Spin-Gap Physics, Ground State Degeneracy, and Bound States on the Depleted Kagomé Lattice

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(Received: )

We analyse the antiferromagnetic spin-$\frac{1}{2}$ Heisenberg model on a depleted kagomé lattice, where some bonds have been reduced to exchange integral $J_2 \ll J_1$. The fully depleted system consists of 1D chains, each with a doubly degenerate singlet-pair ground state and a spectral gap (like the Majumdar-Ghosh model). There are localised and itinerant low-energy excitations. The modes from the lowest branch of excitations are incapable of lifting the 2D system’s ground state degeneracy at finite $J_2/J_1 \ll 1$. Low-energy excitations of the 2D system are dominated by coherently propagating bound states of the 1D excitations.

PACS No: 75.10.Jm

INTRODUCTION.

In recent years, interest in systems exhibiting a spin gap in the excitation spectrum has been fuelled by the appearance of spin-gap phenomena in various situations, including frustrated spin systems [1]. The analysis of toy models of spin-gap physics is noticeably easier in one spatial dimension, so considerable attention has been devoted to this line of work.

Despite the well known distinction between integer and half-integer spin excitation spectra, some spin-$\frac{1}{2}$ systems with intermediate interaction ranges have a spin gap: the Majumdar-Ghosh (MG) model [2,3] and several related models [4,5] exhibit a rich variety of behaviour. The study of the low-lying excitations of the MG model has proved a non-trivial task [6–10], and we need a spin-gapped model analogous to the MG one, but in which the low-lying excitations are easily tractable. We present such a model, obtained by removing certain bonds from the spin-$\frac{1}{2}$ Heisenberg model on a kagomé lattice (cf. the approach of [11] to the full 2D kagomé antiferromagnet).

Under this depletion, the lattice decouples into a set of one-dimensional chains, which have exact singlet-pair ground states (like the MG model) and whose low-lying excitation spectrum can be obtained analytically. The ground state of each chain is doubly degenerate, and consequently the ground state of the whole system has an degeneracy exponential in the number of chains.

We then reinstate the removed bonds at a strength $J_2 \ll J_1$, where $J_1$ is the on-chain exchange integral. This introduces a branch of domain wall–domain wall bound states which propagate coherently on the 2D lattice, and have lower energy than the on-chain modes. Furthermore, we show that the ground state degeneracy obtained for $J_2/J_1 = 0$ is not lifted by the modes in the lowest-lying band for finite $J_2/J_1 \ll 1$.

THE MODEL.

The Hamiltonian of our model is given by

$$H = J_1 \sum_{(i,j) \not\in A} S_i \cdot S_j + J_2 \sum_{(i,j) \in A} S_i \cdot S_j,$$

where the $S_i$ are vectors of spin-$\frac{1}{2}$ operators. It represents the system shown in Fig. 1, where the set $A$ contains the bonds on the edges of the grey triangles. These are the bonds that have been weakened to strength $J_2/J_1$ with respect to the remainder.

FIG. 1. The depleted kagomé lattice. The grey triangles of bonds have been weakened to exchange integral $J_2$; the remainder have exchange integral $J_1 \gg J_2$.

THE ONE-DIMENSIONAL CHAINS.

Ground States. In the limit $J_2/J_1 = 0$, the 2D system decouples into a set of 1D chains. Each chain has doubly degenerate ground states made up of nearest-neighbour singlet pairs. One ground state (called the ‘red’ ground state for convenience) is shown in Fig. 2. The other (‘blue’) ground state is obtained by a mirror reflection of the red state about the grey bar in the figure.

FIG. 2. The red ground state of the chain. Reflection about the grey bar yields the degenerate blue ground state.

These are clearly eigenstates of the on-chain part of the Hamiltonian ([), since each bond is either occupied by a singlet, or part of a triangle with a singlet on one side; see the work of Klein [12] and Affleck et al. [13] on the relationship between total-spin projection operators...
and valence bond crystal states. In the former case, an elementary calculation gives  
\[ S_1 \cdot S_2 \left[ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \right] = -\frac{3J_1}{4} \left[ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \right], \]
whereas the contributions of the other two sides of the triangle cancel out:  
\[ (S_1 \cdot S_3 + S_2 \cdot S_3) \left[ \frac{1}{\sqrt{2}} (|\uparrow\downarrow X \rangle - |\downarrow\uparrow X \rangle) \right] = 0, \]
where \( X = \uparrow, \downarrow \). Notice that the ground states of Fig. 2 are orthogonal to each other only in the limit when the number of spins on the chain tends to infinity, since \((\text{blue} | \text{red}) \sim 2^{-N}\), where \(3N\) is the number of spins.

The bonds at the top of the chain are occupied by singlet pairs in both ground states. If we ignore them for the time being (see below), we are left with a model rather like a Majumdar-Ghosh chain, except that only alternate sites have next-nearest-neighbour interactions.

