Ground state of the spin-\(\frac{1}{2}\) Heisenberg antiferromagnet on an Archimedean 4-6-12 lattice

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An investigation of the Néel Long Range Order (NLRO) in the ground state of antiferromagnetic Heisenberg spin system on the two-dimensional, uniform, bipartite lattice consisting of squares, hexagons and dodecagons is presented. Basing on the analysis of the order parameter and the long-distance correlation function the NLRO is shown to occur in this system. Exact diagonalization and variational (Resonating Valence Bond) methods are applied.

Due to the recent renewal of interest in low dimensional quantum antiferromagnetism, caused mainly by its possible connection with the mechanism of the high-\(T_c\) superconductivity, one has to notice a great progress in the understanding of the nature of the ground state of quantum Heisenberg antiferromagnets for low values of spin variables on low-dimensional lattices. One of the basic issues in the investigations concerning this subject is the question whether a Néel Long Range Order (NLRO) exists in the ground state of an antiferromagnetic spin-\(\frac{1}{2}\) system on a given lattice and how it can be destroyed. This is also the question about the result of the nontrivial and subtle interplay between quantum fluctuations and other mechanisms which can destroy or stabilize NLRO in the ground state. At least two such mechanisms seem to be relevant, namely the local singlet formation tendency and frustration. For example, the first mechanism which breaks the NLRO is present in the
spin system on 1/5-depleted square lattice (being the prototype of the \(CaV_4O_9\) lattice) and it manifests in continuous quantum phase transition with critical exponents which seem to belong to three-dimensional classical Heisenberg universality class \([1,2]\). On the other hand, in a case of a generic model of frustrated antiferromagnet, see e.g., Ref. \([3,4]\), namely \(J_1 - J_2\) model, the growing frustration \((J_2/J_1)\) gives rise to the continuous phase transition. Remarkably, there also may exist systems in which two above competing mechanisms are being built in, like the spin system on Shastry-Sutherland lattice \([5]\) (being the prototype of \(SrCu_2(BO_3)_2\) lattice). The question about the nature of the phase transition in this system remained for some time a puzzle and finally it came out that in the very small area of the parameter space there exists a novel spin-gap phase between the dimerized and long range ordered phases \([6]\) and a continuous transition occurs in the vicinity of a discontinuous one. Another example of this type is the \(J - J'\) model (see, e.g., Ref. \([7]\) and references therein).

Although it is rather widely accepted that spin systems with antiferromagnetic interactions on lattices with low coordination numbers and frustrated ones are the best candidates for disordered ground state, the general question about the NLRO remains not completely answered.

In this paper we focus on a spin-\(\frac{1}{2}\) system with equal, antiferromagnetic, nearest neighbor interactions:

\[
H = \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j. 
\]

(1)
on one of the Archimedean lattices - on the 4-6-12 (square-hexagonal-dodecagonal - SHD) lattice. Note, that in the spin system on the SHD lattice, opposite to the honeycomb lattice (the same coordination number), the nearest neighbors are not equivalent. This, in the natural way, favors the formation of the local singlets i.e., acts against the NLRO. Since our earlier conclusion \([13]\) concerning the existence of NLRO was made basing on the results of a method which seem to overestimate the tendency towards NLRO, we present here a more extensive exact diagonalization and variational study.

To reexamine the problem of the existence of the magnetic order in the ground state
of the spin system on the bipartite SHD lattice the RVB approach developed originally by Anderson [8] and reformulated later by Liang, Doucot and Anderson [11,12] was applied. This procedure seems to be well suited to spin systems on bipartite lattices. At the beginning, however, let us describe the results of exact diagonalization procedure applied to a 36-spin system with periodic boundary conditions on SHD lattice, shown in Fig. 1. Those results were subsequently used to estimate the quality of applying the RVB method to the same system. To diagonalize the 36-spin Hamiltonian the Lanczos algorithm was applied. After using all possible point symmetries and spin reflection the dimension of the $S^z_{\text{tot}}$ sector still amounted to 126,108,405. The ground state energy per bond of this system is $E_0/\text{bond} = -0.373118$ and the correlation functions are collected in Table I. In addition, in Fig. 2 the lowest energy levels of this system vs. quantum numbers are presented. According to Anderson [9] and Bernu et al. [10] the Néel long range order which breaks the rotational invariance in the thermodynamic limit can occur if for small $S$ the lowest energy level for each $S$ sector is linearly dependent on $S(S + 1)$. This kind of dependence is rather clearly seen in Fig. 2. This and the behavior of the averaged correlation function with distance, seen in Fig. 3, form rather strong evidence that the ground state in this spin system is long range ordered. Let us also add that finite size analysis of the gap (based on ED results for 12, 24 and 36-spin systems) gives small negative value ($-0.055$) of the spin gap for infinite system and supports the above conclusion.

