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A bipartite spin $\frac{1}{2}$ Heisenberg model with a gap to excitations

M W Long

School Of Physics, Bath University, Claverton Down, Bath BA2 7AY, UK

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Abstract. We consider the nearest neighbour quantum mechanical Heisenberg model acting on two simple one-dimensional chains of spin $\frac{1}{2}$ atoms. By showing that these models can be mapped onto a chain of spin 1 composites, we deduce that the spectrum has a gap, provided that the spin 1 chain has a gap. This result is in contrast to that found for the chain of spin $\frac{1}{2}$ atoms and suggests that a distinction between integer and half-integer spins is restricted to the linear chain. We present a simple interpretation for the spin correlations of the low energy excitations and give new numerical evidence for a gap in the spectrum of the spin 1 chain. The lowest lying spin $\frac{1}{2}$ chain excitation is a domain wall, but the lowest lying spin 1 chain excitation has previously been suggested to have spin-wave properties, we test this hypothesis numerically.

1. Gapped spin $\frac{1}{2}$ Heisenberg models

Exact results on the quantum mechanical Heisenberg model are both rare and very important. One such result is that half-integer spin chains are gapless whereas integer spin chains have gaps [1]. This important result might lead one to believe that the two classes of spins behave quite generally in different ways. This short note is simply pointing out that more exotic connectivities of atoms can alter this result, and in particular we find a one-dimensional half-integer system with a gap.

The model we discuss has had a short history in the literature [2]. A detailed mathematical treatment can be found in this previous work and we will restrict ourselves to a brief interpretation of the physical content of the model.

The first topology of interest is depicted in figure 1, and may be found in the body centre cubic lattice. The simplest geometric interpretation is of two interpenetrating lines of squares, with the edges of one set of squares passing through the centres of the other squares. Each atom has four nearest neighbours which compose its closest square. The two lines of squares make up two natural sublattices, and since all the nearest neighbours of one line of squares are on the other, the lattice is bipartite.

The nearest neighbour Heisenberg model is:

$$H = J \sum_{[ii']} S_i \cdot S_{i'} \tag{1}$$



Figure 1. The bipartite topology. (a) The two interpenetrating lines of squares. (b) The nearest neighbour bonds which form connected octohedra.

where [ii'] denote nearest neighbours, J is the interaction strength and S_i are quantum mechanical spin $\frac{1}{2}$ operators. For the present geometry we may rewrite the Hamiltonian as:

$$H = J \sum_{[EE']} S_E \cdot S_{E'}$$
(2)

where E denotes an edge which passes through the centre of a square, $S_E = S_{i_1} + denotes$ the total spin of the pair of spins, S_{i_1} and , which sit on the edge above and below a square and [EE'] denote pairs of edges with nearest neighbour spins.

It is clear from (2), that for each relevant edge, the square of the total edge spin, $S_E \cdot S_E$, commutes with the Hamiltonian and is therefore conserved. If we elect to use the representation where these operators are diagonal, viz $S_E \cdot S_E = S_E(S_E + 1)$, then the problem is reduced to finding the configuration of values for S_E which yields the ground state.

The only two possible values for the total edge spin are, $S_E = 0$ and 1. If an edge spin is singlet, then the two neighbouring edge bonds yield zero and the chain is effectively cut, with the two neighbouring edge spins being completely decoupled. Since there is a large energy gain from bonding neighbouring triplet spins, singlet edge spin states are highly excited states and are therefore irrelevant to the low energy physics. The low energy spectrum is dominated by states where all the edge spins are triplet, and this is just the linear chain of spin 1 objects.

The low energy excitation spectrum of the spin 1 chain is gapped, and so the present system also has a gap, in contrast to the spin $\frac{1}{2}$ chain.

