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String correlation functions of the spin-1/2 Heisenberg *XXZ* chain

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Abstract

We calculate certain string correlation functions, originally introduced as order parameters in integer spin chains, for the spin-1/2 *XXZ* Heisenberg chain at zero temperature and in the thermodynamic limit. For small distances, we obtain exact results from Bethe Ansatz and exact diagonalization, whereas in the large-distance limit, field-theoretical arguments yield an asymptotic algebraic decay. We also make contact with two-point spin-correlation functions in the asymptotic limit.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Haldane's work [1, 2] on the different ground-state properties of integer-S and half-integer-S spin chains triggered efforts to seek for a quantitative understanding of the gapped ground state of integer-S chains. Among these are the works of den Nijs and Rommelse [3] as well as Oshikawa [4], where the following generalized string correlation function was considered:

$$\mathcal{O}(n,\theta) \equiv -4\left\langle S_1^z \exp\left[\mathrm{i}\theta\sum_{k=2}^{n-1} S_k^z\right] S_n^z\right\rangle. \tag{1.1}$$

The authors of [3] introduced $\lim_{n\to\infty}\mathcal{O}(n,\pi)$ as an order parameter that characterizes the gapped ground state of the $S = 1$ Heisenberg chain and acquires a nonzero value there. Kennedy and Tasaki [5] introduced a transformation showing that this is due to a broken hidden $Z_2 \times Z_2$ symmetry of the model. In [4], an attempt was made to generalize this argument to integer $S > 1$ chains. In the same reference, the den Nijs–Rommelse order parameter was considered for $\theta \neq \pi$. Several subsequent works considered the generalized string correlation functions (1.1) for integer spin $S > 1$ and generic θ, where $\lim_{n\to\infty} \mathcal{O}(n, \theta)$ acquires nonzero values. The exact calculation of the valence bond solid (VBS) state shows that the correlation takes its maximum values near $\theta = \pi/S$ [4, 6].

Whereas in these works, the focus was mainly on integer spin chains motivated by Haldane's conjecture, interest at the same time rose for $\mathcal{O}(n, \pi)$ in half-integer spin chains. Hida [7] studied $\mathcal{O}(n, \pi)$ for alternating $S = 1/2$ systems, as this model describes a crossover between the gapped $S = 1$ phase and the isotropic $S = 1/2$ Heisenberg chain. In that paper, he reported the asymptotic form of $\mathcal{O}(n, \pi) \sim \text{const}\, n^{-1/4}$ close to the uniform, isotropic $S = 1/2$ chain by means of a field-theoretical approach (the constant was not known there). This means that the string correlation function for the $S = 1/2$ Heisenberg chain $\mathcal{O}(n, \pi)$ decays in an algebraic way much slower than the usual spin–spin correlation function. Hida also considered the generalization of $\mathcal{O}(n, \theta)$ to more general values of θ for an alternating chain, but did not discuss its algebraic decay in this case [8].

Recently, a related string correlation function

$$\rho(n, \theta) \equiv \left\langle \exp\left[\mathrm{i}\theta \sum_{k=1}^{n} S_k^z \right] \right\rangle \tag{1.2}$$

was introduced by Lou *et al* [9]. They came to the conclusion that asymptotically, for spin $S = 3/2$, $\mathcal{O}(n, \theta)|_{S=3/2} \sim -\sin^2(\theta/2)\rho(n, \theta)|_{S=1/2}$. This means that the scaling behaviour of $\rho(n, \theta)|_{S=1/2}$ is also important for $S = 3/2$, which is supported by the fact that the $S = 3/2$ and $S = 1/2$ chains are considered to belong to the same universality class [10, 11]. Using a field-theoretical approach, the authors of [9] found $\rho(n, \theta)|_{S=1/2} \sim \text{const}\, n^{-\theta^2/(4\pi^2)}$ with an unspecified constant, again for the isotropic $S = 1/2$ chain. As far as two-point correlation functions of the $S = 1/2$ chains are concerned, enormous progress has been made in the last decade to obtain exact expressions from Bethe Ansatz [12–14] for short distances [15–29] and from field-theory for both the amplitudes and the exponents of the leading terms in the asymptotic limit [30–33]. These results are not restricted to the isotropic point, but cover the critical anisotropic regime as well,

$$H = J \sum_{l=1}^{N} \left(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z \right), \tag{1.3}$$

with periodic boundary conditions and $J > 0$. In the following, we use the anisotropy parameter γ to parameterize the anisotropy $\Delta =: \cos\gamma$, with $0 < \gamma < \pi$, such that the isotropic points $\gamma = 0, \pi$ are excluded.

Given those technical tools from Bethe Ansatz and field theory, in this work we calculate $\rho(n, \theta)$ and $\mathcal{O}(n, \theta)$, both for short distances and in the asymptotic limit. We thus obtain the exponents and the amplitudes of the leading uniform and alternating parts and verify them by the Bethe Ansatz results. Interestingly, the leading asymptotics of the alternating part can be directly obtained from those of the uniform part. We furthermore study the limiting values $\theta \to 0, 1 - \gamma/\pi$ in the asymptotic limit, where contact is made with $\langle S_1^z S_n^z \rangle$ and $\langle S_1^x S_n^x \rangle$.

This paper is organized as follows. In the following section, we present the Bethe Ansatz calculation of $\rho(n, \theta)$ and $\mathcal{O}(n, \theta)$, as well as results from exact diagonalization that we obtained additionally. The third part contains the field-theoretical approach. Numerical comparisons between the Bethe Ansatz and field-theoretical results are included in an appendix. Calculations not immediately necessary for the understanding of the main text are deferred to further appendices.

2. Exact short distance string correlation functions

The Hamiltonian (1.3) has been solved exactly by the Bethe Ansatz [12–14]. In fact the eigenfunctions can be constructed in a form of superposition of plane waves, which are called the Bethe Ansatz wavefunctions. The corresponding eigenenergies are obtained by solving the Bethe Ansatz equations

$$e^{ik_jN} = (-1)^{M-1}\prod_{l\neq j}\frac{e^{i(k_j+k_l)}+1-2\Delta\, e^{ik_j}}{e^{i(k_j+k_l)}+1-2\Delta\, e^{ik_l}}, \qquad (j=1,\ldots,M), \tag{2.1}$$

where M is the number of the down spins. With a solution of the Bethe Ansatz equations (2.1), the corresponding eigenenergy is expressed as

$$E = \frac{JN\Delta}{4} + J\sum_{j=1}^{M}(\cos k_j - \Delta). \tag{2.2}$$

Especially the ground state is given by a solution in the sector $M = N/2$. In the critical region $-1 < \Delta = \cos\gamma < 1$, its value per site in the thermodynamic limit $N \to \infty$ becomes

$$e_0 = \frac{J\Delta}{4} - \frac{J\sin^2\gamma}{4}\int_{-\infty}^{\infty}\frac{dx}{(\cosh\gamma x - \cos\gamma)\cosh\pi x/2}. \tag{2.3}$$

Enormous works have been contributed to evaluate the physical quantities of the model based on the Bethe Ansatz equations (2.1) [14]. They, however, are usually limited to the bulk quantities. Especially, the exact calculation of correlation functions still is a difficult problem. Only for $\Delta = 0$, where the system reduces to a lattice free-fermion model after a Jordan–Wigner transformation, arbitrary correlation functions can be calculated by means of Wick's theorem [36, 37]. Especially, the two-point spin–spin correlation function is simply given by $\langle S_j^z S_{j+k}^z\rangle = -(1-(-1)^k)/(2\pi^2k^2)$.

There have been many attempts to evaluate the correlation functions for general Δ. However, explicit exact evaluations of the correlation functions have become attainable only recently. For example, the following exact values for the spin–spin correlation functions $\langle S_j^z S_{j+k}^z\rangle$ were obtained up to $k = 7$ for $\Delta = 1$ [25] and up to $k = 8$ for $\Delta = 1/2$ [38]:

- $\Delta = 1$

$$\begin{aligned}
\langle S_j^z S_{j+1}^z\rangle &= \frac{1}{12} - \frac{1}{3}\ln 2 = -0.147\,715\,726\,853\,315\ldots,\\
\langle S_j^z S_{j+2}^z\rangle &= \frac{1}{12} - \frac{4}{3}\ln 2 + \frac{3}{4}\zeta(3) = 0.060\,679\,769\,956\,435\ldots,\\
\langle S_j^z S_{j+3}^z\rangle &= \frac{1}{12} - 3\ln 2 + \frac{37}{6}\zeta(3) - \frac{14}{3}\ln 2\cdot\zeta(3) - \frac{3}{2}\zeta(3)^2 - \frac{125}{24}\zeta(5) + \frac{25}{3}\ln 2\cdot\zeta(5)\\
&= -0.050\,248\,627\,257\,2352\ldots,\\
\langle S_j^z S_{j+4}^z\rangle &= \frac{1}{12} - \frac{16}{3}\ln 2 + \frac{145}{6}\zeta(3) - 54\ln 2\cdot\zeta(3) - \frac{293}{4}\zeta(3)^2\\
&\quad - \frac{875}{12}\zeta(5) + \frac{1450}{3}\ln 2\cdot\zeta(5) - \frac{275}{16}\zeta(3)\cdot\zeta(5) - \frac{1875}{16}\zeta(5)^2\\
&\quad + \frac{3185}{64}\zeta(7) - \frac{1715}{4}\ln 2\cdot\zeta(7) + \frac{6615}{32}\zeta(3)\cdot\zeta(7)\\
&= 0.034\,652\,776\,982\,7281\ldots,\\
\langle S_j^z S_{j+5}^z\rangle &= -0.030\,890\,366\,647\,6093\ldots,\\
\langle S_j^z S_{j+6}^z\rangle &= 0.024\,446\,738\,327\,9589\ldots,\\
\langle S_j^z S_{j+7}^z\rangle &= -0.022\,498\,222\,763\,3722\ldots.
\end{aligned} \tag{2.4}$$

