

Correlation amplitude for the $S = \frac{1}{2}$ XXZ spin chain in the critical region: Numerical renormalization-group study of an open chain

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(Received 13 March 1998)

The density-matrix renormalization-group technique is used to calculate the spin-correlation functions $\langle S_j^x S_k^x \rangle$ and $\langle S_j^z S_k^z \rangle$ of the one-dimensional $S = \frac{1}{2}$ XXZ model in the gapless regime. The numerical results for open chains of 200 spins are analyzed by comparing them with correlation functions calculated from a low-energy field theory. This gives precise estimates of the amplitudes of the correlation functions in the thermodynamic limit. The exact amplitude recently conjectured by Lukyanov and Zamolodchikov and the logarithmic correction in the Heisenberg model are confirmed numerically. [S0163-1829(98)51326-4]

The quantum spin chains have been a subject of very active research over the many years. Among others, the one-dimensional $S = \frac{1}{2}$ XXZ model,

$$\mathcal{H} = \sum_{j=1}^{L-1} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z), \quad (1)$$

is a simplest nontrivial model and has served as a test ground of various theoretical techniques. These include the exact calculation via the Bethe ansatz,¹ numerical computations such as the exact diagonalization studies,² and the conformal field theory (CFT).³ Although each approach alone is often not powerful enough to provide sufficient information we need, employing these techniques together has proven to be very successful to study, e.g., finite-size energy spectra and spin-correlation functions. It is well known that the equal-time correlation functions of the XXZ chain show the power-law decay in the critical regime ($-1 < \Delta \leq 1$) at zero temperature. In the thermodynamic limit ($L \rightarrow \infty$) they have the asymptotic form

$$\langle S_j^x S_k^x \rangle = (-1)^{j-k} \frac{A_x}{|j-k|^\eta} - \frac{\tilde{A}_x}{|j-k|^{\eta+1/\eta}}, \quad (2a)$$

$$\langle S_j^z S_k^z \rangle = (-1)^{j-k} \frac{A_z}{|j-k|^{1/\eta}} - \frac{1}{4\pi^2 \eta (j-k)^2}, \quad (2b)$$

where only the leading oscillating and nonoscillating terms are written. The exact expression of the parameter η appearing in the exponents,

$$\eta = 1 - \frac{1}{\pi} \cos^{-1} \Delta, \quad (3)$$

was obtained by comparing the result of the effective-field-theory description (Abelian bosonization) with the Bethe ansatz solution.⁴ On the other hand, little had been known⁵ on

the correlation amplitudes, until recently Lukyanov and Zamolodchikov⁶ (LZ) conjectured the exact form of A_x :

$$A_x^{\text{LZ}} = \frac{(1+\xi)^2}{8} \left[\frac{\Gamma\left(\frac{\xi}{2}\right)}{2\sqrt{\pi} \Gamma\left(\frac{1}{2} + \frac{\xi}{2}\right)} \right]^\eta \times \exp \left\{ - \int_0^\infty \frac{dt}{t} \left(\frac{\sinh(\eta t)}{\sinh(t) \cosh[(1-\eta)t]} - \eta e^{-2t} \right) \right\}, \quad (4)$$

where $\xi = \eta/(1-\eta)$. This result was then used in Refs. 7 and 8 to obtain the correlation amplitude for the antiferromagnetic Heisenberg model ($\Delta = 1$) with the logarithmic correction predicted earlier from the renormalization-group argument.⁹⁻¹² The aim of this paper is to numerically determine the correlation amplitudes (A_x , \tilde{A}_x , and A_z) for broad ranges of the anisotropy Δ in the critical regime. To this end we apply the density-matrix renormalization-group (DMRG) method^{13,14} to compute the spin-correlation functions for spin chains of $L = 200$, and fit the numerical data to functional forms expected from the effective-field theory (Abelian bosonization). Indeed, the idea of fitting the correlation functions of finite periodic systems to the CFT form has been applied successfully to the Heisenberg case ($\Delta = 1$) to examine the logarithmic correction.¹⁵⁻¹⁷ In the present study we use open spin chains instead of periodic ones, not only because of the better performance of the DMRG method for open chains, but because the boundary effects provide useful information. We numerically verify the LZ formula (4) and give numerical data for the yet analytically unknown amplitudes \tilde{A}_x and A_z .

