Gapless Singlet modes in the Kagomé strips: A study through DMRG and strong coupling analysis

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Recently Azaria et al have studied strips of the Kagomé-lattice in the weak-coupling limit, where they consist of two spin-half chains on the outside weakly coupled to an array of half-integer spins in the middle. Using a number of mappings they have arrived at the interesting result that in this system all spin excitations are gapped but there are gapless spinless modes. Here we study these Kagomé strips in the limit where the interchain couplings are comparable to the coupling to the middle spins by density matrix renormalization group and by a strong coupling analysis. In the limit when the coupling to the middle-spin dominates, the 5-spins of the unit-cell reduce to a single $S=3/2$ spin, and the overall system has well known gapless spin excitations. We study the phase transition from this phase to the weak-coupling phase. We also carry out a strong coupling analysis away from the $S=3/2$ limit, where the five-spin blocks have four degenerate ground states with $S=1/2$, which can be thought of as two spin and two pseudospin degrees of freedom. A numerical study of this strong coupling model also suggests a finite spin-gap.

The spin-half Kagomé-lattice antiferromagnet has proven to be a very fascinating system. Studies based on exact diagonalization of finite systems \[\text{and series expansions}\] strongly suggest that the system has a quantum disordered ground state. Finite size studies show a gap to spin excitations, but the most fascinating aspect of these numerical studies is the existence of a large number of spin-zero excitations below the lowest triplet state. Their number appears to grow exponentially with the size of the system \[\text{and series expansions}\]. The question of whether these spin-zero excitations are gapped or gapless and whether they form a well defined excitation mode of the system has not been resolved.

In this respect an interesting system was recently studied by Azaria et al [8]. They considered a 3-chain strip of the Kagomé-lattice shown in Fig. 1. This is a one-dimensional system with half-integral spin per unit cell, and is thus subject to the Lieb-Schultz-Mattis (LSM) theorem \[\text{and series expansions}\]. Most interestingly, Azaria et al find that the system has no broken symmetries, a spin-gap but gapless spin-zero excitations. This is a rather unusual possibility, but permitted by the LSM theorem. Azaria et al study the system perturbatively in the weak coupling limit, where the Kagomé strip reduces to two spin-half chains on the outside with couplings $J_{\parallel}$ on the chains, coupled weakly with the array of middle spins, with couplings $J_{\perp}$. Using a Majorana fermion representation for the low energy degrees of freedom on the spin-chains and employing a number of mappings, they conclude that these Kagomé strips have a spin-gap, which is exponentially small in $J_{\perp}/J_{\parallel}$, and there are gapless spin-zero modes. The importance of these studies to the Kagomé-strip limit $J_{\perp} = J_{\parallel}$, and furthermore to the Kagomé-lattice antiferromagnets remains unclear. Given the large number of approximate mappings, an independent numerical study of the model is clearly desirable and is performed here.

The limit $\lambda = J_{\perp}/J_{\parallel} \to 0$ is particularly difficult for a numerical study as the spin-gap becomes exponentially small in that limit. In the opposite limit, $\lambda \to \infty$, the five-spin unit cell of the system reduces to spin-3/2 and the system reduces to a spin-3/2 chain. This system is well known to have gapless spin excitations. Thus there must be a phase transition in the model as a function of $\lambda$. We study this system by the density matrix renormalization group (DMRG) and find that the phase transition occurs at $\lambda_c = 1.20(2)$. For $\lambda < \lambda_c$, the system has a spin-gap and gapless spin-zero modes. The Kagomé strips corresponding to $\lambda = 1$ belong to the spin-gap phase.

We have also studied the system of weakly coupled 5-spin blocks, where the ground state in the blocks are different from the $\lambda \to \infty$ limit. For large $\lambda$, the ground states of the block are the four states of a spin-3/2 spin. However at $\lambda = 2$, there is a level crossing in the 5-spin blocks and for $1 < \lambda < 2$, a new set of fourfold degenerate states become ground states. These states have spin-half. They correspond to a singlet pair on one of the chains and a triplet pair on the other chain, which is combined with the middle spin into a spin-half. Thus in addition to spin there is an additional two-fold degeneracy in every block that corresponds to an Ising like degree of freedom. We generate an effective Hamiltonian for the kagome strips by treating the coupling between blocks in degenerate perturbation theory. A numerical study of this strong coupling Hamiltonian also suggests the existence of a spin-gap. Whether this strong coupling phase is the same as the weak-coupling phase studied by Azaria et al remains to be seen.