- $\Delta = 1/2$

$$
\begin{aligned}
\langle S^z_j S^z_{j+1}\rangle &= -\frac{1}{8} = -0.125,\\
\langle S^z_j S^z_{j+2}\rangle &= \frac{7}{256} = 0.027\,343\,75,\\
\langle S^z_j S^z_{j+3}\rangle &= -\frac{401}{16\,384} = -0.024\,475\,097\,656\,25,\\
\langle S^z_j S^z_{j+4}\rangle &= \frac{184\,453}{16\,777\,216} = 0.010\,994\,255\,542\,7551\ldots,\\
\langle S^z_j S^z_{j+5}\rangle &= -\frac{952\,149\,49}{858\,993\,459\,2} = -0.011\,084\,478\,930\,5701\ldots,\\
\langle S^z_j S^z_{j+6}\rangle &= \frac{1758\,750\,082\,939}{281\,474\,976\,710\,656} = 0.006\,248\,335\,477\,248\,9\ldots,\\
\langle S^z_j S^z_{j+7}\rangle &= -\frac{302\,836\,107\,396\,770\,93}{461\,168\,601\,842\,738\,7904} = -0.006\,566\,711\,310\,9326\ldots,\\
\langle S^z_j S^z_{j+8}\rangle &= \frac{502\,021\,884\,974\,051\,534\,3761}{120\,892\,581\,961\,462\,917\,470\,6176} = 0.004\,152\,627\,703\,2786\ldots.
\end{aligned}
\tag{2.5}
$$

Here $\zeta(2k+1)$ is the Riemann zeta function at odd arguments. Note that the nearest-neighbour correlation function $\langle S^z_j S^z_{j+1}\rangle$ can be derived immediately from the ground-state energy (2.3). So these values have been known long before. We also remark $\langle S^z_j S^z_{j+2}\rangle$ for $\Delta = 1$ was obtained some decades ago by Takahashi [39] by his ingenious study of the half-filled Hubbard chain in the strong coupling limit. Other results are due to recent developments of the study of the correlation functions. Note that even for general Δ, the exact analytic expressions have been obtained up to $k = 3$ [22]. Such progress has enabled comparison with the field-theoretical prediction of the asymptotic behaviour as well as other numerical methods such as numerical diagonalization.

It is interesting to note that the calculation of the spin–spin correlation functions (2.4) and (2.5) rely on the generating function, defined by

$$
P^\kappa_n \equiv \left\langle \prod_{j=1}^{n} \left\{ \left(\frac{1}{2} + S^z_j\right) + \kappa \left(\frac{1}{2} - S^z_j\right) \right\} \right\rangle. \tag{2.6}
$$

Here κ is a parameter. Once the generating function (2.6) is calculated, the two-point spin–spin correlation function can be obtained by the formula

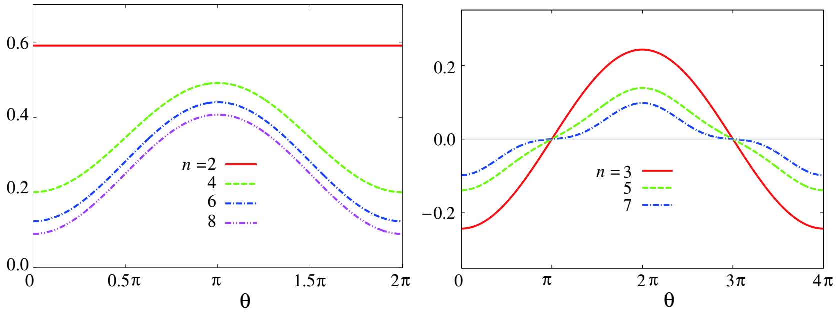
$$
\langle S^z_1 S^z_n\rangle = \frac{1}{2}\frac{\partial^2}{\partial\kappa^2}\left\{P^\kappa_n - 2P^\kappa_{n-1} + P^\kappa_{n-2}\right\}\Big|_{\kappa=1} - \frac{1}{4}. \tag{2.7}
$$

The generating function (2.6) together with its relation to the two-point spin–spin correlation function (2.7) was introduced by Izergin and Korepin [40, 41] (see also the book [13]). Subsequently it was utilized to discuss a certain long-distance asymptotic behaviour [42, 43] as well as to obtain several different forms of multiple integral formulae [18, 19]. However, it was only quite recently that the generating function P^κ_n was *explicitly* calculated for $\Delta \neq 0$, namely, up to $n = 8$ for $\Delta = 1$ [25] and up to $n = 9$ for $\Delta = 1/2$ [38].

Now one will readily find P^κ_n, equation (2.6) and the string correlation function $\rho(n,\theta)$, equation (1.2) are connected as

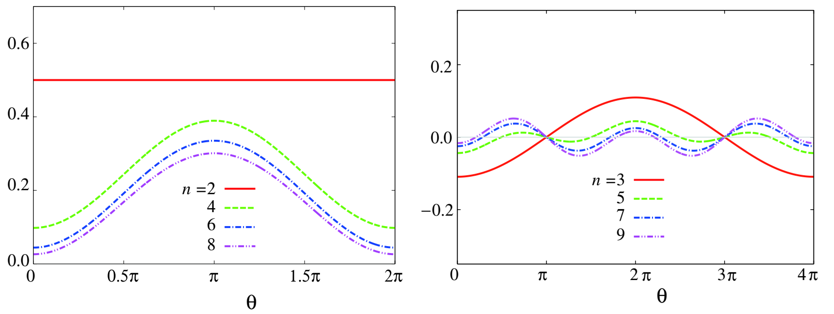
$$
\rho(n,\theta) = \kappa^{-\frac{n}{2}} P^\kappa_n \Big|_{\kappa = \mathrm{e}^{-\mathrm{i}\theta}}. \tag{2.8}
$$

Then we can calculate some exact values of $\rho(n,\theta)$ for $\Delta = 1$ and $\Delta = 1/2$. Moreover, since



(a) $n =$ even (b) $n=$ odd

Figure 1. $\mathcal{O}(n, \theta)$ for $\Delta = 1$.



(a) $n =$ even (b) $n =$ odd

Figure 2. $\mathcal{O}(n, \theta)$ for $\Delta = 1/2$.

the generalized string correlation function $\mathcal{O}(n, \theta)$ (1.1) is related to $\rho(n, \theta)$ as

$$\mathcal{O}(n, \theta) = \frac{1}{\sin^2 \frac{\theta}{2}} \left[\rho(n, \theta) - 2 \left(\cos \frac{\theta}{2} \right) \rho(n-1, \theta) + \left(\cos^2 \frac{\theta}{2} \right) \rho(n-2, \theta) \right], \tag{2.9}$$

we can also evaluate the generalized string correlation functions for $\Delta = 1$ and $\Delta = 1/2$ (cf appendix A). They are plotted in figures 1 and 2. From the figures one observes the following.

- For even n $(\geqslant 4)$, $\mathcal{O}(n, \theta)$ is always positive with a period 2π. It has a single maximum at $\theta = \pi$ and a minimum at $\theta = 0$. Recall that $\mathcal{O}(n, \pi) = (2\mathrm{i})^n \langle \prod_{k=1}^n S_k^z \rangle$ and $\mathcal{O}(n, 0) = -4 \langle S_1^z S_n^z \rangle$.
- For odd n, $\mathcal{O}(n, \theta)$ has a rather complicated structure with a period 4π. In this case, $\mathcal{O}(n, \pi)$ and $\mathcal{O}(n, 3\pi)$ are always zero as they should be.

