Excited state correlations of the finite Heisenberg chain

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Abstract

We consider short range correlations in excited states of the finite XXZ and XXX Heisenberg spin chains. We conjecture that the known results for the factorized ground state correlations can be applied to the excited states too, if the so-called physical part of the construction is changed appropriately. For the ground state we derive simple algebraic expressions for the physical part; the formulas only use the ground state Bethe roots as an input. We conjecture that the same formulas can be applied to the excited states as well, if the exact Bethe roots of the excited states are used instead. In the XXZ chain the results are expected to be valid for all states (except certain singular cases where regularization is needed), whereas in the XXX case they only apply to singlet states or group invariant operators. Our conjectures are tested against numerical data from exact diagonalization and coordinate Bethe Ansatz calculations, and perfect agreement is found in all cases. In the XXX case we also derive a new result for the nearest-neighbour correlator $\langle \sigma_1^z \sigma_2^z \rangle$, which is valid for non-singlet states as well. Our results build a bridge between the known theory of factorized correlations, and the recently conjectured TBA-like description for the building blocks of the construction.

1 Introduction

The Heisenberg spin chain is a model of magnetism in one-dimensional or quasi one-dimensional materials. The study of the original XXX model goes back to its famous solution by Hans Bethe in 1931 [1], whereas the anisotropic version (also called the XXZ model) was first solved by Orbach in 1958 [2]. These spin chains play a central role in the field of integrable models: they are truly interacting models whose solution displays the full arsenal of integrability, yet their relative simplicity make them an ideal testing ground to develop new ideas and methods.

By now a large body of literature has been devoted to the study of the equilibrium properties of the spin chain. The exact eigenstates can be constructed using various forms of the Bethe Ansatz [3], and the thermodynamic properties can be computed using the so-called Thermodynamic Bethe Ansatz (TBA) or the Quantum Transfer Matrix (QTM) methods [4, 5]. On the other hand, for a long time it was believed that the correlation functions can not be computed in a practical way. The correlators are important physical quantities: they are experimentally relevant, and a system can not be considered to be exactly solved until (at least some of the) correlators can be computed. This motivated a long series of works by different groups to study the correlators of the Heisenberg spin chain.

The first results were multiple integral representations for the ground state correlations, which were derived using representation theory of quantum algebras [6, 7, 8] or the Algebraic Bethe Ansatz [9, 10]. Later it was realized in the papers [11, 12, 13, 14] that for the ground state of the infinite XXX model these multiple integrals can be factorized, i.e. expressed as polynomials of a single function in two variables. An exponential formula was found in [15, 16] for the reduced density matrix of a finite sub-chain, whose form was conjectured to be valid even in the finite temperature or finite length cases [17, 18]. Afterwards a new

fermionic structure was found on the space of local operators of the XXZ model [19, 20, 21], which led to easily manageable expressions for the short range correlators including the finite temperature or finite length cases [22, 23, 24, 25]. In practical terms these developments can be summarized as follows: In both the XXX and XXZ cases the correlations can be expressed as a polynomial of only one or two functions, respectively[1]. The algebraic part of the construction provides this polynomial, whereas the physical part specifies the functions themselves depending on the physical situation, which might be the infinite chain at finite temperature, or the ground state of the finite chain. We should also note, that an independent derivation of these results was given later in [26] using discrete functional equations.

The previously mentioned results pertain to equilibrium situations. However, recently there has been considerable interest in the far from equilibrium physics of integrable models, including and especially the Heisenberg spin chains [27, 28]. One of the main questions was whether an integrable model equilibrates to some kind of Generalized Gibbs Ensemble [29, 28]. Regarding the Heisenberg chain this question has been investigated in a series of works [30, 31, 32, 33, 34] leading to [35] (see also [36]), where a conclusive answer was given: the asymptotic states can indeed be described by a generalized statistical physical ensemble, if the recently discovered quasi-local charges are also included [37, 38, 39, 40]. However, the addition of all charges completely fixes all the string root densities of the spin chain [35, 27], therefore it is a question of interpretation whether there is any kind of statistical physics emerging in the long time limit.

In all of these studies it was of central importance to give predictions for the long-time limit of local observables, so that the analytic results could be compared to independent simulations [33, 34] or possibly to experimental data. In out-of-equilibrium situations the system is typically very far from the ground state and there is need to calculate the correlations in highly excited states too. In the spin chain literature the first such results were presented in [41], where it was conjectured that in the thermodynamic limit the known factorized formulas are valid even for the highly excited states if the physical part is computed using a new set of TBA-like integral equations. This conjectured result was used in the works [33, 34], it successfully passed a number of tests, however it was not clear how it relates to the physical part of the finite temperature situation [21, 22]. In the latter problem all ingredients are computed using single contour integrals, whereas [41] uses an infinite system of equations based on the string hypothesis. It is important that the results of [41] are valid for arbitrary smooth string distributions, and not only for the thermal cases. For the the free energy of the finite T case it is known how to connect the TBA equations to the single non-linear integral equation of the QTM method [42], but up to now no such link was known for the factorized correlation functions.

Here we make a step towards filling this gap by investigating the correlations of the excited states of the finite spin chain; this problem has not yet been considered in the literature. We derive algebraic expressions for the physical part of the factorized correlation functions; the results are expected to be valid for all excited states. In the thermodynamic limit these results could lead to a proof of the formulas of [41].

The structure of this article is as follows. In Section 2 we present one of the main conjectures, namely that factorization holds for all excited states of the XXZ model. Also, we present a formula for the physical part, which is a simple algebraic expression that uses the exact Bethe roots. Section 3 deals with the correlations of the XXX model; the focus is on singlet states and singlet operators. In Section 4 we derive a simple but new result for the nearest neighbour $z - z$ correlator of the XXX chain, which is valid for arbitrary Bethe states and not only for the singlets. Section 5 includes our conclusions, and also an outlook to open problems. Finally, Appendices A and B include numerical data and simple coordinate space calculations to support our results, whereas in Appendix C we compare a result of the paper [17] to one of our finite size formulas.

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[1]This applies to spin-reflection invariant operators. In the generic case (including for example the magnetization operator) one more function is needed.

2   Excited state correlations of the XXZ model

In this section we consider the homogeneous XXZ spin chain for generic anisotropy. The model is defined by the Hamiltonian

$$H = \sum_{j=1}^{L} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta(\sigma_j^z \sigma_{j+1}^z - 1)). \tag{2.1}$$

In this work we only consider periodic boundary conditions and assume that L is even. For the anisotropy we will use the parametrization $\Delta = \cosh(\eta)$.

As usual we introduce the monodromy matrix as

$$T(u) = R_{L0}(u) \dots R_{10}(u), \tag{2.2}$$

where the $R_{j0}(u)$ operators are acting on the quantum space at site j and an auxiliary space denoted by 0. The matrix elements of $R_{j0}(u)$ are identical to the well known R-matrix of the XXZ type:

$$R(u) = \frac{1}{\sin(u+i\eta)} \begin{pmatrix} \sin(u+i\eta) & & & \\ & \sin(u) & \sin(i\eta) & \\ & \sin(i\eta) & \sin(u) & \\ & & & \sin(u+i\eta) \end{pmatrix}. \tag{2.3}$$

The trace of the monodromy matrix is called the transfer matrix:

$$\tau(u) = A(u) + D(u).$$

The transfer matrices form a commuting family:

$$[\tau(u), \tau(v)] = 0.$$

It is also known that the Hamiltonian and the higher charges of the model can be obtained as the logarithmic derivative of the transfer matrix around $u = 0$:

$$Q_j = \left(\frac{d}{du} \right)^{j+1} \log \tau(iu) \Big|_{u=0}.$$

It can be shown that with these conventions $H = 2\sinh(\eta)Q_0$.

Eigenstates of the model can be constructed by various forms of the Bethe Ansatz. The coordinate Bethe Ansatz solution can be written as follows. We define N-particle states as

$$|\{u\}_N\rangle = \sum_{y_1 < y_2 < \dots < y_N} \phi_N(\{u\}_N | y_1, \dots, y_N) \sigma_{y_1}^- \dots \sigma_{y_N}^- |0\rangle, \tag{2.4}$$

where $|0\rangle$ is the reference state with all spins up. Then the wave functions can be written as

$$\phi_N(\{u\}_N | \{y\}) = \sum_{P \in S_N} \left[\prod_{1 \le m < n \le N} \frac{\sin(u_{P_m} - u_{P_n} + i\eta)}{\sin(u_{P_m} - u_{P_n})} \right] \left[\prod_{l=1}^{N} \left(\frac{\sin(u_{P_l} + i\eta/2)}{\sin(u_{P_l} - i\eta/2)} \right)^{y_l} \right]. \tag{2.5}$$

Here u_j are the rapidities of the interacting spin waves and they satisfy the Bethe equations, which follow from the periodicity of the wave function:

$$\left(\frac{\sin(u_j - i\eta/2)}{\sin(u_j + i\eta/2)} \right)^L \prod_{k \ne j} \frac{\sin(u_j - u_k + i\eta)}{\sin(u_j - u_k - i\eta)} = 1. \tag{2.6}$$

The energy eigenvalues are

$$E = -\sum_j \frac{2\sinh^2 \eta}{\sin(u_j + i\eta/2)\sin(u_j - i\eta/2)}. \tag{2.7}$$

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In the regime $\Delta > 1$ we have $\eta \in \mathbb{R}$ and the solutions to the Bethe equations (2.6) are either real or they form strings that are centered at the real axis. On the other hand, for $\Delta < 1$ the parameter η is purely imaginary, and as an effect we have a rotation in the complex plane: if we use the same formulas (2.5)-(2.6) even in this regime, then the Bethe roots are either on the imaginary axis or they form strings centered around it[2]. Usually an explicit rotation is performed for $|\Delta| < 1$ by using hyperbolic functions instead of the trigonometric ones. However, in the present work we intend to treat the two regimes together, therefore we use the trigonometric formulas for arbitrary $\Delta \neq 1$.

With the convention (2.5) the norm of the state (2.4) is given by [43]

$$\langle \{u\}_N | \{u\}_N \rangle = \prod_j \frac{\sin(u_j + i\eta/2)\sin(u_j - i\eta/2)}{\sinh(\eta)} \prod_{j<k} \frac{\sin(u_{jk} + i\eta)\sin(u_{jk} - i\eta)}{\sin^2(u_{jk})} \times \det G, \tag{2.8}$$

where G is the Gaudin matrix:

$$G_{jk} = \delta_{jk} \left(L \frac{\sinh(\eta)}{\sin(u_j + i\eta/2)\sin(u_j - i\eta/2)} + \sum_{l=1}^{N} K(u_{jl}) \right) - K(u_{jk}), \tag{2.9}$$

with $u_{jk} = u_j - u_k$ and K is the scattering kernel of the XXZ model:

$$K(u) = -\frac{\sinh(2\eta)}{\sin(u + i\eta)\sin(u - i\eta)}. \tag{2.10}$$

We stress that (2.8) is only valid when the rapidities satisfy the Bethe equations. In the non-physical off-shell cases the norm is a more complicated function of the variables $\{u\}$.

