A Monte Carlo Study of Correlations in Quantum Spin Ladders

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We study antiferromagnetic spin–1/2 Heisenberg ladders, comprised of \( n_c \) chains (2 \( \leq n_c \leq 6 \)) with ratio \( J_\perp/J_\parallel \) of inter– to intra–chain couplings. From measurements of the correlation function we deduce the correlation length \( \xi(T) \). For even \( n_c \), the static structure factor exhibits a peak at a temperature below the corresponding spin gap. Results for isotropically coupled ladders \((J_\perp/J_\parallel = 1)\) are compared to those for the single chain and the square lattice. For \( J_\perp/J_\parallel \leq 0.5 \), the correlation function of the two–chain ladder is in excellent agreement with analytic results from conformal field theory, and \( \xi(T) \) exhibits simple scaling behavior.

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Low–dimensional quantum Heisenberg antiferromagnets (QHA) exhibit many fascinating properties. In 1931, Bethe demonstrated for the one–dimensional (1D) spin \( S = 1/2 \) nearest–neighbor Heisenberg chain that quantum fluctuations prevent the existence of an ordered ground state \( [4] \). Instead, this system exhibits power–law correlations with gapless excitations. Haldane suggested in 1983 that all non–integer–spin chains are gapless, but that integer–spin chains should have a spin gap \( [5] \). By now, there is much evidence for the correctness of this famous conjecture \( [3] \). For the two–dimensional (2D) analog of the spin chains, the square–lattice nearest–neighbor QHA, it has been established over the past decade that an ordered ground state exists even in the extreme quantum limit of \( S = 1/2 \) \( [6] \).

Spin ladders are arrays of coupled chains, and thus present interpolating structures between 1D and 2D \( [3] \). These systems are thought to be realized, with \( S = 1/2 \), in the materials \((VO)_2P_2O_7 \) \( [3] \) and \( Sr_{n-1}Cu_n+1O_{2n+2} \) \( [5] \). They allow the study of the dimensional crossover from the power–law correlations of the \( S = 1/2 \) chain to the long–range order of the square lattice. Interestingly, ladders with an odd number \( n_c \) of chains have power–law spin correlations in their ground state, while those with even \( n_c \) exhibit exponentially decaying correlations due to the presence of a spin gap \( [3] \). In analogy to the general \( S \) chain \( [3] \), the fundamental difference between even and odd ladders is thought to be of topological nature \( [3,3] \).

In this Letter we investigate isotropically coupled ladders as well as the two–chain ladder in the regime of weak inter–chain couplings. The former systems are directly relevant to the known experimental systems which are approximately isotropic \( [3] \). Moreover, the crossover from 1D to 2D is most naturally studied in this case. We perform numerical simulations which allow us to determine both the correlation length and the static structure factor down to very low temperatures. Our results provide a basis for comparison with future neutron scattering and NMR experiments. The two–chain ladder at weak inter–chain couplings allows us to investigate the formation of a spin gap away from the unstable \( T = 0 \) fixed point of the gapless \( S = 1/2 \) chain \( [10] \), and indeed serves to demonstrate the extreme fragility of the \( S = 1/2 \) chain power–law correlations. Our data for the intra– and inter–chain correlation functions at low temperature are in excellent agreement with a recent theoretical prediction \( [1] \). Moreover, we discover that in this regime the correlation length exhibits universal scaling behavior with respect to the inter–chain coupling.

The Hamilton operator for a Heisenberg system of \( n_c \) \( S = 1/2 \) chains forming a ladder is

\[
H = J_{\parallel} \sum_{\langle ij\rangle_{\parallel}} \mathbf{S}_i \cdot \mathbf{S}_j + J_\perp \sum_{\langle ij\rangle_\perp} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{1}
\]

Here, \( \mathbf{S}_i = \frac{1}{2} \sigma_i \) is the quantum spin operator located at the point \( i \), while \( \langle ij\rangle_{\parallel} \) and \( \langle ij\rangle_\perp \) denote nearest neighbors along and between chains, respectively. We consider antiferromagnetic couplings, that is \( J_{\parallel}, J_\perp > 0 \), and periodic boundary conditions along the chains. We use units in which \( \hbar = k_B = 1 \) and, unless noted otherwise, \( J_{\parallel} = 1 \).