We consider a finite XXZ chain of L spins with open boundaries, Eq. (1). We assume L to be an even integer so that the ground state is singlet. According to the standard

Abelian bosonization method,^{3,18} the low-energy dynamics of the XXZ model is described by the Gaussian model

$$H_0 = \frac{1}{2} \int_0^{L+1} dx \left[\left(\frac{d\phi}{dx} \right)^2 + \left(\frac{d\tilde{\phi}}{dx} \right)^2 \right], \quad (5)$$

where $\phi(x)$ and $\tilde{\phi}(x)$ are bosonic fields. We identify the site index j with the continuous variable x , and impose boundary conditions $\phi(0) = \phi(L+1) = \text{const}$ to respect the fact that there is no spin at $j=0, L+1$. The fields have the mode expansions

$$\phi(x) = \pi R + \frac{\hat{Q}x}{L+1} + \sum_{n=1}^{\infty} \frac{\sin(q_n x)}{\sqrt{\pi n}} (a_n + a_n^\dagger), \quad (6a)$$

$$\tilde{\phi}(x) = \tilde{\phi}_0 + i \sum_{n=1}^{\infty} \frac{\cos(q_n x)}{\sqrt{\pi n}} (a_n - a_n^\dagger), \quad (6b)$$

where $q_n = \pi n / (L+1)$, $R = (\eta/2\pi)^{1/2}$, $[\tilde{\phi}_0, \hat{Q}] = i$, and $[a_m, a_n^\dagger] = \delta_{m,n}$. This leads to the commutation relation $[\phi(x), \tilde{\phi}(y)] = -i/2 [1 + \text{sgn}(x-y)]$. The ground state $|0\rangle$ is the singlet vacuum state of the bosons: $a_n|0\rangle = \hat{Q}|0\rangle = 0$. The spin operators in the original Hamiltonian (1) can be expressed in terms of the phase fields as

$$S_j^z = \frac{1}{2\pi R} \frac{d\phi(x)}{dx} + a(-1)^j \sin \frac{\phi(x)}{R}, \quad (7a)$$

$$S_j^- = e^{-2\pi i R \tilde{\phi}(x)} \left[b \sin \frac{\phi(x)}{R} + c(-1)^j \right], \quad (7b)$$

where a , b , and c are real constants. It follows that

$$S_j^x = c(-1)^j \cos[2\pi R \tilde{\phi}(x)] - ib \sin[2\pi R \tilde{\phi}(x)] \sin \frac{\phi(x)}{R}. \quad (7c)$$

Note that the second term in Eq. (7c) is Hermitian because $[\phi(x), \tilde{\phi}(x)] = -i/2$. These formulas are slightly modified from those in Refs. 18–20 for reasons which will become clear below. It is then straightforward to evaluate the correlation functions for the ground state $|0\rangle$, yielding

$$\begin{aligned} \langle S_j^x S_k^x \rangle &= \frac{f_{\eta/2}(2j) f_{\eta/2}(2k)}{f_{\eta}(j-k) f_{\eta}(j+k)} \left\{ (-1)^{j-k} \frac{c^2}{2} \right. \\ &\quad - \frac{b^2}{4 f_{1/2\eta}(2j) f_{1/2\eta}(2k)} \left[\frac{f_{1/\eta}(j+k)}{f_{1/\eta}(j-k)} + \frac{f_{1/\eta}(j-k)}{f_{1/\eta}(j+k)} \right] \\ &\quad \left. - \frac{bc}{2} \text{sgn}(j-k) \left[\frac{(-1)^j}{f_{1/2\eta}(2k)} - \frac{(-1)^k}{f_{1/2\eta}(2j)} \right] \right\}, \quad (8a) \end{aligned}$$

