Susceptibility and low-temperature thermodynamics of spin-$\frac{1}{2}$ Heisenberg ladders

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(Received 13 May 1996)

The temperature dependence of the uniform susceptibility and the ground-state energy of antiferromagnetic Heisenberg ladders with up to six legs has been calculated, using the Monte Carlo loop algorithm. The susceptibilities of even-leg ladders show spin gaps while those of odd-leg ladders remain finite in the zero-temperature limit. For small ratios of intra- to interleg couplings, odd-leg ladders can be mapped at low temperatures to single chains. For equal couplings, the logarithmic corrections at low temperatures increase markedly with the number of legs. [S0163-1829(96)50630-2]

Recently, antiferromagnetic Heisenberg spin-1/2 ladder systems have attracted much interest, following the discovery of a finite spin gap in the two-leg ladder.[1] Later investigations showed that the crossover from the single Heisenberg chain to the two-dimensional (2D) antiferromagnetic 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 (chains), n_l, show a completely different behavior than odd-leg ladders. While even-leg ladders have a spin gap and short range correlations, odd-leg ladders have no gap and power-law correlations. Based on density matrix renormalization group (DMRG) studies, White *et al.*[3] gave an explanation of this fundamental difference in the framework of the resonant valence bond (RVB) picture.[4] These theoretical predictions have been verified experimentally, in materials such as $(VO)_2P_2O_7$ (Ref. 5) and the homologous series of cuprates $Sr_{n-1}Cu_{n+1}O_{2n}$,[6] which contain weakly coupled arrays of ladders.

Previous numerical studies, using exact diagonalization,[1,7] the quantum Monte Carlo (QMC) world line algorithm,[8] or the quantum transfer matrix method[9] were restricted to small systems or could not be applied at low temperatures. Using the new QMC loop algorithm,[10] we overcome these limitations and are able to investigate the systematical dependency of the physical behavior on n_l, including very low temperatures and five- and six-leg ladders. We study the mapping of the three- and five-leg ladders to single chains. In the low-temperature regime, for small ratios of intra- to interleg coupling, odd-leg ladders can be mapped to nearest-neighbor chains, while for equal couplings an effective model with longer range interactions is needed. In the zero-temperature limit, we find that the susceptibility per rung of the odd-leg ladders remains approximately constant independently of n_l. This means that in this limit, the susceptibility per site goes to zero for both even- and odd-leg ladders as n_l increases, in contrast to the finite value of the susceptibility per site for the 2D lattice.

In this paper we consider ladders with n_l legs ($n_l=1,2,\ldots,6$) of length L. The Hamiltonian of such spin-1/2 systems

$$H=J\sum_{\leftrightarrow}\vec{S}_i\cdot\vec{S}_j+J_\perp\sum_{\updownarrow}\vec{S}_i\cdot\vec{S}_j \tag{1}$$

is defined on $L\times n_l$ lattices. The sum marked by $\leftrightarrow$ ($\updownarrow$) runs over nearest neighbors along the legs (rungs). We assumed periodic boundary conditions in the longitudinal direction of the ladder. J and $J_\perp$ are positive, corresponding to antiferromagnetic coupling.

Using the QMC loop algorithm with improved estimators, we have calculated the temperature dependence of the uniform susceptibility χ and the internal energy E. The QMC loop algorithm was first developed by Evertz *et al.*[10] for the six-vertex model, but can also be applied to quantum spin systems.[11,12] The QMC loop algorithm is an improved world line algorithm. The updates are global and no longer local as in the conventional Metropolis world line algorithm. This has the great advantage that the autocorrelation times are reduced by several orders of magnitude. It was thus possible to simulate very long ladders to very low temperatures. We considered systems up to 100×6 sites and reached temperatures down to $T=J/50$ without major problems. All results are extrapolated to a Trotter time interval $\Delta\tau\to 0$. The application of improved estimators (see, e.g., Ref. 12), further reduces the variance of the measured observables dramatically.