We give some exact values of $\mathcal{O}(n, \pi) = (2\mathrm{i})^n \langle \prod_{k=1}^n S_k^z \rangle$ for $\Delta = 1$ and $\Delta = 1/2$ in the following:

- $\Delta = 1$

$$\mathcal{O}(2, \pi) = -\frac{1}{3} + \frac{4}{3} \ln 2 = 0.590\,862\,907\,413\,2604 \ldots$$

$$\mathcal{O}(4, \pi) = \frac{1}{5} - \frac{16}{3} \ln 2 + \frac{232}{15} \zeta(3) - \frac{32}{3} \ln 2 \cdot \zeta(3) - \frac{21}{5} \zeta(3)^2 - \frac{95}{6} \zeta(5) + \frac{70}{3} \ln 2 \cdot \zeta(5) = 0.491\,445\,392\,361\,5522 \ldots$$

$$\mathcal{O}(6,\pi) = 0.440\,301\,669\,702\,6268\ldots$$
$$\mathcal{O}(8,\pi) = 0.407\,242\,414\,759\,6208\ldots \tag{2.10}$$

- $\Delta = 1/2$

$$\begin{aligned}
\mathcal{O}(2,\pi) &= \frac{1}{2}\\
\mathcal{O}(4,\pi) &= \frac{1595}{4096} = 0.389\,404\,296\,875\\
\mathcal{O}(6,\pi) &= \frac{719\,423\,395}{2147\,483\,648} = 0.335\,007\,624\,235\,0041\ldots\\
\mathcal{O}(8,\pi) &= \frac{346\,891\,287\,109\,196\,331}{1152\,921\,504\,606\,846\,976} = 0.300\,880\,229\,680\,0668\ldots.
\end{aligned} \tag{2.11}$$

One observes that $\mathcal{O}(n,\pi)$ for $n =$ even decays very slowly as n increases. Namely as mentioned in the introduction, for $\Delta = 1$, the asymptotic decay $\mathcal{O}(n,\pi) \sim n^{-1/4}$ was given by Hida [7] and more generally

$$\mathcal{O}(n,\theta) \sim n^{-\frac{\theta^2}{4\pi^2}} \tag{2.12}$$

by Lou [9]. In the next section, we shall both generalize this asymptotic formula to the more general $-1 < \Delta < 1$ case and determine the amplitude by making use of field theory. Furthermore since the formula (2.12) does not explain the difference of the periodicity with respect to the parity of n, we shall consider some subleading terms more carefully. We remark that $\rho(n,\theta)$, equation (1.2), shares periodicity properties analogous to $\mathcal{O}(n,\theta)$. In fact it is easy to see that $\rho(n,\theta)$ is expanded as

$$\rho(n,\theta) = \sum_{j=1}^{n} P_{n,j} \cos\left[\left(\frac{n}{2} - j\right)\right]\theta, \tag{2.13}$$

where the coefficients $P_{n,j}$ are the summation of the diagonal density matrix elements in the sector with j down spins. Note that $P_{n,j} = P_{n,n-j}$. From equation (2.13), one can immediately find

$$\rho(n,\theta + 2\pi) = (-1)^n \rho(n,\theta). \tag{2.14}$$

Let us now make some comments on the string correlation functions for $\Delta = 0$. In this case, a simple determinant formula for $\rho(n,\theta)$ exists (cf [44]). Namely let us define an n-by-n matrix A, whose components are given by

$$\begin{aligned}
A_{j,k} &= \left(\cos\frac{\theta}{2}\right)\delta_{j,k} + \left(\mathrm{i}\sin\frac{\theta}{2}\right)M_{j,k}, \qquad (1 \leqslant j,k \leqslant n)\\
M_{j,k} &\equiv \begin{cases} 0 & : \text{if } j-k = \text{even}\\ \dfrac{2}{\pi}\dfrac{(-1)^{\frac{j-k+1}{2}}}{j-k} & : \text{if } j-k = \text{odd}. \end{cases}
\end{aligned} \tag{2.15}$$

Then $\rho(n,\theta)$ is represented simply as

$$\rho(n,\theta) = \det A. \tag{2.16}$$

Using this formula one can evaluate the exact numerical values up to the order of $n \simeq 10\,000$ easily, for example, by *Mathematica* on a standard PC. We give the exact values in table 1 up to $n = 1000$. This determinant is also expressed as a Toeplitz determinant

$$\rho(n,\theta) = \mathrm{e}^{\mathrm{i}n\theta/2} \det \tilde{A}, \tag{2.17}$$

Table 1. Exact values of $\rho(n,\theta)$ for $\Delta = 0$.

n	5	10	20	50	100	200	500	1000
$\rho(n,\pi/4)$	0.884 857	0.866 761	0.848 076	0.824 090	0.806 421	0.789 137	0.766 860	0.750 428
$\rho(n,\pi/2)$	0.605 461	0.564 975	0.516 684	0.459 997	0.421 580	0.386 481	0.344 597	0.315 979
$\rho(n,3\pi/4)$	0.289 075	0.291 125	0.234 367	0.177 503	0.144 555	0.118 072	0.090 6455	0.074 3400

Table 2. Numerical values obtained from the asymptotic formula $\rho_{\mathrm{Asym}}(n,\theta)$ for $\Delta = 0$.

n	5	10	20	50	100	200	500	1000
$\rho_{\mathrm{Asym}}(n,\pi/4)$	0.884 970	0.866 783	0.848 081	0.824 091	0.806 421	0.789 137	0.766 860	0.750 428
$\rho_{\mathrm{Asym}}(n,\pi/2)$	0.605 720	0.565 076	0.516 705	0.460 000	0.421 581	0.386 481	0.344 597	0.315 979
$\rho_{\mathrm{Asym}}(n,3\pi/4)$	0.289 328	0.291 316	0.234 403	0.177 507	0.144 555	0.118 072	0.090 6455	0.074 3400

where the components of the n-by-n Toeplitz matrix $\tilde{A}$ are given by

$$\tilde{A}_{j,k} = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{\mathrm{i}(j-k)q}\sigma(q)\,\mathrm{d}q, \qquad \sigma(q) \equiv \begin{cases} \mathrm{e}^{-\mathrm{i}\theta} : 0 < q < \frac{\pi}{2} \\ 1 \quad\;\; : \frac{\pi}{2} < q < \frac{3\pi}{2} \\ \mathrm{e}^{-\mathrm{i}\theta} : \frac{3\pi}{2} < q < 2\pi. \end{cases} \tag{2.18}$$

There are some mathematical results known on the asymptotic behaviours of Toeplitz determinants as $n \to \infty$. Assume $\theta \neq 0, 2\pi$, then 'the generating function' $\sigma(q)$ of the Toeplitz determinant has jump singularities at $q = \pi/2$ and $q = 3\pi/2$. In such a case, we can invoke the (generalized) Fisher–Hartwig conjecture [45, 46], which brings about an asymptotic formula for $0 < \theta < 2\pi$ as

$$\begin{aligned} &\rho(n,\theta) \simeq \rho^{(0)}_{\mathrm{Asym}}(n,\theta) + (-1)^n \rho^{(1)}_{\mathrm{Asym}}(n,\theta), \\ &\rho^{(k)}_{\mathrm{Asym}}(n,\theta) = n^{-2(-\frac{\theta}{2\pi}+k)^2} 4^{-(-\frac{\theta}{2\pi}+k)^2} \left[G\left(1+\frac{\theta}{2\pi}-k\right) G\left(1-\frac{\theta}{2\pi}+k\right)\right]^2. \end{aligned} \tag{2.19}$$

Here $G(z)$ is the Barnes G-function defined by

$$G(z+1) = (2\pi)^{\frac{1}{2}z} \exp\left(-\frac{1}{2}z - \frac{1}{2}(\gamma+1)z^2\right) \prod_{k=1}^{\infty} \left\{ \left(1+\frac{z}{k}\right)^k \exp\left(-z+\frac{z^2}{2k}\right)\right\}$$

where $\gamma = 0.577\,215\,6649\ldots$ is the Euler–Mascheroni constant. Each term $\rho^{(k)}_{\mathrm{Asym}}(n,\theta)$ decays algebraically with the exponent $-2\left(-\frac{\theta}{2\pi}+k\right)^2$. Then the dominant term is $\rho^{(0)}_{\mathrm{Asym}}(n,\theta)$ for $0 < \theta < \pi$, and is $(-1)^n \rho^{(1)}_{\mathrm{Asym}}(n,\theta)$ for $\pi < \theta < 2\pi$. We refer the reader also to [47, 48] for more information about the (generalized) Fisher–Hartwig conjectures.

Numerical values calculated from equation (2.19) are listed in table 2. Good agreement is found with the data in table 1. In this context, it is remarkable that they coincide within at least three digits even for small distance as $n = 10$. Finally let us note a further exact result for $\rho(n,\pi)$ at $\Delta = 0$. Since $\rho(2m-1,\pi) = 0$, we consider $\rho(2m,\pi)$, which is given more explicitly as

$$\begin{aligned} \rho(2m,\pi) &= (-1)^m 2^{2m} \left\langle \prod_{j=1}^{2m} S^z_j \right\rangle = (-1)^m \det[M_{j,k}]^{2m}_{j,k=1} \\ &= \left(\frac{2}{\pi}\right)^{2m} \prod_{k=1}^{m}\prod_{j\neq k}^{m} \left(\frac{j-k}{j-k-1/2}\right)^2 = \prod_{k=1}^{m} \frac{\Gamma^4(k)}{\Gamma^2\left(k-\frac{1}{2}\right)\Gamma^2\left(k+\frac{1}{2}\right)} \end{aligned}$$

$$= \exp\left[-\frac{1}{2}\int_0^\infty \frac{dt}{t}\frac{1-e^{-mt}}{\cosh^2(t/4)}\right]$$
$$= c_0 m^{-1/2}\exp\left[-\frac{1}{2}\int_0^\infty \frac{dt}{t}\, e^{-t}\tanh^2\left(\frac{t}{4m}\right)\right]$$
$$= c_0 m^{-1/2}\left(1-\frac{1}{32}m^{-2}+\frac{17}{2048}m^{-4}-\frac{379}{65\,536}m^{-6}+\cdots\right), \quad (2.20)$$

where

$$c_0 = \exp\left[\frac{1}{2}\int_0^\infty \frac{dt}{t}\left(e^{-4t}-\frac{1}{\cosh^2 t}\right)\right] = \left[G\left(\frac{1}{2}\right)G\left(\frac{3}{2}\right)\right]^2.$$

Here we have used an integral formula for the logarithm of the Euler gamma function,

$$\log\Gamma(z) = \int_0^\infty \left[(z-1)-\frac{1-e^{(-z+1)t}}{1-e^{-t}}\right]\frac{e^{-t}}{t}\,dt, \qquad (\mathrm{Re}(z)>0). \quad (2.21)$$

Thus we can obtain the asymptotic expansion to an arbitrary order in this case. Note that the leading term is consistent with the formula (2.19) with $\theta = \pi$.

