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Numerical renormalization-group study of the correlation functions of the antiferromagnetic spin-$\frac{1}{2}$ Heisenberg chain

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We use the density-matrix renormalization-group technique developed by White to calculate the spin correlation functions $\langle S^z_{n+l}\, S^z_n\rangle = (-1)^l \omega(l,N)$ for isotropic Heisenberg rings up to $N=70$ sites. The correlation functions for large l and N are found to obey the scaling relation $\omega(l,N)=\omega(l,\infty) f^{\alpha}_{XY}(l/N)$ proposed by Kaplan *et al.*, which is used to determine $\omega(l,\infty)$. The asymptotic correlation function $\omega(l,\infty)$ and the magnetic structure factor $S(q=\pi)$ show logarithmic corrections consistent with $\omega(l,\infty)\sim a\sqrt{\ln cl}/l$, where c is related to the cut-off dependent coupling constant $g_{\rm eff}(l_0)=1/\ln(cl_0)$, as predicted by field theoretical treatments.

Although the exact ground state of the spin-1/2 chain is explicitly known, the Bethe-Ansatz wave function is far too complex to derive directly the spin-correlation functions. Other methods like bosonization or conformal field theory have to be used to get information about the asymptotic behavior of these functions. In general quantum spin chains and in particular their continuum versions are very active fields of research, because they serve as a testing ground of various analytical approaches.[1] Recent field-theoretical studies predict the existence of logarithmic corrections to the finite-size scaling of the energies of these systems and also to the power-law behavior of the spin-correlation functions stemming from marginally irrelevant operators . The modification of the power law originally derived by Luther and Peschel[2] has its physical origin in umklapp scattering processes which appear in the fermionic representation of the model after Jordan-Wigner transformation and has been anticipated a few years ago.[3] Logarithmic corrections to the scaling of the energies and to the correlation functions were obtained by Affleck *et al.*[4] applying conformal field theory to Wess-Zumino-Witten nonlinear-σ models. Giamarchi and Schulz[5] and Singh *et al.*[6] used a renormalization technique to study the sine-Gordon Hamiltonian and obtained to leading order $(-1)^l(\ln l)^{1/2}/l$ for the asymptotic decay of the spin-correlation function in the case of the isotropic Heisenberg chain.

In spite of this analytical progress, numerical attempts have given contradictory results. Kubo, Kaplan and Borysowicz[7] found a small logarithmic correction of the form $(\ln l)^{\sigma}/l$ with an exponent $0.2<\sigma<0.3$ instead of 0.5 as predicted by theory. Later attempts to check the theoretical prediction were made by Liang[8] and by Lin and Campbell,[9] who reported the absence of logarithmic corrections ($\sigma\cong 0$) for spin-1/2 chains, whereas Sandvik and Scalapino[10] report an exponent $\sigma\simeq 1/2$.

Progress on the numerical side was hampered mainly because highly accurate diagonalization results could be obtained only up to $N=30$, while Monte Carlo data for larger systems had too large statistical errors. An equally important reason was that it had been assumed that the data can be analyzed using the universal asymptotic law $(\ln l)^{\sigma}/l$.[7–10] In this paper we clarify and conclude this long dispute on the numerical evidence of the logarithmic corrections by considering the nonuniversal scaling of the coupling constant.

We use the density-matrix algorithm (DMA) (Ref. 11) to study the large-distance decay of the correlation functions and find that they can be calculated with such high precision for sufficiently large systems that the subtle logarithmic corrections to the correlation functions can be resolved. This technique leads to highly accurate results for much larger systems than those which can be solved by straightforward exact diagonalization. The DMA allows for a systematic truncation of the Hilbert space by keeping the most relevant states in describing a state (e.g., the ground state) of a larger system, instead of the lowest energy states usually kept in previous real space renormalization techniques. A general iteration of the method consists of (i) The effective Hamiltonian defined for the superblock $1+2+1'+2'$ (where the blocks 1 and $1'$ come from previous iterations and blocks 2 and $2'$ are new added ones) is diagonalized to obtain the ground state $|\psi\rangle$ (other states could be also kept). (ii) The density matrix $\rho_{ii'}=\Sigma_j \psi_{ij}\psi_{i'j}$ is constructed, where $\psi_{ij}=\langle i\otimes j|\psi\rangle$, the states $|i\rangle(|j\rangle)$ belonging to the Hilbert space of blocks 1 and 2 ($1'$ and $2'$). The eigenstates of ρ with the highest eigenvalues (equivalent to the most probable states of blocks $1+2$ in the ground state of the superblock) are kept up to a certain cutoff. (iii) These states form a new reduced basis to which all the operators have to be changed and the block $1+2$ is renamed as block 1. (iv) A new block 2