The ladder systems are investigated with a very efficient loop cluster algorithm \( [12,13] \) which allows access to very low temperatures and the implementation of improved estimators in order to reduce statistical errors of observables. We simulate lattices large enough, both along the chains and in Euclidean time, so that finite size and finite Trotter number effects are comparable to the statistical errors. In particular, the length of the ladders is kept \( \sim 15 \) times larger than the correlation length. Typically, \( 4 \times 10^4 \) loop updates are performed for equilibration, followed by \( 4 \times 10^5 \) measurements.

In order to obtain information about the gap \( \Delta(n_c, J_\perp) \) for even \( n_c \), we measure the uniform susceptibility

\[
\chi(n_c, J_\perp; T) \sim T^{-1} \langle (\sum_i S_i^\perp)^2 \rangle. \tag{2}
\]

Gap values extracted from fits to the low–\( T \) form \( [14] \).
are shown in Fig. 1. For \( J_1 \geq 2 \), we find very good agreement with strong–coupling expansion results for \( n_c = 2 \) and 4 [15], shown as solid lines. Our susceptibility data for the isotropically coupled ladders (\( J_1 = 1 \)) agree well with recent Monte Carlo work [13], and we obtain \( \Delta(n_c, 1) = 0.502(5), 0.160(5) \), and \( 0.055(6) \) for \( n_c = 2, 4 \), and 6, respectively. In an earlier study [8], \( \Delta_1 = 0.190 \) was found. For \( n_c = 2 \), we are able to access the weak–coupling regime characterized by \( \Delta(2, J_1) \sim J_1 \) [14,17]. We find \( \Delta(2, J_1)/J_1 = 0.41(1) \), which is somewhat smaller than \( \Delta(2, J_1)/J_1 = 0.47(1) \) obtained previously [17].

\[ \chi(n_c, J_\perp; T) \sim T^{-1/2}e^{-\Delta(n_c, J_\perp)/T} \]  

(3)

Next we compute the staggered correlation function

\[ C(i, j) = (-1)^{\text{sign}(i, j)}\langle S_i \cdot S_j \rangle, \]  

(4)

where \( \text{sign}(i, j) = 1(-1) \) if the spins at \( i \) and \( j \) are separated by an even (odd) number of couplings. For a system of two weakly coupled chains at \( T = 0 \), conformal field theory predicts \[ C = G_+(r)G_-(r)[G_-(r)G_-(3r) \pm G_+(r)G_+(3r)], \]  

(5)

and this form is claimed to be exact in the continuum limit at small \( J_\perp \). The sign of the last term is plus for intra– and minus for inter–chain correlations, and \( r \) measures the distance of two spins along the ladder. The functions

\[ G_\pm(r) = r^{-1/4}F_\pm(r/\xi)[1 \pm 2^{-3/2}\xi^{-1}] + O(r^{-5/4}) \]  

(6)

are correlation functions of the 2D Ising model, with scaling functions \( F_\pm \) [8]. In Eq. (6) \( \xi \) denotes the spin–spin correlation length of the ladder system. The intra– and inter–chain correlation functions differ only at short distances. At large distances \( r/\xi \gg 1 \), \( C(r) \) decays as

\[ C(r) \sim r^{-\lambda}e^{-r/\xi} \]  

(7)

with \( \lambda = 1/2 \), which is equivalent to the 2D Ornstein–Zernike (OZ) form. Figure 2 shows the low–\( T \) correlation function for \( n_c = 2 \) at a weak coupling of \( J_1 = 0.2 \). The lines are the result of a fit to Eq. (5) with only two fitting parameters: \( \xi \) and an overall amplitude. The fit is excellent over the entire range, and we obtain \( \xi = 19.4(2) \). As is evident in Fig. 2, Eq. (5) correctly captures the crossover from the short– to the long–distance behavior with a concomitant change in length scales by \( \sim 3 \).

[FIG. 1. Dependence of the spin gap on the inter–chain coupling. The solid lines represent strong–coupling results [15], and the dashed line indicates the weak–coupling behavior \( \Delta(2, J_\perp \to 0) = 0.41(1)J_\perp \).]

[FIG. 2. Intra– and inter–chain correlation functions at \( T = 0.01 \) for a \( S = 1/2 \) two–chain Heisenberg ladder of length 300 with \( J_\perp = 0.2 \). Note that periodic boundary conditions were employed along the chains and that for clarity \( C(r) \) is shown only for even \( r \). The lines are the result of a fit to Eq. (5) in the symmetrized form \( [C(r) + C(300 - r)] \).]