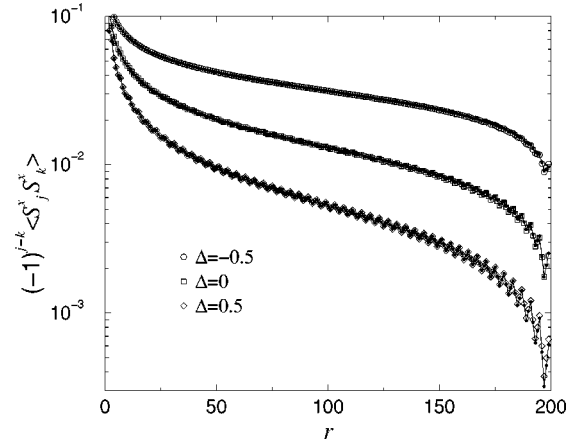


FIG. 1. $(-1)^{j-k} \langle S_j^x S_k^x \rangle$ versus $r = |j-k|$ for $\Delta = -0.5, 0$, and 0.5 (from above). The open symbols are the DMRG data and the small dots connected by lines are the fits, Eq. (8a).

$$\begin{aligned} \langle S_j^z S_k^z \rangle &= \frac{(-1)^{j-k} a^2}{2 f_{1/2\eta}(2j) f_{1/2\eta}(2k)} \left[\frac{f_{1/\eta}(j+k)}{f_{1/\eta}(j-k)} - \frac{f_{1/\eta}(j-k)}{f_{1/\eta}(j+k)} \right] \\ &\quad - \frac{1}{4\pi^2 \eta} \left(\frac{1}{f_2(j-k)} + \frac{1}{f_2(j+k)} \right) \\ &\quad - \frac{a}{2\pi \eta} \left\{ \frac{(-1)^j}{f_{1/2\eta}(2j)} [g(j-k) + g(j+k)] \right. \\ &\quad \left. - \frac{(-1)^k}{f_{1/2\eta}(2k)} [g(j-k) - g(j+k)] \right\} \quad (8b) \end{aligned}$$

with

$$f_a(x) = \left[\frac{2(L+1)}{\pi} \sin \left(\frac{\pi|x|}{2(L+1)} \right) \right]^\alpha, \quad (9a)$$

$$g(x) = \frac{\pi}{2(L+1)} \cot \left(\frac{\pi x}{2(L+1)} \right). \quad (9b)$$

In deriving Eqs. (8a) and (8b) we used the following regularization: $\sum_{n=1}^{\infty} [1 - \cos(q_n x)] / n = \ln[f_1(x)]$. Note that Eqs. (8a) and (8b) reduce to Eqs. (2a) and (2b) with $A_z = a^2/2$, $A_x = c^2/2$, and $\tilde{A}_x = b^2/4$ in the limit $L \rightarrow \infty$ with $|j-L/2| \ll L$ and $|k-L/2| \ll L$. It is also important to observe that Eqs. (8a) and (8b) have exactly the same j and k dependence at the Heisenberg point ($\eta=1$) in accordance with the SU(2) spin symmetry. In fact, under the given boundary conditions, it is essential to use the boson representation (7a) and (7c) to have this SU(2) property. Equation (8b) has another nice feature that, when $\eta=1/2$ and $a=1/\pi$, it coincides with the exact correlation function $\langle S_j^z S_k^z \rangle$ of the XY model. We use Eqs. (8a) and (8b) to analyze the numerical data.

We calculated the spin-spin correlation functions $\langle S_j^\alpha S_k^\alpha \rangle$ ($\alpha=x, z$) for the ground state of $L=200$ spin chains using the DMRG method with the improved algorithm.^{13,14} We employed the finite system method, and the maximum number of kept states m is 80. From the difference between the data at $m=80$ and $m=60$, we estimate the numerical error due to the truncation of the Hilbert space to be of order 10^{-5} for $\langle S_j^x S_k^x \rangle$ and 10^{-6} for $\langle S_j^z S_k^z \rangle$. Figures 1 and 2 show some of our numerical data of the correlations between S_j^α and S_k^α ,