The second geometry of interest to us is the chain of edge sharing tetrahedra, depicted in figure 2 and found in the face centre cubic lattice. The fundamental unit is the tetrahedron, which is well known to be topologically frustrated. This connectivity is very similar to the previous case, with the simple addition of a bond connecting the two atoms on a shared edge, leading to five nearest neighbours to each spin. We may rewrite the Hamiltonian as:

$$H = J \sum_{\{EE'\}} S_E \cdot S_{E'} + \frac{J}{2} \sum_E S_E \cdot S_E - \frac{3J}{4} N_E$$
(3)



Figure 2. The frustrated topology. (a) Connected cubes of face centre cubic atoms. (b) The nearest neighbour bonds which form edge sharing tetrahedra.

where N_E is the number of shared edges. Once again we can choose to use the representation where the squares of total edge spins are conserved, and then the problem reduces to minimizing:

$$H = J \sum_{[EE']} S_E \cdot S_{E'} + \frac{J}{2} \sum_E S_E(S_E + 1) - \frac{3J}{4} N_E$$
(4)

over the possible edge spin values of $S_E = 0$ or 1 for each spin, and then minimizing the energy of the residual segments of spin 1 chain. The only difference from the previous case, is that singlet bonds are now more favourable, gaining a full J from their internal bond. This in turn lowers the energy of the excitations with singlet edge spins, but a numerical study should convince the reader that there is still a gap to the state with the first singlet edge bond. The low energy excitations are therefore *still* those of the infinite spin 1 chain, and this system therefore has a gap to excitations.

In table 1 we present the results of exact diagonalization studies of finite chain segments using the Lanczos algorithm. Finite size scaling applied to the gap to the first excitation is ambiguous, but we have the exact result of Haldane [1] providing a gap. When we consider the gap to the first excitation with a singlet edge spin, viz $S_E = 0$, we predict a gap of $\sim 2.5J$ and $\sim 1.5J$ for the bipartite and frustrated topologies respectively. The periodic calculation for this gap involves comparing the periodic ground state energy with the free ground state energy for the chain which is one spin shorter. The free calculation for this gap involves comparing the ground state of a chain with the sum of the energies of the two ground states of the two halves of the chain.

In conclusion, we have presented two simple one-dimensional connectivities, one bipartite, the other topologically frustrated, both of which yield a gap in the low energy excitation spectrum of the spin $\frac{1}{2}$ Heisenberg model.

The distinction between integer and half-integer spins presented by Haldane [1] may simply be peculiar to the one-dimensional chain.

Table 1. Numerical calculations for finite lengths of spin 1 chains in units of J. The
chains are too short to deduce the true gap, but the gap to the first singlet bond
excitation is clearly large in comparison with the low energy triplet excitation gap.
All gaps are measured with respect to the ground state energy. Note that there are
two low energy states for free boundary conditions.

Noof	No of	Coord state	Finat	First singlet excitation		
atoms	bonds	energy	excitation	Bipartite	Frustrated	
Periodic	boundary	conditions				
2	2	-4.0000	2.0000	4.0000	3.0000	
3	3		1.0000	1.0000	0.0000	
4	4	→6,0000	1.0000	3.0000	2.0000	
5	5	-5.5667	0.2501	0.9210	0.0790	
6	6	-8.6174	0.7206	2.7871	1.7871	
7	7	-9.5722	0.8568	2.2019	1.2019	
8	8	-11.3369	0.5935	2.7023	1.7023	
9	9	-12.4800	0.7702	2.3554	1.3554	
10	10	-14.0941	0.5248	2.6612	1.6612	
11	11	-15.3367	0.7045	2.4421	1.4421	
12	12	-16.8696	0.4842	2.6392	1.6392	
13	13	-18.1697	0.6541	2.4957	1.4957	
14	14	-19.6551	0.4589	2.6269	1.6269	
Free bou	indary con	ditions				
2	1	-2.0000	1.0000	2.0000	1.0000	
3	2	-3.0000	1.0000	3.0000	2.0000	
4	3	-4.6457	0.5091	2.6457	1.6457	
5	4	-5.8303	0.5467	1.8303	0.8303	
6	5	-7.3703	0.3078	2.3703	1.3703	
7 '	6	-8.6346	0.3310	2.6346	1.6346	
8	7	-10.1246	0.2018	2.4889	1.4889	
9	8	-11.4329	0.2127	2.1415	1.1415	
10	9	-12.8946	0.1384	2.4186	1.4186	
11	10	-14.2304	0.1418	2.5698	1.5698	
12	11	-15.6740	0.0971	2.4734	1.4734	
13	12	-17.0282	0.0967	2.2876	1.2876	

