Low-energy sector of the S=1/2 Kagome antiferromagnet

F. Mila
Laboratoire de Physique Quantique, Université Paul Sabatier, 118 Route de Narbonne, 31062 Toulouse Cedex, France.

Starting from a modified version of the S=1/2 Kagome antiferromagnet to emphasize the role of elementary triangles, an effective Hamiltonian involving spin and chirality variables is derived. A mean-field decoupling that retains the quantum nature of these variables is shown to yield a Hamiltonian that can be solved exactly, leading to the following predictions: i) The number of low lying singlet states increase with the number of sites \( N \) like \( 1.15^N \); ii) A singlet-triplet gap remains in the thermodynamic limit; iii) Spinons form bound states with a small binding energy. By comparing these properties with those of the regular Kagome lattice as revealed by numerical experiments, we argue that this description captures the essential low energy physics of that model.

Despite a very intense activity over the past 10 years, the magnetic properties of the S=1/2 Kagome antiferromagnet remain an open problem. If a number of facts seem to be rather firmly established by now thanks to the very extensive numerical simulations that have been performed on that system, a simple theoretical picture that accounts for the basic findings has not emerged yet. The most striking feature is probably the presence of many, low–lying singlet states. The first indication that this might be the case was the appearance of a low temperature peak in the specific heat. While the evolution of this peak with the size of the system is not clear yet, the numerical determination of all the low-lying singlet states for systems with up to 36 sites shows that their number increases like \( 1.15^N \), where \( N \) is the number of sites of the system. The best candidate to explain this proliferation of low-lying singlets is a short-range RVB description of the low-energy sector based on dimer coverings of the Kagome lattice with nearest-neighbour singlets. The main problem with this approach is that the number of dimer states increases like \( 1.26^N \), i.e. much too fast, and no convincing criterion could be found that allows one to select the relevant singlet states. The other important, although less accurately established, findings of the numerical simulations are the absence of long-range magnetic order in the ground-state and the presence of a singlet–triplet gap in the thermodynamic limit. Finally the role of spin 1/2 excitations, as well as the consistency of the numerical results with some exotic types of order, is still under investigation.

In this paper, we propose a simple explanation of these properties. We start from the following observation: The exponential increase of the number of these low–lying states suggest that they originate from the partial lifting of a local degeneracy that would be present if some of the couplings were set to zero. Now the natural bricks to construct the Kagome lattice are triangles, and spins 1/2 on a triangle lead to a fourfold degenerate groundstate: two doublets that differ by their chirality. So let us investigate how this degeneracy is lifted if one constructs the Kagome lattice by coupling triangles. This amounts to studying the modified Kagome lattice depicted in figure 1 starting from the limit \( J'/J \ll 1 \). This can be seen as a triangular lattice of triangles with \( N_t = N/3 \) sites, where \( N \) is the number of sites of the Kagome lattice.

The first step is to derive an effective Hamiltonian in the subspace of the groundstates of the triangles, as in Subrahmanyam’s block spin perturbation approach to the non-dimerized Kagome lattice. Following Schulz’s approach to the problem of three coupled Heisenberg chains with periodic boundary conditions, we describe the four groundstates of a triangle with two Pauli matrices: \( \vec{\sigma} \) for the spin of the doublet, the eigenstates of \( \sigma_z \) being denoted \( \uparrow \) and \( \downarrow \), and \( \vec{\tau} \) for its chirality, the eigenstates of \( \tau_z \) being denoted \( R \) for right and \( L \) for left. In terms of the original spins \( \vec{S} \), these states can be written.
\[ |\alpha R| = \frac{1}{\sqrt{3}} (|\alpha a\alpha a \tau_{ij} + \omega |\alpha a \alpha a + \omega^{2} |\alpha a\alpha a >) \]
\[ |\alpha L| = \frac{1}{\sqrt{3}} (|\alpha a\alpha a \tau_{ij} + \omega^{2} |\alpha a\alpha a + \omega |\alpha a\alpha a >) \] (1)

where \( \omega = \exp(2\pi i/3) \) and \( \alpha = \uparrow \) or \( \downarrow \). \( |\alpha_1\alpha_2\alpha_3 > \) represents a configuration of the original spins \( S \) within one triangle, the indices corresponding to the convention of Fig. 1. Note that the total spin is now given by \( \sum_{ij} \langle \sigma_{ij} \rangle^{2} \), where the prime means that the sum runs over the triangular lattice. Each triangle has an energy \(-3J/4\), and energies will be measured with respect to the groundstate energy \(-3J/4)N_{t} \) of the \( J'/J = 0 \) case. Then, to first order in \( J' \), the effective Hamiltonian \( \hat{H} \) on the triangular lattice is given by:

\[
\hat{H} = (J'/9) \sum_{<i,j>} \hat{H}_{ij} \bar{H}_{ij}, \quad \bar{H}_{ij} = \sum_{<i,j>} \hat{\sigma}_{i} \hat{\sigma}_{j}, \\
\hat{H}_{ij} = (1 - 2(\alpha_{ij} \tau_{i}^{+} - \alpha_{ij} \tau_{j}^{+}))(1 - 2(\beta_{ij} \tau_{i}^{-} + \beta_{ij} \tau_{j}^{-})) \] (2)

where \( <i,j> \) denotes pairs of nearest neighbors. In \( \hat{H}_{ij} \), \( \alpha_{ij} \) and \( \beta_{ij} \) are complex parameters that depend on the type of bond: \( \alpha_{ij} \) (resp. \( \beta_{ij} \)) equals 1, \( \omega^{2} \) or \( \omega \) when the original spin in triangle \( i \) (resp. \( j \)) involved in the bond \( (i,j) \) sits at site 1, 2 or 3 with the convention of Fig. 1. In the basis \( |RR> \), \( |RL> \), \( |LR> \), \( |LL> \) the eigenstates of \( \bar{H}_{ij} \) can be easily calculated:

\[
|\phi_{1}^{\uparrow}(i,j) > = \frac{1}{2}(1, -\beta_{ij}, -\alpha_{ij}, \alpha_{ij}, \beta_{ij}) \quad E_{1} = 9 \\
|\phi_{2}^{\uparrow}(i,j) > = \frac{1}{2}(1, \beta_{ij}, \alpha_{ij}, \alpha_{ij}, \beta_{ij}) \quad E_{2} = 1 \\
|\phi_{3}^{\uparrow}(i,j) > = \frac{1}{2}(1, -\beta_{ij}, \alpha_{ij}, -\alpha_{ij}, \beta_{ij}) \quad E_{3} = -3 \\
|\phi_{4}^{\uparrow}(i,j) > = \frac{1}{2}(1, \beta_{ij}, -\alpha_{ij}, -\alpha_{ij}, \beta_{ij}) \quad E_{4} = -3 \] (3)

while the eigenstates of \( \bar{H}_{ij} \) are denoted \( |\phi_{S,m}^{\uparrow}(i,j) > \) with energies \(-3/4\) for the singlet \( S = 0, m = 0 \) and \( 1/4 \) for the triplets \( S = 1, m = 0, \pm 1 \).

\[
\hat{H}_{MF} = \sum_{<i,j>} (a_{ij}^{\sigma} \hat{H}_{ij}^{\sigma} + a_{ij}^{\alpha} \hat{H}_{ij}^{\alpha} - a_{ij}^{\sigma} a_{ij}^{\alpha}) \] (4)

where the parameters \( a_{ij}^{\sigma} \equiv < \hat{H}_{ij}^{\sigma} > \) and \( a_{ij}^{\alpha} \equiv < \hat{H}_{ij}^{\alpha} > \) have to be determined self-consistently. Note that this mean-field problem is still very complicated a priori since it involves \( S = 1/2 \) Heisenberg like models on a triangular lattice.

Remarkably enough, the low-energy solutions of this problem can be determined analytically. Let us concentrate for the moment on clusters with an even number of sites and with periodic boundary conditions, and let us consider a dimer covering of the triangular lattice by nearest-neighbor dimers. Denoting by \( D \) the set of nearest-neighbor pairs that enter this covering, we can construct a wavefunction \( |\Phi_{0}(D) > \) in the following way:

\[
|\Phi_{0}(D) > = \prod_{<i,j> \in D} |\phi_{S,m}^{\uparrow}(i,j) > \otimes |\phi_{S,m}^{\uparrow}(i,j) > \] (5)