It is important that even though the Bethe Ansatz seems to be complete, the regular solutions of the Bethe equations (2.6) do not produce all eigenstates of the XXZ chain [44]. For example, for arbitrary Δ there are singular states whose Bethe roots include the rapidities $u = \pm i\eta/2$ [45, 46, 47, 48, 49, 50]. The existence of these states is related to a special property of the Bethe Ansatz wave function (2.5): if the state is an eigenvector of the space reflection operator, then the corresponding eigenvalue is always equal to the eigenvalue of the one-site shift operator, whereas there must be states where these two eigenvalues are different and this is produced by the singular rapidities [47]. Other types of singular states appear at the "root of unity points" $\Delta = \cos(\gamma\pi)$ with $\gamma = p/q$ and $p, q \in \mathbb{Z}$ being relative primes; these states are related to additional degeneracies in the spectrum caused by the sl_2 loop algebra [51, 52, 53, 44]. In the present work we concentrate on the regular states and give only a few remarks about the singular cases.

Regarding the correlations our focus is on the short range operators, for example

$$\mathcal{O} = E_1^{ab} E_n^{cd}, \tag{2.11}$$

where E_j^{ab} is the $\mathbb{C}^2 \to \mathbb{C}^2$ elementary matrix acting on site j with a single nonzero matrix element at position (a, b). Our aim is to compute the excited state mean values

$$\langle \{u\}_N | \mathcal{O} | \{u\}_N \rangle. \tag{2.12}$$

The explicit expression for the wave function gives a direct way to compute the correlators in arbitrary Bethe states. For example

$$\langle \{u\}_N | E_1^{22} E_2^{22} | \{u\}_N \rangle = \\ \sum_{3 \leq y_2 < y_3 < \cdots < y_N \leq L} \phi_N^*(\{u\}_N | \{1, 2, y_2, \ldots, y_N\}) \phi_N(\{u\}_N | \{1, 2, y_2, \ldots, y_N\}). \tag{2.13}$$

In order to study the analytic properties of the correlators it is useful to introduce the parameters

$$a_j = e^{ip_j} = \frac{\sin(u_j + i\eta/2)}{\sin(u_j - i\eta/2)}. \tag{2.14}$$

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[2]The so-called "negative-parity" strings with $\mathcal{R}u = \pi/2$ can also be considered to be centered around the imaginary axis due to the π-periodicity.

Here p_j can be identified as the one-particle pseudo-momentum and a_j is the one-particle eigenvalue of the one-site translation operator. In terms of the a-variables the wave function can be written as

$$\phi_N(\{a\}_N|\{y\}) = \sum_{P \in S_N} \left[\prod_{1 \le m < n \le N} \frac{1 - 2\Delta a_{P_m} + a_{P_m} a_{P_n}}{a_{P_n} - a_{P_m}} \right] \left[\prod_{l=1}^{N} a_{P_l}^{y_l} \right]. \tag{2.15}$$

We are interested in correlations in the physical states. The solutions to the Bethe equations are self-conjugate [54], therefore, in terms of the a-variables the conjugate wave function can be written as

$$\phi_N^*(\{a\}_N|\{y\}) = \sum_{P \in S_N} \left[\prod_{1 \le m < n \le N} \frac{1 - 2\Delta a_{P_n} + a_{P_m} a_{P_n}}{a_{P_m} - a_{P_n}} \right] \left[\prod_{l=1}^{N} a_{P_l}^{-y_l} \right]. \tag{2.16}$$

The direct real space calculations lead to expressions that contain powers of a_j^L, $j = 1 \ldots N$. After substituting the Bethe equations in the form

$$a_j^L = \prod_{k \ne j} - \frac{1 - 2\Delta a_j + a_j a_k}{1 - 2\Delta a_k + a_j a_k}$$

all normalized correlators can be written as

$$\langle \{a\}|\mathcal{O}|\{a\} \rangle = \frac{\sum_{j=1}^{N} L^j C_j(\{a\})}{\sum_{j=1}^{N} L^j D_j(\{a\})}, \tag{2.17}$$

where C_j and D_j are polynomials that don't depend on the volume L anymore. The denominator in (2.17) is proportional to the Gaudin determinant, whereas the polynomials C_j are related to the infinite volume form factors of the operator in question [55].

The real space calculations are of course cumbersome and it is not clear how to get useful formulas for arbitrary N and L. An alternative and well established method is the Algebraic Bethe Ansatz (ABA), which provides a systematic way towards the correlators, see [56] and references therein. Previous works concentrated mostly on the ground states, both at zero and finite magnetic fields, with the aim of taking the thermodynamic limit. However, they also include a number of intermediate results for finite chains involving the Bethe roots as arbitrary parameters [18], which are valid for the excited states as well.

In the ABA the correlators are first obtained in the form of multiple integrals. Quite remarkably, these multiple integrals can be factorized, i.e. expressed as a polynomials of simple integrals. In the following subsection we summarize the known results for the XXZ chain, following the presentation of [18, 57, 24].

2.1 Factorization of correlation functions

The construction for the factorized correlation functions consists of two parts: the algebraic part, which deals with the space of operators and expresses their mean values using two functions, and the physical part, which computes these functions depending on the physical situation. The calculations are valid both for the finite size ground state and at finite temperature in the thermodynamic limit.

As a first step we define the auxiliary function $\mathfrak{a}$ through

$$\log \mathfrak{a}(u) = a_0(u) + \int_C \frac{d\omega}{2\pi} K(u - \omega) \log(1 + \mathfrak{a}(\omega)). \tag{2.18}$$

The source of the integral equation and the contour depend on the physical situation. Here we only consider the finite volume ground state case, where

$$a_0(x) = L \log \frac{\sin(x - i\eta/2)}{\sin(x + i\eta/2)}, \tag{2.19}$$

and C is a narrow contour around the segment $[-\pi/2, \pi/2]$ of the real axis, so that it encircles all Bethe roots.

We also define two functions $H(x, y)$ and $\tilde{H}(x, y)$ through the linear integral equations[3]

$$H(u, x) = -q(u, x) - \int_C \frac{d\omega}{2\pi} K(u - \omega) \frac{H(\omega, x)}{1 + \mathfrak{a}(\omega)} \tag{2.20}$$

and

$$\tilde{H}(u, x) = -\tilde{q}(u, x) - \int_C \frac{d\omega}{2\pi} \tilde{K}(u - \omega) \frac{H(\omega, x)}{1 + \mathfrak{a}(\omega)} - \int_C \frac{d\omega}{2\pi} K(\lambda - \omega) \frac{\tilde{H}(\omega, x)}{1 + \mathfrak{a}(\omega)},$$

where

$$\tilde{K}(u) = \frac{\sin(2u)}{\sin(u + i\eta) \sin(u - i\eta)}$$

and

$$q(u, x) = -i(\cot(u - x - i\eta) - \cot(u - x))$$
$$\tilde{q}(u, x) = -i \cot(u - x - i\eta).$$

In these definitions it is assumed that the parameter x lies within the contour C, and in all other cases an analytic continuation is understood. This requirement follows from the derivation of the multiple integrals [10, 18], where as a first step an "inhomogeneous transfer matrix" has to be considered. Here we only treat the homogeneous limit.

For $x, y \in C$ Let the functions $\Psi(x, y)$ and $P(x, y)$ be given by

$$\Psi(x, y) = \int_C \frac{d\omega}{\pi} q(\omega, x) \frac{H(\omega, y)}{1 + \mathfrak{a}(\omega)} \tag{2.21}$$

$$P(x, y) = \int_C \frac{d\omega}{\pi} \left[q(\omega, y) \frac{\tilde{H}(\omega, x)}{1 + \mathfrak{a}(\omega)} + \tilde{q}(\omega, y) \frac{H(\omega, x)}{1 + \mathfrak{a}(\omega)} \right]. \tag{2.22}$$

The behaviour of these functions in the limits $x, y \to i\eta/2$ or $x, y \to 0$ determines the correlations in finite volume or at finite temperature, respectively. Here we are only interested in the finite volume case, therefore we define

$$\Psi_{a,b} = \frac{\partial^a}{\partial x^a} \frac{\partial^b}{\partial y^b} \Psi(ix, iy) \Big|_{x,y=\eta/2}, \qquad P_{a,b} = \frac{\partial^a}{\partial x^a} \frac{\partial^b}{\partial y^b} P(ix, iy) \Big|_{x,y=\eta/2}. \tag{2.23}$$

As a final step we define

$$\omega_{a,b} = -\Psi_{a,b} - (-1)^b \frac{1}{2} \left(\frac{\partial}{\partial u} \right)^{a+b} K(iu) \Big|_{u=0}$$
$$W_{a,b} = -P_{a,b} + (-1)^b \frac{1}{2} \left(\frac{\partial}{\partial u} \right)^{a+b} \tilde{K}(iu) \Big|_{u=0}. \tag{2.24}$$

The objects $\Psi_{a,b}$ and $\omega_{a,b}$ are symmetric, whereas $P_{a,b}$ and $W_{a,b}$ are anti-symmetric with respect to the exchange of indices.

All short distance correlators can be expressed as finite combinations of the numbers $\omega_{a,b}$ and $W_{a,b}$. Explicit formulas can be found in the papers [57, 24] [4]. Simple examples for short

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[3]In the literature the function H was denoted by G. Here we changed the notation to avoid confusion with the Gaudin matrix.