2. Correlations in the spin 1 chain

It is generally believed that the chain of spin 1 atoms has a gap to excitations [3]. As well as the basic theoretical argument [1], there are now a few numerical results which are being used to support the assertion that the gap exists and has a value of $\sim 0.4J$ [4]. These numerical calculations are based on periodic boundary conditions, and our results ennumerated in table 1 for the case of free boundary conditions lead us to reexamine the numerical calculations and seek a deeper understanding.

A lot of effort has been expended on trying to find both the gap to excitations and the correlation length of spin-spin correlations [4]. We will not pursue this problem. Our motivation is to try to understand the sense in which the spin 1 chain is *anomalous*. Firstly we will examine the correlations found in the excitations, with a view to classical and quantum interpretations using the infinite spin and spin $\frac{1}{2}$ chains as analogues. Secondly we will point out two fundamental differences which we cannot as yet interpret.

Bipartite spin $\frac{1}{2}$ Heisenberg model

2.1. Spin-spin correlations and classification of states

The two lowest energy states for free boundary conditions do not seem to exhibit the Haldane gap. A continuous variation of one of the bonds in the chain from zero to J demonstrates that the ground state and first excited state do not exchange with any other states in the system as the boundary conditions are changed, and therefore have identical quantum numbers. The state with periodic boundary conditions which has an excitation worth $\sim 0.4J$ corresponds to a degenerate ground state for free boundary conditions. How can we interpret these states?

Table 2. The spin-spin correlation functions, $(S_i \cdot S_{i'})$, for various states in the spin $\frac{1}{2}$ and spin 1 chains. The values should be interpreted loosely as the average value of $|S|^2 \cos \theta$ between the relevant spins with a vanishing value indicating that the spins are uncorrelated. (a) Periodic boundary conditions. (b) Free boundary conditions.

			Spin $\frac{1}{2}$		Spin 1			
i	i'	Ground state	First spin wave	First ZB spiral state	Ground state	First spin wave	First 2C spiral state	First ZB spiral state
1	2	-0.4490	-0.4193	-0.3982	-1.4056	-1.3654	-1.2492	-1.2258
1	3	0.1879	0.1743	0.0898	0.7775	0.8071	0.5414	0.5902
l	4	-0.1658	-0.1143	-0.0049	-0.6322	-0.6670	-0.2022	-0.3323
1	5	0.1209	0.0902	~0.1035	0.5044	0.5801	-0.1164	0.0123
1	6	-0.1224	-0.0576	0.1269	-0.4621	-0.5361	0.2069	0.0634
L	7	0.1070	0.0701	-0.1703	0.4363	0.5293	-0.3612	-0.2162
L	8	-0.1224	-0.0576	0.1269	-0.4621	-0.5361	0.2069	0.0634
t	9	0.1209	0.0902	~0.1035	0.5044	0.5801	-0.1164	0.0123
	10	-0.1658	-0.1143	-0.0049	-0.6322	-0.6670	-0.2022	-0.3323
L	11	0.1879	0.1743	0.0898	0.7775	0.8071	0.5414	0.5902
l	12	-0.4490	-0.4193	-0.3982	-1.4056	-1.3654	-1.2492	-1.2258

(6)

(a)