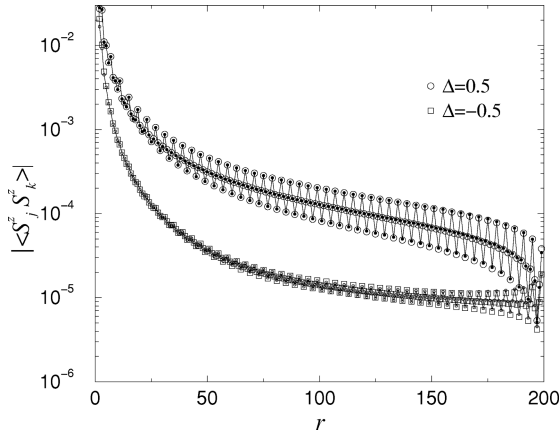


FIG. 2. $|\langle S_j^z S_k^z \rangle|$ versus $r = |j - k|$ for $\Delta = 0.5$ (above) and -0.5 . The open symbols are the DMRG data and the small dots connected by lines are the fits, Eq. (8b).

where $j = (L - r + 1)/2$ and $k = (L + r + 1)/2$ for odd r and $j = (L - r)/2$ and $k = (L + r)/2$ for even r . The DMRG results are shown by open symbols, whose size is, however, made larger than the numerical error for illustration. Taking a , b , and c as free parameters and using the exact exponent Eq. (3), we fit the data²¹ using Eq. (8a) and (8b). The small dots connected by lines in Figs. 1 and 2 are the results of the fitting. From the relation $A_x = c^2/2$, $\tilde{A}_x = b^2/4$, and $A_z = a^2/2$, we obtain the correlation amplitudes, and the results are summarized in Table I. The excellent agreement between the LZ's conjecture A_z^{LZ} and the value obtained from the fitting clearly demonstrates that Eq. (4) is indeed exact, and that there is little finite-size correction left in a , b , and c because Eqs. (8a) and (8b) correctly account for most of the finite-size effect. We also note that the numerical estimate of

TABLE I. Correlation amplitudes estimated from the fitting of the numerical data. A_x^{LZ} is the conjectured amplitude, Eq. (4). The figures in parentheses indicate the error bar on the last quoted digits.

Δ	A_x^{LZ}	A_x	\tilde{A}_x	A_z
-0.9	0.15567	0.15560(3)	***	***
-0.8	0.15904	0.1589(1)	***	***
-0.7	0.15968	0.1595(1)	***	0.008(1)
-0.6	0.15912	0.1589(2)	0.0048(14)	0.0133(1)
-0.5	0.15786	0.1576(2)	0.0076(9)	0.0184(4)
-0.4	0.15617	0.1558(2)	0.0099(7)	0.0235(2)
-0.3	0.15417	0.1538(3)	0.0122(4)	0.02921(3)
-0.2	0.15196	0.1515(3)	0.0144(2)	0.03556(3)
-0.1	0.14958	0.1491(3)	0.0164(2)	0.0425(2)
0.0	0.14709	0.1466(4)	0.0182(2)	0.0501(5)
0.1	0.14451	0.1440(4)	0.01995(7)	0.0588(3)
0.2	0.14187	0.1414(3)	0.02154(5)	0.0683(6)
0.3	0.13921	0.1388(3)	0.02296(4)	0.0791(8)
0.4	0.13656	0.1362(3)	0.02420(4)	0.0918(9)
0.5	0.13400	0.1339(1)	0.02525(6)	0.1063(9)
0.6	0.13164	0.1320(1)	0.0261(2)	0.1236(5)
0.7	0.12973	0.1308(5)	0.0267(3)	0.145(1)
0.8	0.12896	0.132(1)	0.0271(7)	0.171(5)
0.9	0.13214	0.138(3)	0.027(2)	0.20(1)