In order to deduce \( \xi(n_c, J_\perp; T) \) for general \( n_c, J_\perp, \) and \( T \), we fit \( C(i, j) \) at large distances \( r \geq 3\xi \) to the asymptotic form Eq. (7). For \( n_c = 4 \) and 6, Eq. (7) with \( \lambda = 0.5 \) describes our low–\( T \) data very well. However, we find that the asymptotic behavior for even \( n_c \) crosses over between \( T \approx 0.2\Delta(n_c, J_\perp) \) and \( T \approx 0.4\Delta(n_c, J_\perp) \) to the 1D OZ form, that is, \( \lambda = 0 \). For odd \( n_c \) we find that the 1D form works very well at all temperatures.

In Fig. 3, the result of this analysis for \( J_\perp = 1 \) is shown together with \( \xi(T) \) for the square lattice as obtained by both Monte Carlo [13] and neutron scattering in \( Sr_2CuO_2Cl_2 \) [4]. Due to the presence of a gap for even \( n_c \), \( \xi(T) \) remains finite in the limit \( T \to 0 \). We estimate that \( \xi(n_c, 1; 0) = 3.24(5) \) and 10.3(1) for \( n_c = 2 \) and 4, respectively. The result for \( n_c = 2 \) is very close to the value \( \xi = 3.19(1) \) obtained previously [8]. However, in Ref. [8] \( \xi = 5 \) to 6 was obtained for \( n_c = 4 \), which is significantly smaller than our result. For \( n_c = 2 \) and 4 we obtain the respective velocities \( c(n_c, 1) = \Delta(n_c, 1)\xi(n_c, 1; 0) = 1.63(2) \) and 1.65(3) which lie in between the 1D and 2D values \( c_{1D} = \pi/2 \) and
$c_{2D} \simeq 1.68$.

The correlation length of the single $S = 1/2$ chain has been determined in a thermal Bethe–ansatz study \[20\]:

\[\xi_{1D}^{-1}(T) \simeq T \left[ 2 - b^{-1} \left( 1 - 0.486b^{-1} \ln(b) \right) \right] \tag{8}\]

with $b = -\ln(0.3733T)$. For $T \leq 0.3$ our data for the chain ($n_c = 1$) agree with this low-$T$ form, indicated by the dashed line in Fig. 3. We observe that with decreasing temperature $\xi$ for $n_c = 3$ and 5 gradually approaches $\xi_{1D}$.

\[\text{FIG. 3. Correlation length of } n_c \text{ isopropically coupled antiferromagnetic } S = 1/2 \text{ chains. The result for the single chain } (n_c = 1) \text{ is compared with the theoretical prediction Eq. (8) (dashed line). Also shown are the results for the square lattice obtained from both Monte Carlo simulations } \[19\] \text{ as well as neutron scattering experiments in } Sr_2CuO_2Cl_2.\]

In Fig. 4 the static structure factor at $(\pi, \pi)$, $C_{\pi,\pi} = \sum_{i,j} C(i,j)$, is shown for the isopropically coupled system. The overall trend with $n_c$ is similar to that for $\xi$. However, $C_{\pi,\pi}(n_c, J_{\perp}; T)$ for even $n_c$ exhibits a peak at a temperature $T_{\text{max}}$ well below the corresponding spin gap. Not surprisingly, $T_{\text{max}}$ appears to coincide with the temperature at which the asymptotic correlation function Eq. (7) begins to cross over from the 1D OZ form at higher temperatures to the low-$T$ 2D form.

\[\text{FIG. 4. Static structure factor at } (\pi, \pi) \text{ for isopropically coupled antiferromagnetic } S = 1/2 \text{ ladders, as well as for the single chain } (n_c = 1) \text{ and the square lattice } \[19\]. For even } n_c, \text{ } C_{\pi,\pi} \text{ exhibits a peak (indicated by arrows) at a temperature below that corresponding to the relevant spin gap.}\]

The temperature dependence of $\xi(2, J_{\perp}; T)$ in the weak–coupling regime primarily results from that of the single chain, Eq. (8). Apart from logarithmic corrections, the latter is simply $\xi_{1D}(T) \sim T^{-1}$. Eq. (9) thus becomes $(\Delta \xi)^{-1} = 2/\pi + A(T/\Delta)e^{-\Delta T/\Delta}$, which suggests plotting $\Delta \xi$ versus $T/\Delta$ to test for the anticipated scaling for $J_{\perp} \leq 0.5$. As shown in the inset of Fig. (5), our correlation length data indeed collapse onto a universal curve. Over the indicated range the effective value for $A$ is $\sim 1.7$ compared to the low–$T$ value of 2.