This model, obtained by removing the top bonds from our depleted kagomé chain, is called the “delta chain”, or “sawtooth lattice”, and has been analysed by several authors. Early work \([14–16]\) was numerical, and established the existence of an energy gap, later studies \([17,18]\) concentrated on analytic work (mainly variational calculations), modelling the low-lying excitations as domain walls of a few spins. We summarise the domain-wall physics of a single chain here, in a notation suitable to the remainder of the letter.

**Low-Energy Excitations.** It is easy to show that a localised excitation introduced into a red ground state will not propagate coherently. To do this, we consider a group of four spins on the chain (1A, 1B, 2A, and 2B — see Fig. 3), and rewrite the local Hamiltonian in a basis consisting of two-spin eigenstates. Namely,
\[
|S\rangle_n = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle), \quad |\rangle_n = |\downarrow\downarrow\rangle, \\
|0\rangle_n = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \quad |+\rangle_n = |\uparrow\rangle,
\]
where the subscript \(n\) refers to the bond between the spins described. In this case, we consider bonds 1 and 2.

Initially, the state of these bonds will be given by \( |S\rangle_1 |S\rangle_2 \). Henceforth we shall drop the subscripts 1 and 2, leaving them implicit in the order of the kets. Now let us consider introducing a local excitation by modifying the state of bond 1. It is easy to show that
\[
\hat{H} (+) |S\rangle = \frac{J_1}{4} |+\rangle |S\rangle + \frac{J_1}{2} |+\rangle |0\rangle - \frac{J_1}{2} |0\rangle |+\rangle, \\
\hat{H} (0) |S\rangle = \frac{J_1}{4} |0\rangle |S\rangle + \frac{J_1}{2} |+\rangle |-\rangle - \frac{J_1}{2} |-\rangle |+\rangle, \\
\hat{H} (-) |S\rangle = \frac{J_1}{4} |-\rangle |S\rangle + \frac{J_1}{2} |0\rangle |-\rangle - \frac{J_1}{2} |-\rangle |0\rangle,
\]
while \(|S\rangle |X\rangle\) is an eigenstate of \(\hat{H}\). Since there is no term on the right hand side of the form \(|S\rangle |X\rangle\), coherent propagation of such a localised excitation cannot occur. These considerations lead us to conclude that the low-energy excitations of this chain are of the domain-wall type. If we begin with an initially red chain, we may introduce a region of blue ground state into it, bounded by two domain walls of distinct natures (see Fig. 3).

The stationary domain wall (boxed in the figure) is flanked by singlets, and hence remains spatially localised. The mobile domain wall (circled) feels the effect of the on-chain Hamiltonian, and so acquires a dispersion.

**FIG. 3. The two types of domain wall on the chain: stationary (boxed) and mobile (circled).**

We take our basis states to be \(|j\rangle\), representing a mobile domain wall at site \(j\) on the chain. The calculation of the dispersion relation is modified by the fact that these basis states are not mutually orthogonal. Consequently, an expansion of our eigenstate in these basis states, \(|\psi\rangle = \sum_j c_j |j\rangle\), yields an equation for the vector \(c_j\) which reads \(\hat{H} |c\rangle = E |c\rangle\), where \(\hat{H}_{ij} = \langle i|\hat{H}_{\text{chains}}|j\rangle\) and \(A_{ij} = \langle i|j\rangle\). The energy spectrum is therefore obtained from the eigenvalues of the effective Hamiltonian \(A^{-1} \hat{H}\).

Hence we find that the dispersion relation for the mobile wall is given by
\[
E(k) = \frac{7J_1}{6} \left( \frac{5}{4} + \cos k \right),
\]
where the ground state is taken to have zero energy. This result is independent of the correlation (singlet or triplet) between the mobile and stationary domain walls, so this branch contains magnetic and non-magnetic modes.

**Local Modes.** As well as these domain wall modes, the spectrum contains modes in which the spin pairs on the top horizontal bonds are excited into a triplet state, whose rôle must be considered. However, compared to the gap of the domain wall band (\(\approx J_1/4\)), the singlet-triplet gap on these bonds (\(\approx J_1\)) is rather large, so we propose to ignore excitations of the top bond singlets when considering low-energy processes on the chain.

**EXCITATIONS OF THE 2D MODEL.**

**Pair-Hopping Amplitude.** Analysing the effect of \(\alpha \neq 0\) on the excitations of the one-dimensional chains leads naturally to the consideration of tunnelling processes; however, it is clear that a single mobile wall cannot tunnel by itself, as this would violate the restriction that the chain states be unchanged at large distance.

