Low-Energy Properties of Antiferromagnetic Spin-1/2 Heisenberg Ladders with an Odd Number of Legs

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An effective low-energy description for multi-leg spin-1/2 Heisenberg ladders with an odd number of legs is proposed. Using a newly developed Monte Carlo loop algorithm and exact diagonalization techniques, the uniform and staggered magnetic susceptibility and the entropy are calculated for ladders with 1, 3, and 5 legs. These systems show a low-temperature scaling behavior similar to spin-1/2 chains with longer ranged unfrustrated exchange interactions. The spinon velocity does not change as the number of legs increases, but the energy scale parameter decreases markedly.

Recently, antiferromagnetic Heisenberg spin-1/2 ladder attracted much interest, following the discovery of a spin gap in the 2-leg-ladder [1]. Also the crossover from the single chain to the two-dimensional (2D) square lattice, obtained by assembling chains to form “ladders” of increasing width, is far from smooth [2]. Heisenberg ladders with an even number of legs, n, have a spin gap and short range correlations, while odd-leg ladders have no gap and power-law correlations. These theoretical predictions have been verified experimentally, in materials such as \((V\,O)_2P_2O_7\) [3] and the homologous series of cuprates \(Sr_{n-1}Cu_{n+1}O_{2n}\) [4], which contain weakly coupled arrays of ladders.

Here, we concentrate on odd-leg ladders. Our goal is to derive a low-energy description in terms of \(S=1/2\) chains with longer range effective interactions, and examine the evolution with increasing number of legs, \(n\). The Heisenberg Hamiltonian for ladders is

\[
H = J_\| \sum_{\leftrightarrow} S_{i,\tau} S_{j,\tau} + J_\perp \sum_{\uparrow \downarrow} \sum_{\tau, \tau'} S_{i,\tau} S_{j,\tau'},
\]

where \(i\) and \(j\) enumerate the rungs, \(\tau, \tau'\) label the legs, and the sum marked by \(\leftrightarrow\) \((\uparrow \downarrow)\) runs over nearest neighbors along legs (rungs). Periodic boundary conditions are chosen along the leg direction and open boundary conditions perpendicular to it. For the known materials we expect the superexchange to be roughly isotropic \((J_\| = J_\perp)\). However, it is educational first to consider the strongly anisotropic limit \((J_\| > J_\perp)\).

In the completely anisotropic limit \((J_\|/J_\perp = 0)\), each eigenfunction is a direct product of one-rung states whose lowest-lying multiplet is a spin doublet, separated by a gap of order \(J_\perp\) from the first excited state. The ground state of the whole system is therefore \(2^L\) -fold degenerate. A finite value of \(J_\|\) lifts this degeneracy. Our goal is to formulate an effective Hamiltonian, \(H_{eff}\), in this \(2^L\)-dimensional subspace \(\mathcal{M}\) of rung doublets which descibes the low-energy properties. For the case of the 3-leg-ladder, to third order in \(J_\|/J_\perp\), we get

\[
H_{eff}^{(3)} = L \sum_{j=1}^{L} \sum_{n=1}^{3} J_n \bar{S}_{j,n}^{tot} \bar{S}_{j+1,n}^{tot} + J((\bar{S}_{j,n}^{tot} \bar{S}_{j+2,n}^{tot} / (\bar{S}_{j+1,n}^{tot} \bar{S}_{j+3,n}^{tot}))) - (\bar{S}_{j,n}^{tot} \bar{S}_{j+2,n}^{tot} / (\bar{S}_{j+1,n}^{tot} \bar{S}_{j+3,n}^{tot})))
\]

where \(\bar{S}_{j,n}^{tot} = S_{j,n}^{1} + S_{j,n}^{2} + S_{j,n}^{3}\) is the total spin of the \(j\)th rung, \(J_n = J_2 \sum \lambda a_{n,\lambda}(J_1 / J_2)^{\lambda}\), with \(a_{1,1} = 1, a_{1,2} = -1/9, a_{1,3} = -103/243, a_{2,1} = 0, a_{2,2} = -8/27, a_{2,3} = -49/162, a_{3,1} = a_{3,2} = 0, a_{3,3} = -32/243\), and \(J = (16/81)J_1^2 / J_2^2\).

