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Spontaneous Magnetization of the Spin-1/2 Heisenberg Antiferromagnet on the Triangular Lattice with a Distortion

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Abstract. The spin-1/2 triangular-lattice Heisenberg antiferromagnet with a $\sqrt{3} \times \sqrt{3}$-type distortion is studied by the numerical-diagonalization method. We examine this model between the two cases, one is the undistorted triangular lattice and the other is the model on the honeycomb lattice with isolated spins. When the distortion is controlled, we find a nontrivial region where the ground states shows spontaneous magnetization; the magnitude increases gradually as the distortion is larger and is smaller than one third of the saturated magnetization.

1. Introduction

The triangular-lattice antiferromagnet is a typical system that has attracted much attention from its behavior owing to frustrations. In particular, such attention has increased explosively since Anderson pointed out that the quantum Heisenberg antiferromagnet on the triangular lattice is a candidate system of the spin liquid state[1]. Nowadays, it is widely believed that the so-called 120-degree structure is realized as a spin structure of its ground state. Extensive studies concerning this system have been carried out from various aspects[2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21]. Some experiments reported that antiferromagnets have the triangular-lattice structure[22, 23, 24, 25]. Some of them, however, include a distortion in the triangular lattice[24, 25]; the type of this distortion is called the $\sqrt{3} \times \sqrt{3}$-type one. Unfortunately, theoretical understanding concerning effects due to the $\sqrt{3} \times \sqrt{3}$-type distortion in the quantum triangular-lattice antiferromagnet is still insufficient.

Under the above mentioned circumstances, a quite recent study[26] reported the spin-1/2 triangular-lattice antiferromagnet with the $\sqrt{3} \times \sqrt{3}$-type distortion shows an interesting intermediate spin state in the ground state between the undistorted case and the case of the dice lattice[27]. The dice-lattice antiferromagnet is a nonfrustrated system having a ferrimagnetic ground state of the up-up-down structure based on the so-called Lieb-Mattis theorem[28]. The intermediate state shows nonzero spontaneous magnetization but its magnitude is smaller than one third which is realized in the dice-lattice case. Unfortunately, the range of such the intermediate state is different from the experimental cases mentioned above[24, 25]. Therefore, it is an urgent task to clarify properties of the quantum system in the range of the distortion corresponding to the experimental cases.

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The purpose of the present study is to clarify effects of the $\sqrt{3} \times \sqrt{3}$-type distortion in the spin-1/2 Heisenberg antiferromagnet on the triangular lattice illustrated in Fig. 1 by means of a numerical-diagonalization method of the Lanczos algorithm. In particular, we examine the model between the two cases, one is the undistorted triangular lattice and the other is the model on the honeycomb lattice with isolated spins. Our numerical results suggest that the ground states in the region close to the two limiting cases do not show a spontaneous magnetization; however, there appear nonzero spontaneous magnetizations in an intermediate region. The spontaneous magnetization is smaller than one third of the saturated magnetization and increases gradually as the distortion is larger.

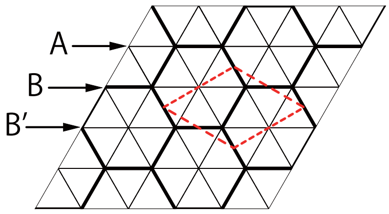

Figure 1. Lattice studied in the present paper. Its unit cell is shown by the red rhombus. The sublattices A, B, and B′ are also illustrated.

This paper is organized as follows. In the next section, the model Hamiltonian treated here and the methods used in this study are explained. The third section is devoted to the presentation and the discussion of our numerical results. In the final section, the summary is given.

2. Model Hamiltonian and methods

The Hamiltonian examined in this study is given by

$$\mathcal{H} = \sum_{i \in \mathrm{B}, j \in \mathrm{B}'} J_1 \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \sum_{i \in \mathrm{A}, j \in \mathrm{B}} J_2 \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \sum_{i \in \mathrm{A}, j \in \mathrm{B}'} J_2 \boldsymbol{S}_i \cdot \boldsymbol{S}_j . \tag{1}$$