Now let us turn to the RVB method. It allows one to find a variational ground state function for a given, finite spin system. Consequently, it is possible to calculate, for a finite spin system, the expectation values of the operators which, after the extrapolation to the thermodynamic limit, can characterize the LRO in the ground state of an infinite spin system. Let us remind the reader three essential steps of this method as applied to quantum spin system on a bipartite lattice. Firstly, the lattice is partitioned into two equivalent sublattices $A$ and $B$. Connecting all spins belonging to $A$ sublattice with arbitrary spins of the $B$ sublattice and assuming that each pair of connected spins is in a singlet state, i.e.,
$|i, j⟩ = \frac{1}{\sqrt{2}}(|↑i ↓j⟩ - |↑j ↓i⟩)$, one produces a covering $|c_α⟩ = \prod_{i \in A, j \in B} |i, j⟩$. The system of all coverings forms, in fact, a new basis which is overcomplete and not orthogonal: the amplitude of probability $⟨c_1 | c_2⟩$ that a system passes from $|c_2⟩$ to $|c_1⟩$ is proportional to $2^{N(c_1, c_2)}$, where $N(c_1, c_2)$ denotes the number of loops arising when one draws the coverings $⟨c_1 |$ and $|c_2⟩$ simultaneously on the same lattice. Note that the Marshall sign rule is fulfilled automatically in this basis. Secondly, the ground state variational function $|Ψ_{trial}⟩$ is expanded into the basis of the functions $|c_i⟩$ and the positive coefficients (amplitudes) in this expansion are just the variational parameters. At this point, however, two important assumptions concerning amplitudes are made: the amplitude for a given covering has a form of a product, i.e., factorizes with respect to singlets entering to this covering. An additional assumption is that the singlets at the same distance contribute to this product in the same way (form resonances - hence the name of the method). Therefore, the trial wave function is assumed to be

$$|Ψ_{trial}⟩ = \sum_α \prod_{i \in A, j \in B} h_{ij}^α |c_α⟩.$$  \hspace{1cm} (2)

Finally, there follows a searching of the minimum of $⟨Ψ_{trial} | H | Ψ_{trial}⟩$ with respect to variational parameters $h_{ij}^α$ and the calculation of the expectation values of the desired operators in the ground state of a spin system under consideration for those $h_{ij}^α$ which minimize $⟨Ψ_{trial} | H | Ψ_{trial}⟩$. For small systems this can be accomplished rigorously by taking into account the whole space of coverings (e.g., for 12 spins there are 720 coverings, each covering consisting of 64 Ising states), for larger ones by the Monte-Carlo method, as proposed by Liang, Doucot and Anderson \[11,12\].

To make an optimal choice of the variational parameters $h_{ij}^α$ we have calculated the variance of the ground state energy for small clusters on some bipartite lattices. The whole basis of coverings was taken into account. The best choice of $h_{ij}^α$ which leads to a minimum value of the variance in the ground state (with not too large dimension of the parameter space) is the following one: $(h_{AA}, h_{AB}, σ)$. Thus $h_{ij}^α = 1$ for $r_{ij} = 1$, $h_{ij}^α = h_{AA}/r_{ij}^σ$ for spins at the distance $r_{ij}$ belonging to the same sublattice, $h_{ij}^α = h_{AB}/r_{ij}^σ$ otherwise, and $r_{ij}$ is the
Manhattan metric (the length of the shortest path over bonds). All the expectation values of operators were calculated for this choice of the variational parameters. It seems to be important to choose not too high a dimension of the variational parameter space. We have observed that the minimum of $\langle \Psi_{\text{trial}} | H | \Psi_{\text{trial}} \rangle$ is rather broad in the parameter space and small changes of $h_{AA}, h_{AB}, \sigma$ lead to relative large changes of $m^2$. It would mean that this method can also account for some disordered singlet states slightly above the ground state.

Table II presents the comparison between the exact diagonalization and variational values of $E_0$/bond and $m^2$ for 12 and 36 spin systems with periodic boundary conditions. RVB method overestimates slightly the tendency towards LRO: variational values of $m^2$ are slightly higher - 0.07% for 12-spin cluster and 5% for 36-spin cluster. The energy is reproduced very well: its underestimation is only 0.4% for the 36-spin system. Those discrepancies result from the singlet factorization assumption and their small values seem to indicate that it is a reasonable one. Let us also note that the parameters $h_{ij}^\alpha$ decay much faster than the spin-spin correlations (for 36 spins $h_{AA} = 0.950$, $h_{AB} = 0.720$, $\sigma = 1.54$).

In Fig. 3 we also present the correlation functions vs. distance obtained from the variational Huse-Elser ground state function [14,15,13]. They are overestimated in comparison to exact values which forms additional motivation to find the RVB ground state and to investigate the squared magnetization calculated from the RVB ground state function in the thermodynamic limit.

