i [S_i \cdot S_{i+3} + \frac{1}{2} (S_i \cdot S_{i+2} + A S_i \cdot S_{i+4})],$$

(1)

where the real constant $A$ is fixed to be unity. Here, $S_i$ is the $S = 1/2$ spin operator at the
site $i$. The numerical study of this system clarified the existence of the ferrimagnetic ground state when the controllable parameter $J'/J$ is changed. In addition, research confirmed that there are two types of ferrimagnetic phases: the phase of the Lieb-Mattis (LM) type and the phase of the non-Lieb-Mattis (NLM) type, which has been found in several frustrated spin systems.\textsuperscript{5–8)}

The purpose of this study is to confirm that the above example is not a special or rare case by investigating other models. In this study, we discuss the ground state of Hamiltonian (1) not only in the case of $S = 1/2$, but also in the case of $S_i$ being an $S = 1$ spin operator. Moreover, we focus on the case of $A = 0.4$, which is different from $A = 1$. Note that energies are measured in units of $J$; we set $J = 1$ hereafter.

We employ two reliable numerical methods, i.e., the density matrix renormalization group (DMRG) method\textsuperscript{9, 10)} and the exact-diagonalization (ED) method. Both methods can give precise physical quantities for finite-size clusters. The DMRG method is very powerful for a one-dimensional system under the open-boundary condition. On the other hand, the ED method does not suffer from the limitation posed by the shape of the clusters; there is no limitation of boundary conditions, although the ED method can treat only systems smaller than those that the DMRG method can treat. Note that, in the present research, we use the “finite-system” DMRG method.

In the present study, two quantities are calculated. One is the lowest energy in each subspace divided by $S_{z\text{tot}}$ to determine the spontaneous magnetization $M$, where $S_{z\text{tot}}$ is the $z$ component of the total spin. We obtain the lowest energy $E(N, S_{z\text{tot}}^z, J')$ for a system size $N$ and a given $J'$. For example, the $S_{z\text{tot}}^z$ dependence of $E(N, S_{z\text{tot}}^z, J')$ in a specific case of $J'$ is presented in the inset of Fig. 1(a). This inset shows the results obtained by our DMRG calculations of the system of $N = 72$ with the maximum number of retained states ($MS$) of 600, and a number of sweeps ($SW$) of 10. One can find the spontaneous magnetization $M$ for a given $J'$ as the highest $S_{z\text{tot}}^z$ among those at the lowest common energy. (See the arrowhead in the inset.) The other quantity is the local magnetization in the ground state for investigating the spin structure of the highest-$S_{z\text{tot}}^z$ state. The local magnetization is obtained by calculating $\langle S_i^z \rangle$, where $S_i^z$ is the $z$-component of the spin at the site $i$ and $\langle O \rangle$ denotes the expectation value of the physical quantity $O$ with respect to the state of interest.

First, let us show the results of the $J'$ dependence of $M/M_s$ in Fig. 1, where $M_s$ is the saturated magnetization. Irrespective of $S = 1/2$ or $S = 1$, we find the nonmagnetic phase ($M/M_s = 0$) and ferromagnetic phase ($M/M_s = 1$). Between the two phases, we also find three regions: the regions of $0 < M/M_s < 1/3$, $M/M_s = 1/3$, and $1/3 < M/M_s < 1$. For $S = 1/2$, ...
one can see that the region of $0 < M/M_s < 1/3$ is much narrower than the distinctly existing region of NLM ferrimagnetism in the case of $S = 1/2$ with $A = 0.4$. The width of the present region for $A = 0.4$ seems to vanish in the limit of $N \to \infty$. One finds that the occurrence of the NLM ferrimagnetism in Hamiltonian (1) requires a fourth-neighbor interaction with $A$ that is larger than the specific value between $A = 0.4$ and $A = 1$. The width of the region of $M/M_s = 1/3$ in both cases of $S = 1/2$ with $A = 0.4$ and $S = 1$ with $A = 0.4$ seems to survive in the limit of $N \to \infty$. The region of $1/3 < M/M_s < 1$ is presumably considered to merge with the ferromagnetic (FM) phase in the thermodynamic limit. The reason for this is that this region appears only near $M/M_s = 1$ and that $M/M_s$ in this region becomes progressively larger with increasing $N$. In addition, we cannot confirm this region in the calculations within $N \leq 30$ of the $S = 1/2$ system under the periodic-boundary condition irrespective of the values of $A$. The issue of whether or not the region of $1/3 < M/M_s < 1$ survives should be clarified in future studies; hereafter, we do not pay further attention to this issue.
Fig. 2. (a) Size dependences of the boundaries of the regions in the case of $S = 1$ with $A = 0.4$. The results presented are those of $N = 24, 36, 48, 60, \text{and } 72$ from the DMRG calculations. (b) Size dependence of the width of each region in the case of $S = 1$ with $A = 0.4$. The width of the region of $0 < M/M_s < 1/3$ and that of $M/M_s = 1/3$ are defined as $|J'_2 - J'_1|$ and $|J'_3 - J'_2|$, respectively.

