The temperature dependence of the uniform susceptibility and the ground state energy of antiferromagnetic Heisenberg ladders with up to 6 legs has been calculated, using the Monte Carlo loop algorithm. The susceptibilities of even-leg-ladders show spin gaps while these of odd-leg-ladders remain finite in the zero temperature limit. For small ratios of intra- to inter-leg 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.

Recently, antiferromagnetic Heisenberg spin-1/2 ladder systems have attracted much interest, following the discovery of a finite spin gap in the 2-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 [3]. 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. [4] gave an explanation of this fundamental difference in the framework of the Resonant Valence Bond (RVB) picture [5]. These theoretical predictions have been verified experimentally, in materials such as \((VO)_2P_2O_7\) [6] and the homologous series of cuprates \(Sr_{n-1}Cu_n+1O_{2n}\) [7], which contain weakly coupled arrays of ladders.

Previous numerical studies, using exact diagonalization [4,6], the Quantum Monte Carlo 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 Quantum Monte Carlo (QMC) loop algorithm [10], we overcome these limitations and are able to investigate very large ladders to much lower temperatures.

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

\[
H = J \sum_{\leftrightarrow} \vec{S}_i \cdot \vec{S}_j + J_\perp \sum_{\downarrow \uparrow} \vec{S}_i \cdot \vec{S}_j \tag{1}
\]

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

Using the Quantum Monte Carlo loop algorithm with improved estimators, we have calculated the temperature dependence of the uniform susceptibility \( \chi \) and the internal energy \( E \). The QMC loop algorithm was first developed by Evertz et al. [11] for the 6-vertex-model, but can also be applied to quantum spin systems [12,13]. The QMC loop algorithm is an improved world line algorithm. The updates in the loop algorithm 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 x 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. [14]), 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. Considering ladders of lengths \( L \), we first extrapolate to \( T \to 0 \). For the odd-leg-ladders we use the form

\[
E_L(T) = E_L(0) + a T^2, \tag{2}
\]

where \( E_L(T) \) is the internal energy of the ladder of length \( L \). This form is motivated by the infinite single chain, which in a low temperature field theory can be described by a massless boson. Our numerical data agree well with Eq. (4) for the finite single chains, as well as for the finite 3- and 5-leg-ladders. The even-leg-ladders, on the other hand, have spin gaps. The internal energy for \( T \) well below the spin gap \( \Delta \) 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 to \( T \to 0 \) we therefore use the form

\[
E_L(T) = E_L(0) + b \left(T^{3/2} + 2\Delta T^{1/2}\right) \exp(-\Delta/T). \]

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 \( 1/L \). The finite size corrections of the ground state energy, however, are negligibly small for ladders with \( L \geq 100 \).

In Fig. 1 we show the susceptibility per rung of \( n_l \) spins, \( \chi(T) \), for the ladders with \( 1 \leq n_l \leq 6 \) 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 well with a third order high temperature 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 $\Delta_{n_l}$ 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. For temperatures $T \ll \Delta$ the susceptibility for the 2-leg-ladder is determined by the thermal occupation of $S = 1$ magnon band with a quadratic dispersion near the zone boundary minimum:

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

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 4- and 6-leg-ladder. We estimate $\Delta_{n_l}$ 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 $\Delta_2$ obtained for the 2-leg-ladder is in perfect agreement with former results. On the other hand, the spin gap obtained by White et al. using DMRG methods for the 4-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 [3]. The spin gap for the 6-leg-ladder $\Delta_6$ is already a factor 10 smaller than $\Delta_2$, suggesting rather an exponential decrease of $\Delta_{n_l}$ 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. 3]. For this we conclude 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 $\sigma$-model or equivalently by a free, massless boson, with a (spin) velocity $v = \pi J/2$. Based on this model $\chi(T = 0)$ and the leading $T$ dependences of $\chi$ have been calculated with the leading marginally irrelevant operator. Two-loop renormalization of the marginal coupling leads to

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

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 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 3- and 5-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 $(s = 1/2)$. 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 $H_{\text{eff}}$ which includes all intra-leg interactions. To first order in $J/J_{\perp}$ we obtain

$$H_{\text{eff}}^{(1)} = J_{\text{eff}} \sum_{j=0}^{\infty} \hat{S}_{j,\text{tot}} \hat{S}_{j+1,\text{tot}}, \quad (5)$$

where $\hat{S}_{j,\text{tot}}$ is the total spin of the $j^{th}$ rung and $J_{\text{eff}} = J$ for the 3-leg-ladder, respectively $J_{\text{eff}} = 1.017 J$ for the 5-leg-ladder. $H_{\text{eff}}^{(1)}$ has just the form of the Hamiltonian of the single chain with an effective coupling $J_{\text{eff}}$ and we can map the low lying energy states of the 3- and 5-leg-ladder to those of the single chain. In the following we will concentrate on the 3-leg-ladder.