3. Asymptotic behaviour of string correlation functions

In this section, we will discuss the asymptotic behaviour of the string correlation functions for the critical region $-1 < \Delta < 1$ (that is $\pi > \gamma > 0$) by use of field theoretical arguments. Thus the aim is to find coefficients D_j and exponents ν_j such that

$$\lim_{n\to\infty}\frac{\rho(n,\theta)-\sum_{j=1}^{m-1}D_j(\theta,\gamma)n^{-\nu_j(\theta,\gamma)}}{n^{-\nu_m(\theta,\gamma)}} =: D_m(\theta,\gamma)\ \text{(finite)}, \qquad m = 1, 2, \ldots. \quad (3.1)$$

The exponents are increasing with j, i.e. $\nu_j < \nu_{j+1}$. The amplitudes and exponents depend on the parameters θ, γ of the model and of the function ρ. Instead of equation (3.1), we use the shorthand notation

$$\rho(n,\theta) \sim \sum_j D_j(\theta,\gamma)n^{-\nu_j(\theta,\gamma)}.$$

The important point to remember is that the asymptotic expansion is defined in the limit $n \to \infty$.

We first present the results obtained so far within the field-theoretical framework and give the details of the derivation in the following section.

3.1. Results

We find the following asymptotic expansion of the string correlation function for $0 < \theta \leqslant \pi$:

$$\begin{aligned}\rho(n,\theta) &\equiv \left\langle \exp\left[i\theta\sum_{k=1}^n S_k^z\right]\right\rangle \\ &\sim D(\theta,\gamma)n^{-\nu_1(\theta,\gamma)}(1+\mathcal{O}(n^{-\delta(\gamma)})) \\ &\quad + (-1)^n D(2\pi-\theta,\gamma)n^{-\nu_1(2\pi-\theta,\gamma)}(1+\mathcal{O}(n^{-\delta(\gamma)})) \\ &\quad + \mathcal{O}(n^{-\nu_1(\theta,\gamma)-2}, (-1)^n n^{-\nu_1(2\pi+\theta,\gamma)}, (-1)^n n^{-\nu_1(2\pi+\theta,\gamma)-2}, (-1)^n n^{-\nu_1(2\pi-\theta,\gamma)-2}),\end{aligned} \quad (3.2)$$

with the exponents of the algebraic decay

$$\nu_1(\theta,\gamma) = \frac{\theta^2}{4\pi^2}\frac{\pi}{\pi-\gamma}, \qquad \delta(\gamma) = 4\frac{\pi}{\pi-\gamma}-4.$$

We conjecture that the coefficient $D(\theta,\gamma)$ takes the following form:

$$D(\theta,\gamma) = \left[\frac{\Gamma\left(\frac{\eta}{2-2\eta}\right)}{2\sqrt{\pi}\,\Gamma\left(\frac{1}{2-2\eta}\right)}\right]^{\theta^2/(4\eta\pi^2)} \times \exp\left[-\int_0^\infty \left(\frac{\sinh^2\frac{\theta}{2\pi}t}{\sinh t\cosh(1-\eta)t\sinh\eta t} - \frac{\theta^2\,\mathrm{e}^{-2t}}{4\eta\pi^2}\right)\frac{\mathrm{d}t}{t}\right] \tag{3.3}$$

$$= \left[\frac{\Gamma\left(\frac{\pi R^2}{1-2\pi R^2}\right)}{2\sqrt{\pi}\,\Gamma\left(\frac{1}{2-4\pi R^2}\right)}\right]^{(\theta/(2\pi R))^2/(2\pi)} \times \exp\left[-\int_0^\infty \left(\frac{\sinh^2\frac{\theta}{2\pi}t}{\sinh t\cosh(1-2\pi R^2)t\sinh 2\pi R^2 t} - \left(\frac{\theta}{2\pi R}\right)^2\frac{\mathrm{e}^{-2t}}{2\pi}\right)\frac{\mathrm{d}t}{t}\right]. \tag{3.4}$$

This conjecture will be justified below. In equation (3.3), Lukyanov's notation is used with $\eta = \frac{\pi-\gamma}{\pi}$, whereas in equation (3.4), the anisotropy is written in terms of the compactification radius R with $2\pi R^2 = \eta$.

Since $\rho(n,\theta) = \rho(n,-\theta)$, the result (3.2) is readily extended to the domain $-\pi \leqslant \theta < 0$. Thus $\rho(n,\theta)$ is known in the fundamental domain $-\pi \leqslant \theta \leqslant \pi$ (note $\rho(n,\theta=0)=1$, trivially). The periodicity equation (2.14) then yields ρ for all values of θ.

We note the following limiting values of the coefficient $D(\theta,\gamma)$:

- $D(\theta = 2\pi\eta,\gamma) = 2(1-\eta)^2 A$, where A is the coefficient of the leading term in an asymptotic expansion of the uniform part of $\langle\sigma_1^x\sigma_n^x\rangle$, namely: $\langle\sigma_1^x\sigma_n^x\rangle_u \sim \frac{A}{n^\eta}$, [33]. Then, as $\nu_1\,(\theta = 2\pi\eta,\gamma) = \eta$, we have the asymptotic equality (note that $1-\eta = \gamma/\pi$) for $\pi/2 < \gamma < \pi$

$$\rho(n,\theta = 2\pi\eta) \sim 2\left(\frac{\gamma}{\pi}\right)^2 \langle\sigma_1^x\sigma_n^x\rangle_u, \qquad \pi/2 < \gamma < \pi \tag{3.5}$$

for the leading order of the uniform part (in order to facilitate comparison with Lukyanov's results, we use the Pauli-matrices $\sigma^\nu = 2S^\nu$). For $\Delta = 0$ ($\gamma = \pi/2$) the alternating part contributes in the same way, which corresponds to

$$\rho(n,\theta=\pi) \sim \{1+(-1)^n\}D(\theta=\pi,\gamma=\pi/2)n^{-1/2} \sim \frac{1+(-1)^n}{2}\langle\sigma_1^x\sigma_n^x\rangle_u. \tag{3.6}$$

This agrees with equation (2.20) (see also appendix C).

- $D(0,\gamma) = 1$, whereas

$$\lim_{\theta\to 0} D(2\pi-\theta,\gamma)\frac{16}{\theta^2} = \frac{A_z}{2} \equiv \frac{4}{\pi^2}\left[\frac{\Gamma\left(\frac{\eta}{2-2\eta}\right)}{2\sqrt{\pi}\,\Gamma\left(\frac{1}{2-2\eta}\right)}\right]^{1/\eta} \times \exp\left[\int_0^\infty \left(\frac{\sinh((2\eta-1)t)}{\sinh(\eta t)\cosh((1-\eta)t)} - \frac{2\eta-1}{\eta}\,\mathrm{e}^{-2t}\right)\frac{\mathrm{d}t}{t}\right]. \tag{3.7}$$

The last equation is proved in appendix B. Following Lukyanov's notation [33], A_z denotes the coefficient of the leading contribution in the alternating part $\langle\sigma_1^z\sigma_n^z\rangle_a$ of the σ^z–σ^z-correlation function, namely

$$\langle\sigma_1^z\sigma_n^z\rangle_a \sim \frac{(-1)^{n-1}A_z}{n^{1/\eta}}. \tag{3.8}$$

In order to obtain the asymptotics of the generalized string correlation function, we first express it in terms of $\rho(n,\theta)$ according to equation (2.9). Then, using the above results, the asymptotic behaviour of $\mathcal{O}(n,\theta)$ is obtained for $0 < \theta \leqslant \pi$:

$$\begin{aligned}\mathcal{O}(n,\theta) &\equiv -4\left\langle S_1^z \exp\left[\mathrm{i}\theta\sum_{k=2}^{n-1} S_k^z\right] S_n^z\right\rangle \\ &\sim D(\theta,\gamma)n^{-\nu_1(\theta,\gamma)}\left[\tan^2\frac{\theta}{4} - \frac{\cos\frac{\theta}{2}}{\cos^2\frac{\theta}{4}}\frac{\nu_1(\theta,\gamma)}{n}\right. \\ &\quad\left. + \frac{\cos\frac{\theta}{2}\left(2\cos\frac{\theta}{2}-1\right)}{\sin^2\frac{\theta}{2}}\frac{\nu_1(\theta,\gamma)(\nu_1(\theta,\gamma)+1)}{n^2} + \cdots\right] \\ &\quad + (-1)^n D(2\pi-\theta,\gamma)n^{-\nu_1(2\pi-\theta,\gamma)}\left[\cot^2\frac{\theta}{4} + \frac{\cos\frac{\theta}{2}}{\sin^2\frac{\theta}{4}}\frac{\nu_1(2\pi-\theta,\gamma)}{n}\right. \\ &\quad\left. + \frac{\cos\frac{\theta}{2}\left(2\cos\frac{\theta}{2}+1\right)}{\sin^2\frac{\theta}{2}}\frac{\nu_1(2\pi-\theta,\gamma)(\nu_1(2\pi-\theta,\gamma)+1)}{n^2} + \cdots\right].\end{aligned} \tag{3.9}$$