The last term in Eq. (3) will be neglected, since the corrections in the energy of the low-lying energy states, due to this term are small. \(H_{eff}^{(3)}\) then has the form of a single chain with effective nearest neighbor (n.n.) coupling \(J_1\), next-nearest neighbor (n.n.n.) coupling \(J_2\), and with exchange coupling \(J_3\) between rung spins separated by three unit cells. Therefore the low-lying energy states of the 3-leg-ladder can be mapped onto those of a \(J_1 - J_2 - J_3\) chain. In this effective system the n.n.n. interaction is \(F = 3J_2 < 0\), while the n.n.n.n. interactions are AF \((J_3 > 0)\). Consequently, both the second and the third term in Eq. (3) enhance the overall AF quasi-long range order. Note, that the third order corrections in Eq. (3) affect \(J_1\) and \(J_2\) strongly since the corresponding coefficients are large. So one must perform the calculations at least up to third order.

To test \(H_{eff}^{(3)}\), we calculate the temperature dependent uniform susceptibility, \(\chi(T)\), for 3-leg ladders [5] using the Quantum Monte Carlo (QMC) loop algorithm [6] [7], and compare to susceptibilities obtained for the effective \(J_1 - J_2 - J_3\) model. We consider large enough systems, such that finite size effects are negligible. All results are extrapolated to a Trotter time interval \(\Delta \tau \to 0\). Further, we compare with recent results obtained by Greven et al. [8] using the same algorithm.

At low temperatures, where only the states in \(\mathcal{M}\) are relevant, the susceptibilities of the 3-leg ladders with small \(J_\|/J_\perp\) coincide with those of the corresponding \(J_1 - J_2 - J_3\) chain. This can be seen in the inset of Fig. 3, where we show the susceptibility per rung of the 3-leg
ladder with \( J_\parallel/J_\perp = 0.2 \) together with the susceptibilities of the corresponding effective models in first, second, and third order in \( J_\parallel/J_\perp \). While the first order effective model (a single chain with only n.n. interactions) gives only a qualitative description of the 3-leg ladder at low temperatures, \( \chi(T) \) of the effective model in third order in \( J_\parallel/J_\perp \) coincides with the susceptibility per rung of the 3-leg ladder up to a crossover temperature. Above this temperature, \( \chi(T) \) of the 3-leg ladder is larger, due to the presence of additional states in the 3-leg ladder which are not included in the subspace \( \mathcal{M} \).

The crossover temperature is of the order of the gap \( \Delta \) to the higher lying states in the 3-leg ladder. It can be estimated best by considering the entropy of both the 3-leg ladder and the corresponding effective model (Fig. 2). Just above the crossover temperature, the additional states lead to a rise \( \propto e^{-\Delta/T} \) in the entropy. Consequently, fitting the form \( e^{-\Delta/T} \) to the difference of the entropy per rung of the 3-leg ladder and the entropy of the corresponding effective model gives a rough estimate of \( \Delta \). We find \( \Delta \approx J_\perp \) more or less independent of \( J_\parallel/J_\perp \).

From Fig. 1, it is clear that with increasing \( J_\parallel/J_\perp \) the quality of the description of the 3-leg ladder by the third order effective model becomes worse. The \textit{qualitative} features of the temperature dependence of the susceptibility, however, are correctly given even in the isotropic case \( J_\parallel/J_\perp = 1 \), e.g. the slope of \( \chi(T) \) is increasing, while the zero-temperature value \( \chi(0) \) remains more or less constant, as \( J_\parallel/J_\perp \) increases (see Fig. 2).

![FIG. 1. Susceptibility of the 3-leg ladder for different \( J_\parallel/J_\perp \) and of the corresponding effective models. The filled symbols show the data for the 3-leg ladders and the open symbols those of the corresponding third order effective model. The crosses show the susceptibility of the corresponding \( J_1-J_2 \) chains in the mapping of the 3-leg ladders to \( J_1-J_2 \) chains (for details see text). The inset shows the susceptibility per rung of the 3-leg ladder with \( J_\parallel/J_\perp = 0.2 \) together with those of the corresponding effective models in first, second and third order in \( J_\parallel/J_\perp \). The error bars are smaller or of the order of the symbols.](image1)

