Exact diagonalization study of the spin-1 two-dimensional $J_1$-$J_3$ Heisenberg model on a triangular lattice

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Abstract

The spin-1 Heisenberg model on a triangular lattice with the ferromagnetic nearest- and antiferromagnetic third-nearest-neighbor exchange interactions, $J_1 = -(1 - p)J$ and $J_2 = pJ$, $J > 0$ ($0 \leq p \leq 1$), is studied with the use of the SPINPACK code. This model is applicable for the description of the magnetic properties of NiGa$_2$S$_4$. The ground, low-lying excited state energies and spin-spin correlation functions have been found for lattices with $N=16$ and $N=20$ sites with the periodic boundary conditions. These results are in qualitative agreement with earlier authors’ results obtained with Mori’s projection operator technique.

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Key words: Heisenberg antiferromagnet, triangular lattice, exact diagonalization

The spin-1 $J_1$-$J_3$ Heisenberg model on a triangular lattice, which takes into account the ferromagnetic nearest- and antiferromagnetic third-nearest-neighbor exchange interactions ($J_1$ and $J_3$, respectively) is of interest as a minimal model for the description of magnetic properties of the compound NiGa$_2$S$_4$ [1]. These properties are mainly determined by the two-dimensional triangular lattice of Ni$^{2+}$ ions with the spin $S = 1$. In particular, the magnetic neutron scattering experiment revealed the incommensurate short-range order [1] - the scattering intensity had a maximum at some incommensurate vector $Q_{\text{exp}}$. The classical version of the $J_1$-$J_3$ model was proposed in Ref. [1], authors of which were able to reproduce the observed incommensurate order with the vector $Q_{\text{exp}}$ by fitting the ratio $J_1/J_3$. The quantum $J_1$-$J_3$ Heisenberg model was investigated in our recent papers [2,3] with the use of Mori’s projection operator technique [1]. It was shown that at zero temperature, depending on the ratio $J_1/J_3$, the system is characterized by the ferromagnetic ordering, spin disorder, incommensurate and commensurate antiferromagnetic ordering. At $J_1/J_3 \approx -0.22$ the model

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describes key features observed [1] in NiGa2S4 - the incommensurate antiferromagnetic short-range order at finite temperature, the quadratic temperature dependence of specific heat and the shape of the uniform susceptibility.

Applying Mori’s method one has to use a number of approximations. Therefore, it is of interest to study the same model with another method and compare obtained results. In this work we employ Schuelenburg’s SPINPACK code [5]. This package is dedicated for exact diagonalization (ED) of finite spin system using Lanczos algorithm.

The Hamiltonian of the model reads

\[ H = \frac{1}{2} \sum_{nm} J_{nm} \left( s_n^z s_m^z + s_n^{+1} s_m^{-1} \right) , \]  

where \( s_n^z \) and \( s_n^\sigma \) are the components of the spin-1 operators \( s_n \), \( n \) and \( m \) label sites of the triangular lattice, \( \sigma = \pm 1 \). As mentioned above, we take into account the nearest-neighbor and third-nearest-neighbor interactions, \( J_{nm} = J_1 \sum_a \delta_{n,m+a} + J_3 \sum_A \delta_{n,m+A} \) with the vectors \( a \) and \( A=2a \) connecting the respective sites. Here the frustration parameter \( p \) is introduced, \( J_1 = -(1-p)J \), \( J_3 = pJ \). \( J > 0 \) will be used below as the unit of energy.

For \( 0 \leq p \leq 1 \) we found energies of the ground, low-lying excited states and spin-spin correlation functions for lattices containing \( N = 16 \) and 20 sites. These lattices are shown in Fig. 1. The periodic boundary conditions were used. From our earlier study of the quantum \( J_1-J_3 \) Heisenberg model on a \( 216 \times 216 \) lattice with Mori’s method [2,3] it is known that the system is ferromagnetically ordered in the interval \( 0 < p < p_{cr} \), \( p_{cr} \approx 0.2 \), when the ferromagnetic coupling \( |J_1| \) is larger than \( J_3 \). We have found the same value also in the classical \( J_1-J_3 \) model on an infinite lattice.

