Diverging Heisenberg spin ladders: ground state and low energy excitations

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Abstract

We consider a two-leg ladder system with interactions varying from constant rung coupling to systematic diminishing of rung interactions leading to diverging chains. We compare and contrast their ground state and excitation characteristics using density matrix renormalization group methods. We find that the finite spin gap in a constant coupling ladder develops into a gapless excitation with slight diminishing of the distance dependent coupling. Varying the spatial range of the rung coupling, we derive the effective length scale of triplet excitations in these ladder classes of systems.

Studies of low dimensional magnetic systems have been the subject of intensive theoretical and experimental research in recent years due to their unique low energy characteristics. For example, while the integer spin Heisenberg chain has a gap in the excitation spectrum together with an exponentially decaying correlation function, its half-integer analogues show gapless excitations with a power-law correlation function [1, 2]. On the other hand, in two dimensions, for a square lattice, the Heisenberg model exhibits long range Néel order in the ground state and has gapless Goldstone modes [3]. Recent interest however lies in systems with intermediate dimensionality and the crossovers between one and two dimensions. One of the approaches to such problems is studying the two-dimensional systems where the interaction along the x-axis is different from that along the y-axis [4]. The way to explore this issue is through the Heisenberg spin ladders consisting of a finite number of chains coupled together, with coupling $j_\parallel$ along the chain and $j_\perp$ between them. There have been many examples of such ladder systems and a series of ladder structures have already been realized, such as vanadyl pyrophosphate $(VO)_2P_2O_7$ [5] and the strontium cuprates $SrCu_2O_3$ [6].

Theoretically, a number of striking prediction have been made for such systems. One clear result from all these studies [7–12] is that ladders with an even number of legs have an energy gap, short range correlation and a 'spin liquid' ground state, while for odd number of legs, the excitation is gapless, with quasi-long range order, and a power-law fall-off of spin–spin correlations. The nature of the ground state has been confirmed experimentally [13]. The thermal and magnetic properties of the integrable $SU(4)$ ladder model have been investigated

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by transfer matrix and high temperature expansion methods. Excellent agreement has been observed between the theoretical results and the experimental data [14]. More recently, ladder models with competing interactions, such as with staggered dimerization and with rung and diagonal coupling, have been introduced and studied in detail. We consider here a conventional two-leg ladder system and study its ground state and excitation characteristics by varying the rung coupling in such a way that the lattice looks like a diverging system. We hereafter call it a diverging ladder. Divergence in coupling turns out to play a crucial role in the excitation characteristics of these ladders. Although such systems have not yet been realized experimentally, recent synthesis of systems with bulky groups in place of hydrogens holds promise for diverging ladder realization with multi-chain characteristics [16].

A very remarkable fact about the spin-1/2 Heisenberg chain is that its excitation spectrum consists of spin-1/2 particles (spinons). Physically such excitations can be created only in pairs because upon flipping one spin the total spin projection is changed by one. Thus in the spin-1/2 Heisenberg chain, the conventional magnons carrying spin 1 are deconfined into spin-1/2 spinons. Putting two spin-1/2 chains together one can observe how spinons are confined back into magnons by studying the dynamical susceptibility. The interchain exchange thus serves here as a control parameter. One can obtain a qualitative understanding of the spinon confinement by considering the strong coupling limit of the spin ladder problem [15]. As the interchain exchange of the spin ladder problem serves as a control parameter for spinon confinement, it would be very interesting to study the ground state and excitation properties of the spin ladder problem by varying the interchain interaction strength gradually in such a way that the ladder system represents various diverging ladders.

There are various numerical and analytical techniques for studying the properties of the spin chain systems. The density matrix renormalization group (DMRG) [17] is perhaps the best numerical tool for handling the spin-1/2 quantum chains and various frustrated spin systems, as it is considered to be the most accurate method for addressing interacting systems in low dimensions [17, 18]. In this work, we have used the DMRG method for studying the Heisenberg ladder with two legs together with various interchain interaction limits.