Let us consider the limit $\theta \to 0$ of the asymptotic formula (3.9). The first two terms of the uniform part in (3.9) vanish in this limit and the third term gives

$$\begin{aligned}&\lim_{\theta\to 0} D(\theta,\gamma)n^{-\nu_1(\theta,\gamma)}\left[\frac{\cos\frac{\theta}{2}\left(2\cos\frac{\theta}{2}-1\right)}{\sin^2\frac{\theta}{2}}\frac{\nu_1(\theta,\gamma)(\nu_1(\theta,\gamma)+1)}{n^2}\right] \\ &\quad = \frac{1}{\pi(\pi-\gamma)n^2} = \frac{1}{\pi^2\eta n^2}.\end{aligned} \tag{3.10}$$

Because of the relation (3.7), the leading alternating part yields

$$\lim_{\theta\to 0}(-1)^n D(2\pi-\theta,\gamma)n^{-\nu_1(2\pi-\theta,\gamma)}\cot^2\frac{\theta}{4} = \frac{(-1)^n A_z}{2n^{1/\eta}}. \tag{3.11}$$

In order to get the correct leading alternating term in the limit $\theta \to 0$, we should also consider the leading alternating part for $-\pi \leqslant \theta < 0$, which reads

$$(-1)^n D(2\pi+\theta,\gamma)n^{-\nu_1(2\pi+\theta,\gamma)}\left[\cot^2\frac{\theta}{4} + \frac{\cos\frac{\theta}{2}}{\sin^2\frac{\theta}{4}}\frac{\nu_1(2\pi+\theta,\gamma)}{n} + \cdots\right] \tag{3.12}$$

in addition to (3.9). Then we have similarly to equation (3.11)

$$\lim_{\theta\to 0}(-1)^n D(2\pi+\theta,\gamma)n^{-\nu_1(2\pi+\theta,\gamma)}\cot^2\frac{\theta}{4} = \frac{(-1)^n A_z}{2n^{1/\eta}} \tag{3.13}$$

in the limit $\theta \to 0$. Collecting the terms (3.10), (3.11) and (3.13) yields

$$\lim_{\theta\to 0}\mathcal{O}(n,\theta) \sim \frac{(-1)^n A_z}{n^{1/\eta}} + \frac{1}{\pi^2\eta n^2}. \tag{3.14}$$

Equation (3.14) coincides with the leading asymptotic behaviour of the two point correlation function $-4\left\langle S_1^z S_n^z\right\rangle = -\left\langle\sigma_1^z\sigma_n^z\right\rangle$.

3.2. Derivation

3.2.1. The string correlation function $\rho(n,\theta)$. An effective field theory describing the low-energy excitations of the *XXZ*-chain in the critical regime $0 < \gamma < \pi$ has been derived by

Lukyanov [32]. At zero magnetic field, the corresponding Hamiltonian density $\mathcal{H}$ reads

$$\mathcal{H} = \frac{v}{2}(\Pi(x)^2 + (\partial_x\varphi(x))^2) + \varepsilon^{1/(\pi R^2)-2}\lambda\cos\frac{2\varphi(x)}{R} + \varepsilon^2\left[\lambda_+ J_L^2(x)J_R^2(x) + \lambda_-\left[J_L^4(x) + J_R^4(x)\right]\right] + \cdots, \tag{3.15}$$

where the dots denote terms with scaling dimensions higher than those given explicitly. The dimensionless constants $v, \lambda, \lambda_\pm$ are known exactly from Bethe Ansatz [32]. The lattice constant ε has the dimension of a length, whereas the dimension of $\mathcal{H}$ is $1/\text{length}^2$. Above, $\mathcal{H}$ is the sum of a Gaussian model and irrelevant operators, the latter with scaling dimensions $1/(\pi R^2)$ and 4. The Hamiltonian is written in terms of the bosonic field φ and its momentum Π, where $[\varphi(x), \Pi(y)] = \mathrm{i}\delta(x-y)$. The left- and right-current operators are then defined as $J_{L,R}(x) = \frac{\mp 1}{\sqrt{4\pi}}(\Pi(x) \pm \varphi(x))$.

Within the same approach, the effective S^z-operator reads

$$S_j^z \equiv S^z(x) \sim \frac{\varepsilon}{2\pi R}\partial_x\varphi(x) + \sum_{m=0}^{\infty}(-1)^m\varepsilon^{(2m+1)^2/(4\pi R^2)}C_m\cos\left(\frac{2m+1}{R}\varphi(x)\right) + \text{descendants}, \tag{3.16}$$

where $x = \varepsilon j$. The constants C_m have been determined in [33]. We do not write down the descendant fields here explicitly, but only note that if a primary field has a scaling dimension Δ, then the descendant fields have a scaling dimension $\Delta + \ell$, where ℓ is a certain positive integer.

To arrive at an asymptotic expression for $\rho(n,\theta)$, we first apply the Euler–MacLaurin formula to the sum in the exponent:

$$\begin{aligned}\sum_{k=1}^{n} S_k^z &= \varepsilon^{-1}\int_0^x S^z(x')\,\mathrm{d}x' - \frac{1}{2}[S^z(0) - S^z(x)] + \mathcal{O}\big(\partial_x^\mu S^z\big)\\ &= \frac{1}{2\pi R}(\varphi(x) - \varphi(0)) + \mathcal{O}(\varepsilon^{(2m+1)^2/(4\pi R^2)+\mu}, \varepsilon^\mu),\end{aligned} \tag{3.17}$$

($\mu \geqslant 1$ integer) from which one concludes that the only cutoff-independent contribution in the integral stems from the first term in the last equation. We expand the exponent with respect to ε and arrive at

$$\rho(n,\theta) \sim \left\langle \exp\left[\mathrm{i}\frac{\theta}{2\pi R}(\varphi(x) - \varphi(0))\right]\left(1 + \mathcal{O}\big(\varepsilon^{2k[(2m+1)^2/(4\pi R^2)+\mu]}, \varepsilon^{2k\mu}\big)\right)\right\rangle \tag{3.18}$$

where the positive integer k originates in the expansion of the exponential function. From this we conclude that the leading exponent of the uniform part is $\nu_1(\theta,\gamma)$, and the leading Euler–MacLaurin corrections to this have exponents $\nu_1(\theta,\gamma) + 2$, $\nu_1(\theta,\gamma) + 1/(2\pi R^2)$.

Thus in order to determine the amplitude of the leading term, we have to calculate $\big\langle\exp\big[\mathrm{i}\frac{\theta}{2\pi R}(\varphi(x) - \varphi(0))\big]\big\rangle$. In the field-theoretical setting of massless Bose fields considered here, this quantity is defined only up to a multiplicative constant Λ with dimension 1/length [33]. It has become custom to choose it such that ('CFT normalization condition')

$$\Lambda^{\alpha^2/(2\pi)}\langle\exp[\mathrm{i}\alpha(\varphi(x) - \varphi(0))]\rangle = |x|^{-\alpha^2/(2\pi)}. \tag{3.19}$$

This means that we have to introduce a constant $D(\theta,\gamma)$ as follows:

$$\rho(n,\theta) \sim D(\theta,\gamma)\left\langle \exp\left[\mathrm{i}\frac{\theta}{2\pi R}(\varphi(x) - \varphi(0))\right]\right\rangle = \frac{D(\theta,\gamma)}{n^{(\theta/2\pi R)^2/(2\pi)}} \tag{3.20}$$

for the leading decay of the uniform part. Because of the symmetry $\rho(n,-\theta) = \rho(n,\theta)$, this result is valid for $-\pi \leqslant \theta \leqslant \pi$. Let us defer the calculation of the coefficient D to the next paragraph and first determine the leading exponent of the alternating part. This is obtained directly by exploiting the periodicity (2.14). Together with equation (3.20), it implies that

$$\rho(n, \pi \leqslant \theta \leqslant 3\pi) \sim D(\theta - 2\pi, \gamma) n^{-\nu_1(\theta-2\pi,\gamma)} \tag{3.21}$$

$$\rho(n, -3\pi \leqslant \theta \leqslant -\pi) \sim D(\theta + 2\pi, \gamma) n^{-\nu_1(\theta+2\pi,\gamma)}. \tag{3.22}$$

The exponents are expected to depend continuously on the parameters θ, γ. Thus for $0 \leqslant \theta \leqslant \pi$ ($-\pi \leqslant \theta < 0$), equation (3.21) (equation (3.22)) yields the leading contribution to the alternating part, which is next-leading with respect to the leading decay given in equation (3.20).