Calculating the effective Hamiltonian of the 3-leg ladders to \( n^{10} \) order leads to a spin-chain Hamiltonian with interaction terms between spins which are separated by up to \( n \) unit cells. All these interactions are invariant under translations and rotations. Consequently, for very low temperatures the 3-leg ladders can be mapped onto the \( k = 1 \) Wess-Zumino-Witten (WZW) nonlinear \( \sigma \)-model \( [10] \), which is determined by a spinon velocity, \( v \), and a energy scale parameter, \( T_0 \). For \( T \ll T_0 \), \( \chi(T) \) of this model reads \( [11] \) up to: \( O(\log T)^{-3} \)

\[
\chi(T) = \frac{1}{2\pi v} + \frac{1}{4\pi v} \left[ \frac{1}{\ln(T_0/T)} - \frac{\ln(\ln(T_0/T) + 1/2)}{2\ln^2(T_0/T)} \right]
\]

\( \chi(T) \) approaches its \( T = 0 \) value \( \chi(0) = 1/(2\pi v) \) with infinite slope. \( T_0 \) should be \( \lesssim \Delta \) and characterizes the interactions between the spinons. The smaller \( T_0 \), the stronger the interactions, and the faster \( \chi(T) \) increases with temperature.

The low temperature regime of the universality class of spin chains with a rotationally and translationally invariant Hamiltonian (to which also the 3-leg ladders belong) is determined by only two parameters, \( v \) and \( T_0 \). However, the determination of \( v \) and \( T_0 \) for the 3-leg ladder is difficult. QMC calculations cannot be performed down to low enough temperatures such that a fit to the above form (3) gives reliable estimates for \( v \) and \( T_0 \). Especially \( T_0 \) is considerably underestimated in all cases.

To overcome this problems we first map the 3-leg ladder to a \( J_1-J_2 \) chain and then study the one-to-one mapping of this \( J_1-J_2 \) chain to the WZW model: \( (J_1, J_2) \leftrightarrow (v, T_0) \). The mapping to \( J_1-J_2 \) chains is always possible since the low-T range is characterized by only two parameters which can be chosen as \( J_1, J_2 \) instead of \( v, T_0 \). The mapping of the 3-leg ladder to \( J_1-J_2 \) chains is done as follows. For small \( J_\parallel/J_\perp \) we can use the third order result for \( J_1 \) and \( J_2 \) (Eq. (3)), neglecting \( J_3 \), since \( J_3 \) is small. Otherwise we fit \( \chi(T) \) of \( J_1-J_2 \) chains
for low $T$ to $\chi(T)$ of the 3-leg ladder (see Fig. [1]) which gives estimates of the values $J_1$ and $J_2$ (see Table [I]).

The mapping $(J_1, J_2) \leftrightarrow (v, T_0)$ can be studied, using exact diagonalisation methods. $v$ and $T_0$ are determined by the finite size scaling of the energy gap between the excited state $E(k = \pi, S_z = 1)$ and the ground state $E(k = 0, S_z = 0)$ [1].

$$E(k = \pi, S_z = 1) - E(k = 0, S_z = 0) = \frac{\pi v}{L} \left( 1 - \frac{1}{2} \frac{1}{\ln(L/L_0)} + \frac{\ln(\ln(L/L_0) + 1/2)}{4 \ln^2(L/L_0)} \right),$$

where $E(k, S_z)$ is the lowest energy with wavevector $k$ and $z$-component of spin $S_z$ for a chain of length $L$. $L_0$ is the characteristic scaling length of the chain. As a consequence of the equivalence of the imaginary time direction and the space direction, $L_0 = v/T_0$. Fitting Eq.(4) for different lengths using exact diagonalisation gives $v$ as well as $T_0$. The results for different fractions $J_2/J_1$ are plotted in Fig.[2]. An alternate possibility to determine $v$ and $T_0$ is to map the $J_1 - J_2$ chains onto the O(3) nonlinear $\sigma$-model with $\theta = \pi$. For the coupling constant $g$ one finds $g = 4 \left( 1 - 4J_2/J_1 \right)^{-1/2}$ [12]. Therefore the spinon velocity can be written as:

$$v = \frac{\pi J_1}{2} \sqrt{1 - 4J_2/J_1}.$$  

Logarithmic corrections, on the other hand, depend on a mass scale $\Lambda$, which is generated dynamically in the $\sigma$-model, and for small $g$, $\Lambda = 1/a \exp(-2\pi/g)$, where $a$ is the lattice spacing [13]. Since $T_0 \propto \Lambda$,

$$T_0 \propto \exp \left[ \frac{\pi}{2} \sqrt{1 - 4J_2/J_1} \right].$$

The results for $v$ and $T_0$ (Eq.[5] and Eq.[6]) are plotted in Fig.[2] together with those obtained by finite size scaling.