The Hamiltonian of our system is given by

$$H = \sum_{n=1}^{N/2} j S_{1,n} \cdot S_{1,n+1} + j S_{2,n} \cdot S_{2,n+1} + j'' S_{1,n} \cdot S_{2,n} \tag{1}$$

where $S_{1,n}$ denotes the $S = 1/2$ spin at the nth site of the first chain and $S_{2,n}$ denotes the $S = 1/2$ spin at the nth site of the second chain. To reduce the finite size effect, we consider the periodic boundary condition so that $S_{1,1} = S_{1,N+1}$ and $S_{2,1} = S_{2,N+1}$. For convenience, we have considered the interaction along the chain as $j = 1.0$. j'' is chosen in such a way that the ladder represents a conventional two-leg system with varying interaction such that $j'' = \frac{j'}{p^{n'-1}}$, where $p = 1, 2, 3$ and 4 and $n' = 1, 2, 3, \ldots$. The schematic diagram is shown in figure 1. Note that the conventional spin ladder is represented when $p = 1$.

In an effort to understand the low energy characteristics, we have varied the j' values from 0.0 to 1.0. We have verified that the DMRG results compare fairly well with the exact diagonalization results for all j' values. In all cases, when $j' = 0.0$, the system is two simple Heisenberg chains without any coupling. In this case, the ground state is highly degenerate. However, with inclusion of nonzero j' for all p, the ground state degeneracy of the system is lifted. The ground state is characterized by the value of the total spin z-component, which is a singlet, with $S_z = 0$. In figure 2, the ground state energy/site is plotted versus j' for $N = 20$, 40 and for infinite system for the conventional as well as for all diverging spin ladders for direct comparison. As can be seen from figure 2, for all cases, the energy/site decreases with increasing j'; however, the rate of decrease in energy is steeper for the Heisenberg ladder than

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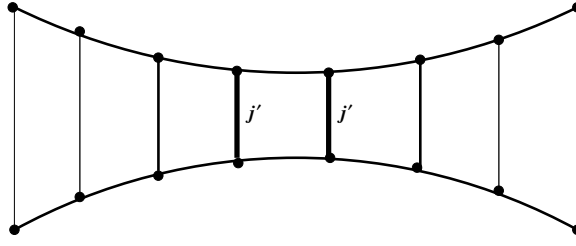
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Figure 1. Schematic diagram of the diverging ladder. The intrachain coupling is fixed as a constant and the interchain coupling weakens as the chain diverges. See the text for details.
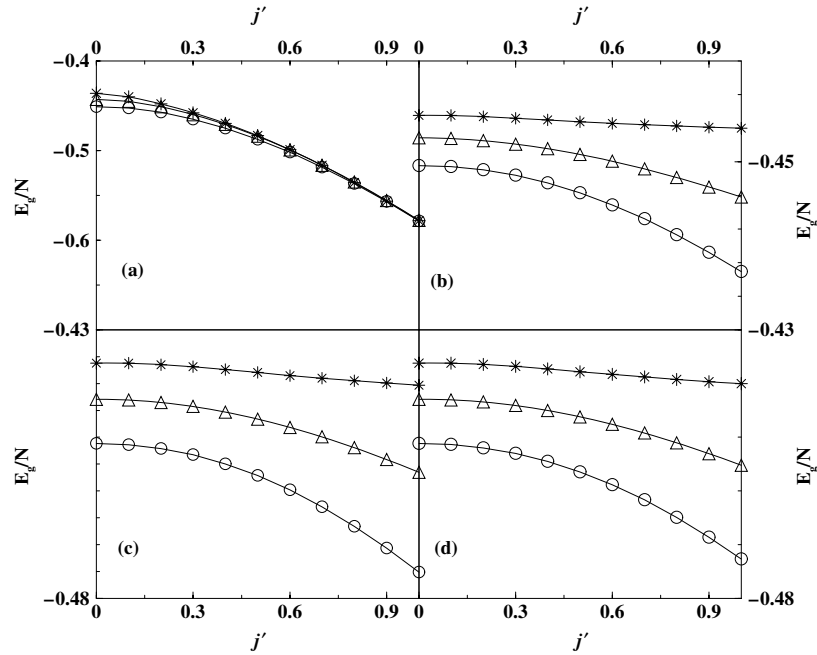

Figure 2. Energy/site versus j' for $N = 20$ (circle), $N = 40$ (triangle) and $N = \infty$ (star) for (a) spin ladder, (b) diverging ladder with $p = 2$, (c) diverging ladder with $p = 3$ and (d) diverging ladder with $p = 4$.

for the diverging ladder. Figure 2 also shows that there is a strong finite size effect, the more so for the diverging cases. In fact, the energy saturation depends strongly on the ladder type.