[4]Our notations differ slightly from [57, 24]: The quantities ω and W correspond to ω and ω'/η of [57, 24].

range correlators are:

$$\langle \sigma_1^z \sigma_2^z \rangle_T = \coth(\eta)\omega_{0,0} + W_{1,0}$$

$$\langle \sigma_1^x \sigma_2^x \rangle_T = -\frac{\omega_{0,0}}{2\sinh(\eta)} - \frac{\cosh(\eta)}{2}W_{1,0}$$

$$\langle \sigma_1^z \sigma_3^z \rangle_T = 2\coth(2\eta)\omega_{0,0} + W_{1,0} + \tanh(\eta)\frac{\omega_{2,0} - 2\omega_{1,1}}{4} - \frac{\sinh^2(\eta)}{4}W_{2,1} \tag{2.25}$$

$$\langle \sigma_1^x \sigma_3^x \rangle_T = -\frac{1}{\sinh(2\eta)}\omega_{0,0} - \frac{\cosh(2\eta)}{2}W_{1,0} - \tanh(\eta)\cosh(2\eta)\frac{\omega_{2,0} - 2\omega_{1,1}}{8} +$$

$$+ \sinh^2(\eta)\frac{W_{2,1}}{8}.$$

2.2 Transforming back to algebraic expressions

The main idea to get the excited state correlations is to find the proper modification of the ground state formulas. In the previous section all the necessary ingredients were presented in the form of contour integrals. In the field of integrable models it is very common that the excited state quantities can be obtained by a simple change of the integration contours; this could be a promising direction even in our case. In particular, it is plausible that with certain changes of integration contours all intermediate results of [18] could be formulated for the finite volume excited states too, thus leading to factorized formulas [58]. However, it could be difficult to define the contours for *all* excited states, or to perform numerical computations in practice. Therefore we choose a different strategy: we transform the contour integrals into algebraic expressions, and perform the generalization to excited states afterwards.

The solution of (2.18) is the well known counting function:

$$\mathfrak{a}(x) = \left(\frac{\sin(x - i\eta/2)}{\sin(x + i\eta/2)}\right)^L \prod_{k=1}^N \frac{\sin(x - u_k + i\eta)}{\sin(x - u_k - i\eta)}. \tag{2.26}$$

The condition $1 + \mathfrak{a}(x) = 0$ encodes the Bethe equations. Therefore all integrals involving the weight function $1/(1 + \mathfrak{a}(x))$ are naturally equivalent to a sum over the Bethe roots. For example (2.20) is transformed into

$$H(x, x_1) = -q(x, x_1) - i\sum_{j=1}^N K(x - u_j)\frac{H(u_j, x_1)}{\mathfrak{a}'(u_j)} + \frac{K(x - x_1)}{1 + \mathfrak{a}(x_1)}. \tag{2.27}$$

Here we used the fact that the only pole of $H(x, x_1)$ within the contour is at $x = x_1$ with residue i. For the correlators we will be interested in the $x_{1,2} \to i\eta/2$ limit (and the first few derivatives) of $H(x_1, x_2)$. It can be seen from (2.26) that $\mathfrak{a}(x)$ has an order-L zero at $x = i\eta/2$, therefore we may substitute $\mathfrak{a}(x_1) \to 0$. This results in

$$H(x, x_1) = -q_+(x, x_1) - i\sum_{j=1}^N K(x - u_j)\frac{H(u_j, x_1)}{\mathfrak{a}'(u_j)}, \tag{2.28}$$

where

$$q_+(u, x) = -i(\cot(u - x + i\eta) - \cot(u - x)). \tag{2.29}$$

Introducing the function $F(x, y) = -iH(x, y)/\mathfrak{a}'(x)$ we have

$$F(x, x_1)(i\mathfrak{a}'(x)) = -q_+(x, x_1) + \sum_{j=1}^N K(x - u_j)F(u_j, x_1). \tag{2.30}$$

Specifying to the points $x = u_j$

$$F(u_j, x_1)(i\mathfrak{a}'(u_j)) = -q_+(u_j, x_1) + \sum_{k=1}^N K(x - u_k)F(u_k, x_1). \tag{2.31}$$

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It is easy to see from (2.26) that

$$i\mathfrak{a}'(u_j) = L\frac{\sinh(\eta)}{\sin(x - i\eta/2)\sin(x + i\eta/2)} + \sum_{k=1}^{N} K(u_j - u_k). \tag{2.32}$$

Therefore (2.31) can be written as

$$G_{jk}F(u_j, x_1) = q_+(u_j, x_1). \tag{2.33}$$

Evaluating the integral (2.21) for the function Ψ leads to

$$\Psi(x_1, x_2) = 2\sum_{j=1}^{N} F(u_j, x_1)q(u_j, x_2) - 2\frac{H(x, y)}{1 + \mathfrak{a}(x)} + 2\frac{q(y, x)}{1 + \mathfrak{a}(y)}. \tag{2.34}$$

This can be transformed using equation (2.28) into

$$\Psi(x_1, x_2) = 2\sum_{j=1}^{N} F(u_j, x_1)q_+(u_j, x_2), \tag{2.35}$$

which is written using (2.33) as

$$\Psi(x_1, x_2) = 2(q_+(u, x_1) \cdot G^{-1} \cdot q_+(u, x_2)). \tag{2.36}$$

Here the multiplication is understood as a summation over the Bethe roots and G^{-1} is the inverse of the Gaudin matrix. The derivatives of Ψ around the points $x_{1,2} = i\eta/2$ are given by

$$\Psi_{n,m} = \partial_{x_1}^n \partial_{x_2}^m \Psi(x_1, x_2)|_{x_{1,2}=i\eta/2} = 2(q_n \cdot G^{-1} \cdot q_m), \tag{2.37}$$

where we defined

$$q_j(u) = \partial_x^j q_+(u, ix)|_{x=\eta/2}. \tag{2.38}$$

Note that the functions $q_j(u)$ are the single-particle eigenvalue functions of the conserved charges. Also, it can be shown that the first row and column of $\Psi_{n,m}$ are related to the conserved charges of the Bethe state in question. Indeed, let e be a vector of length N with all elements equal to 1. It is easy to see from the definition of G that

$$Lq_0 = -G \cdot e. \tag{2.39}$$

It follows that the first row and first column of the matrix $\Psi_{n,m}$ contain the charge densities:

$$\Psi_{0,n} = \Psi_{n,0} = 2(q_n \cdot G^{-1} \cdot q_0) = -2\frac{1}{L}(q_n \cdot e) = -2\frac{1}{L}\sum_{j=1}^{N} q_n(u_j) = -2\frac{Q_n}{L}. \tag{2.40}$$

With similar steps the following algebraic representation can be derived for the function P:

$$P(x, y) = 2(-\tilde{q}_+(u, x) \cdot G^{-1} \cdot q_+(u, y) + q_+(u, x) \cdot G^{-1} \cdot \tilde{q}_+(u, y) - \\ - q_+(u, x) \cdot G^{-1} \cdot \tilde{G} \cdot G^{-1} \cdot q_+(u, y)), \tag{2.41}$$

where $\tilde{G}$ is an other $N \times N$ matrix with elements

$$\tilde{G}_{jk} = \tilde{K}(u_j - u_k) \tag{2.42}$$

and

$$\tilde{q}_+(u, x) = -i\cot(u - x + i\eta). \tag{2.43}$$

2.3 Conjectures for excited states

The factorization procedure for the correlation functions consists of the algebraic part and the physical part. Although the factorization for the excited states has not yet been considered in the literature, it is very natural to expect that the algebraic part of the construction holds also for the excited state of the model [58], especially in the light of the intermediate results of [18].

Regarding the physical part, formulas (2.36) and (2.41) are algebraic expressions that compute the physical part for the ground state wave function. Using these expressions, and supplied with the algebraic part, any correlation function can be expressed as a function of the ground state Bethe roots. Although the resulting formulas were not obtained by a direct algebraic manipulation of the coordinate space expressions, it is plausible that for any correlator there is a specific set of algebraic steps, that transforms the "raw" real space formulas into the factorized form, and these would just as well work for the excited states too. Similarly, for any correlator there is a specific set of manipulations that transform the contour integrals into the factorized form [17, 18], and with a change of contours they would provide the excited state quantities.

Based on the above arguments we formulate the following conjecture:

Conjecture 1. *In the XXZ chain the correlation functions of all regular states are given by the factorized formulas, provided that the physical part of the construction is computed via (2.37)-(2.41) using the exact excited state Bethe roots.*

The singular states including the rapidities $u_j = \pm i\eta/2$ are excluded from the conjecture. Their true wave function differs from (2.5), which becomes ill-defined. Similarly, the expression (2.37) for the building blocks $\Psi_{a,b}$ becomes singular. Similarly, we excluded the singular states of the root of unity points that also lead to ill-defined expressions due to the exact n-strings. It is plausible that factorization itself holds for such states, but the calculation of the physical part needs to be regularized. These cases will be considered in a future publication.

We performed numerical tests of conjecture 1. The methods and some examples of the numerical results are presented in Appendix A. In all cases perfect agreement was found.

3 Excited state correlations of the XXX model

In this section we treat the $SU(2)$-symmetric Heisenberg spin chain, which is defined through the Hamiltonian

$$H = \sum_{j=1}^{L} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \sigma_j^z \sigma_{j+1}^z - 1). \tag{3.1}$$

The coordinate space eigenstates and the Bethe equations can be obtained either as a scaling limit of the XXZ formulas, or independently by the Bethe Ansatz of the XXX type. For the sake of completeness here we summarize the relevant formulas.

The coordinate space wave functions can be written as

$$\phi_N(\{u\}_N|\{y\}) = \sum_{P \in S_N} \left[\prod_{1 \le m < n \le N} \frac{u_{P_m} - u_{P_n} + i}{u_{P_m} - u_{P_n}} \right] \left[\prod_{l=1}^{N} \left(\frac{u_{P_l} + i/2}{u_{P_l} - i/2} \right)^{y_l} \right]. \tag{3.2}$$

The Bethe equations take the form

$$\left(\frac{u_j - i/2}{u_j + i/2} \right)^L \prod_{k \ne j} \frac{u_j - u_k + i}{u_j - u_k - i} = 1, \tag{3.3}$$

and the energy eigenvalues are

$$E = - \sum_j \frac{2}{u_j^2 + 1/4}.$$

With the normalization given by (3.2) the norm of the Bethe state is

$$\langle \{u\}_N | \{u\}_N \rangle = \prod_j (u_j^2 + 1/4) \prod_{j<k} \frac{u_{jk}^2 + 1}{u_{jk}^2} \times \det G, \qquad (3.4)$$

where the XXX-type Gaudin matrix G is of the form

$$G_{jk} = \delta_{jk} \left(L \frac{1}{u_j^2 + 1/4} + \sum_{l=1}^{N} \varphi(u_{jl}) \right) - \varphi(u_{jk}), \qquad (3.5)$$

and

$$\varphi(u) = -\frac{2}{u^2 + 1}. \qquad (3.6)$$

It is known that in the XXX chain the Bethe states are highest weight states with respect to the $SU(2)$ symmetry and singlet states are obtained when $N = L/2$ [59]. The remaining states can be constructed using the global spin lowering operator S^-, which can be embedded naturally into to the Algebraic Bethe Ansatz framework [59]. In fact, the action S^- is equivalent to adding a Bethe particle with infinite rapidity. However, in the present paper we will only consider the highest weight cases.