What are the exponents of the next-leading contributions? In equation (3.20) we have tacitly assumed that the expectation value is taken with respect to the unperturbed Gaussian part of the Hamiltonian (3.15). However, there are additional contributions in equation (3.15), with scaling dimensions $\Delta = 1/(\pi R^2), 4$. As argued in [35], they lead to exponents $\nu_1(\theta, \gamma) + k(\Delta - 2)$ in $\left\langle \exp\left[\mathrm{i}\frac{\theta}{2\pi R}(\varphi(x) - \varphi(0))\right]\right\rangle$, where the integer k denotes the order of the perturbational expansion. Since there is no contribution of the cos-operator for $k = 1$, the next-leading exponent stemming from this contribution is $\nu_2(\theta, \gamma) = \nu_1(\theta, \gamma) + \delta(\gamma)$ with $\delta(\gamma) = 4\pi/(\pi - \gamma) - 4$. On the other hand, the first-order contribution of the $\lambda_\pm$-operators yields an exponent $\nu_1(\theta, \gamma) + 2$. This latter one is always larger than $\nu_1(\theta, \gamma)$, $\nu_1(\theta - 2\pi, \gamma)$ (for $0 < \theta < \pi$) and we discard it here. Thus $\nu_2(\theta, \gamma)$ yields the next-leading exponent in the uniform part. According to the periodicity argument, the next-leading exponent in the alternating part for $0 < \theta < \pi$ is then $\nu_2(\theta - 2\pi, \gamma)$.

We now focus on the coefficient $D(\theta, \gamma)$. The result given in equation (3.3) is a conjecture based on the work [34]. The following tests of this conjecture have been performed.

- For $\gamma = \pi/2$, one can show that $D(\theta, \pi/2)$ reduces to (2.19), namely

$$D(\theta, \pi/2) = 4^{-\frac{\theta^2}{4\pi^2}} \left[G\left(1 + \frac{\theta}{2\pi}\right) G\left(1 - \frac{\theta}{2\pi}\right)\right]^2. \tag{3.23}$$

  This equality can be checked by means of an integral representation of the Barnes G-function (see appendix C).
- Numerical comparisons for $\Delta = 1/2$ between the exact data from the Bethe Ansatz (for $n = 9$) and the asymptotic results (3.2) and (3.9) have been performed for $\theta = \pi/4, \pi/2, 3\pi/4, \pi$. In all cases, very good agreement is found. Similarly, we compared with the data obtained by numerical diagonalization up to a system size of $N = 28$ lattice sites for general Δ (see appendix A).

Our conjecture for D is based on arguments similar to the conjecture for the coefficient of the leading decay of $\left\langle\sigma_1^x \sigma_n^x\right\rangle$, cf [33, 34]. In [34], the expectation value of $\langle \exp[\mathrm{i}\alpha\vartheta]\rangle$ in a *massive* sine-Gordon model with an operator $\cos(\beta\vartheta)$ is determined,

$$\langle \exp[\mathrm{i}\alpha\vartheta]\rangle = (\varepsilon m)^{\alpha^2/(4\pi)} N(\alpha, \beta), \tag{3.24}$$

where m is the particle mass associated with the field ϑ and $N(\alpha, \beta)$ a function of both the parameters α and β. Since in that problem, $\sigma^x \sim \mathrm{e}^{\mathrm{i}2\pi R\vartheta}$ with an *a priori* unknown amplitude, calculating the amplitude of the leading decay of $\left\langle\sigma_1^x \sigma_n^x\right\rangle$ with respect to a sine-Gordon model with an operator $\cos(\beta\vartheta)$ is very similar to our problem of determining D.

An explicit value for $N(\alpha, \beta)$ in equation (3.24) is conjectured and confirmed explicitly in certain limiting cases in [34]. The authors then calculate $\left\langle\sigma_1^x \sigma_n^x\right\rangle \sim A(\eta) N(1/\eta, 2/R) n^{-\eta}$ by making use of the fact that this correlation function is known *explicitly* for the massive *XYZ*-model close to the critical *XXZ*-point, namely $\left\langle\sigma_1^x \sigma_n^x\right\rangle_m \sim A_m(\varepsilon m)^{-\eta}$ with a known coefficient A_m. This allows for the deduction of $A(\eta)$.

In our case, the field φ is related to ϑ by $\partial_t\varphi = \partial_x\vartheta$. However, the problem of calculating D is completely analogous to the calculation of $A(\eta)$ sketched above, with a sine-Gordon-term $\cos(2\varphi/R)$ in the Hamiltonian. The only unknown is the string function $\rho_m(\theta)$ in the massive *XYZ*-regime. We know that

$$\rho_m(\theta) = C_m(R)(\varepsilon m)^{(\theta/(2\pi R))^2/(2\pi)} \tag{3.25}$$

with an unknown constant C_m depending on R. Note that in the massive regime, we cannot relate $2/R$ to γ, but rather take it as the constant in the sine-Gordon term $\cos(2\varphi/R)$. On the other hand, the results in [34] tell us that

$$\rho_m(\theta) = DN(\theta/(2\pi R), 2/R)(\varepsilon m)^{(\theta/(2\pi R))^2/(2\pi)} \tag{3.26}$$

with a known coefficient $N(\theta/(2\pi R), 2/R)$. By comparing equation (3.26) with equation (3.25), one obtains D in terms of θ, R and the unknown $C_m(R)$. We find that $C_m(R) = 2(1-\eta)^2 = 2(1-2\pi R^2)^2$ yields excellent agreement with the numerical data as described above. This results in the coefficient $D(\theta,\gamma)$ as given in equations (3.3) and (3.4).

We finally comment on the isotropic case, $\gamma = 0$. Here, $\nu_1(\theta, \gamma = 0) = \theta^2/(4\pi^2)$, in agreement with the result of [9]. However, we expect that a logarithmic dependence of the amplitude on the distance occurs, similarly to what happens for the two-point functions [31–33]. We leave the study of this case as a project for future research.

3.2.2. The generalized string correlation function $\mathcal{O}(n,\theta)$. From equation (2.9), the asymptotics of $\mathcal{O}(n,\theta)$ is obtained once the asymptotics of $\rho(n,\theta)$ is known. It is nevertheless instructive to perform a consistency check of this result by calculating the asymptotics of $\mathcal{O}$ directly by using field-theoretical arguments.

Therefore, one might be tempted to take the asymptotic expansion of $S^z(x)$, equation (3.16), and insert it into equation (1.1). However, in such a calculation the leading terms given in equation (3.2) would be absent. We are thus led to use the following asymptotic expansion for the S^z-operators at sites 1 and n involved in $\mathcal{O}(n,\theta\neq 0)$:

$$S^z(x) \sim s_0 + \frac{\varepsilon}{2\pi R}\partial_x\varphi(x) + \sum_{m=0}^{\infty}(-1)^j\varepsilon^{(2m+1)^2/(4\pi R^2)}C_m\cos\left(\frac{2m+1}{R}\varphi(x)\right) + \text{descendants}, \tag{3.27}$$

with $x = \varepsilon j$. The asymptotic expansion starts with a finite constant s_0. For the asymptotics of the phase factor in $\mathcal{O}(n,\theta)$, we still use equation (3.16). Carrying out the same calculations as above, one finds $s_0^2 = \tan^2(\theta/4)$, which vanishes for $\theta = 0$. The intriguing point is that we have to modify the asymptotic expansion for the spins at sites 1 and n in $\mathcal{O}(n,\theta)$ without modifying the Hamiltonian, and that the parameter θ enters in the constant s_0. Namely, it looks as if in the asymptotic limit, the phase operator in $\mathcal{O}(n,\theta)$ acts as a local field on the edge spins.

4. Conclusion and outlook

We evaluated the string correlation functions $\rho(n,\theta)$ and $\mathcal{O}(n,\theta)$ for the critical anisotropic spin $S = 1/2$ chain. For small n, exact results were obtained from the Bethe Ansatz, whereas in the asymptotic limit, both the amplitudes and the exponents of the leading decay could be determined from field theory. The field-theoretical results agree well with the Bethe Ansatz

Table A1. Exact values of string correlation functions for $\Delta = 1$.

n	2	3	4	5	6	7	8
$\rho(n, \pi/4)$	0.940 083	0.915 627	0.925 111	0.910 171	0.917 092	0.90616	0.911707
$\rho(n, \pi/2)$	0.795 431	0.685 542	0.744 898	0.671 293	0.718 266	0.660 85	0.700 65
$\rho(n, 3\pi/4)$	0.650 78	0.362 761	0.565 509	0.349 604	0.521 325	0.339 972	0.492 564
$\rho(n, \pi)$	0.590 863	0	0.491 445	0	0.440 302	0	0.407 242
$\mathcal{O}(n, \pi/4)$	0.590 863	−0.224 243	0.243 53	−0.120 692	0.170 343	−0.078 639 1	0.137 344
$\mathcal{O}(n, \pi/2)$	0.590 863	−0.171 628	0.346 22	−0.078 7594	0.282 725	−0.038 569	0.250 4
$\mathcal{O}(n, 3\pi/4)$	0.590 863	−0.092 8846	0.448 91	−0.035 2563	0.394 313	−0.009 179 44	0.361 674

Table A2. Exact values of string correlation functions for $\Delta = 1/2$.

n	2	3	4	5	6	7	8
$\rho(n, \pi/4)$	0.926 777	0.909 081	0.909 299	0.900 034	0.899 811	0.893 662	0.893 337
$\rho(n, \pi/2)$	0.75	0.668 437	0.692 139	0.644 847	0.661 899	0.628 299	0.641 883
$\rho(n, 3\pi/4)$	0.573 223	0.346 957	0.477 542	0.325 21	0.429 591	0.310 018	0.398 987
$\rho(n, \pi)$	0.5	0	0.389 404	0	0.335 008	0	0.300 88
$\mathcal{O}(n, \pi/4)$	0.5	−0.101 049	0.140 59	−0.028 550 5	0.088 0858	−0.005 091 66	0.068 9805
$\mathcal{O}(n, \pi/2)$	0.5	−0.077 3398	0.243 652	0.000 467 493	0.192 033	0.029 311 8	0.168 568
$\mathcal{O}(n, 3\pi/4)$	0.5	−0.041 856	0.346 715	0.012 332	0.293 62	0.033 798	0.263 161

data. Especially, for $\Delta = 0$, the asymptotics could be confirmed directly from the Bethe Ansatz results.