Here, $\boldsymbol{S}_j$ represents the $S = 1/2$ spin operator at site j. Let us consider, in this study, the case of isotropic interaction in spin space. The site j is assumed to be the vertices of the lattice depicted in Fig. 1. The number of spin sites is represented by N_{s}. Note here that the vertices are divided into three sublattices A, B, and B′; each site j_{A} in the A sublattice is linked by six interaction bonds J_2 denoted by thin lines; each site j_{B} in the B or $j_{\mathrm{B}'}$ in the B′ sublattice is linked by three interaction bonds J_2 and three interaction bonds J_1, denoted by thick lines. The ratio of J_2/J_1 is denoted by r. All interactions are supposed to be antiferromagnetic, namely, $J_1 > 0$ and $J_2 > 0$. Energies are measured in units of J_1; hereafter, we set $J_1 = 1$. In particular, we examine the case of $J_2 \leq J_1$ in this study. Note that for $J_1 = J_2$, namely, $r = 1$, the present lattice is identical to the triangular lattice; the ground state of the system on this lattice is understood as the so-called 120-degree structure illustrated in Fig. 2(a). Therefore, this state clearly has no spontaneous magnetization. Just for $r = 0$, on the other hand, the network of the vertices becomes the honeycomb lattice accompanied by isolated spins. At zero temperature, the system shows degenerate ground states. One of the states is illustrated in Fig. 2(c). This state corresponds to the highest magnetization among the degenerate ground states. Note however that when infinitesimally small J_2 is switched on, it is a nontrivial issue whether or not the state illustrated in Fig. 2(c) becomes the lowest-energy state as a result of the perturbative effect of small J_2. Note also that, in the case of $J_2 \geq J_1$, a nontrivial intermediate phase was found between $r = 1$ for the triangular lattice and $r \to \infty$ for the dice lattice[26].

The finite-size clusters that we treat in the present study are depicted in Fig. 3(a)-(d). We examine the cases of $N_{\mathrm{s}} = 12$, 21, 27, and 36 under the periodic boundary condition. In all the cases, $N_{\mathrm{s}}/3$ is an integer; therefore, the number of spin sites in a sublattice is the same

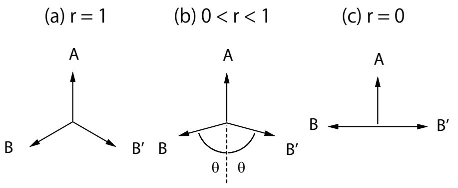

Figure 2. Possible spin states based on a classical picture for $r = 1$, $0 < r < 1$, and $r = 0$, respectively.

irrespective of sublattices. The clusters are rhombic and have an inner angle $\pi/3$; this shape allows us to capture two dimensionality well.

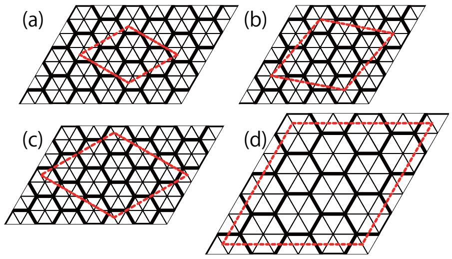

Figure 3. Finite-size clusters treated in the present study. Panels (a), (b), (c), and (d) denote cases for $N_s = 12$, 21, 27, and 36, respectively.

We calculate the lowest energy of $\mathcal{H}$ in the subspace characterized by $\sum_j S_j^z = M$ by numerical diagonalizations based on the Lanczos algorithm and/or the Householder algorithm. The numerical-diagonalization calculations are unbiased against any approximations; thus we are able to obtain reliable information of the system. We denote the energy by $E(N_s, M)$, where M takes an integer or a half odd integer up to the saturation value M_{sat} $(= N_s/2)$. We focus our attention on spontaneous magnetization M_{spo}; our calculations can determine M_{spo} as the largest value of M among the lowest-energy states. Note that for cases of odd N_s, the smallest M_{spo} cannot rigorously vanish; the result of $M_{spo} = 1/2$ in the ground state indicates that the system shows no spontaneous magnetization. Part of the Lanczos diagonalizations were carried out using an MPI-parallelized code, which was originally developed in the study of Haldane gaps[29]. The usefulness of our program was confirmed in several large-scale parallelized calculations[30, 31, 32, 33].

3. Results and discussion

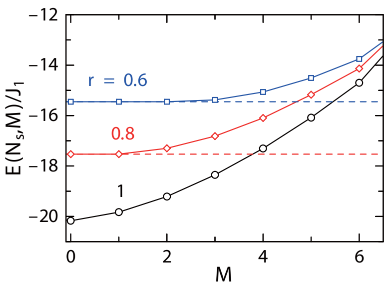

Figure 4. M-dependence of the ground-state energy for $N_s = 36$ when the distortion in the lattice is switched on. Black circles, red diamonds, and blue squares denote results for $r = 1$, 0.8, and 0.6, respectively.

