Antiferromagnetic Heisenberg ladders in a staggered magnetic field

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We study the low-energy excitations of the spin-1/2 antiferromagnetic Heisenberg chain and $N$-leg ($N=2,3,4$) ladders in a staggered magnetic field $h_s$. We show that $h_s$ induces gap and midgap states in all the cases and examine their field scaling behavior. A modified boundary scheme is devised to extract accurate bulk excitation behavior. The gap values converge rapidly as $N$ increases, leading to a field scaling exponent $\gamma = 1/2$ for both the longitudinal and transverse gaps of the square lattice ($N \to \infty$). The midgap states induced by the boundary edge effects share the bulk gap scaling exponents but their overall scaling behavior in the large-$N$ limit needs further investigation.

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Heisenberg spin ladders have attracted considerable interest for their fascinating properties due to strong quantum fluctuations and their unique structural character as a crossover platform from one to two dimensions. It is known that spin ladders with odd and even numbered legs have drastically different behavior; the former have gapless spin excitation spectra while the latter have finite spin gaps. This disparity complicates considerably attempts to extrapolate the results of ladders to two-dimensional systems. An important development in the study of low-dimensional spin systems is the observation of an unexpected magnetic field induced gap in the low-energy excitation spectrum of copper benzoate, a quasi-one-dimensional spin chain material. Recently, the field induced gap has been reported in more spin chain materials such as Yb$_4$As$_3$, CuCl$_2$2(dimethylsulfoxide)$_2$, and [Pyrimidine-Cu(NO$_3$)$_2$(H$_2$O)$_2$]$_n$(CuPM). A gap in the low-energy excitation spectrum of a spin-1/2 Heisenberg chain can be induced by an effective staggered magnetic field. The staggered field may originate from the staggered gyromagnetic tensor or/and the Dzyaloshinskii-Moriya (DM) interaction when an external magnetic field is applied. Using a local gauge transformation and neglecting small anisotropic terms in both the Heisenberg exchange and the Zeemann splitting terms, an effective Hamiltonian for spin chain materials with the DM interaction can be written as:

$$\hat{H}_{eff} = \sum_i \left[ i\hat{S}_i \cdot \hat{S}_{i+1} - HS_i^z - h_s(-1)^iS_i^z \right],$$

where $H$ and $h_s$ are the uniform and staggered magnetic field, respectively. This effective Hamiltonian has been mapped onto the sine-Gordon model using the bosonization technique to obtain an analytic form for the spin gap as a function of the magnetic field. Furthermore, it was shown that the uniform field does not change the qualitative scaling behavior induced by the staggered field and the scaling function derived for $H=0$ provides a good explanation for the experimental results at the low-field region and its validity is supported by the density matrix renormalization group (DMRG) calculations. However, the effective field theory is only applicable when the field is not too strong. The recent DMRG calculations unveiled different field-dependence at higher fields and a crossover in the intermediate field regime.

Additional intriguing phenomena induced by the staggered field have been recently reported for quasi-one-dimensional spin chain materials BaCu$_2$Si$_2$O$_6$ and CuCl$_2$·2(dimethylsulfoxide) ($CDC$). The neutron scattering measurement on CDC and electron spin resonance measurement on BaCu$_2$Si$_2$O$_6$ show that the field dependence of the induced gap deviates from the sine-Gordon model prediction for the spin chains. It suggests that the interchain interaction may play an important role. Studies on the effect of the interchain interaction is therefore needed to clarify the fundamental physics and to establish the nature of the low-energy excitation in these new materials. Moreover, there is also considerable interest in searching for a reliable extrapolation from multi-leg ladders to the square lattice. This should be achievable for spin chain materials with the DM interaction since, unlike the $h_s=0$ case, ladders with both odd and even numbered legs show field induced gaps with similar scaling behavior under the staggered field.

In the present work, we study spin-1/2 antiferromagnetic Heisenberg ladders with the following Hamiltonian:

$$\hat{H} = \sum_{a=1}^{N} \sum_{i=1}^{L-1} J_{\perp} \hat{S}_{a,i} \cdot \hat{S}_{a,i+1} + \sum_{a=1}^{N-1} \sum_{i=1}^{L} J_{\parallel} \hat{S}_{a,i} \cdot \hat{S}_{a+1,i} + \sum_{a=1}^{N} \sum_{i=1}^{L} (-1)^i h_s S_{a,i}^z,$$

where $N$ ($L$) is the number of legs (rungs). We consider the case of isotropic coupling, i.e., $J = J_\perp = 1$, and employ the DMRG method to study its low-energy properties. We kept up to 800 states for ladders with up to 300 rungs in our computations. The truncation
errors are less than $10^{-8}$ in all the cases. Although the staggered field breaks the SO(3) symmetry, the total $S^z$ remains conserved. The spin gaps for the longitudinal and transverse branches, $\Delta_L$ and $\Delta_T$, are defined as:

$$\Delta_L(L) = E_1(L,0) - E_Q(L,0)$$
$$\Delta_T(L) = E_0(L,1) - E_0(L,0)$$

where $E_0(L,S_z)$ and $E_1(L,S_z)$ are the ground-state and first excitation energy in the $S_z$ sector. In DMRG calculations, numerical accuracy is usually much higher with the use of the open boundary condition (OBC) than that with the periodic boundary condition (PBC). Recent studies reveal that there generally exist midgap states induced by the edge excitations in open-end spin chains in the presence of a staggered magnetic field. Our calculations show that midgap states also exist in spin ladders (see below). This complicates the process of extracting the bulk excitations. To address this issue, we devised a modified boundary scheme (MBS) to first identify and then move the midgap states away from the low-energy spectrum. It ensures a reliable extraction of the bulk excitation gap while allowing an accurate description of the midgap states.

The idea behind the MBS is to push the edge excitations up in energy and leave only the bulk excitations in the low-energy spectrum. This is achieved by introducing an edge parameter in the Hamiltonian that systematically drives up the edge excitation. Similar treatments have been proposed in previous DMRG calculations with OBC. Here we introduce a continuous monotonic function $f(x), 0 \leq x \leq 1$, where $f(0) > 1$ and $f(1) = 1$, to rescale the Hamiltonian parameters

$$Y_i/Y = \begin{cases} 
  c_1, & 1 \leq i \leq M \\
  1, & M < i < L - M \\
  c_{L+1-i}, & L - M + 1 \leq i \leq L
\end{cases},$$

where $Y$ represents $J$, $h_s$, or $J_\perp$ and $c_m = f(m/M)$, $1 \leq m \leq M$ where $M$ is the number of the edge sites on which the parameters are adjusted. We choose the functional form $f(x) = 1 + \alpha(1 + \cos(\pi x))$ where $\alpha \geq 0$ is the only adjustable parameter ($\alpha = 0$ corresponds to OBC). This choice is certainly not unique, but it satisfies the requirement for simplicity and effectiveness in removing edge excitations from the low-energy spectrum. We have run extensive tests and found this scheme work very well for ladders with both ferromagnetic and antiferromagnetic couplings at all field strengths.

We demonstrate the implementation of MBS in the case of the two-leg ladder. Figure shows the gap and midgap states versus $1/L$ with various $\alpha$ at $h_s = 0.6$. The gap obtained under PBC represents the bulk value. A midgap state appears in the open-end (OBC) case due to topological edge effects. As $\alpha$ increases, the midgap state is gradually pushed up in energy and eventually enters the continuum spectrum, leaving the bulk gap state as the lowest excitation in the large-$L$ limit. We performed the same calculations on the three- and four-leg ladders and found that midgap states exist for all the cases. With MBS one can clearly identify these bound states inside the field induced gap for a detailed study and then systematically push them up in energy and extract the bulk excitations with proper values of $\alpha$. It is noted that a large $\alpha$ is needed for cases where the edge state lies well below the bulk gap. In some special cases where the edge states are degenerate in the large-$L$ limit with the ground state as in spin-1 and 2 Heisenberg chains, special measures need to be taken to eliminate the degeneracy before applying MBS. In the calculations presented below we use $\alpha = 2.0$ with $M = 10$ to ensure good convergence in all the cases.

![Figure 1](image1.png)

**FIG. 1:** The longitudinal (top) and transverse (bottom) gap and midgap states versus $1/L$ at various $\alpha$ values for the two-leg ladder at $h_s=0.6$ with $M = 10$.

![Figure 2](image2.png)

**FIG. 2:** The longitudinal and transverse gap versus the staggered magnetic field $h_s$ for the spin-1/2 chain ($N=1$) and $N$-leg ($N = 2, 3, 4$) ladders. The fitted scaling curves are also shown for $N = 1, 3, 4$ as the dashed, dotted and solid lines, respectively. The insets illustrate the gaps for $h_s \in [0, 0.1]$.

We now turn to the study of the staggered field induced gaps in the spin chain and ladders and the extrapolation toward the square lattice. Figure shows the longitudinal and transverse gaps for the chain ($N=1$) and $N$-leg...
are given in Table I. From this procedure, we obtain the longitudinal and transverse gaps for the isotropic antiferromagnetic Heisenberg square lattice with a staggered magnetic field
\[ \Delta_L = (4.03 \pm 0.09)h_s^{0.50 \pm 0.01}, \]
\[ \Delta_T = (2.27 \pm 0.01)h_s^{0.50 \pm 0.01}. \]

Our numerical results suggest a common exponent \( \gamma \) for both branches. It is also interesting to note that a recent field-theoretical study of coupled spin-1/2 antiferromagnetic Heisenberg chains with a leg-independent staggered field also shows that the field induced gap scales with the staggered magnetic field as \( h_s^{1/2} \). Possible connections and general implications of the common scaling behavior in these different spin lattice models deserve further analytical investigation.