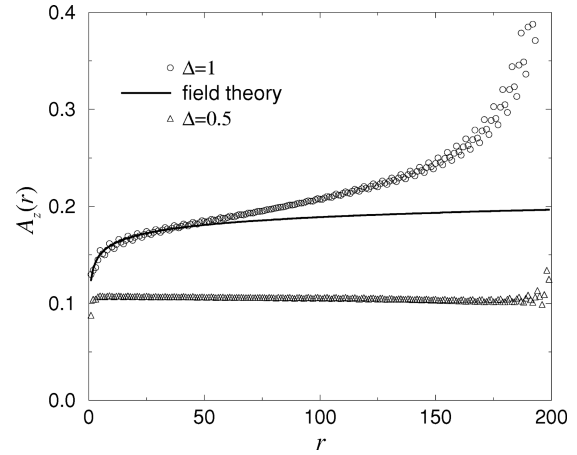


FIG. 3. Effective correlation amplitude $A_z(r)$ as a function of r for $\Delta = 1$ and 0.5 . The solid line represents the $\sqrt{\ln r}$ correction [Eq. (10)] predicted from a field-theory calculation. $A_z(r)$ is almost constant (~ 0.1) at $\Delta = 0.5$.

A_z at $\Delta = 0$ agrees with the exact value, $1/2\pi^2$. For $\Delta \leq -0.7$, it is difficult to estimate \tilde{A}_x and A_z because the exponent $1/\eta$ for these terms becomes so large that they give only a negligible contribution to the correlation functions. As seen in Figs. 1 and 2, for $-1 < \Delta \leq 0.6$ Eqs. (8a) and (8b) can fit the numerical data extremely well including the oscillations of period 4, which are characteristic of open chains.

As Δ becomes closer to 1, however, the quality of the fitting becomes poor. This is due to the irrelevant operator $\cos(2\phi/R)$ ignored in Eq. (5). Roughly speaking, this operator gives rise to corrections of order $r^{-4(1/\eta-1)}$ to the amplitudes, and at $\Delta = 1$ this turns into the logarithmic correction.^{7,8} Since this type of correction is not taken into account in Eqs. (8a) and (8b), they cannot describe the correlation functions completely for the parameter regime where the effect of the leading irrelevant operator becomes important. To elucidate this, we plot in Fig. 3 the effective amplitude $A_z(r)$ given by $A_z(r) = a^2(r)/2$, where $a(r)$ is obtained by solving Eq. (8b) for each $r = |j - k|$. We see that $A_z(r)$ is constant for $\Delta = 0.5$, which is another indication that the fitting works well. At $\Delta = 1$, on the other hand, $A_z(r)$ is roughly an increasing function of r . This result is compared with the recent analytical result valid in the limit $L \rightarrow \infty$,⁸

$$A_z(r) = \frac{1}{\sqrt{8\pi^3}g} \left(1 - \frac{3}{16}g^2 + \frac{156\zeta(3) - 73}{384}g^3 \right), \quad (10)$$

where g is determined from

$$\frac{1}{g} + \frac{1}{2} \ln g = \ln(2\sqrt{2\pi} e^{\gamma+1} r) \quad (11)$$

with $\gamma = 0.5772 \dots$. Equation (10) is shown as a solid line in Fig. 3, which goes on top of the numerical data for $r \leq 50$. Thus, our numerical result is consistent with the recent analytic calculation,^{7,8} $\langle S_j^\alpha S_k^\alpha \rangle = [\ln(2\sqrt{2\pi} e^{\gamma+1} r)/8\pi^3]^{1/2}/r$ for $r \gg 1$. The discrepancy at larger r in Fig. 3 would be due to the finite-size effect or the boundary effect. The numerical estimates of the amplitudes for $\Delta = 0.8$ and 0.9 also suffer from the correction coming from the irrelevant operator and have larger error bars than for $\Delta \leq 0.6$.

In summary, we have demonstrated that the spin-correlation functions of open XXZ chains in the critical regime can be fitted very well with the correlation functions calculated from the effective low-energy theory (free bosons), if the effect of the irrelevant operator is not severe. From the fitting, we obtained the correlation amplitudes for broad ranges of the parameter Δ with high precision and numerically verified the Lukyanov and Zamolodchikovs con-

jecture. We hope that our numerical estimates for A_z and \tilde{A}_x will be confirmed in turn by analytic calculations in the future.

The numerical computation was carried out at the Yukawa Institute Computer Facility, Kyoto University. A.F. was supported by a Monbusho Grant for overseas research.

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