		Spin $\frac{1}{2}$		Spin 1		
i	ť'	Ground state	First excitation	Ground state	First excitation	
1	2	-0.6563	-0.5598	-1.6371	-1.5950	
1	3	0.1982	0.2189	0.8952	0.8685	
1	4	-0.2206	-0.1304	-0.8121	-0.7023	
1	5	0.1095	0.1163	0.6266	0.5094	
1	6	-0.1293	0.0333	~0.6146	-0.3830	
1	7	0.0726	0.0573	0.5277	0.2808	
1	8	-0.0899	0.0103	~0.5730	-0.1698	
1	9	0.0512	0.0155	0.5128	0.1089	
1	10	-0.0677	0.0304	-0.6369	0.0009	
1	11	0.0340	-0.0082	0.5231	-0.0193	
1	12	-0.0517	0.0329	-0.8125	0.1331	

A study of the spin-spin correlations ennumerated in table 2 leads to an explanation for the change. The first excited state with free boundary conditions gains a twist, with the spin at the opposite end of the chain being on average antiparallel to its relative direction in the ground state with free boundary conditions.

This capacity for the spins to achieve a twist is very important in the study of the spin chain. For the classical limit such spiral states form very low energy gapless excitations which are quite distinct from classical spin waves.

Classical spin waves involve three spin dimensions and are small displacements of the spins away from their classical directions. The displacements precess in the two dimensions which are perpendicular to the classical ground state quantization direction. The quantum analogue of these states can be found by studying the spin correlations of the excitations. A spin-wave excitation has the same basic pattern of spin correlations as the ground state, but with a minor modification in the magnitude of the correlations. The spin correlations of the lowest lying excitations for periodic boundary conditions ennumerated in table 2 are of this type. Such an excitation has spin 1 and is well modelled by a Holstein-Primakoff description.

The classical spiral states involve only two spin dimensions and are also found in the XY model. All the spins lie in one plane and precess by a constant angle as one proceeds along the chain. A simple interpretation of such an excitation is that of a *domain wall*. Two ground states at each end of the chain with different quantization directions can be smoothly connected by such a spiral. The quantum analogue of these states can also be found by a study of the spin correlations. Although the *local* correlations retain the same pattern as the ground state, at longer distances the relative phase of the correlations becomes reversed.

For spin $\frac{1}{2}$ systems domain walls seem to take an even more central role [5]. The low lying excitations are *not* spin waves but are in fact domain walls carrying spin $\frac{1}{2}$. Spin waves may then be interpreted as bound states of pairs of domain walls, which can break up at low temperatures in collisions.

The fact that free boundary conditions facilitate the inclusion of a twist, suggests that the low lying excitations may well be domain walls and not spin waves even for the spin 1 chain. It is then quite natural to suggest the possibility that although the spin waves might have a gap, maybe the domain walls do not. It is clear from table 2 that the lowest lying excitation for the periodic systems considered are spin-wave like.

The natural way to test the above hypothesis numerically, is to attempt to perform finite size scaling on domain wall excitations, but can we find such excitations?

It seems clear that domain walls are topological excitations and can only be created in pairs. The reason that the even membered chains have a spin wave as a lowest excitation, may then be interpreted as one spin wave being cheaper than two domain walls for these small systems. One of the consequences of this topological property is that odd membered rings must have one such excitation and so perhaps a comparison of odd and even membered rings might yield the energy of a domain wall. Furthermore, a recent study of some exactly soluble geometries, with only short range order in their ground states, demonstrates that domain wall excitation energies can be found from a comparison of odd and even membered chains for some systems [6]. Any such comparison for the spin 1 chain suggests that odd and even membered rings are directly comparable and there is no additional energy for odd membered rings as we shall show in the next subsection. Unfortunately, one cannot then deduce that a domain wall costs nothing, because for a system with only short range correlations. the odd membered chain may also yield the unique ground state in the limit. The odd membered rings do have total-spin 1 ground states, further suggesting that there is an extra 'object' present, corresponding possibly to a spin 1 domain wall,

If one accepts that a study of odd membered chains is ambiguous, then one is forced to look for spiral states in the even membered chains. Fortunately it is quite easy to interpret the low energy excitations in these systems. The ground state is a total spin singlet with zone centre phase coherence. There is an energy band at low energy corresponding to a single spin wave. The spin-wave states have total spin 1 and exist all across the zone except at the zone centre. At the zone centre, the lowest lying excitation is a spin 2 state which may be interpreted as two spin waves. The first spiral state is the lowest lying spin 0 excitation across the zone. The spin-spin correlations for these states are also ennumerated in table 2 and it is clear that there is one full twist along the chain.