The Hamiltonian corresponding to the Kagomé strip...
can be written as
\[ H = \sum_{\alpha=1,2} \sum_{i} [J_{\|}(S_{\alpha,2i}S_{\alpha,2i+1}) + J_{\perp}S_{2i+1/2}(S_{\alpha,i} + S_{\alpha,2i+1})] \tag{1} \]

where there are two chains with index \( \alpha = 1, 2 \) and the \( S_{2i+1/2} \) is the middle spin which interacts with the four sites, two from each chain (see Fig.1).

We have carried out an extensive DMRG [10,11] calculation on this Kagomé strip Hamiltonian, for various parameter ranges as well as for various system sizes with periodic boundary conditions. Apart from conserving the \( z \)-component of the total spin (\( S^z_{\text{tot}} \)), we have also used spin-parity (up-down symmetry) to divide the total spin spectrum into even and odd total spin subspaces for accurate description of the states in singlet and triplet branches.

The unit cell contains 5 spin-half sites, so it will be error-prone to put one or two unit cells in every DMRG iteration. Instead, we have increased the system size by 2 spin-half sites in every iteration. However, this creates new difficulties if we introduce the sites in the conventional way. At intermediate stages of DMRG we need to introduce couplings between sites which are not coupled in the true system. This problem is reduced as far as possible by inserting sites in a particular order, closely resembling the true system. Furthermore, the intermediate stage configurations and couplings, for every value of \( \lambda \), are optimized by comparing the DMRG results for smaller systems with exact diagonalization. As accuracies in the energy are very important, we have taken extra precautions to check energies at every intermediate DMRG step. The DMRG accuracy depends on \( m \), the number of density matrix eigenstates kept per block as well as the ratio \( \lambda \). We use \( m \) between 100 to 200. In the spin-3/2 (large \( \lambda \)) phase small values of \( m \) suffice, while large values of \( m \) are necessary for the calculation of properties in the spin-gap phase. Finite size DMRG algorithm has been implemented for even numbers of 5-spin blocks, and depending on the energy convergence we have performed 2 to 3 finite-system sweeps. Truncation errors, defined by the sum of the discarded density matrix eigenvalues, ranged from zero to \( 10^{-6} \) for \( \lambda = 1 \). As has been discussed in various DMRG studies, this discarded density matrix weight roughly measures the absolute error in the DMRG energies. The largest system that we have studied varies from 50 to 100 spin-half sites. We have set \( J_{\perp} = 1 \) and varied the coupling, \( J_{\|} \), from 0 to 2.

We begin with the DMRG results on the ground state properties. The ground state of the system is a non-degenerate spin singlet over the entire parameter range. The ground state energy is a continuous function of \( J_{\|}/J_{\perp} \). However, its 2nd derivative with respect to the \( J_{\|}/J_{\perp} \), has a kink at \( J_{\|}/J_{\perp} = 0.8 \pm 0.05 \), signalling a continuous phase transition. To study this transition further, we plot nearest neighbour correlation function between the spins in a chain, within a unit cell, as a function of \( J_{\|}/J_{\perp} \) in Fig.2. This correlation is positive when the system is an effective spin-3/2 chain, and the outer spins in a block are all parallel. When the chain couplings dominate, all nearest neighbor chain correlations become antiferromagnetic. The change in sign occurs precisely at this transition. Let us call the phase for \( J_{\|}/J_{\perp} < 0.8 \pm 0.05 \) phase I and the phase for \( J_{\|}/J_{\perp} > 0.8 \pm 0.05 \) phase II.