In Table [I] the estimated values $v$, $T_0$ (following the above described procedure) are given for various 3-leg ladders. The spinon velocity increases, while $T_0$ decreases with increasing $J_1/J_\perp$.

The values for $v$ and $T_0$ can now be put back into Eq.[6] which gives the low temperature susceptibilities of the corresponding 3-leg ladders. This is shown at the example of $J_1/J_\perp = 0.2$ in Fig.[3]. Together with the QMC data for the 3-leg ladder itself and its third order effective model, we get the susceptibility for the 3-leg ladder with good precision on the whole temperature range from zero temperature to high $T$.

![Graph](image)

**FIG. 3.** Spinon velocity, $v$, and energy scale parameter, $T_0$, of the $J_1 - J_2$ chains, determined by finite size scaling analysis (circles) respectively by mapping to the O(3)-non linear $\sigma$-model.

In Table [I] for low temperatures, 3-leg ladders can be mapped onto $J_1 - J_2$ chains. The corresponding coupling constants, $J_1$ the 3-leg ladders are also listed. The value enclosed in bracket was obtained by fitting the $\xi$-data to Eq.[8].

| $J_1/J_\parallel$ | $J_2/J_\parallel$ | $J_2/J_\perp$ | $v/J_\parallel$ | $T_0/J_\parallel$ |
|------------------|------------------|----------------|----------------|-----------------|
| 0                | 1                | 0              | $\pi/2$        | 2.6             |
| 0.1              | 0.985            | -0.033         | 1.61           | 1.64            |
| 0.2              | 0.961            | -0.071         | 1.63           | 1.28            |
| 0.4              | 0.86             | -0.17          | 1.63           | 0.78            |
| 0.6              | 0.76             | -0.30          | 1.65           | 0.57            |
| 0.8              | 0.67             | -0.47          | 1.73           | 0.47            |
| 1.0              | 0.61             | -0.61          | 1.81           | 0.41 (0.34)     |

**TABLE I.** For low temperatures, 3-leg ladders can be mapped onto $J_1 - J_2$ chains. The corresponding coupling constants, $J_1$ the 3-leg ladders are also listed. The value enclosed in bracket was obtained by fitting the $\xi$-data to Eq.[8].

Greven et al. recently calculated the correlation length $\xi$ of isotropic ladders [11], using also the QMC loop algorithm. For $T \ll T_0$ the inverse of the correlation length in the WZW-model can be written as [14]

$$\frac{1}{\xi(T)} \approx T \left( 2 - \frac{1}{\ln(T_0/T)} + \frac{1}{2} \frac{\ln(\ln(T_0/T) + 1/2)}{\ln^2(T_0/T)} \right).$$

![Graph](image)

**FIG. 4.** Susceptibility of the 3-leg ladder with $J_1/J_\perp = 0.2$ and its effective models. The error bars are smaller or of order of the symbols.
Fitting the data \( n_1 = 3 \) to the above form (Eq.\( \text{(2)} \)) also gives an estimate of \( T_0 \). In the isotropic case we find \( T_0 = 0.34 J_0 \), which is in good agreement with our result (see Table \( \text{(1)} \)). For the 5-leg-ladder \( T_0 \) is already \( \lesssim 0.1 J_0 \).