A finite size scaling study of small chains is ambiguous because of the small size of the systems involved. It is our belief that a comparison between spin $\frac{1}{2}$ systems and spin 1 systems is the most convincing analysis, because the spin $\frac{1}{2}$ chain can be solved and understood analytically.

Apart from an interchange of the zone centre and zone boundary for half of the spin $\frac{1}{2}$ chains, the type of states and their correlations are surprisingly similar for the two types of chains. In our investigations, only the finite size scaling characteristics have exhibited any significant differences, the classification of the states being analogous.

In figures 3(a) and 3(b) we plot the energies of both the first excited state and the lowest lying zone boundary spiral state for each type of spin. The interpretation of the spin $\frac{1}{2}$ system is easy given the analytic solution. The spiral state involves two phase boundaries and hence two topological excitations. Dividing this energy in two indicates that one topological excitation costs less energy than one spin wave, in perfect agreement with the analytic results. The two types of state finite size scale towards zero energy as they should do. The analogous states for the spin 1 system behave in a quite different way. Not only is it very difficult to argue that the excitation energies scale towards zero, the spiral state is much more than twice the single-spin-wave energy, suggesting that spin waves would be the dominant thermodynamic excitations at low temperatures, opposite to the behaviour predicted for the spin $\frac{1}{2}$ system. Also of some concern is the negative curvature of the spiral state energies, which weakens the argument for the gap for these states in comparison to the spin-wave states.

In figure 3(c) we plot the energies of the lowest spin 2 excitation and the zone centre spiral state. The lowest spin 2 excitation seems to finite size scale towards a finite value, exhibiting positive curvature like the lowest energy spin 1 excitation. It is quite natural to interpret this state as having two of the spin 1 excitations. The zone centre spiral produces the first real surprise; *it does not appear to scale towards the same gap as the other excitations.* There is however evidence of the positive curvature found for the other excitations indicating a gap. Naive estimates would suggest that in the absence of new effects it would become the lowest excitation at about $N \sim 50$. This state has all the properties one might expect of two low energy domain walls in the infinite chain limit.

We have found much evidence which supports the Haldane gap. However, the lowest lying excitation being finite size scaled in the cluster calculations may not be the lowest lying excitation. In fact the lowest lying excitation could well be a domain boundary as it is for the spin $\frac{1}{2}$ chain.

We believe that the low energy excitations of the spin $\frac{1}{2}$ and spin 1 chain have quite different local spin correlations, and should be interpreted as quite different types of excitations.



1/N

Figure 3. The Excitation energies of small loops of atoms. The symbols denote: X, the lowest energy spin-wave excitation; O, the lowest energy spiral excitation; +, half the spiral excitation energy; *, the lowest energy spin 2 state. (a) Spin $\frac{1}{2}$. (b) Spin 1: the states analogous to those in (a). (c) Spin 1: some other low energy states.

2.2. Anomalous behaviour for the spin 1 chain

Although we are calling the lowest energy excitation of the spin 1 chain a spin wave, a careful comparison of the correlations in table 2 shows that this excited state has more Néel order for more distant spins than the ground state, in complete contrast to both the spin $\frac{1}{2}$ case and the spin-wave interpretation. One can interpret this fact with the suggestion that the quantum analogue of the Néel state is an excited state and excitations of the ground state can locally excite extra Néel order. This is an analogous interpretation to that applied to the exactly soluble models with only short range correlations in the ground state [6], where the analogy is clear cut.

The spin correlation functions for our small clusters are not representative of the infinite chains. A comparison between excitations is more likely to survive into the infinite system however. The physical phenomena which stabilize the ground state do not change, and unless there is a *reversal* of behaviour with an excitation becoming

the ground state the relative characteristics can be believed.