TABLE I: Fitting coefficients and exponents for \( N = 1, 2, 3, 4 \) and \( \infty \). Those for the two-leg ladder are taken from Fig. 2 at \( N = 2 \) and \( \beta \) and \( \gamma \) for \( N = \infty \) from Fig. 3 (see text).

| \( N \) | \( 1 \) | \( 2 \) | \( 3 \) | \( 4 \) | \( \infty \) |
|---|---|---|---|---|---|
| \( \beta_L^{\infty} \) | 2.97 | 3.84 | 3.98 | 4.02 | 4.03 ± 0.09 |
| \( \gamma_L^{\infty} \) | 0.68 | 0.56 | 0.53 | 0.52 | 0.50 ± 0.01 |
| \( \beta_T^{\infty} \) | 1.88 | 2.10 | 2.16 | 2.19 | 2.27 ± 0.01 |
| \( \gamma_T^{\infty} \) | 0.61 | 0.56 | 0.54 | 0.53 | 0.50 ± 0.01 |

We extrapolate the longitudinal and transverse gaps \( \gamma_{L,T}^{N} \) and \( \beta_{L,T}^{N} \) toward the large-\( N \) (two dimensional) limit using the second order polynomial fitting: \( a(N) = a_0 + a_1 N^{-1} + a_2 N^{-2} \), where \( a \) denotes either \( \gamma_{L,T}^{N} \) or \( \beta_{L,T}^{N} \) given in Table I with \( N = 1, 3, 4 \). This fitting is illustrated in Fig. 3 and the extrapolated \( \gamma_{L,T}^{\infty} \) and \( \beta_{L,T}^{\infty} \) are shown in Fig. 2. Meanwhile, due to the large gap at \( h_s = 0 \), a good fitting using Eq. (5) cannot be achieved for \( N = 2 \); instead, the scaling parameters for \( N = 2 \) are obtained from the extrapolation curves obtained from fitting the results for \( N = 1, 3, 4 \) (see below).

Finally, we examine the scaling behavior of the midgap states in spin ladders with a staggered magnetic field. As shown in Fig. 4, midgap states exist in all the cases studied and the scaling exponents \( \gamma_L^{N} \) and \( \gamma_T^{N} \) for the bulk gaps provide a good fit for the midgap states. However, the scaling coefficients \( \beta_L^{N} \) and \( \beta_T^{N} \) show an oscillatory pattern with increasing \( N \) (up to \( N = 4 \) studied here). It indicates that these coefficients have not properly converged at \( N = 4 \), probably due to a different (compared to the bulk excitations) energy scale associated with the boundary edge excitations. Consequently, the question of whether the midgap states would persist in the large-\( N \) limit remains open at present. Meanwhile, we observe that although the bulk low-energy behaviors of the spin-1/2 two-leg ladder are similar to those of a spin-1 chain their boundary edge excitations and the field scaling behaviors are quite different. The spin-1 chain has a four-fold degenerate ground state that splits in a staggered field and turns (partly) into the lowest midgap states. The two-leg ladder has a non-degenerate ground state and its transverse midgap states come from the boundary edge excitations that originally
FIG. 4: The scaling fit for the transverse and longitudinal overlaps with the bulk excitation continuum. However, when one adds other interactions to the standard two-leg ladder, the resulting low-energy properties, i.e. gap and midgaps, in the Haldane phase can be the same as the $S = 1$ chain\cite{11}.

In summary, we have carried out a systematic study of the low-energy excitations of spin-1/2 antiferromagnetic Heisenberg chain and ladders in a staggered magnetic field and obtained the field scaling behavior of both longitudinal and transverse gaps. A modified boundary scheme has been devised to extract the bulk excitation behavior using the more accurate open boundary option in the DMRG calculations. The calculated bulk gaps converge rapidly with increasing number of legs above weak field regime; it allows a reliable extrapolation to obtain the field scaling behavior of the gaps for the isotropic square lattice. We also examined the midgap states in the spin ladders induced by the topological edge effect. The midgap states share the same scaling exponents with the bulk gaps but the scaling coefficients show an oscillatory pattern with increasing number of legs (up to $N=4$). As a result, the overall scaling behavior of the midgap states in the large-$N$ limit needs further investigation.

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