However, there exists an amplitude for pair hopping of a stationary and a mobile domain wall. To describe it, let us introduce a set of basis states more general than those used in the 1D analysis. In our new notation, \(|i, j\rangle_1\)
represents a state of chain 1 with a stationary domain wall at site \(i\), and a mobile domain wall at site \(j\). Our previous basis states \(|j\rangle\) are now represented by \(|0, j\rangle_1\).

Let us deal with the case where both chains are in the red ground state at large distance. There is a term of perturbation theory, first order in \(J_2/J_1\), that connects the states \(|i, j\rangle_1\) (red) and \(|\text{red}\rangle_2\) and \(|\text{red}\rangle_1|k, j\rangle_2\). This term is represented diagrammatically in Fig. [4].

![Diagram](image)

**FIG. 4.** A pictorial representation of the steps in the inter-chain tunnelling process. Those triangles through which the grey bar passes have bonds with exchange integral \(J_2\).

Using the standard formulae of Rayleigh-Schrödinger perturbation theory, and approximating the energy of the local mode by \(\epsilon\), perturbation theory, first order in \(J_2/J_1\), we make a simple Ansatz: we assume the self-energy \(\Gamma\) is the unit step function. The precise value of the prefactor depends on the value we use for the local mode gap, but the linearity in the case where the two ground states are blue. Both of our qualitative results to be altered by the introduction of the effective Hamiltonian is

\[
\hat{H}_{\text{eff}} = \frac{J_2}{20} |i-j| |k-j| \Theta ((i-j)(k-j)),
\]

where \(\Theta(z)\) is the unit step function. The precise value of the prefactor depends on the value we use for the local mode gap, but the linearity in the case where the two ground states are blue. Both of these cases will be called ‘non-reflective hopping’, since the sign of \(k\) is preserved in the hopping process. The alternative situation, ‘reflective hopping’, will be taken up in a forthcoming publication [13]. We do not expect our qualitative results to be altered by the introduction of reflective hopping (see concluding discussion).

**Bound States (Non-Reflective Hopping).** To analyse the non-reflective case, we formulate an effective model by introducing creation and annihilation operators for the mobile \(|c_{n,i}\rangle\) and stationary \(|d_{n,i}\rangle\) domain walls; here, \(n\) and \(i\) are chain and site indices respectively. It is clear that the domain walls must obey an exclusion principle, but this still leaves a choice of statistics: fermions or hard-core bosons? In the dilute limit, the exchange statistics are not relevant to the calculation; conventionally, we choose the operators \(\{c, c^\dagger, d, d^\dagger\}\) to obey Fermi statistics.

In these terms, the effective Hamiltonian is

\[
\hat{H}_{\text{eff}} = t \sum_{n,i} \left( c^\dagger_{n,i} c_{n,i+1} + \text{h.c.} \right) + (\epsilon - \mu) \sum_{n,i} c^\dagger_{n,i} c_{n,i} + \mu \sum_{n,i} d^\dagger_{n,i} d_{n,i} + \sum_{n,i,j,k} \left( V_{ijk}^{n-1,n} c^\dagger_{n,i} d^\dagger_{n,k} d_{n-1,j} c_{n-1,i} + \text{h.c.} \right) \]  

(6)

where \(t = \frac{1}{2} J_1\), \(\epsilon = \frac{3}{2} J_1\), and \(V_{ijk}\) is just the amplitude \(A_{\text{non-refl}}\) from Eq. [5], with \(i\) being the position of the mobile wall, \(j\) that of the stationary wall before hopping, and \(k\) that of the stationary wall after hopping.

Because of the translational invariance in the \(x\) (parallel to the chains) and \(y\) (transverse to the chains) directions, we may Fourier transform and work in momentum space. The action is given by

\[
S = \sum_{\omega, p, h} c_{\omega ph}^\dagger (\omega - \epsilon - 2t \cos p + \mu) c_{\omega ph} + \sum_{\omega, p, h} d_{\omega ph}^\dagger (\omega - \mu) d_{\omega ph} + \sum_{\omega_1 \omega_2 \omega_3} \Gamma^{(0)}_{pq} \frac{h}{\omega_1 \omega_2 \omega_3} \frac{p}{\omega_4} c_{\omega_2 ph}^\dagger d_{\omega_1 ph} c_{\omega_1 ph},
\]

(7)

where \(\omega_4 \equiv \omega_1 + \omega_2 - \omega_3\), \(s \equiv p + q - r\), and \(c_{\omega ph}^\dagger\), \(c_{\omega ph}\), \(d_{\omega ph}^\dagger\), \(d_{\omega ph}\) now represent Grassmann fields. The \(\omega_i\) are fermionic Matsubara frequencies, \(p, q, r, s\) are momenta along the chains, and \(h\) is the transverse momentum. Recall that, in the case we consider, all momenta are restricted to positive values. The bare vertex part, \(\Gamma^{(0)}\), is given by

\[
\Gamma^{(0)} = \frac{J_2}{20} \frac{h \cos \frac{\omega}{2}}{2\pi} \left( f(q) f(-s) + f(-q) f(s) \right),
\]

(8)

where the function \(f(q)\) is the Fourier transform of the hopping amplitude’s spatial dependence, given in Eq. [3].

