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The ground state of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on an Archimedean 4–6–12 lattice

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Abstract

An investigation of the Néel long-range order (NLRO) in the ground state of the antiferromagnetic Heisenberg spin system on the two-dimensional, uniform, bipartite lattice consisting of squares, hexagons and dodecagons is presented. On the basis of the analysis of the order parameter and the long-distance correlation function, 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 high-T_c superconductivity, one cannot fail to notice the 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 of 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 a 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 (i) the tendency towards local singlet formation and (ii) frustration. For example, the first mechanism which breaks the NLRO is present in the spin system on a one-fifth-depleted square lattice (which is the prototype of the CaV_4O_9 lattice) and it manifests itself in a continuous quantum phase transition with critical exponents which seem to belong to the three-dimensional classical Heisenberg universality class [1, 2]. On the other hand, in the case of a *generic* model of a frustrated antiferromagnet—see, e.g., reference [3, 4]—namely the J_1–J_2 model, the growing frustration (J_2/J_1) gives rise to the continuous phase transition. Remarkably, there may also exist systems in which the two above competing mechanisms are built in, like the spin system on the Shastry–Sutherland lattice [5] (which is the prototype of the $SrCu_2(BO_3)_2$ lattice). The question of the nature of the phase transition in this system remained for some time a puzzle, and finally it emerged that in a very small area of the parameter space

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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., reference [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 showing the disordered ground state, the general question concerning the NLRO remains not completely answered.

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

$$H = \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \tag{1}$$

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, oppositely to the case for the honeycomb lattice (with the same coordination number), the nearest neighbours are not equivalent. This, in a natural way, favours the formation of the local singlets, i.e., acts against the NLRO. Since our earlier conclusion [13] concerning the existence of NLRO was made on the basis of the results from a method which seem to overestimate the tendency towards NLRO, we present here a more extensive exact-diagonalization and variational study.

To re-examine 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 examining spin systems on bipartite lattices. First, however, let us describe the results of an exact-diagonalization procedure applied to a 36-spin system with periodic boundary conditions on a SHD lattice, shown in figure 1. These results were subsequently used to estimate the quality achieved by 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_{tot}-sector still amounted to 126 108 405. The ground-state energy per bond of this system is $E_0/\text{bond} = -0.373\,118$ and the correlation functions are collected in table 1. In addition, in figure 2 the lowest energy levels of this system versus 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

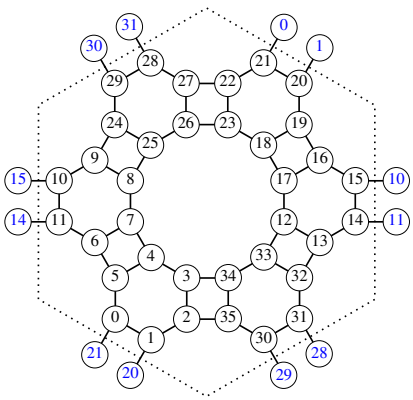

Figure 1. The 36-spin system on a bipartite square–hexagonal–dodecagonal lattice.

Table 1. 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 figure 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		

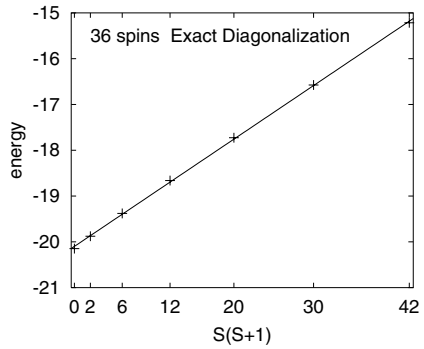

Figure 2. The lowest energy levels of the spin system from figure 1 versus quantum numbers $S(S+1)$. The straight line is the fit to the lowest energy in each sector.

clearly seen in figure 2. This and the behaviour of the averaged correlation function with distance, seen in figure 3, constitute 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 a small negative value (−0.055) of the spin gap for an 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 recall three essential steps of this method as applied to a quantum spin system on a bipartite lattice. Firstly, the lattice is partitioned into two equivalent sublattices A and B. Connecting all spins belonging to the A sublattice with arbitrary spins of the B sublattice and assuming that each pair of connected spins is in a singlet state, i.e., $|i, j\rangle = (1/\sqrt{2})(|\uparrow_i\downarrow_j\rangle - |\uparrow_j\downarrow_i\rangle$, one produces a covering $|c_\alpha\rangle = \prod_{i\in \mathrm{A},\, j\in \mathrm{B}} |i, j\rangle$. The system of all coverings forms, in fact, a new basis which is overcomplete and not orthogonal: the amplitude of the probability $\langle c_1|c_2\rangle$ that a system passes from $|c_2\rangle$ to $|c_1\rangle$ 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 $\langle c_1|$ and $|c_2\rangle$ simultaneously on the same lattice. Note that the Marshall sign rule is fulfilled automatically in this basis. Secondly, the ground-state