Let us now describe our results for larger systems. The variational values of $E_0$ and $m^2$ for 48-, 108-, and 192-spin systems with periodic boundary conditions are collected in Table II and their finite size analysis is presented in Figs. 4, 5. Since these quantities have a finite-size correction (for small $N$ corrections of higher orders may be important), we decided to take into account only the data for $N = 48$, 108 and 192 spins in the extrapolation. The ground state energy per bond scales [14] like $N^{-3/2}$: fitting the data from Table II leads to $E(N) = E_\infty + aN^{-3/2}$ with $E_\infty = -0.3688$ and $a = -0.8805$. Note that $E_\infty$ is slightly lower than that obtained by Huse-Elser approach ($E_{\infty,HE} = -0.3605$) (see Ref. [13]). The square of order parameter scales [14] like $N^{-1/2}$. This leads to the following form of the square of
sublattice magnetization as a function of $N$: $m^2(N) = m_{\infty}^2 + bN^{-1/2}$ with $m_{\infty}^2 = 0.0648$ and $c = 0.5136$. Note that $m_{\infty}$ is only 50% of its classical value (1/2) - which should be compared to 63% resulting from Huse-Elser ground state variational function.

Finally, in Fig. 6, the correlation function vs. the Euclidean distance is plotted. It decays to about 0.09 for $r \sim 6$ and further almost does not change with the distance. This provides an additional argument that the long-range magnetic order persists in the ground state of this spin system.

To conclude, we have presented the results of the investigation of the ground state of the antiferromagnetic spin system on SHD lattice. The behavior of the low-energy levels obtained from exact diagonalization, the value of $m_{\infty}^2$ and the finite value of the correlation function on higher distances represent an evidence for the existence of two-sublattice Néel long-range magnetic order in this system.

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**FIG. 1.** The 36-spin system on bipartite square-hexagonal-dodecagonal lattice.

**FIG. 2.** The lowest energy levels of the spin system from Fig. 1 vs. quantum numbers $S(S + 1)$. Straight line is the fit to the lowest energy in each sector.

**FIG. 3.** The dependence of the sublattice correlation function on the Euclidean distance for the spin system shown in Fig. 1. Comparison between exact diagonalization and variational results.

**FIG. 4.** Variational energy per bond $E_0/bond$ of the spin system on the SHD lattice as a function of $N^{-3/2}$ extrapolated to the thermodynamic limit. Only three values (for $N = 48$, 108 and 192 spins) were used in this extrapolation.

**FIG. 5.** Squared sublattice magnetization $m^2$ of the spin system on the SHD lattice as a function of $N^{-1/2}$ extrapolated to the thermodynamic limit. Only three values (for $N = 48$, 108 and 192 spins) were used in this extrapolation.
FIG. 6. The dependence of the sublattice correlation function on the Euclidean distance for the 192-spin system.

TABLE I. The values of the correlation $\langle S_0^z S_i^z \rangle$ resulting from the exact diagonalization of the 36-spin system depicted in Fig. 1.

| $i$ | $\langle S_0^z S_i^z \rangle$ | $i$ | $\langle S_0^z S_i^z \rangle$ | $i$ | $\langle S_0^z S_i^z \rangle$ |
|-----|-----------------|-----|-----------------|-----|-----------------|
| 1   | -0.1381         | 13  | -0.0338         | 25  | -0.0360         |
| 2   | 0.0561          | 14  | 0.0350          | 26  | 0.0386          |
| 3   | -0.0533         | 15  | -0.0352         | 27  | -0.0436         |
| 4   | 0.0561          | 16  | 0.0386          | 28  | 0.0350          |
| 5   | -0.1033         | 17  | -0.0374         | 29  | -0.0354         |
| 6   | 0.0521          | 18  | 0.0413          | 30  | 0.0356          |
| 7   | -0.0474         | 19  | -0.0474         | 31  | -0.0354         |
| 8   | 0.0365          | 20  | 0.0742          | 32  | 0.0335          |
| 9   | -0.0354         | 21  | -0.1317         | 33  | -0.0354         |
| 10  | 0.0356          | 22  | 0.0521          | 34  | 0.0413          |
| 11  | -0.0389         | 23  | -0.0460         | 35  | -0.0460         |
| 12  | 0.0340          | 24  | 0.0340          |     |                 |
TABLE II. The ground state energy per bond $E_0/bond$ and the squared sublattice magnetization $m^2$, for some finite spin systems on SHD lattice. For the 12- and 36-spin systems the results of exact diagonalization are also included. In the case of the 12-spin cluster the variational values were obtained in the whole basis of coverings, for larger clusters the Monte-Carlo method was applied. Statistical errors, in parentheses, are the last two digits.

| N   | $E_0/bond$   | $m^2$     |
|-----|--------------|-----------|
| 12  | exact -0.3850 | 0.2913    |
|     | variational -0.3850 | 0.2915    |
| 36  | exact -0.3731 | 0.1632    |
|     | variational -0.3718(15) | 0.1707(30) |
| 48  | -0.3715(15) | 0.1402(37) |
| 108 | -0.3698(16) | 0.1104(50) |
| 192 | -0.3691(15) | 0.1044(54) |
36 spins  Exact Diagonalization

energy

S(S+1)

0 2 6 12 20 30 42

-15 -16 -17 -18 -19 -20 -21
36 spins

\[ \langle S(0)S(r) \rangle \]

RVB WF
Huse-Elser WF
ED

\( r \)

1 1.5 2 2.5 3 3.5 4 4.5 5

0 0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4