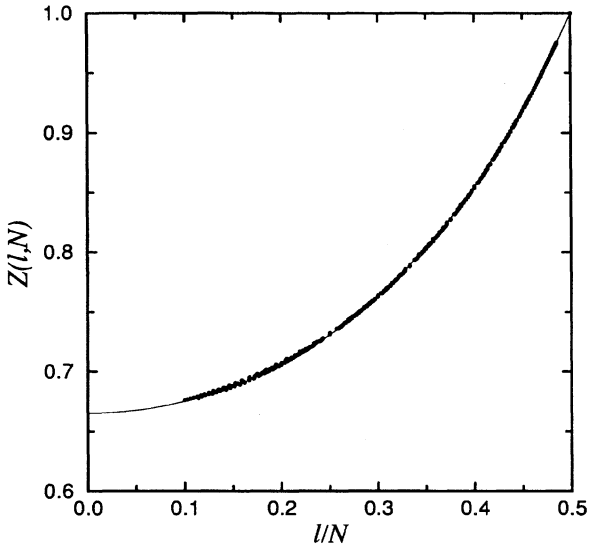

FIG. 1. The ratio $Z(l,N)=\bar{\omega}(l,N)/\bar{\omega}(l,2l)$ versus l/N for $l\geq 7$ and $14\leq N\leq 70$. The scaling function (4) with $\alpha=1.805$ is shown as a solid line.

is added (one site in our case) and the new superblock $(1+2+1'+2')$ is formed as the direct product of the states of all the blocks (the blocks $1'$ and $2'$ are identical to blocks 1 and 2, respectively).

The method has been applied successfully to several problems such as the Haldane gap of spin-1 chains,[12] the one-dimensional Kondo insulator,[13] and the two-chain Hubbard model.[14]

We used the DMA method keeping up to 200 states per block, one target state (the ground state), and periodic boundary conditions. The ground-state energy has a relative error of $\sim 10^{-6}$ for a system with $N=70$ sites and $\sim 10^{-5}$ for $N=100$, as compared to the exact finite-size energies calculated using the Bethe ansatz. The error in the spin-correlation function for large distances is almost two orders of magnitude larger than the error in the energy, as we estimated by comparing our calculations with exact results for 30 sites.[9] Because of this we present results up to $N=70$ so as to have a large enough accuracy.

In the following we consider the average value $\bar{\omega}(l,N)=\frac{1}{4}[\omega(l-1,N)+2\omega(l,N)+\omega(l+1,N)]$ [where $\langle S^z_{n+l}S^z_n\rangle=(-1)^l\omega(l,N)$] to remove the even-odd-l oscillations of the spin-correlation function, which are of order l^{-2} in ω and $\sim l^{-4}$ in $\bar{\omega}$.[15] To extract the values of the correlation function for the infinite system, we adopt the scaling relation of Kaplan *et al.*[16]

$$\bar{\omega}(l,N)=\bar{\omega}(l,\infty)f(l/N), \tag{1}$$

which is expected to hold for sufficiently large l and N. The scaling function is given by $f(l/N)=f_{XY}{}^{\alpha}(l/N)$ in terms of the scaling function of the XY model