Clearly \( |\Phi_{0}(D) > \) will be a solution of the problem if \( a_{ij}^{\sigma} = a_{ij}^{\alpha} = 0 \) as soon as \( < i,j > \notin D \). This turns out to be true thanks to the following properties

\[
< \phi_{S,m}^{\uparrow}(i,j) \phi_{S,m}^{\uparrow}(k,l) | \hat{H}_{jk} | \phi_{S,m}^{\uparrow}(i,j) \phi_{S,m}^{\uparrow}(k,l) > = 0 \\
< \phi_{S,0}^{\sigma}(i,j) \phi_{S,0}^{\alpha}(k,l) | \hat{H}_{jk} | \phi_{S,0}^{\sigma}(i,j) \phi_{S,0}^{\alpha}(k,l) > = 0 \] (6)

which can be easily checked directly with the expressions of the wavefunctions. So \( |\Phi_{0}(D) > \) is a solution characterized by \( a_{ij}^{\sigma} = 9, a_{ij}^{\alpha} = -3/4 \) if \( < i,j > \in D \) and 0 otherwise, its energy is given by \( E_{0}(S = 0) = -(3J'/8)N_{t} \), and it is a singlet [22]. To prove that is minimizes the energy of Eq. (4), we have solved the mean-field problem numerically on small clusters with up to 3 \times 4 \) sites. This has been done by iteration starting from random values of \( a_{ij}^{\sigma} \) and \( a_{ij}^{\alpha} \), and we found that the lowest energy is always equal to \(-(3J'/8)N_{t}\). In fact, solutions like...
\( \Phi_0(D) \) exist most of the time for such mean-field Hamiltonians, but they are usually significantly higher in energy than uniform solutions. In the present case however, other solutions involving \( |\phi_0^\sigma(i,j)\rangle \) are very bad energetically because \( E_2 = E_1/9 \). Note that the wavefunction \( |\phi_0^\sigma(i,j)\rangle \) corresponds neither to ferromagnetic nor antiferromagnetic ordering of the chiral variables since it is a linear combination of the four basis states \( |RR\rangle, |RL\rangle, |LR\rangle, |LL\rangle \). So there is no chiral ordering of the type discussed by Baskaran [26] for the triangular lattice even locally.

Similarly, triplet solutions can be constructed for a given dimer covering of the triangular lattice. Choose two neighbouring sites \((i_0, j_0)\), and consider a dimer covering \( D(i_0, j_0) \) of the remaining sites. The wavefunction with lowest energy is of the form

\[
|\Phi_0(D(i_0, j_0))\rangle = |\phi_0^\sigma(i_0, j_0)\rangle \otimes |\phi_0^\tau_m(i_0, j_0)\rangle
\]

In this expression, \( m = 0, \pm 1 \) and \( n \) can take the values 3 or 4. The energy of this state is \( E_0(S = 1) = E_0(S = 0) + (2/3)J' \). Again it was checked numerically on a \( 3 \times 4 \) cluster that this is indeed the lowest energy in the triplet sector. So this mean-field approach predicts that there is a singlet-triplet energy gap \( \Delta \) equal to \( (2/3)J' \).

Another class of low-lying states exist in the triplet sector. They can be constructed in the following way: Choose two sites \((k, l)\) that are not nearest neighbours, denote by \( D(k, l) \) a dimer covering of the remaining sites, and consider the wavefunction

\[
|\Phi_0(D(k, l))\rangle = |\sigma_k \tau_k\rangle \otimes |\sigma_l \tau_l\rangle
\]

where \( |\sigma_k \tau_k\rangle \) (resp. \( |\sigma_l \tau_l\rangle \)) can be any configuration at site \( k \) (resp. \( l \)). Then similar arguments show that this is a solution with energy \( E_1(S = 1) = E_0(S = 1) + J'/12 \). Each unpaired site correspond to a \( S = 1/2 \) excitation and can be interpreted as a spinon. This mean-field approach predicts that spinons form triplet bound states on neighbouring sites with a binding energy equal to \( J'/12 \). In fact, if we consider a cluster with an odd number of sites, the groundstate can be shown to consist of one unpaired site - i.e. one spinon - times \( |\Phi_0(D)\rangle \), where \( D \) is a dimer covering of the remaining sites.

Now let us turn to the very interesting question of the groundstate degeneracy. The energy \( E_0(S = 0) \) does not depend on the particular dimer covering \( D \) used to construct the wavefunction \( |\Phi_0(D)\rangle \). So, for a given cluster, the degeneracy is controlled by the number of dimer coverings. This number can be calculated using standard techniques [25,26]. For the triangular lattice, we found that it increases with the number of sites \( N \) like \( \alpha N^2 \) with

\[
\ln \alpha = \frac{1}{16\pi^2} \int_0^{2\pi} \int_0^{2\pi} \ln(4 + 4 \sin x \sin y + 4 \sin^2 y) dx dy.
\]

A numerical integration yields \( \ln \alpha = 0.4286 \), or \( \alpha = 1.5351 \). In terms of the original Kagome lattice, this corresponds to a degeneracy that increases like \( (\alpha^{1/3})^N = 1.1536^N \) since \( N = 3N_0 \).