3.1 Factorized correlation functions of the XXX chain

Here we present the known factorized results for the correlators of the finite XXX chain; we follow the presentation of [18, 17, 60]. It is important that the corresponding results do not follow from a scaling limit of the factorized XXZ formulas. In fact, the building blocks $\omega_{a,b}$ and $W_{a,b}$ defined in (2.24) become singular in the XXX limit and only the special combinations for the correlators remain finite. In other words, the physical and algebraic parts of the construction mix with each other. Nevertheless, certain basic objects such as the auxiliary functions $\mathfrak{a}(x)$, $H(x,y)$ and the function $\Psi(x,y)$ have simple scaling limits.

The auxiliary function of the XXX model is defined as

$$\log \mathfrak{a}(x) = a_0(x) + \frac{1}{2\pi} \int_{\mathcal{C}} \varphi(x-y) \log(1 + \mathfrak{a}(y)) dy, \qquad (3.7)$$

where $\varphi(x)$ is given by (3.6) and $\mathcal{C}$ is a closed contour around the real axis, which lies within the strip $|\Im z| < 1/2$. For the finite volume ground state the source term is

$$a_0(x) = L \log \frac{x - i/2}{x + i/2}. \qquad (3.8)$$

We define the functions

$$\Psi^{XXX}(x_1, x_2) = \frac{1}{\pi} \int_{\mathcal{C}} \frac{dy}{1 + \mathfrak{a}(y)} \frac{H(y, x_1)}{(y - x_2)(y - x_2 - i)}$$
$$\omega(x_1, x_2) = \frac{1}{2} + \frac{1}{2}((x_1 - x_2)^2 - 1)\Psi^{XXX}(ix_1, ix_2), \qquad (3.9)$$

where H is the solution to the linear integral equation

$$H^{XXX}(x, x_1) = -\frac{1}{(x - x_1)(x - x_1 - i)} + \frac{1}{\pi} \int_{\mathcal{C}} \frac{dy}{1 + \mathfrak{a}(y)} \frac{H^{XXX}(y, x_1)}{1 + (x - y)^2}. \qquad (3.10)$$

In the previous definitions it is important that the parameters $x_{1,2}$ are assumed to lie within the contour C.

For the finite volume ground state (or in the finite temperature case with zero magnetic field) all reduced density matrix elements can be expressed using the functions ω or Ψ alone. For the finite volume situation we define

$$\omega_{n,m} = \partial_{x_1}^n \partial_{x_2}^m \omega(x_1, x_2)|_{x_1, x_2 = 1/2} \qquad \Psi_{n,m}^{XXX} = \partial_{x_1}^n \partial_{x_2}^m \Psi^{XXX}(x_1, x_2)|_{x_1, x_2 = i/2} \qquad (3.11)$$

Then all ground state correlators can be expressed as a finite combination of the quantities $\Psi_{n,m}^{XXX}$, for example the simplest $z-z$ correlators read[5]

$$\langle \sigma_1^z \sigma_2^z \rangle = \frac{1}{3}(1 - \Psi_{0,0}^{XXX}) \tag{3.12}$$

$$\langle \sigma_1^z \sigma_3^z \rangle = \frac{1}{3}(1 - 4\Psi_{0,0}^{XXX} + \Psi_{1,1} - \frac{1}{2}\Psi_{2,0}^{XXX}) \tag{3.13}$$

$$\langle \sigma_1^z \sigma_4^z \rangle = \frac{1}{108}(36 + 288\Psi_{1,1}^{XXX} - 15\Psi_{2,2}^{XXX} + 10\Psi_{3,1}^{XXX} + \Psi_{2,0}^{XXX}(-156 + 12\Psi_{1,1}^{XXX} - 6\Psi_{2,0}^{XXX})$$
$$+ 2\Psi_{0,0}^{XXX}(-162 - 42\Psi_{1,1}^{XXX} + 3\Psi_{2,2}^{XXX} - 2\Psi_{3,1}^{XXX}) +$$
$$+ \Psi_{1,0}^{XXX}(84\Psi_{1,0}^{XXX} - 12\Psi_{2,1}^{XXX} + 4\Psi_{3,0}^{XXX})). \tag{3.14}$$

It is important that in the finite temperature case these formulas only hold if the magnetization is zero [17]. At finite magnetic field the resulting formulas are more complicated, because they involve additional objects that were called "moments" in [17]. They are defined through

$$\Phi_j(x) = \frac{1}{\pi} \int_{\mathcal{C}} dy \frac{y^{j-1} H(y,x)}{1 + \mathfrak{a}(y)}. \tag{3.15}$$

It can be shown that for the ground state in the thermodynamic limit

$$\lim_{L \to \infty} \Phi_j(x) \equiv \Phi_j^0(x) = (-i\partial_y)^{(j-1)} \left. \frac{2e^{iyx}}{1 + e^y} \right|_{y=0}. \tag{3.16}$$

The first few cases are

$$\Phi_1^0(x) = 1 \qquad \Phi_2^0(x) = x + \frac{i}{2} \qquad \Phi_3^0(x) = x^2 + ix. \tag{3.17}$$

The normalized moments are defined as

$$\tilde{\Phi}_j(x) = \Phi_j(x) - \Phi_j^0(x). \tag{3.18}$$

The first normalized moment is special because for the finite volume ground state (or the finite T case with $h = 0$) it vanishes for arbitrary x [17, 18]. It is also useful to introduce the symmetric combinations

$$\Delta_n(x_1, \ldots, x_n) = \frac{\det_n\left(\tilde{\Phi}_j(x_k)\right)}{\prod_{1 \le j \le k \le n} x_{jk}}. \tag{3.19}$$

It was conjectured in [17] that for $T, h \ne 0$ all local correlators can be expressed using the functions Ψ^{XXX} and the Δ_n. However, in contrast to the zero magnetization case it is not known how to compute the algebraic part for an arbitrary operator. In [17] the reduced density matrices up to length 3 were computed explicitly, but a general theory is still missing. An exponential form for the reduced density matrix is only available for zero magnetization, where all Δ_n vanish [17]. This fact has implications also for the excited state correlations.

Returning to the finite volume ground state, all of the previous integral formulas can be transformed into algebraic expressions, in the same way as in the XXZ case. We refrain from repeating the calculation and just present the final result for the function Ψ^{XXX}:

$$\Psi^{XXX}(x_1, x_2) = 2(q_+^{XXX}(u, x_1) \cdot G^{-1} \cdot q_+^{XXX}(u, x_2)), \tag{3.20}$$

where

$$q_+^{XXX}(u, x) = -\frac{1}{(u - x + i)(u - x)}. \tag{3.21}$$

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[5]In [60] the correlators are given in terms of ω, but for convenience we present them as a function of Ψ. In formula (11) of [60] there is a misprint in the case of $\langle \sigma_1^z \sigma_4^z \rangle$: the coefficient of the term $(1,0)(3,0)$ is written as -4/27, whereas correctly it is 4/27.

Also, the moments can be expressed as

$$\Phi_j(x) = 2(u^{(j-1)} \cdot G^{-1} \cdot q_+^{XXX}(u,x)) + 2\frac{x^{j-1}}{1+\mathfrak{a}(x)}. \qquad (3.22)$$

Note that (3.20) has the same structure as the corresponding formula (2.36) of the XXZ chain.

3.2 Excited state correlations

Here we formulate our conjecture for the excited states of the XXX model. In this case some care needs to be taken due to the $SU(2)$-symmetry of the model. Both the states and the operators organize themselves into $SU(2)$-multiplets, and the mean values within each multiplet can be calculated using the Wigner-Eckart theorem. The regular Bethe states are highest weight states, and the finite volume ground state is a singlet. A priori there is no reason to expect that the factorized formulas for the ground state should describe the correlations in an arbitrary $SU(2)$-multiplet. For example the $z-z$ and $x-x$ correlators are typically different. However, the factorized formulas could hold if the state is a singlet, or if the operator is a singlet. Regarding the second option it is useful to define the $SU(2)$-averaged operators

$$\bar{\mathcal{O}} = \int_{U \in SU(2)} \mathcal{D}U \; U\mathcal{O}U^\dagger,$$

where $\mathcal{D}U$ is the Haar-measure. Examples are given by the operators

$$\sigma_{1n} \equiv \frac{1}{3}\left(\sigma_1^x\sigma_n^x + \sigma_1^y\sigma_n^y + \sigma_1^z\sigma_n^z\right). \qquad (3.23)$$

For the group-invariant operators we formulate the following conjecture:

Conjecture 2. *For any regular Bethe state of the XXX chain the mean values of the $SU(2)$-invariant operators $\bar{\mathcal{O}}$ are given by the known factorized formulas, provided that the physical part of the construction is computed via (2.37) using the exact excited state Bethe roots.*

This conjecture includes those cases where the Bethe state is a singlet and the operator $\mathcal{O}$ is not, because in singlet states the mean values of $\mathcal{O}$ and $\bar{\mathcal{O}}$ coincide. We note that the present situation (namely that relatively simple results hold for group invariant operators) is analogous to the case of the quantum group invariant operators of the XXZ chain considered in [16].

We tested this conjecture for the operators σ_{1n} for $n = 2, 3, 4$. We performed exact diagonalization and found perfect agreement on chains with length up to $L = 12$; examples of our data is presented in Appendix A. Also, we performed coordinate Bethe Ansatz calculations for $N = 1$ and $N = 2$ and arbitrary L, and this also confirms the conjecture. The calculations are presented in Appendix B.

It is an interesting open question whether some kind of factorization holds for the mean values of an arbitrary operator $\mathcal{O}$ in non-singlet states. The results of [17, 18] suggest that the multiple integrals can indeed be factorized, and the generic case involves the moments too. In the following section we derive a new result for $\sigma_1^z\sigma_2^z$ which is valid for arbitrary eigenstates, and this result confirms the expectations.

4 The $\Delta \to 1$ limit

The goal of this section is to determine the local correlator $\sigma_1^z\sigma_2^z$ in non-singlet states of the XXX chain. To this order we employ a careful $\Delta \to 1+$ (or equivalently $\eta \to 0$) limit in finite size.