Finally, we examine the static structure factor \( C(\pi, \pi) \), defined by (\( N_s = \text{number of sites} \))

\[
C(k_x, k_y) = \frac{1}{N_s} \sum_{i,j,\tau,\tau'} e^{ik_x(i-j)+ik_y(\tau-\tau')} < \vec{S}_{i,\tau} \vec{S}_{j,\tau'} >
\]

and show that it can be calculated from the effective model without introducing additional physical parameters. \( C(\pi, \pi) \) can be written as \( \sum_{i,j} (-1)^{i+j} < \vec{S}_{i,\pi} \vec{S}_{j,\pi} > /3L \), where \( \vec{S}_{i,\pi} = \vec{S}_{i,1} - \vec{S}_{i,2} + \vec{S}_{i,3} \) is the staggered spin of one rung. In the limit \( J_{||} = 0 \) the correlations of the staggered rung-spins is simply related to those of the uniform rung-spins by:

\[
< \vec{S}_{i,\pi} \vec{S}_{j,\pi} >_{i \neq j} = \lambda < \vec{S}_{i,\pi} \vec{S}_{j,\pi} >_{i \neq j}, \tag{8}
\]

with \( \lambda = 25/9 \) for all temperatures, where only the states in \( \mathcal{M} \) are relevant. For \( J_{||} \neq 0 \) the “wave function” of the spin-1/2 degree of freedom at each rung is spread out over a certain number of unit cells. On one hand, this gives rise to the longer range interactions, described above, and on the other hand, it affects the correlations \( < \vec{S}_{i,\pi} \vec{S}_{j,\pi} > \) and \( < \vec{S}_{i,\pi} \vec{S}_{j,\pi} > \). For large distances \( |i-j| \gg 1 \), however, \( < \vec{S}_{i,\pi} \vec{S}_{j,\pi} > \) and \( < \vec{S}_{i,\pi} \vec{S}_{j,\pi} > \) are still related by Eq.\( \text{(8)} \) but with a renormalized value of \( \lambda \).

Here, we calculate \( \lambda \) numerically, using QMC simulations. The values are plotted in Fig.\( \text{3} \) for different \( J_{||}/J_{\perp} \) and extrapolating to \( J_{||} = 0 \) leads to a value \( \lambda = 2.78 \) which agrees with the analytical result 25/9. At low \( T \), the correlation length \( \xi \gg 1 \) and \( C(\pi, \pi) \), as well as \( C(\pi, 0) = \sum_{i,j} (-1)^{i+j} < \vec{S}_{i,\pi} \vec{S}_{j,\pi} > /3L \), are dominated by correlations with \( |i-j| \gg 1 \). Additionally, \( C(\pi, 0) \) per rung of the 3-leg ladder differs only slightly from \( C(\pi) \) of the single chain. Consequently at low temperature, \( C(\pi, \pi)_{3\text{-leg}} = \lambda C(\pi, 0)_{3\text{-leg}} \approx \lambda C(\pi)_{\text{single chain}} /3 \). Greven et al. have calculated \( C(\pi, \pi)_{3\text{-leg}} \) for \( J_{||} = J_{\perp} \) and \( C(\pi)_{\text{single chain}} \). From their data we determine \( C(\pi, \pi)_{3\text{-leg}} / C(\pi)_{\text{single chain}} = 2.55 \), which is in good agreement with our value \( \lambda/3 = 2.64 \) (see Fig.\( \text{3} \)).

The above considerations can be generalized to an arbitrary odd-leg ladder with \( n_1 \) legs. There are no qualitative differences. The overall AF quasi-long range order, however, increases with increasing \( n_1 \). Therefore, especially the ratio \( |J_{||}/J_{\perp}| \) of the effective Hamiltonian \( H_{\text{eff}} \) is larger. The logarithmic corrections increase markedly (\( T_0 \) decreases) and the \( T \to 0 \) behavior sets in at lower temperature as \( n_1 \) increases. The zero temperature value \( \chi(0) \), on the other hand, is almost independent of \( n_1 \). This implies that the spinon velocity of odd-leg ladders depends only slightly on the number of legs.

In conclusion, we have proposed an effective spin-1/2 chain model which describes the low-energy properties of odd-leg ladders. The temperature dependence of \( \chi \), \( \xi \), and \( C(\pi, \pi) \) for the effective system is shown to be consistent with that of the original model at low enough temperatures. The effective model requires two parameters, e.g. a spinon velocity \( v \) and an energy scale, \( T_0 \). With an increasing number of legs, \( v \) does not change, but \( T_0 \) decreases rapidly. The exchange interactions of the corresponding effective model become longer ranged, and antiferromagnetic correlations are enhanced.

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![Graph](image-url)