The formation of bound states is signalled by the appearance of divergences in the dressed vertex part, \(\Gamma\). Being unable to solve the full set of Schwinger-Dyson equations, we make a simple Ansatz: we assume the self-energies of the two propagators to be zero. Our defence is that the gap in the unperturbed model is quite large.

The remaining bound state condition can be solved analytically only near two lines in the Brillouin zone, \(h = \pm \frac{\pi}{2}\). Setting \(h = \frac{\pi}{2} - \delta\), we find that

\[
\epsilon = \frac{J_2 \delta}{10t} \left( \frac{2 \cos^2 P - 4 \cos P + 3}{(4 \cos P - 5)^2} \right),
\]

(9)
where $P$ is the on-chain momentum, and $\frac{1}{2} c^2$ is the distance that the bound state lies below the band of unperturbed modes, i.e. $E_{\text{bound}} = \frac{1}{2} c^2 J_1 - \frac{1}{2} \epsilon^2$. Similar behaviour is found near the line $h = -\frac{\pi}{2}$. We tentatively conclude that the branch of bound states exists throughout the Brillouin zone, touching the bottom of the continuum band tangentially along the lines $h = \pm \frac{\pi}{2}$.

**GROUND STATES OF THE 2D MODEL.**

In the limit $J_2/J_1 = 0$, the double degeneracy of each chain in the system leads to a total degeneracy $g = 2L$, where $L$ is the number of chains.

It is noteworthy that we have been unable to find a process (within the manifold of domain wall states) that lifts this ground state degeneracy in the $\alpha \neq 0$ case. Any such process consists of a finite number of inter-chain hopping events. Each such hop between two chains of the same ground state has a counterpart hop between two chains of different ground states, the only difference being that in the latter case the left-to-right order of the stationary and mobile domain walls is reversed. Due to a combination of the spatially extended nature of the domain wall states (see above) and the imposition of periodic boundary conditions, such a reversal cannot make a difference to the amplitude of the process. Hence all perturbation theory corrections to the energy of a given ground state of the two-dimensional lattice have counterparts of equal magnitude and sign for any other ground state.

Although no explicit calculation has been performed, the degeneracy is almost certainly lifted by perturbative processes involving the excitation of local modes on the ‘top’ horizontal bonds of the chains. Nonetheless, it is interesting to note that, because of the effective screening of the chains from one another due to the singlets on the top bonds, the modes in our low-energy manifold are incapable of lifting the ground state degeneracy of the $\alpha = 0$ case.

**CONCLUSION.**

We have presented a quasi-1D chain with nearest-neighbour antiferromagnetic exchange and a spin-gapped excitation spectrum that can be treated analytically in the low-energy limit. This chain was obtained by a natural depletion of the 2D kagomé antiferromagnet, and as well as itinerant and localised domain walls (obtained in [17,18] by similar methods to ours) it has local modes with a gap larger than that of the itinerant excitations.

Recoupling these chains weakly, we have obtained a pair-hopping amplitude of the itinerant and localised 1D modes that arises naturally from the nature of the 1D ground states. Furthermore, we have shown that the ground state degeneracy of the 2D system (which is exponential in the number of chains) is not lifted by processes in the lowest branch for finite $J_2/J_1 \ll 1$; this effect is due to symmetry properties of the ground states and the nature of the interchain coupling. As regards the excitations, the pair hopping amplitude leads to a band of bound states of the 1D domain walls; these bound states propagate coherently on the 2D lattice, and have lower energy than the on-chain excitations.

While our model is not proposed as a starting point for treating the isotropic 2D kagomé antiferromagnet, it has several novel and interesting features, notably the inability of the domain wall modes to lift the ground state degeneracy [20] and the formation of a band of coherently propagating 2D states for arbitrarily small $J_2/J_1 \neq 0$.

Finally, one might ask whether the consideration of reflective rather than non-reflective hopping will change our results. Qualitatively, one may argue that it will not: since bound states already form in the non-reflective system, the existence of reflective hopping will act only to strengthen the tendency to bind, perhaps modifying the prefactor in [20]. These topics, along with a semiclassical method of treating the non-reflective case, will be taken up in a forthcoming publication [19].

**ACKNOWLEDGMENTS.**

We are pleased to acknowledge useful discussions with J. T. Chalker, C. Lhuillier, P. Lecheminant, P. Azaria, R. Siddharthan, and A. Campbell-Smith. One of us (CH) acknowledges financial support from EPSRC (UK) studentship 96305551.