Most interestingly, the leading decay of the two-point xx-correlation function was recovered, equation (3.5). Whether this result has a physical background has to be clarified. As far as the limit $\theta \to 0$ in $\mathcal{O}(n, \theta)$ is concerned, we have recovered the expected result (3.14). However, the rather heuristic expansion (3.27) in the field-theory for $\theta \neq 0$ deserves further investigations in the future.

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Appendix A. Numerical values of string correlation functions

For $\Delta = 1$ and $1/2$, the string correlation functions $\rho(n, \theta)$ and $\mathcal{O}(n, \theta)$ can be evaluated analytically up to $n = 8$ and $n = 9$, respectively. Here firstly, we list their precise numerical values for $\theta = \pi/4, \pi/2, 3\pi/4, \pi$ up to $n = 8$, based on these analytical expressions (see tables A1 and A2). Note that $\rho(1, \theta) = \cos\frac{\theta}{2}$ irrespective of Δ and therefore we have

$$\rho\left(1, \frac{\pi}{4}\right) = \cos\frac{\pi}{8} = 0.923\,880, \qquad \rho\left(1, \frac{\pi}{2}\right) = \cos\frac{\pi}{4} = 0.707\,107,$$
$$\rho\left(1, \frac{3\pi}{4}\right) = \cos\frac{3\pi}{8} = 0.382\,683, \qquad \rho(1, \pi) = 0.$$

Note also that $\mathcal{O}(2, \theta) = -4\langle S_1^z S_2^z\rangle$ irrespective of θ by its definition.

Table A3. Asymptotic formulae of string correlation functions for $\Delta = 1/2$.

n	2	3	4	5	6	7	8
$\rho_{\mathrm{Asym}}(n, \pi/4)$	0.926 694	0.909 865	0.909 106	0.900 388	0.899 692	0.893 859	0.893 259
$\rho_{\mathrm{Asym}}(n, \pi/2)$	0.751 733	0.669 839	0.692 208	0.645 454	0.661862	0.628 622	0.641843
$\rho_{\mathrm{Asym}}(n, 3\pi/4)$	0.577 912	0.348 016	0.478 151	0.325 667	0.429 729	0.310 258	0.399 020
$\rho_{\mathrm{Asym}}(n, \pi)$	0.506 119	0	0.390 271	0	0.335 222	0	0.300 940
$\mathcal{O}_{\mathrm{Asym}}(n, \pi/4)$	0.306 262	−0.081 2361	0.116 753	−0.020 490 5	0.079 3274	−0.000 774 240	0.064 4446
$\mathcal{O}_{\mathrm{Asym}}(n, \pi/2)$	0.402 260	−0.072 2680	0.233 892	0.002 756 05	0.188 836 0	0.030 538 8	0.167 037
$\mathcal{O}_{\mathrm{Asym}}(n, 3\pi/4)$	0.477 679	−0.041 3030	0.344 917	0.012 869 4	0.293 024	0.034 1302	0.262 857

Table A4. Numerical values of $\rho(n, \theta)$ for $\Delta = 0.3$.

n	2	3	4	5	6	7	8
$\rho_{\mathrm{Num}}(n, \pi/4)$	0.921 405	0.905 433	0.902 971	0.894 779	0.892 836	0.887 437	0.885 867
$\rho_{\mathrm{Asym}}(n, \pi/4)$	0.921 707	0.905 979	0.902 974	0.894 999	0.892 828	0.887 552	0.885 852
$\rho_{\mathrm{Num}}(n, \pi/2)$	0.731 659	0.658 904	0.671 538	0.631 168	0.640 067	0.612 185	0.619 215
$\rho_{\mathrm{Asym}}(n, \pi/2)$	0.734 432	0.659 884	0.672 036	0.631 562	0.640 252	0.612 384	0.619 276
$\rho_{\mathrm{Num}}(n, 3\pi/4)$	0.541 914	0.338 150	0.444 087	0.312 623	0.395 710	0.295 270	0.365 120
$\rho_{\mathrm{Asym}}(n, 3\pi/4)$	0.548 200	0.338 908	0.445 270	0.312 938	0.396 134	0.295 431	0.365 265

Table A5. Numerical values of $\rho(n, \theta)$ for $\Delta = 0.7$.

n	2	3	4	5	6	7	8
$\rho_{\mathrm{Num}}(n, \pi/4)$	0.932 056	0.912 068	0.915 471	0.904 519	0.906 536	0.899 088	0.900 492
$\rho_{\mathrm{Asym}}(n, \pi/4)$	0.931 684	0.913 012	0.915 038	0.905 020	0.906 242	0.899 399	0.900 275
$\rho_{\mathrm{Num}}(n, \pi/2)$	0.768 025	0.676 242	0.712 563	0.656 541	0.683 506	0.642 401	0.664 320
$\rho_{\mathrm{Asym}}(n, \pi/2)$	0.768 824	0.677 927	0.712 076	0.657 389	0.683 096	0.642 903	0.663 983
$\rho_{\mathrm{Num}}(n, 3\pi/4)$	0.603 994	0.354 168	0.511 302	0.335 990	0.464 170	0.322 975	0.433 890
$\rho_{\mathrm{Asym}}(n, 3\pi/4)$	0.607 173	0.355 419	0.511 188	0.336 608	0.463 845	0.323 332	0.433 544

Table A6. Numerical values of $\rho(n, \theta)$ for $\Delta = -0.3$.

n	2	3	4	5	6	7	8
$\rho_{\mathrm{Num}}(n, \pi/4)$	0.903 373	0.887 893	0.878 937	0.870 856	0.865 109	0.859 693	0.855 477
$\rho_{\mathrm{Asym}}(n, \pi/4)$	0.903 927	0.887 947	0.879 042	0.870 896	0.865 149	0.859 714	0.855 487
$\rho_{\mathrm{Num}}(n, \pi/2)$	0.670 096	0.613 07	0.597 811	0.569 629	0.559 974	0.541 915	0.534 903
$\rho_{\mathrm{Asym}}(n, \pi/2)$	0.674 020	0.613 330	0.598 582	0.569 822	0.560 266	0.542 024	0.535 013
$\rho_{\mathrm{Num}}(n, 3\pi/4)$	0.436 818	0.295 804	0.332 446	0.256 666	0.283 712	0.232 404	0.253 962
$\rho_{\mathrm{Asym}}(n, 3\pi/4)$	0.446 622	0.296 198	0.334 401	0.256 936	0.284 437	0.232 560	0.254 249

For $\Delta = 1/2$ let us compare the results above with the numerical value of the asymptotic formulae (3.2) and (3.9) with $\gamma = \pi/3$ in table A3.

We find the exact values and the asymptotic formulae are in good agreement especially for $\rho(n, \theta)$. The deviation is somewhat larger for $\mathcal{O}(n, \theta)$, for which we probably need higher order corrections to the asymptotic formulae to achieve better agreement.

To confirm our asymptotic formula further, we have calculated $\rho(n, \theta)$ numerically for several values of $\Delta\,(= \pm 0.3, \pm 0.7, -0.5)$ by means of the exact diagonalization for finite systems $N = 20$–28. Then we have applied an extrapolation according to $c_0 + c_1/N^2 + c_2/N^3 + c_3/N^4 + c_4/N^5$ and estimated $\rho_{\mathrm{Num}}(n, \theta)$ in the thermodynamic limit. These values are compared with our asymptotic formula $\rho_{\mathrm{Asym}}(n, \theta)$ in tables A4–A8. We

Table A7. Numerical values of $\rho(n,\theta)$ for $\Delta = -0.5$.

n	2	3	4	5	6	7	8
$\rho_{\mathrm{Num}}(n,\pi/4)$	0.895 942	0.877 985	0.866 417	0.857 132	0.849 944	0.843 718	0.838 522
$\rho_{\mathrm{Asym}}(n,\pi/4)$	0.895 477	0.877 611	0.866 290	0.857 039	0.849 893	0.843 674	0.838 481
$\rho_{\mathrm{Num}}(n,\pi/2)$	0.644 723	0.587 178	0.562 522	0.535 287	0.520 367	0.503 241	0.492 689
$\rho_{\mathrm{Asym}}(n,\pi/2)$	0.646 724	0.586 707	0.562 879	0.535 292	0.520 512	0.503 266	0.492 719
$\rho_{\mathrm{Num}}(n,3\pi/4)$	0.393 503	0.271 884	0.284 932	0.226 344	0.236 472	0.199 498	0.207 607
$\rho_{\mathrm{Asym}}(n,3\pi/4)$	0.402 915	0.271 927	0.286 782	0.226 578	0.237 163	0.199 648	0.207 867

