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# The Ground-State of the Quantum Spin-$\frac{1}{2}$ Heisenberg Antiferromagnet on *Square-Kagomé* Lattice: Resonating Valence Bond Description

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In this paper we report on some ground-state properties of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on the two-dimensional *square-kagomé* lattice. Finite $N$-spin systems were investigated with the use of the resonating valence bond method. Like in the case of spin system on *kagomé* lattice we find the almost flat dependence of mean singlet length on $1/N$.

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## 1. Introduction

In recent years, because of fascinating quantum effects discovered in novel magnetic materials, the low-dimensional antiferromagnetic quantum spin systems have been attracting a lot of attention [1–6]. Mainly the ground-state properties are being discussed in the literature, but finite temperature behavior also has unresolved aspects. Currently, a subject of experimental and theoretical interest are

two-dimensional quantum Heisenberg spin systems with strong frustration which do not exhibit long-range magnetic order in the ground state.

One of the most interesting examples is the spin-$\frac{1}{2}$ Heisenberg antiferromagnet (HAFM) on the *kagomé* lattice, a two-dimensional lattice of corner-sharing triangles with hexagonal voids. Despite intensive studies during the last decade its ground state properties are not completely understood yet (see the reviews [7–9] and references therein). As the first Zeng and Elser [10] pointed out that the ground state of the spin-$\frac{1}{2}$ HAFM on *kagomé* lattice may be disordered. All approaches based on either exact diagonalization (ED) [11, 12], on perturbation series expansions [13] or on high temperature expansions [14] point a disordered ground state. This system is a quantum spin liquid with very short-ranged spin, dimer, chirality correlations [7–9] and a large number of singlet states below the first triplet state [15–17]. Let us also stress that in classical spin system on *kagomé* lattice there exists an infinitely degenerated ground state.

We focus here on the ground state properties of HAFM on *square-kagomé* lattice [18–20] (similar to *kagomé* lattice but of different symmetry, see Fig. 1). This is a two-dimensional network of corner-sharing triangles, too. However, the voids in between are alternately squares and octagons rather than hexagons (like in the case of *kagomé* lattice). In contrast with the *kagomé* lattice, this lattice is not a uniform tiling [21] because it is not built by regular polygons only. Moreover, it possesses two non-equivalent sites. In spite of this, one finds some significant geometrical similarities to the *kagomé* lattice. Besides "corner-sharing triangles" the both lattices have the same coordination number (equal to four) and additionally the even regular polygons are surrounded only by triangles. The *square-kagomé* lattice is also strongly frustrated and shows an infinite nontrivial degeneracy of the classical ground state. The above properties suggest that one can expect that the HAFM on this lattice is another candidate for a quantum paramagnetic ground state [22].

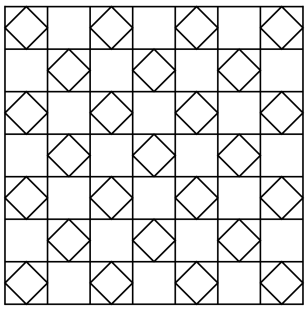

Fig. 1. The *square-kagomé* lattice.

As usual, two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet is described by the following Hamiltonian:

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

The sum runs over all pairs of nearest neighbors on the lattice under consideration and the unit of energy is set to $J = 1$ in what follows.

The aim of this investigation was to elucidate the nature of the ground states in spin-$\frac{1}{2}$ systems on both above-mentioned lattices (*square-kagomé* and *kagomé*) and using an ED approach in RVB basis to answer the question whether these states may be properly described within short-range resonating valence bond (SRRVB) method. Similar task was undertaken by Mambrini and Mila [23] for spin system on *kagomé* lattice (spectrum of non-magnetic excitation within a singlet–triplet gap is continuous, SRRVB description captures essentially the low--temperature physics of this system) and earlier by Zeng and Elser [24] (excitation energy scale in the singlet sector is very small), but no definite conclusion has been drawn.