In Table I the ground-state energies of the different ladders in the isotropic case ($J=J_\perp$) are presented. The energies were obtained as follows: considering ladders of lengths L, we first extrapolate to $T\to 0$. For the odd-leg ladders we use the form

$$E_L(T)=E_L(0)+aT^2, \tag{2}$$

where $E_L(T)$ is the internal energy of the ladder of length L. This form is motivated by the infinite single chain, which

TABLE I. Ground-state energies per site for the different ladders in the isotropic case. For the single chain we have perfect agreement with the analytical result $\frac{1}{4}-\ln 2$ from the Bethe ansatz (Ref. 13). Furthermore, the result for the two-leg ladder coincides with the ground-state energy calculated by Barnes *et al.*,[8] using Lanczos techniques. With increasing width the results approach to the ground-state energy per site of the infinite 2D square lattice, which was calculated by various methods. For an overview see Ref. 14. The reference value given here was recently obtained by Wiese and Ying (Ref. 12) using the QMC loop algorithm.

Number of legs	Obtained ground-state energy	Reference value
1	−0.4432(1)	−0.44315 . . . (Ref. 13)
2	−0.5780(2)	−0.578 (Ref. 8)
3	−0.6006(3)	
4	−0.6187(3)	
5	−0.6278(4)	
6	−0.635(1)	
2D lattice		−0.6693(1) (Ref. 12)

in a low-temperature field theory can be described by a massless boson. It has to be kept in mind that, due to the finite length, also the odd-leg ladders have a small gap in the excitation spectrum, which is up to logarithmic corrections equal to $\pi v/L$, where v is the spin velocity. Therefore Eq. (2) is only valid for $\pi v/L \ll T \ll J$. In this temperature range our numerical data agree well with Eq. (2) for the finite single chains, as well as for the three- and five-leg ladders. The even-leg ladders, on the other hand, have spin gaps even in the infinite system. The internal energy for T well below the spin gap Δ is determined by the thermal occupation of the lowest lying $S=1$ magnon band with a quadratic dispersion near the zone boundary minimum. For the extrapolation $T\rightarrow 0$ we therefore use the form $E_L(T)=E_L(0)+b(T^{3/2}+2\Delta T^{1/2})\exp(-\Delta/T)$. In a second step the ground-state energies $E_L(0)$ for the finite systems are extrapolated to the bulk limit $E_{L=\infty}(0)$, fitting $E_L(0)$ to a polynomial in $1/L$. However, the finite size corrections are negligibly small for $L\geqslant 100$.

In Fig. 1 we show the susceptibility per rung of n_l spins, $\chi(T)$, for the ladders with $1\leqslant n_l \leqslant 6$ in the isotropic case $J=J_\perp$. We always consider ladders long enough such that finite size corrections are negligible. For $T>J$ the results agree well with a third order high-T expansion. At low temperatures, we observe the predicted behavior. Ladders with even n_l show an exponential drop of the susceptibility indicating a gap in the excitation spectrum. For larger n_l, the drop sets in at smaller T and is steeper. The gap Δ_{n_l} decreases substantially with increasing n_l. For odd n_l on the other hand, $\chi(T)$ remains finite also at $T\ll J$, as in the single chain.

Ladders with even n_l were already investigated in detail.[3,9,15] For temperatures $T\ll\Delta$ the susceptibility for the two-leg ladder is determined by the thermal occupation of $S=1$ magnon band with a quadratic dispersion near the zone boundary minimum[9]:

$$\chi(T)\propto T^{-1/2}e^{-\Delta/T}, \quad T\ll\Delta. \tag{3}$$

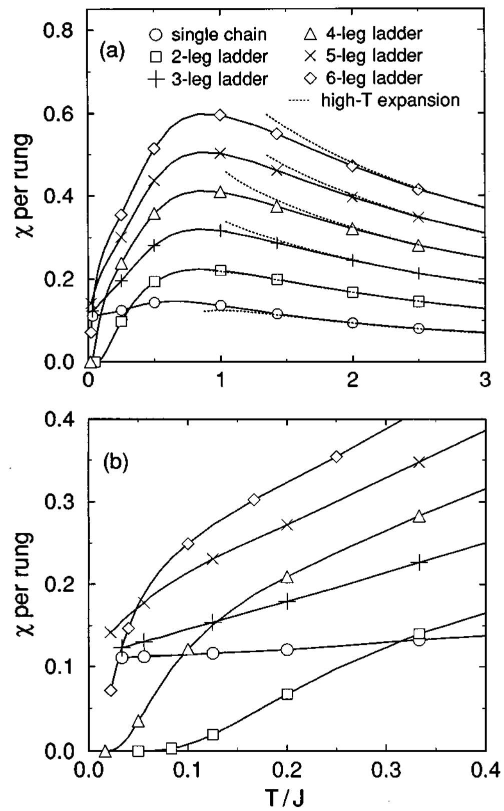

FIG. 1. Susceptibility as a function of the temperature for the single chain and the Heisenberg ladders with up to six legs. At high temperatures the result agree well with a third order high-temperature expansion. The low-temperature region is shown in (b) in a larger scale. To distinguish the curves some data points are marked by symbols. The error bars are smaller than the symbols.

Provided a quadratic dispersion for the lowest lying magnon branch in the excitation spectrum near its minimum is assumed, Eq. (3) also holds for the four- and six-leg ladder. We estimate Δ_{n_l} by fitting the numerical QMC data for low temperatures and find in the isotropic case $\Delta_2=0.51(1)J$ for $n_l=2$, $\Delta_4=0.17(1)J$ for $n_l=4$, and $\Delta_6=0.05(1)J$ for $n_l=6$. The value Δ_2 obtained for the two-leg ladder is in perfect agreement with former results.[3,8,9] On the other hand, the spin gap obtained by White *et al.*,[3] using DMRG methods for the four-leg ladder $\Delta_4=0.190J$ is slightly larger than our value.

The decrease of the spin gap with increasing n_l can be explained by delocalization of RVB singlets not only along but more and more also across the ladder. The decrease of the spin gap, however, is much faster than $\Delta_{n_l}\propto 1/n_l$, suggested in Ref. 3. The spin gap for the six-leg ladder Δ_6 is already a factor 10 smaller than Δ_2, suggesting rather an exponential decrease of Δ_{n_l} with increasing n_l.

The susceptibility per rung of the odd-leg ladders remains finite in the low-temperature limit and tends to a zero-temperature value approximately independent of n_l [see Fig. 1(b)]. This indicates that the odd-leg ladders belong to the same universality class as the single chain.

The single chain can be described in a low-temperature field theory by the $k=1$ Wess-Zumino-Witten nonlinear σ model or equivalently by a free, massless boson, with a

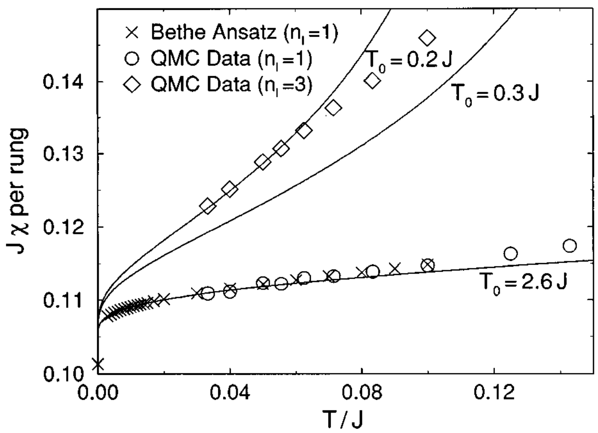

FIG. 2. Renormalization group improved field theory (solid lines) [Eq. (4)] for different cutoff temperatures T_0 versus Bethe ansatz data (Ref. 16) and QMC results for $\chi(T)$ at low temperature. The error bars are smaller than the symbols.