$$f_{XY}(x)=1+0.288\,22\,\sinh^2(1.673x). \tag{2}$$

To check the scaling we plot in Fig. 1

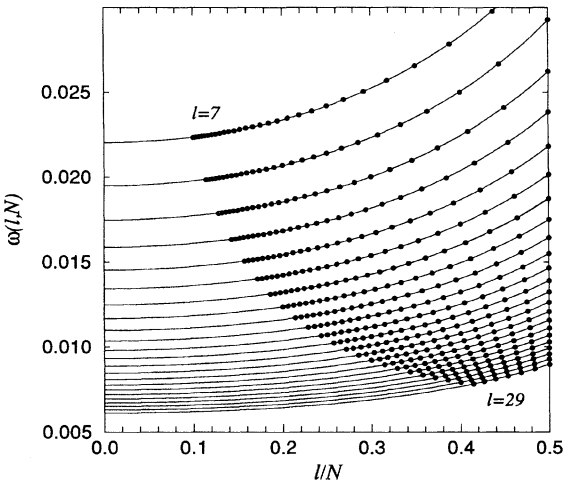

FIG. 2. Correlation function $\bar{\omega}(l,N)$ versus l/N for $l=7-29$. The solid curves are single parameter fits using the scaling relation (1) with $\bar{\omega}(l,\infty)$ as free parameter.

$$Z(l,N)=\bar{\omega}(l,N)/\bar{\omega}(l,2l) \tag{3}$$

as a function of l/N. We find that all the curves coincide within 0.3% in a unique curve for $l\geq 7$, which confirms the scaling hypothesis. Following the proposal of Ref. 16 we performed a least-squares fit for these curves using the function

$$Z(l,N)=\left[\frac{f_{XY}(l/N)}{f_{XY}(1/2)}\right]^{\alpha} \tag{4}$$

and obtained for the exponent $\alpha=1.805_2$ (the small error is determined from the dispersion of the fitted exponents considering all the curves). The fit is also shown in Fig. 1. This implies that the scaling function defined in Eq. (1) is

$$f(x)=[1+0.288\,22\,\sinh^2(1.673x)]^{1.805}. \tag{5}$$

The surprising quality of the scaling is shown in Fig. 2 where we plot the averaged $\bar{\omega}(l,N)$ as a function of l/N for several values of l. From Eq. (1) we see that the size dependence of the correlation function is given by the function $f(l/N)$ rather than the normally used $1/N^2$ behavior. We have fitted these curves with a one-parameter fit using Eq. (1) with $\bar{\omega}(l,\infty)$ as the free parameter. We use these extrapolated values $\bar{\omega}_e(l,\infty)$ to study the logarithmic corrections below.

There are very small deviations from scaling which cannot be seen in Fig. 2 , which look systematic and are probably not due to the Hilbert-space truncation. They appear as a small N dependence of $\bar{\omega}(l,N)/f(l/N)$. These deviations are less than 0.4% of the value at $l/N=1/2$. We note that these deviations could induce an error on $\bar{\omega}(l,\infty)$ of at most 1% for the largest l values.

To display the logarithmic behavior of the correlation function we have plotted $l\bar{\omega}(l,N)/f(l/N)$ as a function of $l(l\geq 7)$ for different N values in Fig. 3. Here we can see the small N dependence for a given l mentioned above, but a clear logarithmic behavior is found. We also show the extrapolated values $l\bar{\omega}_e(l,\infty)$. To visualize the magnitude of

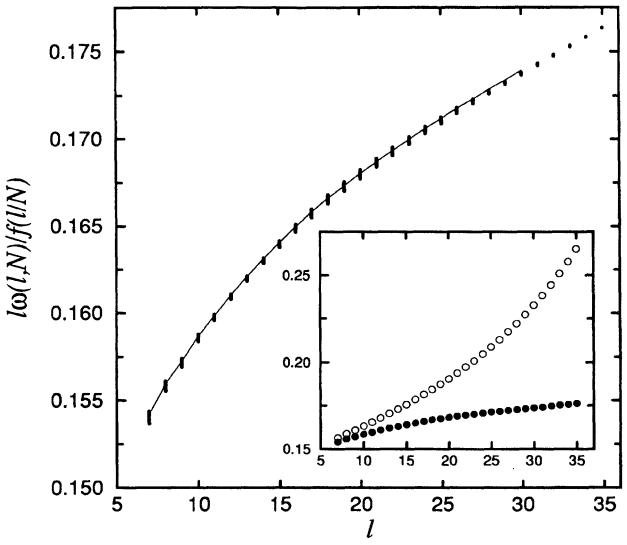

FIG. 3. Comparison of $l\tilde{\omega}(l,N)/f(l/N)$ versus l for $N=14-70$ with $l\tilde{\omega}_e(l,\infty)$ (solid curve). In the inset $l\tilde{\omega}(l,N)/f(l/N)$ (filled circles) and $l\tilde{\omega}(l,N)$ (open circles) are shown for $N=70$ showing how $f(l/N)$ corrects the finite-size effects.

the finite-size correction to the correlation functions, we show in the inset the bare data for a finite system, $l\tilde{\omega}(l,N)$ as compared to the finite-size corrected values $l\tilde{\omega}(l,N)/f(l/N)$. We see that the corrections are largest for $l\simeq N/2$ [as can also be seen from Eq. (5)].