## 2. The RVB method

Let us briefly remind the reader essential aspects of RVB approach [25, 26] as applied to quantum spin-$\frac{1}{2}$ systems: matrix elements of the Hamiltonian are calculated not in the Ising basis but in the (complete) basis taken from an over--complete, not orthogonal set of *dimer coverings* $|c_k\rangle$:

$$\langle c_k | \, \boldsymbol{S}_i \cdot \boldsymbol{S}_j | c_l \rangle = (-1)^d \left( \pm \frac{3}{4} \right) \langle c_k | c_l \rangle, \tag{2}$$

where $\langle c_k | c_l \rangle = 2^{\mathcal{N}}$ with $\mathcal{N}$ being a number of loops arising when one draws the coverings $\langle c_k|$ and $|c_l\rangle$ simultaneously on the same lattice. All dimers in the system are oriented; $d$ denotes the number of *disoriented* dimers that one meets passing along the loop containing $i$ and $j$. Finally, $+\frac{3}{4}$ is taken if there is even number of dimers between $i$ to $j$, $-\frac{3}{4}$ in the opposite case. In order to find the ground state of Hamiltonian (1) we transform it into an orthogonal basis which we find solving eigenproblem for the matrix of scalar products $\langle c_k | c_l \rangle$:

$$H_O = O^\dagger H O, \tag{3}$$

subsequently we solve the eigenproblem for $H_O$ (or, equivalently, one can solve the generalized eigenproblem $H|\Psi\rangle = EC|\Psi\rangle$, with $C$ being the matrix formed from $\langle c_k | c_l \rangle$) and finally, express the ground state in the original basis of *dimer coverings* $|c_i\rangle$:

$$|\Psi_{\mathrm{GS}}\rangle = \sum_i \alpha_i |c_i\rangle. \tag{4}$$

Although, due to nonorthogonality, this procedure is more complicated from mathematical point of view, it has great advantage because of its clear physical meaning: one can characterize the ground state, in addition to energy, order parameter, correlations, etc., by some *geometrical* quantities. One of them is a mean singlet length ($SL$), defined as follows:

$$\langle SL\rangle = \sum_{i,j} \alpha_i^* \alpha_j x_{ij} \langle c_i | c_j \rangle, \tag{5}$$

similarly to

$$\langle \Psi_{\rm GS} | H | \Psi_{\rm GS} \rangle = \sum_{i,j} \alpha_i^* \alpha_j \langle c_i | H | c_j \rangle. \tag{6}$$

In Eq. (5) $x_{ij} = M_{ij}/O_{ij}$ — $M_{ij}$ stands for total Manhattan length of all loops which enter to the scalar product $\langle c_i | c_j \rangle$. Similarly, $O_{ij}$ denotes total order of all loops in such a case. Clearly, $M_{ij}/O_{ij}$ informs us about the number of bonds *per* dimer for given $i$ and $j$ ($x_{ij}$ are numbers, not operators); in the case if the basis is constructed from short-range coverings only $M_{ij}/O_{ij} = 1$ for all $i$, $j$.

## 3. Results and conclusions

We present in Table I the values of $\langle SL\rangle$ for some finite spin systems with periodic boundary conditions. The largest system $N = 18$ required a full diagonalization of a matrix in dimension 4862. All these data are shown in Fig. 2. Although it is rather not possible to obtain scaling dependences — the lines are only guides for an eye — one can observe qualitatively different behavior of $\langle SL\rangle$ vs. $1/N$: for systems on *kagomé* and *square-kagomé* lattices this dependence is almost flat, whereas for linear system and system on square lattice one can notice that $\langle SL\rangle$ increases more rapidly with the size of the system. This can be interpreted as follows.

TABLE I

Mean singlet lengths, $\langle SL\rangle$, in the ground state of spin-½ HAFM for linear chain ($N = 12$, 14, 16, 18), square lattice ($N = 16$, 18) *kagomé* and *square-kagomé* lattices ($N = 12$, 18) calculated by exact diagonalization in the RVB basis. The dimension of the complete RVB basis, i.e., the number of independent dimer coverings, is also given.

| Lattice | $N = 12$ | 14 | 16 | 18 |
|---|---|---|---|---|
| Complete RVB basis | 132 | 429 | 1430 | 4862 |
| linear chain | 1.496 | 1.572 | 1.618 | 1.674 |
| square | – | – | 1.300 | 1.360 |
| *kagomé* | 1.390 | – | – | 1.430 |
| *square-kagomé* | 1.269 | – | – | 1.355 |