As seen from Figs. 2 and 3, the ground state (GS) of the \( N \)-site lattice is transformed from the classic ferromagnet (S=N) to the singlet state at some critical value of the frustration parameter \( p \). For the lattices with \( N=16 \) and \( N=20 \) these critical values are \( p_{16} \approx 0.45 \) and \( p_{20} \approx 0.28 \), respectively. It can be supposed that with the rise of the lattice size this critical value will tend to the value \( p_{cr} \) obtained in [2]. According to [2] a transition from the ferromagnetically ordered state to a spin disorder occurs at this value of the frustration parameter \( p_{cr} \). In Figs. 2a and 3a the dependencies of the GS energy (\( E_{GS} \), S=N) and the first excited state (\( E_1 \), S=15 and S=19, correspondingly) on \( p \) are presented. These dependencies are linear. Differences between the GS and excited-state energies disappear at the critical values \( p_{16} \) and \( p_{20} \). For \( p > p_{16} \) and \( p > p_{20} \) the energies of the low-lying states are shown in Figs. 2b and 3b. The GS is characterized by \( S=0 \). The lowest excited states are characterized by \( S=0 \) (\( E_2 \)) and \( S=1 \) (\( E_3 \)). Notice that relative positions of the curves for the first singlet \( E_2 \) and the first triplet \( E_3 \) excitations are different for \( N=16 \) and \( N=20 \). Apparently the difference is related to the small size of the lattices and difference in their shapes.

The spin gap - the energy difference between the first excited triplet and the singlet ground state - is shown in Fig. 4 for \( N=16 \) and \( N=20 \).
In Fig. 5 we compare the dependencies of the GS energy per site on the frustration parameter $p$ in the $N=20$, $N=16$ lattices, obtained by ED, and in a $216 \times 216$ lattice obtained by Mori’s projection operator technique [2]. As a whole these dependencies are similar. As one can see, all these plots are linear in the ferromagnetic region ($p < p_{16}$, $p_{20}$ or $p_{cr}$). Besides, $p_{cr} < p_{20} < p_{16}$. This sequence of the critical values of $p$ seems reasonable because Mori’s result was obtained in the largest lattices. For $p > p_{16}$, $p_{20}$ or $p_{cr}$ all curves have maxima. However, positions of the maxima are different: $p \approx 0.7$ for $N=16$ and $p \approx 0.9$ for $N=20$.

Spin correlation functions for nearest- and third-nearest-neighbors are shown in Fig. 6. The data were obtained by the exact diagonalization in the $N=20$ lattice and by Mori’s technique in a $216 \times 216$ lattice. In panels (a) and (b) ED correlations are constant and equal to unity in the ferromagnetic phase for $p < p_{20}$. In this region correlation functions obtained by Mori’s method are also constant. However, they are somewhat smaller than one due to approximations made in the $S=1$ case [2]. The interaction between nearest neighbor spins vanishes at $p = 1$, which manifests itself in the vanishing correlation $\langle S_0 S_a \rangle$. The correlation $\langle S_0 S_{2a} \rangle$ depends only weakly on $p$ in the range $p > p_{20}$ and $p > p_{cr}$. Analyzing condensation parameters, in Ref.[2] it was shown that at $T = 0$ in the range $p_{cr} < p \lesssim 0.31$ there exists a spin-disordered phase. For larger frustration parameters the system becomes an antiferromagnet with an incommensurate ordering vector, which varies with $p$. Notice that the phase transition at $p \approx 0.31$ does not reveal itself in Fig. 6. As seen from the figure, curves obtained in the larger lattice are more smooth than those in the $N=20$ lattice, which, at least partly, may be connected with finite-size effects. However, spin correlations calculated in the two lattices by two different methods are in general close and behave similarly with changing the frustration parameter. We can conclude that results obtained with the approximate approach based on Mori’s projection operator technique are in reasonable agreement with the exact-diagonalization data.