As the $\Delta \to 1$ limit is performed from above, the states organize themselves into $SU(2)$ multiplets. We follow one of these states with N particles and assume that the state vector evolves analytically as a function of Δ. We apply the Hellmann-Feynman theorem in the form

$$L(\langle \Psi_{XXX}|\sigma_1^z\sigma_2^z|\Psi_{XXX}\rangle - 1) = \lim_{\Delta\to 1}\frac{E_{XXZ}(\Delta) - E_{XXX}}{\Delta - 1}. \qquad (4.1)$$

At finite η the Bethe roots u_j are solutions to the equations

$$\left(\frac{\sin(u_j - i\eta/2)}{\sin(u_j + i\eta/2)}\right)^L \prod_{k \neq j} \frac{\sin(u_j - u_k + i\eta)}{\sin(u_j - u_k - i\eta)} = 1. \tag{4.2}$$

The energy is given by

$$E_{XXZ}(\Delta) = \sum_{j=1}^{N} -2i \sinh(\eta) \left(\cot(u_j + i\eta/2) - \cot(u_j - i\eta/2)\right). \tag{4.3}$$

We assume that the roots u_j scale smoothly into the XXX rapidities with the usual behaviour[6]

$$u_j \to \eta x_j, \tag{4.4}$$

such that x_j is a solution of the Bethe equations (3.3).

At the XXX point the energy becomes

$$E_{XXX} = \sum_{j=1}^{N} -2i \left(\frac{1}{x_j + i/2} - \frac{1}{x_j - i/2}\right). \tag{4.5}$$

The leading order correction in Δ is

$$\Delta - 1 = \frac{\eta^2}{2} + \dots, \tag{4.6}$$

therefore we need the $\mathcal{O}(\eta^2)$ corrections in the energy (4.3). The scaling (4.4) gives the correct leading behaviour, but the first corrections to the rapidities also need to be calculated. We write

$$u_j = \eta \tilde{u}_j, \qquad \tilde{u}_j = x_j + \eta^2 y_j + \mathcal{O}(\eta^4). \tag{4.7}$$

The y_j parameters can be determined from the Bethe equations. After taking the logarithm of (4.2) we perform the expansions

$$\log \frac{\sin(\eta(\tilde{u}_j - i/2))}{\sin(\eta(\tilde{u}_j + i/2))} = \log \frac{x_j - i/2}{x_j + i/2} + i\eta^2 \frac{1}{x_j^2 + 1/4} y_j + i\frac{\eta^2}{3} x_j + \mathcal{O}(\eta^4) \tag{4.8}$$

and

$$\log \frac{\sin(\eta(\tilde{u}_j - \tilde{u}_k + i/2))}{\sin(\eta(\tilde{u}_j - \tilde{u}_k - i/2))} =$$
$$\log \frac{x_j - x_k + i/2}{x_j - x_k - i/2} - i\eta^2 \frac{2}{(x_j - x_k)^2 + 1}(y_j - y_k) - 2i\frac{\eta^2}{3}(x_j - x_k) + \mathcal{O}(\eta^4). \tag{4.9}$$

This results in

$$0 = G_{jk} y_k + \frac{1}{3}\left((L - 2N)x_j + 2\sum_l x_l\right), \tag{4.10}$$

which fixes the y_j parameters.

The XXZ energy can be expanded as

$$E_{XXZ}(\Delta) = \left(1 + \frac{\eta^2}{6}\right)E_{XXX} - \frac{2}{3}\eta^2 N - \eta^2 \sum_{j=1}^{N} 2q_1(x_j)y_j + \mathcal{O}(\eta^4) \tag{4.11}$$

with

$$q_1(x) = -\frac{2x}{(x^2 + 1)^2}. \tag{4.12}$$

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[6]The states that are not highest weight are obtained when some of the u_j don't scale to 0: this results in infinite x_j parameters. However, here we only consider the highest weight cases.

Putting everything together

$$\langle \Psi_{XXX} | \sigma_1^z \sigma_2^z | \Psi_{XXX} \rangle =$$

$$= \frac{L + E_{XXX}}{3L} + \frac{2(L - 2N)}{3L} \left[1 + 2 \sum_{j,k=1}^{N} q_1(x_j) G_{jk}^{-1} x_k \right] + \frac{2}{3L} \left(\sum_j x_j \right) \sum_{j,k=1}^{N} 4q_1(x_j) G_{jk}^{-1}. \tag{4.13}$$

This is a new result of the present work. It is interesting to compare it to equation (29) of [17], which states, that in the finite temperature case with a finite magnetic field the corresponding correlator can be expressed as

$$\langle \sigma_1^z \sigma_2^z \rangle_{T,h} = \frac{2}{3} \Delta_2(i/2, i/2) + \frac{1}{3}(1 - \Psi_{0,0}^{XXX}), \tag{4.14}$$

where $\Delta_2(i/2, i/2)$ is the homogeneous limit of the function defined in (3.19). In Appendix C it is shown that if we substitute our finite volume formulas (2.37) and (3.22) into (4.14), then we obtain our result (4.13). This is an independent confirmation of the conjecture that the formulas of [17] with the non-vanishing moments could work for all excited states of the XXX model.

It is also interesting to specify the result (4.13) to singlet states. The derivation holds also in this case, but as a result of the $SU(2)$-invariance the $z - z$ correlator is related directly to the energy, and the correlator is given simply by the first term of (4.13). On the other hand, the second term vanishes automatically due to $N = L/2$. It follows that (4.13) can be valid only if

$$\left(\sum_j x_j \right) \left(\sum_{j,k=1}^{N} 4q_1(x_j) G_{jk}^{-1} \right) = 0. \tag{4.15}$$

Quite interestingly both factors are zero for all singlet states, and this can be shown using the following arguments.

The vanishing of the first factor follows from the sum rules originally discovered by Baxter in the context of the XYZ model [61][7]. In the XYZ model the sum of the rapidities in an arbitrary eigenstate with $N = L/2$ is an integer multiple of $\pi/2$, and this property survives also in the XXZ limit, see for example equation (17) of [62] or (151) of [44]. In the $\Delta \to 1$ limit the rapidities get rescaled as (4.4), and if all the resulting XXX rapidities are finite (ie. the state is really a singlet), then the only possibility is that this integer multiple of $\pi/2$ is actually zero.

The vanishing of the second factor follows from the fact, that at zero magnetization the first moment $\Phi_1(x)$ vanishes for arbitrary x [17], and from (3.22) we have

$$0 = \partial_x \tilde{\Phi}_1(x)|_{x \to i/2} = \sum_{j,k=1}^{N} 4q_1(x_j) G_{jk}^{-1}. \tag{4.16}$$

5 Conclusions and Outlook

In this work we have studied factorized formulas for the excited state mean values of the XXZ and XXX spin chains. The main idea was that the known construction for the ground state correlators should give correct results for the excited states as well, if the physical part is calculated through certain algebraic expressions, that can be obtained from the integral representations. Our main conjectures 1 and 2 were tested using exact diagonalization and real space calculations with low particle numbers $N = 1, 2$. The findings can be summarized as follows:

- In the XXZ case the simple generalization of the ground state formulas to excited states works for almost all states and arbitrary $\Delta \neq 1$ values. The only exclusions are Bethe

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[7]The idea of this proof was first suggested to us by Andreas Klümper.

states with the pair of singular rapidities $\pm i\eta/2$, and the special states of the root of unity points $\Delta = \cos(p\pi/q)$. However, we expect that the exclusion of these states is a just a technical difficulty, which can be easily circumvented by a proper regularization.

- At the XXX point the factorized formulas give correct answers for group-invariant operators. This is true for all states except those with singular rapidities $\pm i/2$, where regularization is needed.

We would like to stress that our results can be applied whenever the algebraic part of the construction is already available. In particular this means that the distance of the correlator is limited to small values; in principle the algebraic part could be computed for any distance, but the resulting expressions become too big and the calculation becomes unfeasible [25].

There are several open questions that deserve further study. First of all, it needs to be shown rigorously whether our main conjectures 1 and 2 are correct. We have presented evidence that supports the conjectures, but a rigorous proof would be desirable. Also, it needs to be sorted out how to regularize the factorized formulas to accommodate the states with singular rapidities. We expect that simple regularization schemes already available in the literature would solve these problems.

An other, more ambitious task is to consider the non-singlet operators in non-singlet states of the XXX model. The situation is analogous to the case of the finite temperature correlations with finite magnetic field. Explicit factorization of multiple integral formulas for this case has been performed earlier in [17], and it was conjectured that all short-range correlators can be expressed using the functions Ψ^{XXX} and Δ_n. Our result (4.13) about the nearest neighbour $z-z$ correlator has the exact same structure as the corresponding formula of [17]. This evidence, together with the fact that the multiple integral formulas in the finite T and finite size problems have the same structure [17, 18] suggest that the generic finite size mean values will take the same form as in the infinite volume, finite T problem with finite magnetic field.

Finally, it would be worthwhile to consider the thermodynamic limit of our finite size formulas. In large volumes the summation over the rapidities leads to integrals over the root densities, and due to the string hypothesis one has to deal with root densities and other auxiliary functions for all string types. Performing this calculation would establish a bridge to the TBA-like description of the physical part conjectured in [41] for $\Delta > 1$. Also, it is important to consider the thermodynamic limit in the $\Delta < 1$ case, because its relevance to quench problems [63, 36].

We hope to return to these questions in future research.

Acknowledgments

A Numerical tests

We performed exact diagonalization in order to check our conjectures. Our procedure included the following steps:

- We numerically constructed the transfer matrices (2.2) (and their XXX counterparts) for a few arbitrarily chosen rapidity parameters. We exactly diagonalized finite sums of transfer matrices. This method has an advantage over diagonalizing the Hamiltonian itself, because it removes all unwanted degeneracies and it immediately provides the Bethe Ansatz states. We considered spin chains up to length $L = 12$.

- For each eigenstate we numerically computed the mean values of certain short range correlators. In the XXZ case we considered the operators $\sigma_1^a \sigma_n^a$ with $a = x, z$ and $n = 2, 3, 4$. On the other hand, in the XXX case we chose the averaged operators σ_{1n}.

- The Bethe roots of the individual states were found with the method originally developed in [52]. The idea is to numerically compute the transfer matrix eigenvalues for a finite set of rapidities, and afterwards use the famous $T - Q$ relations to find the Q function and the Bethe roots. For the formulas relevant to the XXX model we refer the reader to [49], which also includes tables of the XXX Bethe roots up to $L = 12$ (tables with $L > 8$ are found in the supplementary material on the arxiv).
- We computed the predictions for the correlators using the factorized formulas, and compared them to the numerics from exact diagonalization.

It is important that this method enabled us to treat all excited Bethe states; even the states with the singular rapidities are found directly.