Next let us try to assess the validity of this mean-field approach. One argument in favour of this kind of approach is that it is qualitatively correct in the case of three coupled chains with periodic boundary conditions: Schulz's analysis based on Renormalization Group argument predicts a dimerized, twofold degenerate groundstate with gapped spin excitations [13,20], and this is exactly the physics of the mean-field solution adapted to that case [21]. To check its validity in cases of higher groundstate degeneracy, we have performed numerical simulations of the effective Hamiltonian of Eq. (2) for finite systems of coupled triangles. For the modified Kagome problem this turns out to be very difficult because the first cluster where dimer coverings can be done properly has \( 3 \times 4 \) sites. To determine the low lying states is then a numerical task comparable to the Kagome problem itself for 36 sites, and this is beyond the scope of the present paper. So we have compared mean-field and exact results for similar but different systems, namely for rings of \( n \) triangles with diagonal bonds up to \( n = 6 \). For \( n = 2 \), the mean-field description is of course exact. For \( n = 4 \) and 6, the structure of the low-energy spectrum is correctly given by the mean-field approach. For instance, for \( n = 4 \), the mean-field approach predicts that the groundstate is threefold degenerate, and the exact results give 3 low-lying singlets at \(-1.72053J'\) (non degenerate) and \(-1.54077J'\) (two-fold degenerate), the next state being a triplet located at \(-1.13942J'\). For \( n = 6 \), the groundstate degeneracy is 6 at the mean-field level, and the exact results also give 6 low-lying singlets. The details will be given elsewhere, but the answer is clear: The mean-field approach is qualitatively correct in predicting the number of low-lying singlets. To go beyond mean-field is expected to partially lift the degeneracy within the groundstate manifold but not to change the number of low-lying singlets.

Finally, let us come to the most important question: What can we learn from this approach concerning the regular (non-dimerized) Kagome lattice? First of all, let us translate our results in terms of the original spins \( \vec{S} \). We know from the analysis of the two triangle problem that the basic brick of our mean-field wavefunction, namely a two-site wavefunction of the type \( |\phi_0^\sigma(i,j)\rangle \otimes |\phi_0^\tau(i,j)\rangle \), corresponds to a dimer mapping of the two triangle problem (see Figure 2). So, the wavefunctions of Eq. (3) correspond to a certain subset of the dimerized wavefunctions of the Kagome lattice used by Zeng and Elser [11]. Next, let us compare the physical properties of this mean-field solution with the numerical results obtained on the Kagome lattice. As we noticed in the introduction, the number of dimerized states increases like \( 1.26^N \), i.e. much too fast. However, the number of states selected with our criterion increases roughly like \( 1.15^N \), in agreement with the numerical results for even clusters [8]. This is probably the most interesting result of the present approach: It provides a simple but nevertheless quantitative explanation of the very numerous low-lying singlet states of the \( S=1/2 \) Kagome antiferromagnet. Their number scales with the number of dimer coverings of the underlying triangular lattice of triangles.
The fact that one can choose triangles pointing upwards or downwards to build the wave-function means that the actual low lying states can have domains with different orientations of the triangles. Elementary energy considerations suggest that these domains are large however, so that they can only marginally contribute to the increase of the number of singlet states with the size of the system. Interestingly enough we can also explain the apparent discrepancy between odd and even clusters in the results of Ref. [8]. For odd clusters, there is an unpaired site, and according to the present theory, the degeneracy results of Ref. [8].

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FIG. 3. Logarithm of the number of dimer coverings of the triangular lattice as a function of the number of sites $N_t$ for small systems with periodic boundary conditions. The slope of $\ln(N_{odd})$ is 1.18, while the slope of both $\ln(N_{even})$ and $\ln(N_{odd}/N_t)$ is 1.15.

To summarize, we have studied a dimerized version of the $S=1/2$ Kagome antiferromagnet by performing a mean-field analysis of the effective hamiltonian that describes its low-energy sector. This approach leads to a transparent picture of the low energy properties which turns out to bear remarkable similarities to those reported for the regular Kagome lattice [5], e.g. the number of low-lying singlets or the presence of a singlet-triplet gap. Besides, these results lead to natural subspaces of dimer wavefunctions to describe the low energy singlet and triplet sectors of the regular Kagome model. A variational study of this model using these wave-functions is in progress to make more precise statements about the low-lying singlet subspace by a factor 25!

$$\ln(N_{\text{odd}})$$

$$\ln(N_{\text{even}})$$

$$\ln(N_{\text{odd}}/N_t)$$

$$N_t$$

$[\text{Cond-mat/9709274}]$

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