We have calculated various equal-time two spin correlation functions for the system. Let us distinguish between four different types of pair correlations, namely, those (i) between the spins in the middle row, (ii) between the middle spins and the spins in the outer chains, (iii) between the spins on the same chain and (iv) between spins on different chains. In the DMRG procedure, we have computed these correlation functions from the sites inserted at the last iteration or it’s previous iteration, to minimize the errors. Two such correlations (type (i) and (iii)) are shown in Fig.3 in the two phases noted above. At small \( J_{\|}/J_{\perp} \) (in phase I), both the correlations decay algebraically with distance, which is consistent with the quasi long range order of the half-odd-integer spin chains. But as we go to phase II, the correlation functions behave differently. In this case, we observe a rapid decay of the correlations. For the middle spin correlations, the decay is quite fast and eventually settles down to a number of order \( 10^{-3} \), which within our numerical uncertainties is consistent with zero. Thus the behavior is suggestive of a short correlation length in phase II.

We now present results on the excitation spectrum. The spin-gap can be defined as the energy difference between the lowest energy states in even and odd parity branches, which is equivalent to the lowest energies in \( S^z_{\text{tot}} = 0 \) and \( S^z_{\text{tot}} = 1 \) sectors respectively. We have targeted lowest few states in the even parity branch and ensured that these are singlet states as they do not appear in \( S^z_{\text{tot}} = 2 \) sector. In Fig.4, we show the excitation gaps to the lowest few excited states from the ground state singlet in phase II. As is clear from the figure, there is a finite gap to the lowest triplet state, but not to the singlets. If we had a system with broken symmetry, as in the Majumdar-Ghosh model, we would expect two singlet states to become degenerate in the thermodynamic limit, but a gap to all other states. This is not the case here. We see that a number of singlets are coming down in energy as the system size is increased, suggesting gapless singlet modes. As we have not done a wavevector resolved calculation, we cannot tell how many gapless singlet modes are present. Our calculations are also not accurate enough to determine the central charge of the system in phase II, which will also give the number of gapless modes.

We have observed a finite spin-gap all the way from \( J_{\|}/J_{\perp} = 0.85 \pm 0.05 \) to 2.0. However, the spin-gap is quite
small over the entire parameter range and the maximum in the spin-gap occurs at around $J_\parallel/J_\perp = 1.1$, with a gap value of $0.15 \pm 0.01$. This spin-gap measurement is quite reminiscent of what White and Affleck had found in the zig-zag chain at large next nearest neighbour coupling $\lambda$. It is difficult to calculate the small gaps accurately. A better alternative was to find the correlation length (instead of gap) by DMRG. Unfortunately, because of our large unit cell, we are not able to go to large enough systems to calculate the correlation length. The spin gap would eventually vanish as $J_\parallel/J_\perp$ becomes large as in that limit there are two isolated spin-1/2 chains and free spin-1/2’s in the middle.

We now turn to a strong-coupling analysis of the Kagomé-strip problem. By the strong coupling limit, we mean a limit in which the Kagomé-strip can be regarded as weakly coupled 5-spin blocks. As discussed earlier, the spin-3/2 phase is clearly well described in the strong-coupling limit. As weakly coupled 5-spin blocks. As discussed earlier, the spin-3/2 phase is clearly well described in the strong-coupling limit. The question we wish to address is whether the spin-gap phase be described by a strong-coupling approach. To this end, we first let the inter-block exchange be zero and vary $\lambda = J_\perp/J_\parallel$ within a block and examine the ground state multiplets. For large $\lambda$, we have a spin-3/2 ground state, which turning on interblock interactions leads to the spin-3/2 chain. At $\lambda = 2$, there is a level crossing transition and for $1 < \lambda < 2$ a different set of four-fold degenerate states becomes the ground state for the block. A potential candidate for the spin-gap phase is one where these four states of a block are coupled by the interblock interactions. Note that these four states have spin-half and consist of singlet on one of the chains and a triplet on the other chain, which is then combined into a spin-half with the spin in the middle. Thus in addition to the spin degree of freedom, there is an additional spin-half ‘pseudospin’ degree of freedom. The pseudospins have Ising-like symmetry which corresponds to interchanging the two chains.