First, let us observe magnetization-dependence of the ground state energy which lets us recognize whether the spontaneous magnetization appears or not and which provides us with information about the magnitude of the spontaneous magnetization M_{spo} if it appears; results for $N_s = 36$ are depicted in Fig. 4. For $r = 1$, the energy for $M = 0$ is lower than any other energies for $M > 0$, which indicates that the spontaneous magnetization does not appear in the ground state, namely, $M_{spo} = 0$. For $r = 0.8$ and 0.6, on the other hand, the ground states are degenerate; the degeneracy is illustrated by broken lines in Fig. 4. These degeneracies indicate that nonzero $M_{\rm spo}$ appears. The largest M in the degenerated ground states corresponds to $M_{\rm spo}$; one finds $M_{\rm spo} = 1$ and $M_{\rm spo} = 2$ for $r = 0.8$ and 0.6, respectively.

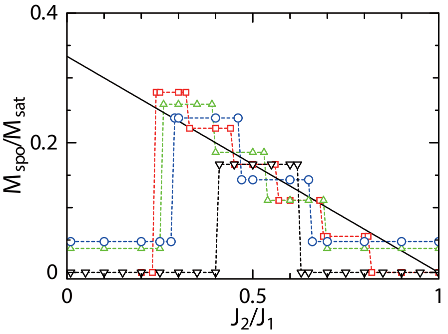

Figure 5. r-dependence of the spontaneous magnetization for various $N_{\rm s}$. Red squares, green triangles, blue circles, and black inversed triangles denote results for $N_{\rm s}$ = 36, 27, 21, and 12, respectively. The line denotes the result from the classical picture illustrated in Fig. 2(b).

Next, we examine the change of the spontaneous magnetization when r is controlled in $0 < r \le 1$; results for various $N_{\rm s}$ are depicted in Fig. 5. For all the cases of $N_{\rm s}$=12, 21, 27, and 36, the region of nonzero $M_{\rm spo}$ certainly exists. Note that the nonzero $M_{\rm spo}$ gradually increases when r is decreased. Note also that all possible values as $M_{\rm spo}$ are realized although the maximum of $M_{\rm spo}$ does not reach $(1/3)M_{\rm sat}$. The r-dependence of $M_{\rm spo}$ is compared with the result from the argument based on a classical picture illustrated in Fig. 2(b). In the region of r with nonzero-$M_{\rm spo}$ up to $M_{\rm spo} = (1/3)M_{\rm sat} - 1$, brief dependence of the quantum case seems to agree with the classical line although step-like behavior owing to a finite-size effect exists. However, it is unclear within the present calculations whether the spin states in the quantum case are certainly understood well by the simple classical picture shown in Fig. 2(b) because such a example is actually known[26]. Intensive examination of the nonzero-$M_{\rm spo}$ spin states should be tackled in future studies. In the viewpoint of the appearance of states with continuously increasing $M_{\rm spo}$, similar behavior was observed in other various systems[34, 35, 36, 37, 38, 39, 40, 41]; these nontrivial states are considered to be so-called *non-Lieb-Mattis* ferrimagnetic ones. The relationship between the nonzero-$M_{\rm spo}$ states and the non-Lieb-Mattis ferrimagnetic states should be tackled in future studies. When r is further decreased, one can noticeably observe that the spontaneous magnetization discontinuously disappears. A marked behavior is that the range of nonzero $M_{\rm spo}$ gradually widens as the system size is increased. With decreasing r, here, we define $r_{\rm c2}$ as the value of r where $M_{\rm spo}$ changes from 0 or 1/2 to larger values and $r_{\rm c1}$ as the value of r where $M_{\rm spo}$ decreases again to 0 or 1/2 from larger values. The system size dependences of $r_{\rm c1}$ and $r_{\rm c2}$ are depicted in Fig. 6. One finds that $r_{\rm c2}$ gradually increases with increasing $N_{\rm s}$ and that it seems to go to a value close to $r = 1$. On the other hand, $r_{\rm c1}$ gradually decreases with increasing $N_{\rm s}$, but it seems to converge to a nonzero value. It is unclear at present whether $r_{\rm c1}$ converges to zero or a nonzero value in the thermodynamic limit, which should be clarified in future studies. As a primary consequence of this study, the present calculations strongly suggest that the presence of the nonzero-$M_{\rm spo}$ region is evident.