(spin) velocity $v=\pi J/2$. Based on this model $\chi(T=0)$ and the leading T dependences of χ have been calculated[16,17] with the leading marginally irrelevant operator. Two-loop renormalization of the marginal coupling leads to

$$\chi(T)=\frac{1}{2\pi v}+\frac{1}{4\pi v}\left[\frac{1}{\ln(T_0/T)}-\frac{\ln(\ln(T_0/T)+1/2)}{2\ln^2(T_0/T)}\right]+O((\ln T)^{-3}),\tag{4}$$

where T_0 is the cut off temperature. The susceptibility approaches its asymptotic zero-temperature value $\chi(0)=(2\pi v)^{-1}=(J\pi^2)^{-1}$ with infinite slope. The field theoretical results can be compared to the exact Bethe ansatz data[16] and one finds that Eq. (4) holds to within 1% for $T<0.1J$. These results are shown in Fig. 2 together with our QMC data for low temperatures.

We turn now to the three- and five-leg ladders. In the limit $J/J_\perp=0$ each eigenfunction is a direct product of one-rung states whose lowest lying multiplet is a spin doublet. The ground state of the whole system is therefore 2^L-fold degenerate. A finite value of J lifts this degeneracy. In this 2^L-dimensional subspace $\mathcal{M}$ we can define an effective Hamiltonian $H_{\rm eff}$ which includes all intraleg interactions. To first order in $J/J_\perp$ we obtain[18]

$$H^{(1)}_{\rm eff}=J_{\rm eff}\sum_{j=0}^{\infty}\vec{S}_{j,\ \rm tot}\cdot\vec{S}_{j+1,\,\rm tot},\tag{5}$$

where $\vec{S}_{j,\rm tot}$ is the total spin of the jth rung and $J_{\rm eff}=J$ for the three-leg ladder, respectively $J_{\rm eff}=1.017J$ for the five-leg ladder. $H^{(1)}_{\rm eff}$ has just the form of the Hamiltonian of the single chain with an effective coupling $J_{\rm eff}$ and we can map the low lying energy states of the three- and five-leg ladder to those of the single chain. In the following we will concentrate on the three-leg ladder:

The susceptibility of the single chain $\chi_1(T/J)$ scales with $1/J$. It follows that for a three-leg ladder with small $J/J_\perp$ and at low temperature, where only the above mentioned low lying states in $\mathcal{M}$ are relevant, the susceptibility per rung χ_3 scales with $1/J_{\rm eff}$ and has the same functional dependence on $T/J_{\rm eff}$ as $\chi_1(T/J)$, according to Eq. (5). This can be seen in Fig. 3, where we show $J\chi_3$ for different ratios $J/J_\perp$ as a function of T/J. For small $J/J_\perp$ the susceptibility per rung χ_3 multiplied by J is very close to $J\chi_1$ until a crossover temperature, which depends on $J/J_\perp$. Above this temperature, the susceptibility of the three-leg ladder is larger, due to the presence of additional states in the three-leg ladder which are not included in the 2^L-dimensional subspace $\mathcal{M}$. These additional states have a finite gap $\tilde{\Delta}$. The susceptibility of the three-leg ladder then reads

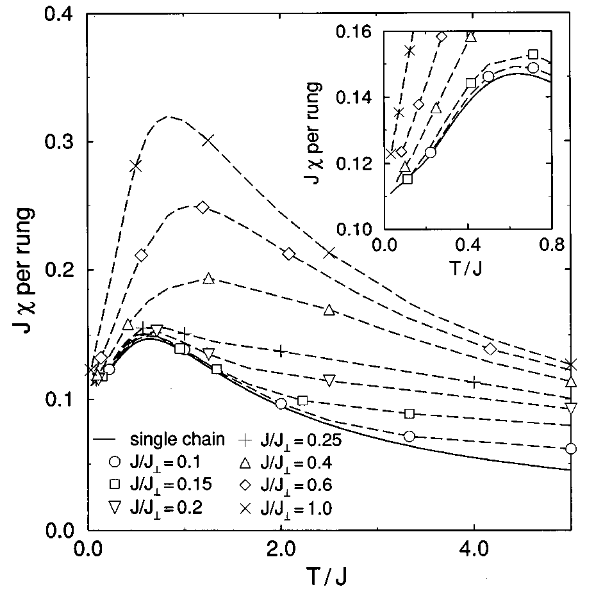

FIG. 3. Susceptibility per rung of the three-leg ladder χ_3 (dashed lines) for different ratios $J/J_\perp$ and of the single chain χ_1 in function of the temperature. The inset shows the low-temperature region in a larger scale. To distinguish the curves some data points are marked by symbols. The error bars are smaller than the symbols.

$$\chi_3=\chi_1(J_{\rm eff})+\tilde{\chi},\tag{6}$$

where $\tilde{\chi}$ is the contribution of the additional states. From our QMC data we find $J_{\rm eff}\approx J$ for all small $J/J_\perp$ and $\Delta_4(J/J_\perp)\lesssim\tilde{\Delta}\lesssim\Delta_2(J/J_\perp)$.