The logarithmic corrections to the correlation function follow from the scaling relation[4-6]

$$\frac{G_i(r)}{G_i(r_0)}=\frac{r_0}{r}\exp\left(-4\pi b_i\int_{r_0}^{r}d(\ln r')g(r')\right), \tag{6}$$

where we use the notation of Ref. 4 with $G_i(r)\equiv\tilde{\omega}(r,\infty)$ and l replaced by the continuous variable r. The r dependence of the coupling constant to one-loop order is given as

$$g(r)=\frac{g(r_0)}{1+\pi b g(r_0)\ln(r/r_0)}\,. \tag{7}$$

For spin-1/2 the parameters are determined by $b=4/\sqrt{3}$ and $4b_i/b=-1/2$. The r dependence of the coupling constant leads after integration to the multiplicative logarithmic correction of the form

$$\frac{G_i(r)}{G_i(r_0)}=\frac{r_0}{r}\sqrt{\frac{g(r_0)}{g(r)}}. \tag{8}$$

For the following analysis we insert Eq. (7) and obtain

$$\frac{G_i(r)}{G_i(r_0)}=\sqrt{g_{\rm eff}}\,\frac{r_0}{r}\left[\ln\left(\frac{r}{r_0}\,e^{1/g_{\rm eff}}\right)\right]^{\frac{1}{2}}, \tag{9}$$

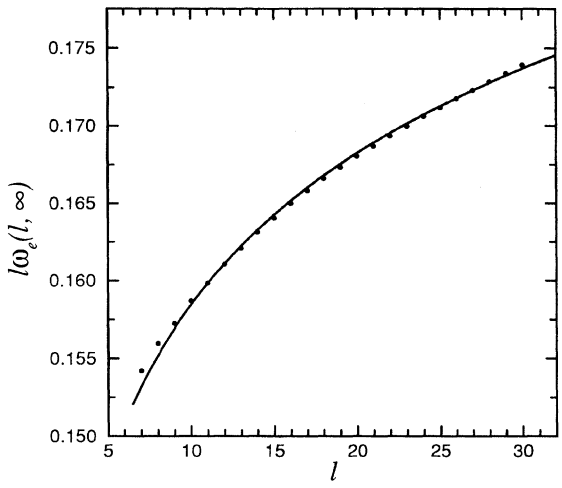

FIG. 4. Logarithmic corrections are clearly seen in the quantity $l\tilde{\omega}_e(l,\infty)$ versus l, which is well fitted by the analytical expression (10) (solid curve).

with $g_{\rm eff}(r_0)\equiv 4\pi g(r_0)/\sqrt{3}$. This equation shows that the universal, i.e., coupling constant independent, asymptotic relation $(1/r)(\ln r)^{1/2}$ is only reached for sufficiently large distances r.

We fitted the curves in Fig. 3 with the dependence predicted by renormalization group

$$l\tilde{\omega}(l,\infty)=a\sqrt{\ln(cl)}, \tag{10}$$

where $c=\exp[1/g_{\rm eff}(l_0)]/l_0$ defines the scale on which the asymptotic behavior $\omega(l,\infty)\sim\sqrt{\ln(l)}/l$ is approached. Figure 4 gives a comparison of the data and our best fit with $a=6.789\times10^{-2}$ and $c=23.21$. This implies that the asymptotic regime, i.e., $\ln(c)/\ln(l)<<1$, is reached only for chains with more than several thousand sites. The small deviations may stem either from remaining uncertainities in the determination of $\tilde{\omega}_e(l,\infty)$ or from the one-loop calculation, which is exact only to order $O(g^2)$. From the value for c we obtain for the coupling constant $g_{\rm eff}(20)=0.163$ at $l_0=20$. This may be compared with an effective coupling constant $g_{\rm eff}(20)\sim0.26$ deduced numerically from the scaling of the ground-state energy and triplet and singlet excitations.[4]