We can now use degenerate perturbation theory to obtain an effective Hamiltonian coupling the spin-pseudospin degrees of freedom on neighboring blocks. Before proceeding with the degenerate perturbation theory, we note that at $\lambda = 1$, these 4-states become degenerate with two other states of the block. These are states, where in both chains the spins are combined into a singlet and the middle spin is free. We note that an extension of Mila’s proposed low energy manifold for the Kagomé lattice [3], will reduce to these 6-states per block for the Kagomé strip. However, for now, we will restrict ourselves to 4-states only and leave the 6-state degenerate perturbation theory for later work.

To proceed, we decompose the full Kagomé-strip Hamiltonian as $H = H_0 + H_1$, where $H_0$ contains parts of the intra-block interactions and $H_1$ contains rest of intra-block and all of the interactions between the blocks. To be concrete, we consider,

$$H_0 = S_{2i+1}^z + S_{2i+1}^z + S_{2i}^z + S_{2i}^z$$

and

$$H_1 = J_{ij}(S_{1,2i+1}^z S_{1,2i+1}^z + S_{2,2i+1}^z S_{2,2i+1}^z)$$

where $S_{k,2i}$ denotes the spin at site $2i$ of the $k$-th chain. And the chain index with a prime indicates that the chain belongs to another block.

The first order effective Hamiltonian turns out to be quite simple and without quantum fluctuation in the pseudospin degrees of freedom.

$$H_{eff}^1 = J_{ij}[-(1/4 + 2/9) \sum_{ij}(S_i S_j + 4S_i T_i^z T_j^z)]$$

where $S_i$ and $T_i$ are the spin and pseudospin operators respectively. The second order effective Hamiltonian is given by,

$$H_{eff}^2 = J_{ij}^2 \sum_{ij}[-0.5817 + 0.1201 S_i S_j + 0.3041 T_i^z T_j^z -0.1126(T_i^z T_j^z - T_j^z T_i^z) -0.1129(T_i^z T_j^z + T_j^z T_i^z) +2.2428 S_i T_i^z T_j^z -0.2334 S_i T_j^z T_i^z + T_i^z T_j^z +0.2344 S_i T_i^z T_j^z + T_i^z T_j^z)]$$

Here, the biquadratic exchanges, which involve four operator terms, could not be made simple. We checked the validity of this perturbation theory by making sure that the Hamiltonian written above produces the correct low-energy spectrum for a two-block system of the original Hamiltonian, $H = H_0 + cH_1$, with small enough $c$.

We now consider a system described by a Hamiltonian $H_{eff}^1 + H_{eff}^2$. In other words, we are considering the perturbations to be of order one but neglecting higher order terms. This Hamiltonian has 4-states per site and can be studied by numerical methods. We use an exact diagonalization method to study the system with up to 10 sites.

The ground state with $2N$ sites has $S^z_{tot} = 0$. Although the sizes studied are small, it strongly suggests a gapped triplet excitation as $N \rightarrow \infty$. Our data are not conclusive enough to identify whether the phase corresponds to a broken symmetry ground state or the Kagomé phase with gapless nonmagnetic excitations. Note that this Hamiltonian has similarities to biquadratic spin-orbital model which has a broken symmetry spin-gap phase [14, 15]. Thus, the question remains open whether the phase II of the Kagomé strip can be obtained within a strong coupling approach.

In conclusion, in this paper we have studied the 3-chain Kagomé strip Hamiltonian by DMRG and by a strong coupling expansion. The results support the work
of Azaria et al that in this model there is a spin-gap phase with gapless singlet modes.

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**Figure Captions:**

Fig.1: Schematic diagram of the Kagomé strip lattice. The corresponding Hamiltonian is given in Eq. 1.

Fig.2: Nearest neighbour two-spin correlation functions between the spins on the chain within a unit cell as a function of $\lambda$, the coupling ratio.

Fig.3: Two-spin correlation functions a) between the spins on an outer chain and b) between the middle spins, in the two phases.

Fig.4: Excitation gaps as a function of system size. The lowest triplet excitation and three lowest singlet excitations are shown.