Firstly, since for all systems $\langle SL\rangle > 1$, the ground state of any of them can be described properly in short-range RVB basis (if it were possible then one would have $\langle SL\rangle = 1$; in such a case $\langle SL\rangle = \langle \Psi_{\rm GS} | \Psi_{\rm GS} \rangle$). This result suggests that longer dimers are also important and the true ground state in this case may be more complicated than that constructed within SR basis [23] — resonance loops in

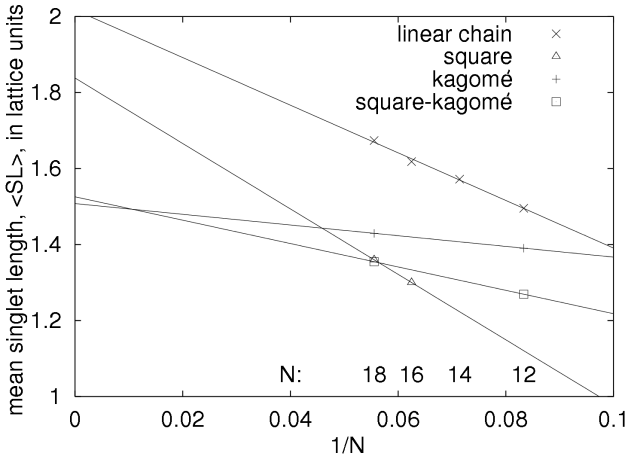


Fig. 2. The $\langle SL \rangle$ dependence on $1/N$.

true ground state contain short dimers which are not necessarily nearest neighbors but longer singlets seem to be excluded. Indeed, the qualitative difference between the linear chain and square lattice systems on one hand and on *kagomé* and *square--kagomé* lattices on the other is that in the former case (both systems are bipartite) there exist longer resonance loops and hence it is possible to write a variational ground state function as a product over dimers; each dimer enters to this product with an amplitude which decays like an inverse power of its length [25, 27]. Let us remind also that the ground state energy $E_{\rm GS}$ is lowered by resonance loops and it is natural to expect that in the case if longer loops are present, the dependence $E_{\rm GS}$ vs. $N$ in finite size scaling should be more pronounced. In fact, for HAFM on *kagomé* and *square-kagomé* lattices this dependence is rather flat, but still present — longer singlets are absent in the ground state. In other words: if $E_{\rm GS}$ is to some extent not sensitive to $N$ in finite size scaling then long range singlets are absent in the ground state, see Fig. 2.20 in [8].

TABLE II

The ground state energy of finite systems on *kagomé* and *square-kagomé* lattices calculated by ED in the basis containing short-range dimer coverings. The data in the last column are taken from [23]. The dimension of the short--range RVB basis is also given.

| Lattice | $N = 12$ | 18 | 24 | 30 | 36 |
|---|---|---|---|---|---|
| SRRVB basis | 12 | 128 | 512 | 2048 | 8192 |
| *kagomé* | –0.226563 | –0.219794 | –0.214725 | – | –0.210908 |
| $E_{\rm SRRVB}/E_{\rm exact}$ | 0.9986 | 0.9812 | 0.9622 | – | 0.9622 |
| *squaré-kagomé* | –0.226563 | –0.219740 | –0.219393 | –0.214266 | – |
| $E_{\rm SRRVB}/E_{\rm exact}$ | 0.9986 | 0.9820 | 0.9819 | 0.9672 | – |

Let us now examine quantitatively the difference between the ground state calculated in complete RVB basis and in the basis of short-range dimer coverings in small system on both "corner-sharing triangles" lattices. The relevant values are given in Table II. One can conclude that the ground state in both systems may be described in SR dimer basis qualitatively only — $E_{\mathrm{GS}}$ is slightly underestimated.

Let us summarize main similarities between antiferromagnetic spin system on *kagomé* and *square-kagomé* lattices which are reported in this paper. In both systems the dependence $\langle SL \rangle$ on $1/N$ is rather flat, contrary to systems on bipartite lattices (linear chain and square lattice). Therefore it is possible to find for the latter systems the variational ground state function which is written in the form of a product — this enables to find approximate amplitudes for each basis state. Such an approach gives poor results in the case of frustrated systems.

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