We stress that our analysis of the data differs from earlier numerical studies where the asymptotic expression $\tilde{\omega}(l,\infty)\cong a(\ln l)^{\sigma}/l$ was considered assuming $c=1$ and with σ as a free parameter.[7-9] Sandvik and Scalapino,[10] on the other hand, suggested that previous numerical studies[7-9] did not succeed in finding the proper exponent since the scaling relation (1) may not hold in the presence of logarithmic corrections. They proposed instead an alternative relation which connects $\omega(l,N)$ with the asymptotic correlation function $\omega(l,\infty)$ and which does not obey (1).[17] After subtracting the oscillatory $1/l^2$ contribution from the correlation function they analyze the ratio $D(l,N)=\omega(l,N)l/\sqrt{\ln l}$, assuming the log corrections are given by $\sqrt{\ln l}$. Given our results $D(l,N)\propto f(l/N)\sqrt{\ln cl}/\sqrt{\ln l}$, i.e., the functional used in Ref. 10 accounts for finite size effects but also for parts of

the log corrections, consequently their analysis concerning the form of these corrections is not conclusive.

Finally it should also be possible to determine the logarithmic corrections from the N dependence of the structure factor $S_N(q=\pi)=\Sigma_l \bar{\omega}(l,N)$. Earlier attempts[7–9,18] were not successful because this expression also involves large finite-size effects as $\bar{\omega}(l,N)\cong\bar{\omega}(l,\infty)f(l/N)$. It is therefore better to consider the quantity

$$S_N(\pi)=\sum_{-N/2+1}^{N/2}\frac{\bar{\omega}(l,N)}{f(l/N)}\,. \tag{11}$$

Given Eq. (10) for $\bar{\omega}(l,\infty)$ at large l one expects $S_N(\pi)\cong\text{const}+\frac{4}{3}a\ln^{3/2}(cN/2)$. From our fit of S_N we find values for a and c which are very close to the parameters deduced from $l\bar{\omega}(l,\infty)$ (see Fig. 5).

In conclusion we have shown that the scaling relation proposed in Ref. 16 provides a very accurate description of finite-size effects for large enough systems and distances ($l\geqslant 7$), and we have obtained an improved value for the exponent entering the expression for the scaling function. Furthermore we have shown that the correlation function $\omega(l,\infty)$ of the infinite system, which can be determined from N-site rings for $l\leqslant N/2$, does not obey the universal asymptotic law $(\ln l)^{\sigma}/l$ as was assumed in previous numerical work, but is governed by the nonuniversal scaling of the coupling constant. Our data confirm the multiplicative logarithmic corrections to the spin correlation function of the form $\omega(l,\infty)\sim a\sqrt{\ln cl}/l$ as derived from quantum field theory,[4–6] and we determine in particular the scale parameter c of the logarithmic term and the related effective coupling constant which has not been obtained by these approaches.

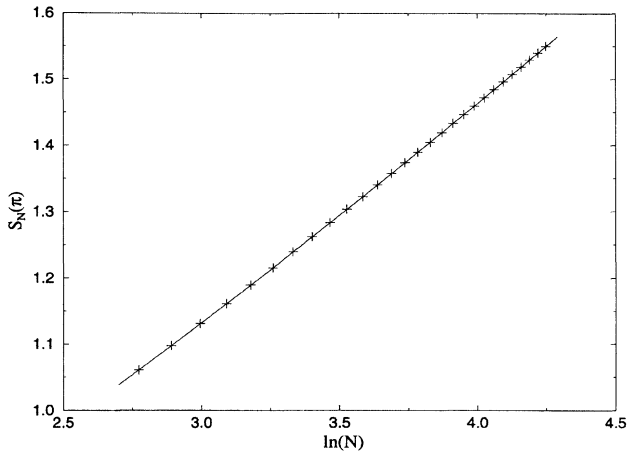

FIG. 5. $S_N(\pi)$[Eq. (11)] vs ln (N). Comparison of data (+) and fit (solid line) using $S_N(\pi)\cong\text{const}+\frac{4}{3}a\ln^{3/2}(cN/2)$ with const $=-4.06\times10^{-2}$, $a=6.67\times10^{-2}$ and $c=25.5$.

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