Fig. 3. Local magnetization $\langle S^z_i \rangle$ under the open-boundary condition: for $J' = 2.1$ in the case of $S = 1$ with $A = 0.4$ from the DMRG calculation for $N = 72$. The site number is denoted by $i$, which is classified into $i = 3n - 2$, $3n - 1$, and $3n$, where $n$ is an integer. Squares, circles, and triangles mean $i = 3n - 2$, $3n - 1$, and $3n$, respectively.

Next, we study the size dependences of the phase boundaries in the case of $S = 1$ with $A = 0.4$ depicted in Fig. 2(a). We present results of four boundaries: $J' = J'_1$ between the nonmagnetic phase and the region of $0 < M/M_s < 1/3$, $J' = J'_2$ between the regions of $0 < M/M_s < 1/3$ and $M/M_s = 1/3$, $J' = J'_3$ between the regions of $M/M_s = 1/3$ and $1/3 < M/M_s < 1$, and $J' = J'_4$ between the region of $1/3 < M/M_s < 1$ and the FM phase. To confirm the behavior up to the thermodynamic limit, we also examine the $N^{-1}$ dependences of the two widths of the regions of $M/M_s = 1/3$ and $0 < M/M_s < 1/3$ in Fig. 2(b). Although the width of the region of $M/M_s = 1/3$ decreases with increasing $N$, this dependence shows a behavior that is convex-downwards for large sizes; the width seems to converge to 0.3. Therefore, the phase of $M/M_s = 1/3$ definitely survives in the limit of $N \to \infty$. On the other hand, the width of $0 < M/M_s < 1/3$ obviously disappears in the limit of $N \to \infty$. An appropriate tuning of the parameters in Hamiltonian (1) of the $S = 1$ system might cause the
NLM ferrimagnetism; such parameter sets should be searched for in future studies.

Finally, we examine the local magnetization $\langle S_z^i \rangle$ in the phase of $M/M_s = 1/3$ in the case of $S = 1$ with $A = 0.4$. In Fig. 3, we present our DMRG result of $\langle S_z^i \rangle$ of the system of $N = 72$. We confirm the up-down-up spin behavior, and this spin structure is consistent with $M/M_s = 1/3$ in the parameter region near approximately $J' = 2.1$ in Fig. 1(b). Thus, this phase is considered to be the LM-type ferrimagnetic phase.

In summary, we study the ground-state properties of a frustrated Heisenberg spin chain by the ED and DMRG methods. Despite the fact that this system consists of only a single spin site in each unit cell determined from the shape of the Hamiltonian, the LM-type ferrimagnetic ground state is realized in a finite region not only in the case of $S = 1/2$ but also of $S = 1$. The present models showing ferrimagnetism indicate that a “multi-sublattice structure” is not required for the occurrence of ferrimagnetism in quantum spin systems with isotropic interactions as a general circumstance.

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