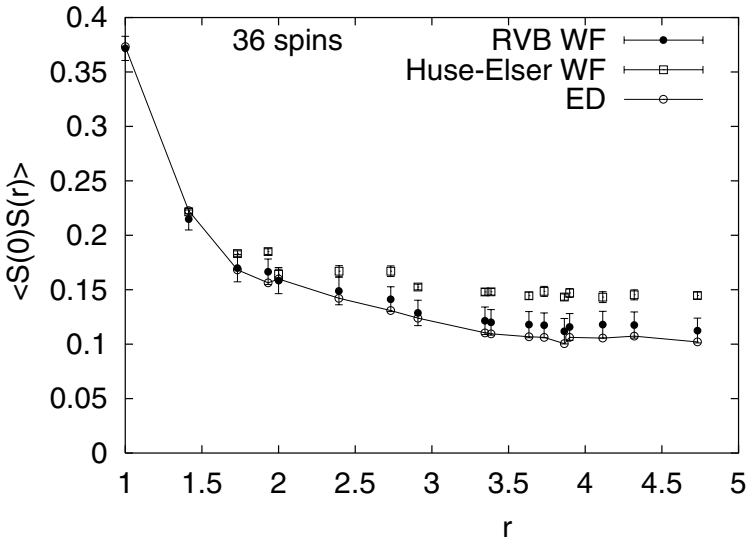

Figure 3. The dependence of the sublattice correlation function on the Euclidean distance for the spin system shown in figure 1. Comparison between exact-diagonalization and variational results.

variational function $|\Psi_{\text{trial}}\rangle$ is expanded in the basis of the functions $|c_i\rangle$, 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 the form of a product, i.e., factorizes with respect to singlets entering into 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

$$|\Psi_{\text{trial}}\rangle = \sum_{\alpha} \prod_{i\in\text{A},\, j\in\text{B}} h_{ij}^{\alpha} |c_{\alpha}\rangle. \tag{2}$$

Finally, there follows a search for the minimum of $\langle\Psi_{\text{trial}}|H|\Psi_{\text{trial}}\rangle$ 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 $\langle\Psi_{\text{trial}}|H|\Psi_{\text{trial}}\rangle$. 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), and 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 a dimension of the parameter space that is not too large) is the following one: $(h_{\text{AA}}, h_{\text{AB}}, \sigma)$. Thus $h_{ij}^{\alpha} = 1$ for $r_{ij} = 1$, $h_{ij}^{\alpha} = h_{\text{AA}}/r_{ij}^{\sigma}$ for spins at the distance r_{ij} belonging to the same sublattice, $h_{ij}^{\alpha} = h_{\text{AB}}/r_{ij}^{\sigma}$ otherwise, and r_{ij} is the Manhattan metric (the length of the shortest path over bonds). All of the expectation values of operators were calculated for this choice of the variational parameters. It seems to be important to choose a dimension of the variational parameter space that is not too high. 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 $h_{\text{AA}}, h_{\text{AB}}, \sigma$ lead to relatively large changes of m^2. This would mean that this method can also account for some disordered singlet states slightly above the ground state.

Table 2 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. The RVB method slightly overestimates the tendency towards LRO: the variational values of m^2 are slightly higher—0.07% for the 12-spin cluster and 5% for the 36-spin cluster. The energy is reproduced very well: its underestimation is only 0.4% for the 36-spin system. These 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}^{α} decay much faster than the spin–spin correlations (for 36 spins $h_{\mathrm{AA}} = 0.950$, $h_{\mathrm{AB}} = 0.720$, $\sigma = 1.54$). In figure 3 we also present the correlation functions versus distance obtained from the variational Huse–Elser ground-state function [13–15]. They are overestimated in comparison to exact values, which provides additional motivation for finding the RVB ground state and investigating the squared magnetization calculated from the RVB ground-state function in the thermodynamic limit.