Let $E_1(N)$ be the lowest eigenvalue of the matrix for $S_z = 1$ (or $S_z = -1$) for N sites system. Then, the singlet–triplet energy gap Δ_{st} is given by $\Delta_{st} = E_1(N) - E_g(N)$. Here $E_g(N)$ is the ground state energy of the N-site system. In figures 3(a) and (c), we have plotted Δ_{st} as a function of j' for $N = 8, 16, 24, \ldots, 40$ for the spin ladder and as well as for the diverging ladder with $p = 2$. In the Heisenberg ladder, the gap decreases up to a certain j', but beyond that it increases with j'. This critical j', however, strongly depends on the system size; the bigger the system size, the smaller the critical j'. Furthermore, the rate of reduction of the finite size gap values is different for different j' values. This is apparent because the thermodynamic gap for the two-leg ladder system is of the order of the interchain coupling, j'. For a j' value comparable to the chain coupling (j), the rate of finite size gap reduction is very low, much less
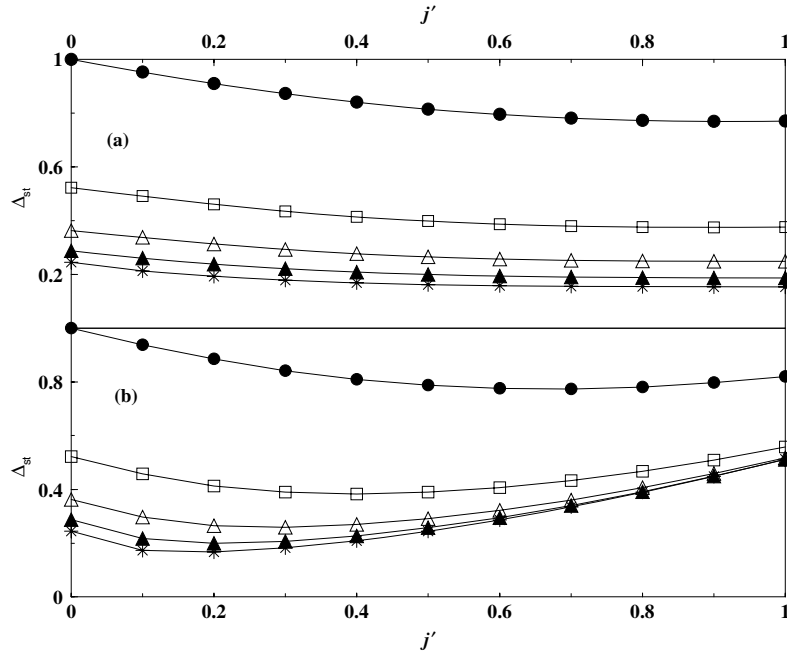
Figure 3. Energy gap versus j' for $N = 8$ (circle), $N = 16$ (square), $N = 24$ (open triangle), $N = 32$ (filled triangle) and $N = 40$ (star) for (a) spin ladder and (b) diverging ladder with $p = 2$.

compared to those for smaller j' values. This shows that the finite size effect is almost absent when the chains are coupled strongly, beyond a certain chain length. Interestingly, it gives us a clue to the extent of spatial length over which the excitation is spread. As the chain length grows, the triplet wavefunction is deconfined into both chains with a spatial length.

On the other hand, in the case of the $p = 2$ diverging ladder, the gap decreases smoothly with j', initially with larger slope for smaller j', but with larger j', it settles at different finite size spin gap values. Unlike in the case of the ideal two-leg ladder, the reduction of the gap with increase in the j' value seems to be consistent for all system sizes that we have considered. However, the magnitude of the finite size gap decreases with increase in system size for all j' values. This points towards an effective length for the excitation with gapless behaviour in the thermodynamic limit. Similar behaviour is also found for other diverging ladders.