In conclusion, we investigeted the spin-1 Heisenberg model on a triangular lattice with the ferromagnetic nearest- and antiferromagnetic third-nearest-neighbor exchange interactions with the use of the exact diagonalization of small lattices with periodic boundary conditions. The SPINPACK code using the Lanczos method was employed to find the energies of the ground and low-lying exited states in the entire range of the frustration parameter $0 < p < 1$, where $p = \frac{J_3}{J_1-J_3}$, $J_1$ and $J_3$ are the nearest- and third-nearest exchange constants. Besides, spin-spin correlation functions between nearest- and third-nearest spins and spin gaps were calculated. We found qualitative and in some cases quantitative agreement between results on the ground-state energy and spin correlations, obtained by exact diagonalization of small lattices and by Mori’s projection technique in larger lattices.

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Figure captions

Fig. 1. The triangular lattices with N=16 and N=20 sites, studied in this work.

Fig. 2. a) The dependencies of the ground state energy ($E_{GS}$, S=N=16, squares, solid line) and the energy of the lowest excited state with S=N-1=15 ($E_1$, circles, dashed line) in the range of the frustration parameter $p \leq 0.45$ on the N=16 lattice. In this interval of $p$, the system is characterized by the ferromagnetic order, b) The dependencies of the ground state energy ($E_{GS}$, S=0, squares, solid line), the energy of the lowest singlet excited state ($E_2$, circles, short-dashed line) and the energy of the lowest triplet excited state ($E_3$, S=1, triangles, dashed line) in the frustration parameter range $p \geq 0.45$.

Fig. 3. a) The dependencies of the ground state energy ($E_{GS}$, S=N=20, squares, solid line) and the energy of the lowest excited state with S=N-1=19 ($E_1$, circles, dashed line) in the range of the frustration parameter $p \leq 0.28$ on the N=20 lattice. In this interval of $p$, the system is characterized by the ferromagnetic order, b) The dependencies of the ground state energy ($E_{GS}$, S=0, squares, solid line), the energy of the lowest singlet excited state ($E_2$, circles, short-dashed line) and the energy of the lowest triplet excited state ($E_3$, S=1, triangles, dashed line) in the frustration parameter range $p \geq 0.28$.

Fig. 4. The dependencies of the spin gap $E_3(S=1) - E_{GS}(S=0)$ on the frustration parameter $p$ for the N=16 (solid line) and the N=20 (dashed line) lattices.

Fig. 5. The dependencies of the ground state energy per site ($E_{GS}/N$) on the frustration parameter $p$ for the N=20 lattice (solid line), the N=16 lattice (dash-dotted line), obtained by ED, and in a $216 \times 216$ lattice, obtained by Mori’s projection operator technique (dashed line). The parameters $p_{20}$, $p_{16}$ and $p_{cr}$ are values of $p$, at which the transition from the ferromagnetic to the singlet GS occurs.

Fig. 6. The nearest-neighbor (a) and third-nearest-neighbor spin correlations, obtained in the N=20 lattice (circles and dashed lines) and in a $216 \times 216$ lattice at $T = 0$ by Mori’s technique (squares and solid lines).
N=16

- $E_1$ (S=15)
- $E_{gs}$ (S=16)

- $E_2$ (S=0)
- $E_{gs}$ (S=0)

ENERGY vs. $\rho$

- N=16
- $E_1$ (S=15)
- $E_{gs}$ (S=16)
- $E_2$ (S=0)
- $E_{gs}$ (S=0)
\[ N = 20 \]
$E_3(S=1) - E_{\text{GS}}$

- $N=16$
- $N=20$