For the two–chain ladder, we have established that $\Delta(2, J_{\perp} \rightarrow 0) = 0.41(1)J_{\perp}$. We can furthermore estimate the weak–coupling behavior for $n_c = 4$. From Fig. 1, it can be inferred that $\Delta(4, J_{\perp} \rightarrow 0) \approx 0.35J_{\perp}$, which leads to $\Delta(4, J_{\perp} \rightarrow 0) = 0.06J_{\perp}$ as a lower bound. From the lowest $J_{\perp}$ for $n_c = 4$, we have $\Delta(4, J_{\perp} \rightarrow 0) = 0.12J_{\perp}$ which constitutes an upper bound. Thus we arrive at the estimate $\Delta(4, J_{\perp} \rightarrow 0) = 0.09J_{\perp}$.

We note that the trend with increasing $n_c$ of the ladder
gap resembles that of the single integer–spin chain as a function of increasing $S$: For $S = 1$, $\Delta S=1 = 0.4105 J_{||}$ is known very accurately [21], while recent estimates for $S = 2$ range between $\Delta S=2 = 0.049(18) J_{||}$ and $0.085(5) J_{||}$ [22]. It has recently been argued that the two–chain ladder with antiferromagnetic inter–chain coupling lies in the same phase as the $S = 1$ single chain [22], and that the weak–coupling physics is independent of the sign of $J_{\perp}$ [11]. Clearly, further numerical and analytical work to establish this correspondence is necessary.

In summary, our Monte Carlo calculations on spin ladders have provided a number of new results. First, our weakly–coupled two–chain system agrees very well with measured low–temperature correlation function for the prototype $S = 1/2$ square–lattice Heisenberg antiferromagnet $Sr_{2}CuO_{2}Cl_{2}$, neutron scattering measurements of the correlation length are in excellent agreement with Monte Carlo simulations and theory [1], as well as high–temperature series expansion [23]. Once sizable single crystals of the ladder systems become available, we intend to extend our neutron scattering work to these interesting systems. We also hope that our Monte Carlo results will motivate future theoretical efforts to predict $C(i,j)$ for general $n_{c}$, $J_{\perp}$, and $T$.

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References:

[1] H.A. Bethe, Z. Phys. 71, 205 (1931).
[2] F.D.M. Haldane, Phys. Lett. 93A, 464 (1983).
[3] See, e.g., I. Affleck, Rev. Math. Phys. 6, 887 (1994).
[4] M. Greven et al., Z. Phys. B 96, 465 (1995).
[5] For a review, see E. Dagotto and T.M. Rice, Science 271, 618 (1996).
[6] D.C. Johnston et al., Phys. Rev. B 35, 219 (1987).
[7] Z. Hiroi et al., J. Solid State Chem. 95, 230 (1991).
[8] S.R. White, R.M. Noack, and D.J. Scalapino, Phys. Rev. Lett. 73, 886 (1994).
[9] G. Sierra (to be published).
[10] T. Barnes et al., Phys. Rev. B 47, 3196 (1993).
[11] D.G. Shelton, A.A. Nersesyan, and A.M. Tsvelik, Phys. Rev. B 53, 8521 (1996).
[12] H.G. Evertz, G. Lana, and M. Marcu, Phys. Rev. Lett. 70, 875 (1993).
[13] U.–J. Wiese and H.–P. Ying, Z. Phys. B 93, 147 (1994).
[14] M. Troyer, H. Tsumetsugu, and D. W" urtz, Phys. Rev. B 50, 13515 (1994).
[15] M. Reigrotzki, H. Tsumetsugu, and T.M Rice, J. Phys. Cond. Matt. 6, 9235 (1994).
[16] B. Frischmuth et al. (to be published).
[17] N. Hatano, Y. Nishiyama, and M. Suzuki, J. Phys. A: Math. Gen. 27, 6077 (1994).
[18] T.T. Wu et al., Phys. Rev. B 13, 316 (1976).
[19] M. Greven, Ph.D. thesis, MIT (1995); see also M. Makivić and H.–Q. Ding, Phys. Rev. B 43, 3562 (1991).
[20] K. Nomura and M. Yamada, Phys. Rev. B 43, 8217 (1991).
[21] S.R. White and D.A. Huse, Phys. Rev. B 48, 3844 (1993); O. Golinelli, Th. Joliceur, and R. Lacace, Phys. Rev. B 50, 3037 (1994).
[22] S. Yamamoto, Phys. Rev. Lett. 75, 3348 (1995), and references herein.
[23] S.R. White, Phys. Rev. B 53, 52 (1996).
[24] N. Elstner et al., Phys. Rev. Lett. 75, 938 (1995).