Table A8. Numerical values of $\rho(n,\theta)$ for $\Delta = -0.7$.

n	2	3	4	5	6	7	8
$\rho_{\mathrm{Num}}(n,\pi/4)$	0.886 810	0.863 491	0.847 596	0.835 540	0.825 990	0.818 029	0.811 263
$\rho_{\mathrm{Asym}}(n,\pi/4)$	0.883 755	0.861 533	0.846 496	0.834 864	0.825 552	0.817 718	0.811 018
$\rho_{\mathrm{Num}}(n,\pi/2)$	0.613 546	0.549 304	0.512 895	0.483 364	0.462 734	0.444 631	0.430 668
$\rho_{\mathrm{Asym}}(n,\pi/2)$	0.610 618	0.545 990	0.511 485	0.482 427	0.462 241	0.444 263	0.430 380
$\rho_{\mathrm{Num}}(n,3\pi/4)$	0.340 281	0.236 892	0.225 198	0.182 532	0.177 268	0.153 088	0.150 087
$\rho_{\mathrm{Asym}}(n,3\pi/4)$	0.348 075	0.235 495	0.226 127	0.182 395	0.177 655	0.153 117	0.150 189

conclude that our asymptotic formula gives fairly precise values for all ranges of Δ in the critical region.

Appendix B. Proof of (3.7)

We prove equation (3.7) in the form

$$\lim_{\theta\to 0} D(2\pi-\theta)\frac{4\pi^2}{\theta^2} = \left[\frac{\Gamma\left(\frac{\eta}{2-2\eta}\right)}{2\sqrt{\pi}\,\Gamma\left(\frac{1}{2-2\eta}\right)}\right]^{1/\eta} \times \exp\left[\int_0^\infty \left(\frac{\sinh((2\eta-1)t)}{\sinh\eta t\cosh((1-\eta)t)} - \frac{2\eta-1}{\eta}\,\mathrm{e}^{-2t}\right)\frac{\mathrm{d}t}{t}\right]. \tag{B.1}$$

By taking the logarithm and introduce a variable $z \equiv \theta/2\pi$, we can calculate the LHS from the definition (3.3) as follows:

$$\lim_{\theta\to 0}\ln\left(D(2\pi-\theta)\frac{4\pi^2}{\theta^2}\right) = \ln\left[\frac{\Gamma\left(\frac{\eta}{2-2\eta}\right)}{2\sqrt{\pi}\,\Gamma\left(\frac{1}{2-2\eta}\right)}\right]^{1/\eta} - \lim_{z\to 0}\left\{\int_0^\infty\left(\frac{\sinh^2(1-z)t}{\sinh t\cosh(1-\eta)t\sinh\eta t} - \frac{(1-z)^2}{\eta}\,\mathrm{e}^{-2t}\right)\frac{\mathrm{d}t}{t} + 2\ln z\right\}. \tag{B.2}$$

Now substitute the function $\ln z$ by its integral represention

$$\ln z = \int_0^\infty (\mathrm{e}^{-t}-\mathrm{e}^{-zt})\frac{\mathrm{d}t}{t} = \int_0^\infty (\mathrm{e}^{-2t}-\mathrm{e}^{-2zt})\frac{\mathrm{d}t}{t}, \qquad (\mathrm{Re}(z)>0) \tag{B.3}$$

we have

$$-\lim_{z\to 0}\left\{\int_0^\infty\left(\frac{\sinh^2(1-z)t}{\sinh t\cosh(1-\eta)t\sinh\eta t} - \frac{(1-z)^2}{\eta}\,\mathrm{e}^{-2t}\right)\frac{\mathrm{d}t}{t} + 2\ln z\right\}$$

$$= -\lim_{z\to 0}\left\{\int_0^\infty\left(\frac{\sinh^2(1-z)t}{\sinh t\cosh(1-\eta)t\sinh\eta t}-2\mathrm{e}^{-2zt}+\left(2-\frac{(1-z)^2}{\eta}\right)\mathrm{e}^{-2t}\right)\frac{\mathrm{d}t}{t}\right\}$$
$$= \int_0^\infty\left(\frac{-\sinh t}{\cosh(1-\eta)t\sinh\eta t}+2-\frac{2\eta-1}{\eta}\mathrm{e}^{-2t}\right)\frac{\mathrm{d}t}{t}$$
$$= \int_0^\infty\left(\frac{\sinh((2\eta-1)t)}{\cosh(1-\eta)t\sinh\eta t}-\frac{2\eta-1}{\eta}\mathrm{e}^{-2t}\right)\frac{\mathrm{d}t}{t}. \tag{B.4}$$

Thus equation (B.1), namely, equation (3.7) is proved.

Appendix C. Proof of (3.23)

If we use the notation $z = \theta/(2\pi)$, the asymptotic amplitude of the string correlation function (3.3) is rewritten as

$$D(\theta,\gamma) = \left[\frac{\Gamma\left(\frac{\eta}{2-2\eta}\right)}{2\sqrt{\pi}\,\Gamma\left(\frac{1}{2-2\eta}\right)}\right]^{z^2/\eta}\exp\left[-\int_0^\infty\left(\frac{\sinh^2 zt}{\sinh t\cosh(1-\eta)t\sinh\eta t}-\frac{z^2\,\mathrm{e}^{-2t}}{\eta}\right)\frac{\mathrm{d}t}{t}\right]. \tag{C.1}$$

Setting the parameters as

$$\gamma = \pi/2, \qquad \Delta = \cos\gamma = 0, \qquad \eta = (\pi-\gamma)/\pi = 1/2, \tag{C.2}$$

we obtain

$$D(\theta,\pi/2) = \left(\frac{1}{2}\right)^{2z^2}\exp\left[-\int_0^\infty\left(\frac{\sinh^2(zt)}{\sinh t\cosh(t/2)\sinh(t/2)}-2z^2\,\mathrm{e}^{-2t}\right)\frac{\mathrm{d}t}{t}\right]$$
$$= 4^{-z^2}\exp\left[-2\int_0^\infty\left(\frac{\sinh^2(zt)}{\sinh^2 t}-z^2\,\mathrm{e}^{-2t}\right)\frac{\mathrm{d}t}{t}\right]. \tag{C.3}$$

On the other hand, the Barnes G-function enjoys the following integral representation [49]

$$\ln G(1+z) = \int_0^\infty\frac{\mathrm{e}^{-t}}{t(1-\mathrm{e}^{-t})^2}\left(1-zt+\frac{z^2t^2}{2}-\mathrm{e}^{-zt}\right)\mathrm{d}t$$
$$-(1+\gamma_E)\frac{z^2}{2}+\left(\log\frac{2\pi}{\mathrm{e}}\right)\frac{z}{2}, \qquad (\mathrm{Re}(z) > -1) \tag{C.4}$$

where γ is the Euler–Mascheroni constant. From this integral representation we have

$$-\ln[G(1+z)G(1-z)] = \int_0^\infty\frac{\mathrm{e}^{-t}}{t(1-\mathrm{e}^{-t})^2}(-2-z^2t^2+2\cosh(zt))\,\mathrm{d}t+(1+\gamma_E)z^2$$
$$= \int_0^\infty\frac{-2-z^2t^2+2\cosh(zt)}{4\sinh^2(t/2)}\frac{\mathrm{d}t}{t}+(1+\gamma_E)z^2$$
$$= \int_0^\infty\frac{-1-2z^2t^2+\cosh(2zt)}{2\sinh^2 t}\frac{\mathrm{d}t}{t}+(1+\gamma_E)z^2$$
$$= \int_0^\infty\frac{\sinh^2(zt)-z^2t^2}{\sinh^2 t}\frac{\mathrm{d}t}{t}+(1+\gamma_E)z^2. \tag{C.5}$$

Now substituting the formula

$$\int_0^\infty\left(\frac{t}{\sinh^2 t}-\frac{\mathrm{e}^{-t}}{\sinh t}\right)\mathrm{d}t = [(\ln(\sinh t)-t\coth t)-(\ln(\sinh t)-t)]_0^\infty$$
$$= \left[\frac{-2t}{\mathrm{e}^{2t}-1}\right]_0^\infty = 1, \tag{C.6}$$

into the standard integral representation of the Euler–Mascheroni constant,

$$\gamma_E = \int_0^\infty \left(\frac{e^{-t}}{1 - e^{-t}} - \frac{e^{-t}}{t} \right) dt \tag{C.7}$$

we can establish another integral formula

$$1 + \gamma_E = \int_0^\infty \left(\frac{t^2}{\sinh^2 t} - e^{-2t} \right) \frac{dt}{t}. \tag{C.8}$$

Substituting equation (C.8) into equation (C.5) yields

$$-\ln[G(1+z)G(1-z)] = \int_0^\infty \left(\frac{\sinh^2(zt)}{\sinh^2 t} - z^2 e^{-2t} \right) \frac{dt}{t}, \tag{C.9}$$

from which we conclude

$$D(\theta, \pi/2) = 4^{-z^2} [G(1+z)G(1-z)]^2, \tag{C.10}$$

which is equivalent to equation (3.23).

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