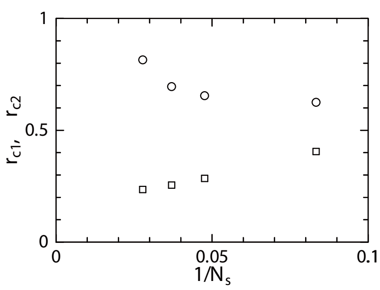

Figure 6. Size dependence of the boundaries of the nonzero-$M_{\rm spo}$ phase. Squares and circles denotes results for $r_{\rm c1}$ and $r_{\rm c2}$, respectively.

Next, let us discuss the behavior around $r = r_{c1}$ under the assumption that r_{c1} converges to a nonzero value in the thermodynamic limit. We consider the M-dependence of the ground-state energy; our numerical results for $N_s = 36$ are depicted in Fig. 7. For $N_s = 36$, our calculations for $r = 0.24$ indicate $M_{spo} = 5$ and those for $r = 0.23$ indicate that M_{spo} vanishes. For $r = 0.23$, however, the degeneracy from $M = 2$ to $M = 5$ still survives, which is illustrated by a broken line in Fig. 7. In our calculations for $r = 0.2$, on the other hand, the degeneracy appears from $M = 4$ to $M = 5$. One finds that the degeneracy gradually collapses from the side of smaller-M. The behavior around $r = r_{c1}$ is absolutely different from the behavior around $r = r_{c2}$ shown in Fig. 3. The spin state in the region of $0 < r < r_{c1}$ is unclear at present. To know the characteristics within numerical calculations, correlation functions for large systems are required. Another possible approach that is applicable to attack this issue may be a perturbation calculation from the case of $r = 0$. Such future studies would give additional information about this state.

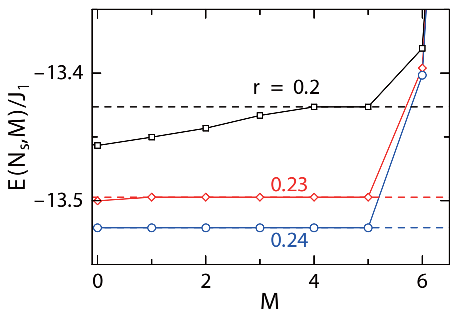

Figure 7. M-dependence of the ground-state energy for $N_s = 36$ in the region near $r = r_{c1}$ where the spontaneous magnetization is vanishing owing to a large distortion. Blue circles, red diamonds, and black squares denote results for $r = 0.24$, 0.23, and 0.2, respectively.

Finally, let us discuss our results based on the experimental results[24, 25]. Neutron scattering experiment in $RbVBr_3$ reported that the ratio of interactions is $r \sim 0.59$[24]. From our results in Fig. 5, $r \sim 0.59$ corresponds to the spontaneous magnetization of $M_{spo}/M_{sat} \sim 0.1$-0.2. Concerning $RbFeBr_3$, on the other hand, ref. [25] concluded $r < 1$ but did not give a specific value for r unfortunately. Our numerical results will be helpful to analyze experimental results of these materials.

4. Summary

We studied the ground state of the spin-1/2 Heisenberg antiferromagnet on the triangular lattice with a $\sqrt{3} \times \sqrt{3}$-type distortion by the numerical-diagonalization method. We find a region of nontrivial states showing spontaneous magnetization between the case of undistorted triangular lattice and the case of the honeycomb-lattice system accompanied by isolated spins. Nontrivial spin states with spontaneous magnetization have been found in various systems of some modified cases from the kagome-lattice antiferromagnet, the square-kagome-lattice antiferromagnet, the Cairo-pentagon-lattice antiferromagnet, the Lieb-lattice antiferromagnet, and so on[39, 40, 42, 43, 44, 45, 46]. Comparison between our present finding and these previously known information contributes much for our understanding of frustration effects in magnetic materials.

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hp170070, and hp170207). Some of the computations were performed using facilities of the Department of Simulation Science, National Institute for Fusion Science; Institute for Solid State Physics, The University of Tokyo; and Supercomputing Division, Information Technology Center, The University of Tokyo. This work was partly supported by the Strategic Programs for Innovative Research; the Ministry of Education, Culture, Sports, Science and Technology of Japan; and the Computational Materials Science Initiative, Japan.

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