Table 2. The ground-state energy per bond E_0/bond and the squared sublattice magnetization m^2, for some finite spin systems on a SHD lattice. For the 12- and 36-spin systems the results from 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 in 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)

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 2 and their finite-size analysis is presented in figures 4, 5. Since these quantities have a finite-size correction (for small N, corrections of higher orders may be important), we decided to

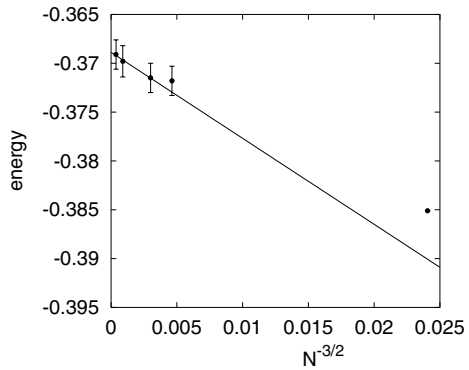

Figure 4. Variational energy per bond E_0/bond of the spin system on the SHD lattice as a function of $N^{-3/2}$ extrapolated to the thermodynamic limit. Only three values (for $N = 48$, 108 and 192 spins) were used in this extrapolation.

take into account only the data for $N = 48$, 108 and 192 spins in the extrapolation. The ground-state energy per bond scales [16] like $N^{-3/2}$: fitting the data from table 2 leads to $E(N) = E_\infty + aN^{-3/2}$ with $E_\infty = -0.3688$ and $a = -0.8805$. Note that E_∞ is slightly lower than that obtained by the Huse–Elser approach ($E_{\infty,HE} = -0.3605$) (see reference [13]). The square of the order parameter scales [16] like $N^{-1/2}$. This leads to the following form of the square of sublattice magnetization as a function of N: $m^2(N) = m^2_\infty + bN^{-1/2}$ with $m^2_\infty = 0.0648$ and $c = 0.5136$. Note that m_∞ is only 50% of its classical value (1/2)—which should be compared to 63% resulting from the Huse–Elser ground-state variational function.

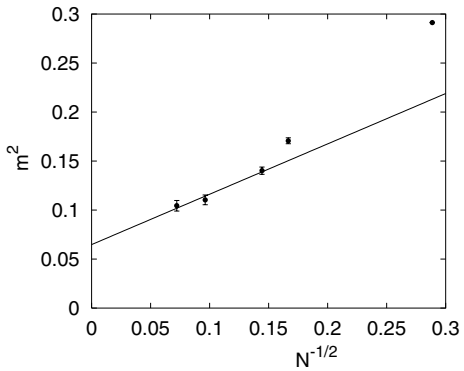

Figure 5. Squared sublattice magnetization m^2 of the spin system on the SHD lattice as a function of $N^{-1/2}$ extrapolated to the thermodynamic limit. Only three values (for $N = 48$, 108 and 192 spins) were used in this extrapolation.

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

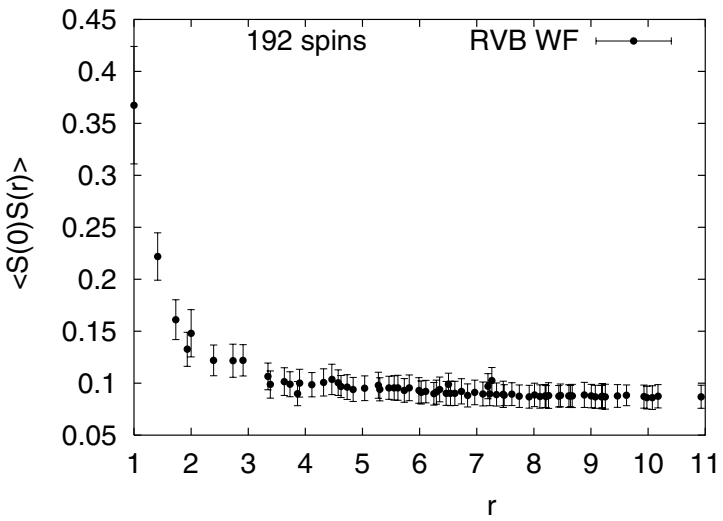

Figure 6. The dependence of the sublattice correlation function on the Euclidean distance for the 192-spin system.

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

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