The susceptibility of the single chain $\chi_1(T/J)$ scales with $1/J$. It follows, that for a 3-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 $\chi_3$ scales with $1/J$ and has the same functional dependence on $T/J_{\perp}$ as $\chi_1(T/J)$, according to Eq. (5). This can be seen in Fig. 6 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 $\chi_3$ 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 3-leg-ladder is larger, due to the presence of additional states in the 3-leg-ladder which are not included in the $2^L$-dimensional subspace $\mathcal{M}$. These additional states have a finite gap $\Delta$. The susceptibility of the 3-leg-ladder then reads

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

where $\tilde{\chi}$ is the contribution of the additional states. From our QMC data we find $J_{\text{eff}} \approx J$ for all small $J/J_{\perp}$ and $\Delta_3(J/J_{\perp}) \lesssim \Delta \lesssim \Delta_2(J/J_{\perp})$.

In the isotropic case $J = J_{\perp}$, the gap $\Delta$ in units of $J$ is indeed smaller than for small $J/J_{\perp}$ but remains finite ($\Delta_4 \lesssim \Delta \lesssim \Delta_2$). For $T \ll \Delta$ we can neglect the contribution $\tilde{\chi}$ of the additional states. Comparing $\chi_3$ to $\chi_1$ for $T \ll \Delta$, we see that their slopes are completely different (see Fig. 3). Therefore we conclude that in this case the simple model, discussed above [Eq. (5)], no longer applies.
As $J/J_\perp \to 1$ also next-nearest neighbor and longer range interactions between rung-spins become important in the effective Hamiltonian $H_{\text{eff}}$. 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 \cite{16}. Therefore, for very low temperatures the susceptibility of the 3-leg-ladder can be described by Eq. (4) also in the isotropic case (see Fig. 3).

The spin velocity in the isotropic 3-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. \cite{3} determined the spin gap of the finite single chain and the finite 3-leg-ladder in function of $1/L$. The slopes of these curves as $1/L \to 0$, $\pi v_1$ and $\pi v_3$, agree, at least within 5%. Assuming $v_1 = v_3$, we get a rough estimate of the cut-off-temperature $T_0$ in the isotropic 3-leg-ladder. The value is much smaller than in the single chain. We conclude therefore, that the effective interactions between the spinons in the 3-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 non linear $\sigma$-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 the zero temperature value of the susceptibility per site $\chi^{(\text{site})}_{n_l}(0)$ 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 $\chi^{(\text{site})}_{n_l}(0) \propto 1/n_l$. For $n_l \to \infty$ the zero temperature value $\chi^{(\text{site})}_{n_l}(0)$ 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 therefore a further example that the crossover from the single chain to the 2D-lattice is not a smooth one.

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| number of legs | obtained ground state energy | reference value |
|----------------|-----------------------------|-----------------|
| 1              | -0.4432(1)                  | -0.44315...     |
| 2              | -0.5780(2)                  | -0.578          |
| 3              | -0.6006(3)                  | -               |
| 4              | -0.6187(3)                  | -               |
| 5              | -0.6278(4)                  | -               |
| 6              | -0.635(1)                   | -               |
| 2D lattice    | -0.6693(1)                  | -               |

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 [13]. Furthermore, the result for the 2-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 [14]. The reference value given here was recently obtained by U.J. Wiese and H.P. Ying [12] using the QMC loop algorithm.

FIG. 1. Susceptibility as a function of the temperature for the single chain and the Heisenberg ladders with up to 6 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.

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

FIG. 3. Susceptibility per rung of the 3-leg-ladder $\chi_3$ (dashed lines) for different ratios $J/J_\perp$ and of the single chain $\chi_1$ 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.
Bethe Ansatz ($n_l=1$)

QMC Data ($n_l=1$) $T_0 = 0.2 J$

QMC Data ($n_l=3$) $T_0 = 0.3 J$

$T_0 = 2.6 J$
\[
\begin{align*}
J \chi \text{ per rung} \\
\frac{J}{J_{\perp}} = 0.1 \\
\frac{J}{J_{\perp}} = 0.15 \\
\frac{J}{J_{\perp}} = 0.2 \\
\frac{J}{J_{\perp}} = 0.25 \\
\frac{J}{J_{\perp}} = 0.4 \\
\frac{J}{J_{\perp}} = 0.6 \\
\frac{J}{J_{\perp}} = 1.0
\end{align*}
\]