For a clear picture of the excitation gaps in the infinite limit and the spatial length of the excitation, we have plotted finite size gap values as a function of inverse system size (N) for all the j'. The solid curves are fits to the data of the form

$$\Delta(N) = \Delta + a_1 N^{-1} + a_2 N^{-2} + \cdots \tag{2}$$

where $\Delta(N)$ is the spin gap of the N-site system.

For the diverging ladders, we find that the system is gapless for all values of j'. However, for the spin ladder, where j' is constant, the energy gap increases with j', as has been reported earlier. Figure 4(a) shows the convergence of the singlet–triplet energy gap with inverse system size for all p values with $j' = 0.5$. Interestingly, as can be seen from figure 4(a), as the system size is increased the spin ladder gap crosses the diverging ladder gap at some N value, which strongly depends on p. For each diverging ladder, and for each j' value, we find the system size where the spin gap is same as the spin ladder gap, which is denoted by $(\alpha_{p,j'}(N))$. This is a direct theoretical observation of quantum-confinement-induced crossover. That is to say,
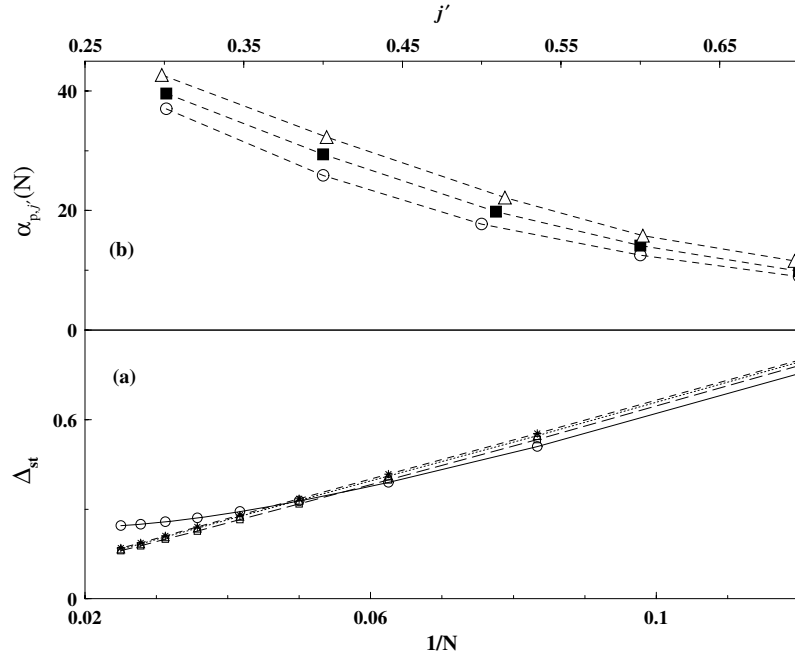
Figure 4. (a) Gap versus $1/N$ for $p = 1$ (circle), $p = 2$ (square), $p = 3$ (triangle) and $p = 4$ (star) diverging ladders; (b) crossing point versus j' with $p = 2$ (circle), $p = 3$ (filled square) and $p = 4$ (triangle).

$(\alpha_{p,j'}(N))$ represents the effective system size over which the triplet excitation is spread. To compare and contrast the $(\alpha_{p,j'}(N))$ values for different values of j', in figure 4(b) we have plotted them as a function of j' for all cases of diverging ladders. As can be seen, $\alpha_{p,j'}(N)$ decreases with increase in j'. Note that, since our system sizes are small (from 8 to 40 sites), for smaller values of j', we do not find any spin gap crossing. In fact, for smaller j', the triplet excitation is spread over a large system size. This shows that the low energy excitation of a ladder system is strongly influenced by interchain coupling and that the excitation itself is spread over two chains [19, 20]. The main point is that the critical system size required for the triplet excitation to be stable depends strongly on the interchain coupling.

In conclusion, we have studied the Heisenberg ladder and as well as the diverging ladders via the density matrix renormalization group method. Our results confirm the existence of the gap in the excitation spectrum of the Heisenberg ladder for even number of legs and gaplessness over all the interaction strengths for the diverging ladders. We have also measured the effective length scale of the triplet excitation over which the excitation is spread in these ladder classes of systems.

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