In the XXZ case we considered both the massive and massless regimes. It was observed that Conjecture 1 holds for all states except the singular ones which include the special rapidities $\pm i\eta/2$. Tables 1-5 include examples of our numerical data; here we chose the points $\Delta = 2$ and $\Delta = 0.7$ with $L = 8$ in both cases. Tables 1 and 4 show the energies, particle numbers, momentum quantum numbers and the correlations of the first few states, and the root content of the states is shown in Tables 3 and 5. The numerical errors in the predictions for the correlators were typically of the order $10^{-14} - 10^{-16}$; examples for the errors are given in table 2. For some states a larger error is observed (up to $\mathcal{O}(10^{-6})$), but this is probably related to failure of our numerical program to accurately resolve degeneracies in the spectrum: it can be seen from the root content that these states are not parity invariant, therefore they have a degenerate partner with negated root content.

In the XXX case it was found that Conjecture 2 indeed holds: the factorized formulas give correct answer for the singlet operators σ_{1n} for all regular states. Table 6 shows the energies, particle numbers, momentum quantum numbers and the correlations in all highest weight states at $L = 8$. Table 7 shows the corresponding rapidities.

B Real space calculations with $N = 1$ and $N = 2$

Here we consider the XXX model and perform real space calculations in the case of low particle numbers $N = 1, 2$. We only consider the $SU(2)$ averaged operators

$$\sigma_{1n} = \frac{1}{3} \left[\sigma_1^z \sigma_n^z + 2(\sigma_1^+ \sigma_n^- + \sigma_1^- \sigma_n^+) \right].$$

Throughout the calculations we will use the parametrization

$$a = e^{ip} = \frac{u + i/2}{u - i/2}, \tag{B.1}$$

where u is the Bethe rapidity and p is the one-particle pseudo-momentum.

B.1 $N = 1$

In the one-particle case the un-normalized wave function can be written as

$$\phi(a|y) = a^y. \tag{B.2}$$

The norm is

$$\langle a|a \rangle = L. \tag{B.3}$$

A simple direct calculation gives the following value for the correlator:

$$\langle a|\sigma_{1n}|a \rangle = \frac{1}{3} \left[\frac{L - 4}{L} + 2\frac{a^{n-1} + a^{-(n-1)}}{L} \right]. \tag{B.4}$$

This result has to be compared to the conjectures of Section 3. In the one-particle case the Gaudin matrix is just a scalar:

$$G = L\frac{1}{u^2 + 1/4}. \tag{B.5}$$

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Then (3.20) gives simply

$$\Psi^{XXX}(x,y) = \frac{2(u^2 + 1/4)}{L((x - i/2 - u)^2 + 1/4)((y - i/2 - u)^2 + 1/4)}. \tag{B.6}$$

It is a straightforward calculation to check that the factorized results (3.12)-(3.14) indeed reproduce (B.4) with $n = 3$ and $n = 4$.

B.2 $N = 2$

Here we choose the following normalization for the wave function:

$$\phi(a,b|x,y) = a^x b^y + a^y b^x S(a,b), \qquad x < y, \tag{B.7}$$

where S is the scattering amplitude which es expressed in the a-variables as

$$S(a,b) = -\frac{1 - 2b + ab}{1 - 2a + ab}.$$

The Bethe equations are

$$a^L S(a,b) = b^L S(b,a) = 1.$$

We performed the real space calculations using the program Mathematica. As a warm up we calculated the norm of the wave function (B.7). After substituting the Bethe equations we obtained

$$\langle a,b|a,b\rangle = L^2 - L\left(1 + \frac{aS(a,b) - bS(b,a)}{a - b}\right).$$

It is easy to check that this is equal to the Gaudin determinant up to the overall normalization differences between (B.7) and (2.4).

Afterwards we performed the real space calculation of the correlators σ_{1n} and obtained them as rational functions of a and b. After substituting the Bethe equations the results take the form (2.17), where the C_j polynomials only depend on n but not on L[8]. The results are lengthy and we refrain from listing them here.

We also calculated the predictions of Conjecture 2. In the present case the Gaudin matrix (3.5) has a simple structure and the function Ψ^{XXX} is easily calculated using two Bethe rapidities u and v as

$$\Psi^{XXX}(x,y) = \frac{2}{\det G} \times$$
$$\times \begin{pmatrix} \frac{1}{(u-x+i/2)^2+1/4} \\ \frac{1}{(v-x+i/2)^2+1/4} \end{pmatrix} \begin{pmatrix} \frac{L}{u^2+1/4} - \frac{2}{(u-v)^2+1} & -\frac{2}{(u-v)^2+1} \\ -\frac{2}{(u-v)^2+1} & \frac{L}{v^2+1/4} - \frac{2}{(u-v)^2+1} \end{pmatrix} \begin{pmatrix} \frac{1}{(u-y+i/2)^2+1/4} \\ \frac{1}{(v-y+i/2)^2+1/4} \end{pmatrix}. \tag{B.8}$$

Using the formulas (3.12)-(3.14) and making the substitutions

$$a = \frac{u + i/2}{u - i/2} \qquad b = \frac{v + i/2}{v - i/2}$$

the predictions can be compared to real space calculations.

For both σ_{13} and σ_{14} we found exact agreement between the resulting formulas.

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[8]It is important that in the present calculation the distance n is simply a parameter. This is in contrast with the multiple integrals of the ABA method, where the number of the integrals grows with n. On the other hand, the ABA results are valid for arbitrary N, whereas the coordinate BA calculations become increasingly complicated as we increase N.

C The correlator $\langle \sigma_1^z \sigma_2^z \rangle$ in finite and infinite volume

Here we evaluate formula (4.14) assuming that the quantities $\Delta_2(0,0)$ and $\Psi^{XXX}(0,0)$ are given by the finite size formulas of Section 3. We recall that

$$\Psi_{0,0}^{XXX} = 2q_0(u) \cdot G^{-1} \cdot q_0(u), \qquad \Phi_j(x) = 2u^{j-1} \cdot G^{-1} \cdot q_+(u-x) + 2\frac{x^{j-1}}{1+\mathfrak{a}(x)},$$

and

$$q_k(u) = (\partial_x)^k q_+(u-x)|_{x=i/2}, \tag{C.1}$$

and the homogeneous limit of the determinants Δ_n can be calculated as

$$\Delta_n(i/2,\ldots,i/2) = \det\left[\frac{\tilde{\Phi}_{j,k}}{(k-1)!} \right],$$

where

$$\tilde{\Phi}_{j,k} \equiv (\partial_x)^{k-1} \tilde{\Phi}_j(x)\Big|_{x=i/2} =$$

$$= 2u^{j-1} \cdot G^{-1} \cdot q_{k-1}(u) + 2(\partial_x)^{k-1} x^{j-1}\big|_{x=i/2} - \left[(\partial_x)^{k-1}(-i\partial_y)^{j-1} \frac{2e^{iyx}}{1+e^y} \right]\Bigg|_{y=0,x=i/2}.$$

In the present case

$$\Delta_2(0,0) = \tilde{\Phi}_{1,1}\tilde{\Phi}_{2,2} - \tilde{\Phi}_{1,2}\tilde{\Phi}_{2,1}.$$

For $k=1$ we have

$$G^{-1} \cdot q_0(u) = -\frac{1}{L}e,$$

where e is a vector with all elements equal 1. It follows that

$$\Psi^{XXX}(0,0) = -\frac{2\sum_j q_0(u_j)}{L} = -\frac{E}{L}, \qquad \Phi_{1,1} = -\frac{2N}{L} + 2, \qquad \Phi_{2,1} = -\frac{2\sum_j u_j}{L}.$$

For the normalized $\tilde{\Phi}$ quantities we have

$$\tilde{\Phi}_{1,1} = -\frac{2N}{L} + 1 \qquad\qquad \tilde{\Phi}_{2,1} = -\frac{2\sum_j u_j}{L}$$

$$\tilde{\Phi}_{1,2} = 2e \cdot G^{-1} \cdot q_1(u) \qquad\qquad \tilde{\Phi}_{2,2} = 2u \cdot G^{-1} \cdot q_1(u) + 1.$$

Putting everything together formula (4.14) indeed yields (4.13).