In the isotropic case $J=J_\perp$, the gap $\tilde{\Delta}$ in units of J is indeed smaller than for small $J/J_\perp$ but remains finite $(\Delta_4\lesssim\tilde{\Delta}\lesssim\Delta_2)$. For $T\ll\tilde{\Delta}$ we can neglect the contribution $\tilde{\chi}$ of the additional states. Comparing $J\chi_3$ to $J\chi_1$ for $T\ll\tilde{\Delta}$, we see that their slopes are completely different, but their zero-temperature values are more or less equal (see inset of Fig. 3 or Fig. 2). Therefore, no $J_{\rm eff}$ can be found to fulfill Eq. (6) and we conclude that in this case the simple model, discussed above [Eq. (6)], no longer applies.

Instead, as $J/J_\perp\to 1$ also next-nearest neighbor and longer range interactions between rung spins become important in the effective Hamiltonian $H_{\rm eff}$. Since these additional interactions respect the SU(2) and translational symmetry, Eq. (4) still applies for some values of v and T_0, according to Ref. 16. Therefore, for very small T the susceptibility of the three-leg ladder can be described by Eq. (4) also in the isotropic case (see Fig. 2).

The spin velocity in the isotropic three-leg ladder v_3 seems to be close to that of the single chain v_1. This can be seen by two facts. First, both of the susceptibilities per rung seem to extrapolate to the same zero-temperature value. Secondly, White *et al.*[3] determined the spin gap of the finite single chain and the finite three-leg ladder in function of $1/L$. The slopes of these curves as $1/L \rightarrow 0$, πv_1, and πv_3, agree, at least within 5%. Assuming $v_1 = v_3$, we get a rough estimate of the cutoff temperature T_0 in the isotropic three-leg ladder from our numerical data. The value is much smaller than in the single chain (see Fig. 2). We conclude therefore, that the effective interactions between the spinons in the three-leg ladder are much stronger than those in the single chain.

We conclude that the odd-leg ladders belong to the same universality class as the single chain and can be described in the zero-temperature limit by a $k=1$ Wess-Zumino-Witten nonlinear σ model with a spin velocity v_{n_l}. These velocities seem to have more or less the same value for all n_l. With increasing n_l, however, we move further away from the conformal point and the logarithmic corrections, due to the leading marginally irrelevant operator, increase markedly.

Finally, we want to point out that also for the odd-leg ladders as well as for the even-leg ladders the $T \rightarrow 0$ behavior sets in at lower temperature as n_l increases and that the zero-temperature value of the susceptibility per site $\chi_{n_l}^{(\mathrm{site})}(0)$ for the odd-leg ladders decreases with increasing n_l. Since the odd-leg ladders seem to have more or less the same zero-temperature value of the susceptibility per rung, it follows that $\chi_{n_l}^{(\mathrm{site})}(0) \propto 1/n_l$. For $n_l \rightarrow \infty$ the zero-temperature value $\chi_{n_l}^{(\mathrm{site})}(0)$ therefore goes to zero for odd n_l as well as for even n_l. The susceptibility per site of a 2D square lattice, however, is finite for $T=0$. This is a further example that the crossover from the single chain to the 2D lattice is not a smooth one.

We wish to thank G. Sierra, H.G. Evertz, D. Würtz, and especially T.M. Rice for very instructive and stimulating discussions. The calculations were performed on the Intel Paragon of the ETH Zürich. The work was partially supported by the Schweizerischen Nationalfond (B.F.) and by an ETH internal grant (B.A.).

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