If we calculate the expectation value of the square of the sublattice magnetization, then we find a sequence of excitations of the spin 1 chain, with increasing total spin, for which the sublattice magnetization *increases*. This is in direct contrast to the spin $\frac{1}{2}$ chain for which the corresponding states show a decrease in sublattice magnetization as the spin-wave interpretation suggests. The first spin wave and the lowest energy spin 2 excitation depicted in figure 3(c) by \times and *, respectively, are the first two states with increasing sublattice magnetization. The relevant states are the lowest energy states for the given total spin, and may be interpreted as having an increasing number of spin 1 excitations, one more for each increment in the total spin. In figure 4 we finite size scale the change in the square of the sublattice magnetization for these 'spin-wave' states. The spin waves on the spin $\frac{1}{2}$ chain clearly involve a loss in magnetization whereas the 'spin waves' for the spin 1 chain clearly involve a gain. It might initially be assumed that once the chain reaches the coherence length of the spin correlations that any gain in the sublattice magnetization might be lost, but the change is clearly increasing, suggesting that each excitation is associated with a local increase in magnetic order.



Figure 4. A finite size scaling calculation of the change in sublattice magnetization of the excitations of the spin $\frac{1}{2}$ and spin 1 chains denoted by \times and O, respectively. The change is calculated from the spin zero ground states of the relevant chains, and the three states scaled are the total spin 1, 2 and 3 ground states which have increasing sublattice magnetizations. The spin $\frac{1}{2}$ system has a loss in sublattice magnetization for these states whereas the spin 1 system has a gain in sublattice magnetization.

There is a physical interpretation of the spin $\frac{1}{2}$ systems for which the sublattice magnetization increases in the excitations. In quantum spin systems there is a competition between two energies; classical ordering energy and quantum fluctuation energy or zero point motion. When geometric considerations destabilize the ordered state, the ground state optimizes quantum fluctuation energy at the expense of classical ordering energy. Excitations then reinstate the ordering energy overcompensated by a loss in the dominant quantum fluctuation energy. This is a possible interpretation for



Figure 5. The ground state energies of odd and even membered loops of spin 1 atoms. The approximate infinite loop limit has been extracted and the residual contribution, $\Delta E = E + 1.4016N$, is plotted. There is clearly no contribution from the domain wall which must be present for the odd membered chains.

the behaviour of the spin 1 chain.

There is a second anomaly which remains a surprising and unexplained feature. When we consider free boundary conditions, we seem to find two ground states and then a gap to higher excitations. The two states which exponentially approach each other in the infinite chain limit have total spin 0 and total spin 1. We have no interpretation of this ground state degeneracy, but we have observed a corresponding result for the chain with periodic boundary conditions. At first sight even and odd chains might be expected to have quite different energies since an odd chain necessitates a domain wall. In figure 5 we depict a careful comparison of the ground state energies of even and odd chains with periodic boundary conditions. The approximate infinite loop limit has been extracted, and the difference between the two loops should correspond to the energy of a single domain wall. To our surprise the domain wall found this way is predicted to be at zero energy. If we recall the correlations found in the two ground states for *free* boundary conditions, then the two spins at opposite ends of the chain are found to be parallel for one and antiparallel for the other on average. It seems natural to associate these two free boundary condition ground states with the periodic boundary condition ground states of the odd and even membered chain respectively. An interpretation of this 'anomaly' might shed some light on the subject.

It would be nice if we could associate each chain end with a spin $\frac{1}{2}$, and then the resulting combination of the two would explain the degeneracy. This explanation is of course nonsense, since it is not possible to make a half-integer spin from only integer spins.

In conclusion, the numerical evidence for the Haldane gap is strong, with only the zone centre spiral causing concern. It is still conceivable that long wave length spirals are gapless.

Note added in proof. The reader is directed to reference [7], which may well prove interesting. Some of the ideas have a strong overlap with the present article.

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