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	E	N	J	$\langle\sigma_1^z\sigma_2^z\rangle$	$\langle\sigma_1^z\sigma_3^z\rangle$	$\langle\sigma_1^z\sigma_4^z\rangle$	$\langle\sigma_1^x\sigma_2^x\rangle$	$\langle\sigma_1^x\sigma_3^x\rangle$	$\langle\sigma_1^x\sigma_4^x\rangle$
1	-36.1577	4	-0	1.00000	-0.77381	0.55947	-0.54364	-0.48605	0.13559
2	-35.1227	4	4	-1.00000	-0.87304	0.75209	-0.75785	-0.32213	0.05255
3	-31.9185	3	4	-0.00000	-0.44530	0.10801	0.14514	-0.54961	0.24317
4*	-30.4979	4	4	1.00000	-0.47190	-0.03764	0.21568	-0.43421	-0.08096
5	-29.4276	3	1	0.00000	-0.46515	0.12383	0.16438	-0.37408	0.01858
6	-29.1610	4	1	-1.00000	-0.44374	-0.03196	0.18650	-0.37882	0.02717
7	-28.3967	4	3	-1.00000	-0.48454	-0.00201	0.24404	-0.29025	0.14360
8	-28.2969	4	-0	1.00000	-0.61733	0.30334	-0.15418	-0.15122	0.20686
9	-27.4782	3	3	-0.00000	-0.40745	0.26602	-0.21529	-0.30994	0.02627
10	-26.9793	3	0	-0.00000	-0.48056	0.36874	-0.26012	-0.20565	0.22899
11	-26.3751	4	2	-1.00000	-0.40264	-0.15462	-0.00260	-0.24581	0.06465
12	-26.2433	3	2	0.00000	-0.39599	0.22330	-0.18488	-0.24422	-0.12448
13	-25.6569	4	3	1.00000	-0.40636	-0.08168	-0.01196	-0.19720	-0.18874
14	-25.2867	4	2	1.00000	-0.41200	-0.03927	0.17598	-0.16842	-0.08671
15	-24.7075	4	2	1.00000	-0.46980	-0.01595	0.20141	-0.07442	0.05612
16	-24.4287	3	2	0.00000	-0.46749	0.11275	0.22015	-0.05931	-0.03089
17	-24.2925	4	1	1.00000	-0.48180	-0.01760	-0.00060	-0.03648	0.18215
18*	-24.0000	4	-0	-1.00000	-0.50000	-0.00000	-0.00000	-0.00000	-0.25000
19	-23.6520	3	1	0.00000	-0.43058	0.22230	-0.10473	-0.04767	0.06131
20	-23.3698	4	4	-1.00000	-0.42333	0.06085	-0.23535	-0.03728	0.03861
21	-23.1266	2	0	0.00000	0.00725	0.10369	0.23868	-0.45266	0.34116
22	-23.0670	3	4	-0.00000	-0.36663	0.17000	-0.00872	-0.07505	0.02696
23	-21.4400	3	3	-0.00000	-0.34113	-0.03974	0.20530	0.00113	-0.13741
24	-21.3810	4	3	-1.00000	-0.35755	-0.04656	0.05623	0.02124	-0.15380
25	-21.2481	4	1	-1.00000	-0.43533	-0.04543	0.22808	0.10733	-0.16686
26	-21.0118	2	2	-0.00000	0.00472	0.09993	0.24151	-0.31796	-0.00000
27*	-20.8791	4	4	1.00000	-0.31781	-0.18963	0.09706	0.01287	-0.21640
28	-20.2925	2	1	-0.00000	0.02467	0.27299	0.20234	-0.29296	-0.01285
29	-20.2844	4	0	1.00000	-0.36483	-0.19859	0.13415	0.09705	0.02393
30*	-20.0000	3	-0	0.00000	-0.00000	-0.25000	0.00000	-0.25000	-0.12500
31	-20.0000	3	0	-0.00000	-0.35714	-0.07143	0.21429	0.10714	-0.03571
32	-19.3685	4	0	1.00000	-0.02885	-0.22253	-0.24533	-0.18168	-0.07996
33	-19.0707	3	1	-0.00000	-0.03722	-0.14017	-0.03592	-0.15470	0.02689
34	-18.9234	4	1	-1.00000	-0.03682	-0.16601	-0.26115	-0.14589	0.05193
35	-18.8157	3	2	-0.00000	-0.01470	-0.24160	-0.01204	-0.16129	-0.15896
36	-18.6357	4	3	1.00000	-0.06897	-0.14533	-0.28570	-0.09576	0.17589
37	-18.5112	4	2	-1.00000	-0.01151	-0.26087	-0.25683	-0.14544	-0.10876
38	-18.4910	3	3	0.00000	-0.06635	-0.09953	-0.06773	-0.08934	0.17045
39	-18.2825	4	4	-1.00000	-0.16403	-0.04601	-0.31077	0.02137	0.37728
40	-17.9394	4	2	1.00000	-0.06788	-0.16993	-0.19477	-0.05333	0.14711
41	-17.8276	3	1	0.00000	0.01651	-0.22108	-0.01696	-0.13074	-0.17328
42	-17.8109	3	4	0.00000	-0.14863	0.04346	-0.17412	0.03545	0.40029

Table 1: List of the correlation functions in the first few eigenstates of the XXZ model for $\Delta = 2$ and $L = 8$. Whenever degenerate states are connected to each other by space or spin reflection we only kept one of them in the list. In the table N denotes the number of Bethe particles, $J = 0 \ldots (L/2)$ is the overall momentum quantum number. States marked with a star include the singular rapidities $\pm i\eta/2$. The factorized formulas correctly reproduce the correlators in all cases except the singular states.

	E	$\langle\sigma_1^z\sigma_2^z\rangle$	$\langle\sigma_1^z\sigma_3^z\rangle$	$\langle\sigma_1^z\sigma_4^z\rangle$	$\langle\sigma_1^x\sigma_2^x\rangle$	$\langle\sigma_1^x\sigma_3^x\rangle$	$\langle\sigma_1^x\sigma_4^x\rangle$
1	-36.1577	2.2×10^{-16}	8.9×10^{-16}	1.8×10^{-14}	2.3×10^{-15}	1.9×10^{-16}	1.5×10^{-14}
2	-35.1227	8.9×10^{-16}	4.4×10^{-15}	5.1×10^{-15}	1.1×10^{-15}	4×10^{-16}	8.4×10^{-15}
3	-31.9185	1.6×10^{-15}	5.5×10^{-15}	2.3×10^{-14}	1.1×10^{-16}	2.2×10^{-15}	1.5×10^{-14}
4*	-30.4979	NaN	NaN	NaN	NaN	NaN	NaN
5	-29.4276	1×10^{-15}	3.1×10^{-15}	3.2×10^{-14}	1.1×10^{-15}	4.4×10^{-16}	2.2×10^{-14}
6	-29.1610	2.1×10^{-15}	7.1×10^{-16}	2.2×10^{-14}	2.4×10^{-15}	9.2×10^{-15}	1.7×10^{-14}
7	-28.3967	8.9×10^{-16}	1.1×10^{-15}	1.3×10^{-14}	2.8×10^{-16}	5.6×10^{-17}	1×10^{-14}
8	-28.2969	8.9×10^{-16}	5.6×10^{-16}	2×10^{-14}	1.1×10^{-15}	3.9×10^{-16}	4.4×10^{-15}
9	-27.4782	2.4×10^{-15}	7.8×10^{-16}	1.1×10^{-14}	5.6×10^{-17}	1×10^{-15}	1.1×10^{-14}
10	-26.9793	1.1×10^{-15}	3.9×10^{-16}	3.6×10^{-15}	4.4×10^{-16}	1.9×10^{-15}	7.7×10^{-16}
11	-26.3751	5.6×10^{-17}	1.7×10^{-16}	1.6×10^{-15}	3.2×10^{-15}	2.6×10^{-15}	8.7×10^{-16}
12	-26.2433	7.8×10^{-16}	5.4×10^{-15}	4.9×10^{-15}	8.6×10^{-16}	2.8×10^{-16}	7.8×10^{-15}
13	-25.6569	3.1×10^{-13}	4.1×10^{-12}	3.6×10^{-13}	2.4×10^{-13}	2.5×10^{-12}	9×10^{-12}
14	-25.2867	1.1×10^{-15}	4.2×10^{-14}	9.6×10^{-14}	2.2×10^{-15}	2×10^{-14}	3.7×10^{-14}
15	-24.7075	1.1×10^{-15}	3.2×10^{-15}	3.7×10^{-15}	1.2×10^{-15}	2×10^{-15}	4.3×10^{-15}
16	-24.4287	3.3×10^{-16}	1.7×10^{-15}	3×10^{-15}	8.3×10^{-16}	5×10^{-16}	3.7×10^{-15}
17	-24.2925	1.3×10^{-15}	1.7×10^{-15}	9×10^{-15}	1.2×10^{-15}	1.7×10^{-16}	7.6×10^{-15}
18*	-24.0000	NaN	NaN	NaN	NaN	NaN	NaN
19	-23.6520	1.3×10^{-15}	1.6×10^{-15}	1.4×10^{-17}	2×10^{-16}	4.9×10^{-16}	6.7×10^{-15}
20	-23.3698	2.8×10^{-14}	5.8×10^{-13}	4.9×10^{-14}	3×10^{-14}	2.7×10^{-13}	2.3×10^{-13}
21	-23.1266	5.3×10^{-16}	6.7×10^{-16}	1.2×10^{-15}	4.9×10^{-15}	4.8×10^{-15}	4.2×10^{-16}
22	-23.0670	7.8×10^{-16}	1.4×10^{-15}	1.5×10^{-14}	1.6×10^{-15}	1.2×10^{-15}	6.7×10^{-15}
23	-21.4400	5×10^{-16}	1.6×10^{-15}	1.4×10^{-14}	3.5×10^{-16}	5.6×10^{-16}	7.4×10^{-15}
24	-21.3810	1.8×10^{-15}	2.2×10^{-15}	1.5×10^{-14}	9.7×10^{-16}	7.8×10^{-16}	1.8×10^{-14}
25	-21.2481	1.1×10^{-10}	3.2×10^{-10}	6.2×10^{-09}	1.1×10^{-10}	5×10^{-10}	1×10^{-08}
26	-21.0118	5.6×10^{-16}	1×10^{-15}	1.8×10^{-14}	4.4×10^{-16}	1.4×10^{-15}	1.5×10^{-14}
27*	-20.8791	NaN	NaN	NaN	NaN	NaN	NaN
28	-20.2925	1.1×10^{-15}	1.8×10^{-15}	9.5×10^{-15}	3.3×10^{-16}	3.5×10^{-18}	1×10^{-15}
29	-20.2844	3.9×10^{-16}	5.6×10^{-17}	5.1×10^{-15}	6.7×10^{-16}	5.6×10^{-16}	3.3×10^{-15}
30*	-20.0000	NaN	NaN	NaN	NaN	NaN	NaN
31	-20.0000	1.7×10^{-16}	3.2×10^{-15}	6.9×10^{-15}	7.2×10^{-16}	6×10^{-16}	1×10^{-14}
32	-19.3685	4.1×10^{-15}	6.6×10^{-13}	1.3×10^{-12}	2.2×10^{-15}	3.6×10^{-13}	4.3×10^{-12}
33	-19.0707	5×10^{-15}	1×10^{-14}	2.7×10^{-14}	2.3×10^{-15}	1.8×10^{-14}	4.1×10^{-14}
34	-18.9234	7.4×10^{-16}	1.5×10^{-15}	8×10^{-15}	4.7×10^{-16}	1.1×10^{-15}	2.8×10^{-15}
35	-18.8157	1.4×10^{-13}	8.3×10^{-14}	3.8×10^{-13}	1.2×10^{-13}	2.7×10^{-13}	4.1×10^{-13}
36	-18.6357	7.5×10^{-16}	6.9×10^{-15}	1×10^{-14}	2.7×10^{-15}	1.1×10^{-14}	1.7×10^{-14}
37	-18.5112	3.3×10^{-15}	2.1×10^{-14}	3.1×10^{-14}	3.8×10^{-15}	3.1×10^{-14}	1.4×10^{-14}
38	-18.4910	6.5×10^{-16}	2.5×10^{-15}	9.5×10^{-15}	1.7×10^{-15}	1.5×10^{-15}	8.3×10^{-15}
39	-18.2825	2.4×10^{-15}	6.7×10^{-15}	1×10^{-14}	4.5×10^{-15}	7.8×10^{-15}	6.4×10^{-15}
40	-17.9394	7.9×10^{-16}	4.7×10^{-16}	1.7×10^{-14}	1.3×10^{-15}	1.1×10^{-16}	1.6×10^{-14}
41	-17.8276	8.3×10^{-09}	4.2×10^{-08}	2.1×10^{-06}	8.5×10^{-09}	4.7×10^{-08}	1.8×10^{-06}
42	-17.8109	1.9×10^{-16}	8.9×10^{-16}	9.4×10^{-15}	2.6×10^{-15}	1.9×10^{-15}	5.1×10^{-15}

Table 2: List of the numerical errors for the calculation of correlation functions in the first few eigenstates of the XXZ model for $\Delta = 2$ and $L = 8$. Whenever degenerate states are connected to each other by space or spin reflection we only kept one of them in the list. States marked with a star include the singular rapidities $\pm i\eta/2$; in these cases the factorized correlations are not computed, because the corresponding expressions are ill defined and need regularization.

1	-0.16931	0.16931	-0.67692	0.67692
2	0	0.36517	-0.36517	-1.57080
3	0	-0.32582	0.32582	
4*	0.18374	-0.18374	-0.65848i	0.65848i
5	0.08677	-0.22094	-0.68609	
6	0.03422	-0.33383	-0.63559+0.65091i	-0.63559-0.65091i
7	0.01707	0.37440	-0.98113+0.61044i	-0.98113-0.61044i
8	-0.15916	0.15916	-1.57080+0.76282i	-1.57080-0.76282i
9	0.03724	0.36952	-0.78636	
10	0.14958	-0.14958	-1.57080	
11	-0.32884	0.38712	-0.81454+0.63423i	-0.81454-0.63423i
12	-0.24837	0.39897	-0.73478	
13	0.16131	0.27757-0.65850i	0.27757+0.65850i	-0.71645
14	-0.18828	-0.70030	0.44429-0.65896i	0.44429+0.65896i
15	0.13162	0.57017	1.21990+0.75972i	1.21990-0.75972i
16	0.10182	0.46175	1.39682	
17	-0.17285	0.57575	1.36934+0.76935i	1.36934-0.76935i
18*	0	-0.65848i	0.65848i	-1.57080
19	-0.17459	0.49080	1.47126	
20	0	1.57080	-1.57080-0.35091i	-1.57080+0.35091i
21	0.13785	-0.13785		
22	0	-0.87010	0.87010	
23	-0.28888	-0.81653	0.91977	
24	-0.32729	1.26917	-1.25634+0.47792i	-1.25634-0.47792i
25	0.38794	-0.17943+0.65848i	-0.17943-0.65848i	1.54172
26	0.08798	0.40130		
27*	-0.65848i	0.65848i	-0.71693	0.71693
28	-0.16404	0.43048		
29	-0.58190	0.58190	1.57080-0.78528i	1.57080+0.78528i
30*	0	0.65848i	-0.65848i	
31	0.52360	-0.52360	-1.57080	
32	0.04168	-0.04168	1.33652i	-1.33652i
33	-0.11381	0.52304-0.65895i	0.52304+0.65895i	
34	-0.10163	0.54749	0.56247-1.32488i	0.56247+1.32488i
35	0.18614	0.41430+0.65859i	0.41430-0.65859i	
36	0.08631	0.98431	1.03549+1.36050i	1.03549-1.36050i
37	0.18214	0.45323	0.46771+1.33824i	0.46771-1.33824i
38	0.07731	0.98921-0.64251i	0.98921+0.64251i	
39	0	-1.57080	-1.57080+1.41573i	-1.57080-1.41573i
40	-0.19570	1.07228	1.13250-1.35314i	1.13250+1.35314i
41	0.33452	-0.12946+0.65848i	-0.12946-0.65848i	
42	0	-1.57080+0.69453i	1.57080-0.69453i	

Table 3: Bethe root content in the first few states at $\Delta = 2$, $L = 8$. Whenever degenerate states are connected to each other by space or spin reflection we only kept one of them in the list. States marked with a star include the singular rapidities $\pm i\eta/2$.

	E	N	J	$\langle\sigma_1^z\sigma_2^z\rangle$	$\langle\sigma_1^z\sigma_3^z\rangle$	$\langle\sigma_1^z\sigma_4^z\rangle$	$\langle\sigma_1^x\sigma_2^x\rangle$	$\langle\sigma_1^x\sigma_3^x\rangle$	$\langle\sigma_1^x\sigma_4^x\rangle$
1	-18.8078	4	0	-0.55523	0.17411	-0.17857	-0.63116	0.30760	-0.29264
2	-17.1789	3	4	-0.37804	0.05519	0.09571	-0.59137	0.34351	-0.26778
3	-16.3463	4	4	-0.70565	0.46055	-0.50445	-0.42467	0.07272	0.15524
4*	-15.3317	4	4	-0.43852	-0.07926	0.18411	-0.45475	-0.05900	0.20029
5	-14.5716	4	1	-0.34075	-0.08169	0.08617	-0.44147	0.12485	0.10379
6	-14.4385	3	1	-0.40282	0.07618	0.11199	-0.41142	0.01125	0.15510
7	-13.5074	3	3	-0.25626	0.10481	-0.15772	-0.40452	0.09997	0.01195
8	-13.0793	4	3	-0.45086	-0.00254	0.21038	-0.30966	0.15167	-0.16087
9	-12.8462	2	0	0.01812	0.11432	0.22837	-0.45923	0.36597	-0.27813
10	-12.3510	3	2	-0.25615	0.07089	-0.13928	-0.33228	-0.05083	-0.07248
11	-12.2647	4	2	-0.29826	-0.29478	-0.01439	-0.31215	0.13104	-0.17247
12	-11.8077	4	3	-0.23238	-0.19759	-0.07003	-0.30665	-0.14760	-0.03699
13	-11.7284	3	0	-0.44022	0.34938	-0.26275	-0.22895	0.23119	-0.00485
14	-11.5032	4	2	-0.20335	-0.11094	-0.04214	-0.29777	-0.07649	0.05979
15	-11.4450	4	0	-0.50248	0.37331	-0.48284	-0.18945	0.18769	0.10722
16	-10.6975	2	2	0.01426	0.11117	0.23182	-0.32358	-0.00000	0.18678
17	-10.3143	2	1	0.06514	0.26935	0.16551	-0.31745	0.03794	0.03011
18	-10.0405	3	2	-0.19673	-0.09617	0.12150	-0.20867	0.08873	0.19586
19	-10.0132	3	4	-0.13796	0.00401	0.09603	-0.22754	-0.00317	-0.09340
20	-9.9144	4	4	-0.19588	-0.02394	-0.37565	-0.20109	0.06464	0.04398
21	-9.6574	4	2	-0.40732	-0.04904	0.12664	-0.11103	0.07340	0.21892
22*	-9.6000	3	0	-0.00000	-0.25000	-0.00000	-0.25000	-0.12500	0.00000
23	-9.5110	3	1	-0.24273	-0.07193	0.10480	-0.15949	0.18795	0.05760
24	-9.1958	4	1	-0.37899	-0.10244	-0.01856	-0.09209	0.18674	0.14175
25	-8.8184	4	3	-0.06300	-0.13441	-0.24467	-0.17910	-0.14975	0.12408
26	-8.7270	3	3	-0.10430	-0.21899	0.08270	-0.15893	-0.14497	-0.01306
27*	-8.4253	4	4	-0.05373	-0.22139	-0.22437	-0.15778	-0.25000	-0.07695
28*	-8.4000	4	0	-0.50000	-0.00000	0.00000	-0.00000	-0.25000	0.00000
29	-8.0873	4	0	-0.24214	-0.05748	-0.21013	-0.07071	-0.18598	-0.20935
30	-7.9465	4	1	-0.07037	-0.06535	-0.25547	-0.12203	-0.00078	-0.09941
31	-7.9343	4	2	-0.02443	-0.30708	-0.24022	-0.13734	-0.15321	0.03579
32	-7.7855	3	1	0.06800	-0.18074	-0.06856	-0.16039	-0.14461	0.07699
33	-7.7574	3	1	-0.17221	0.08450	-0.15357	-0.07457	-0.07944	-0.15130
34	-7.6784	2	0	0.13829	0.20570	0.01856	-0.17830	-0.21003	0.08810
35	-7.5238	3	2	-0.25121	-0.05371	0.05552	-0.03231	-0.23776	-0.12077
36	-7.4061	2	3	0.03020	0.27341	0.19640	-0.12345	0.00431	-0.13014
37	-7.0942	3	0	-0.06867	-0.23635	-0.02045	-0.06936	0.00256	0.07524
38	-7.0588	3	3	-0.11784	0.05867	-0.19845	-0.04993	0.12789	0.04083
39	-6.9067	4	3	-0.20247	-0.03306	-0.26446	-0.01080	0.18554	0.06709
40	-6.8721	4	1	-0.29782	-0.15369	0.18784	0.02473	-0.21028	-0.02506
41	-6.8651	2	2	0.11190	0.23114	0.01427	-0.11823	-0.00000	-0.05325
42	-6.8000	1	4	0.50000	0.50000	0.50000	-0.25000	0.25000	-0.25000

Table 4: List of the correlation functions in the first few eigenstates of the XXZ model for $\Delta = 0.7$ and $L = 8$. Whenever degenerate states are connected to each other by space or spin reflection we only kept one of them in the list. In the table N denotes the number of Bethe particles, $J = 0\ldots(L/2)$ is the overall momentum quantum number. States marked with a star include the singular rapidities $\pm i\eta/2$. The factorized formulas correctly reproduce the correlators in all cases except the singular states.

1	0.10290i	-0.10290i	-0.41679i	0.41679i
2	0	-0.21412i	0.21412i	
3	0	-0.19828i	0.19828i	-1.57080
4*	-0.11284i	0.11284i	0.39770	-0.39770
5	0.05523i	-0.13596i	-0.45671i	1.57080+0.53745i
6	0.03604i	-0.16484i	-0.57849i	
7	0.01595i	0.22953i	-0.62652i	
8	0.02501i	0.22723i	-0.50508i	-1.57080+0.25284i
9	0.09368i	-0.09368i		
10	-0.17550i	0.24105i	-0.59845i	
11	-0.15054i	0.24671i	-0.47828i	-1.57080+0.38211i
12	0.09671i	-0.39772+0.17721i	0.39772+0.17721i	-0.45113i
13	0.08816i	-0.08816i	1.57080	
14	-0.11623i	-0.44009i	-0.39811+0.27816i	0.39811+0.27816i
15	-0.08831i	0.08831i	-1.57080-0.67395i	1.57080+0.67395i
16	0.07157i	0.30728i		
17	-0.10461i	0.32066i		
18	0.05874i	0.27040i	-1.57080-0.20712i	
19	0	0.64966i	-0.64966i	
20	0	0.54135i	-0.54135i	-1.57080
21	0.06005i	0.26612i	1.57080+0.46830i	-1.57080-0.79448i
22*	0	-0.39770	0.39770	
23	-0.10375i	0.28673i	1.57080-0.11375i	
24	-0.10232i	0.28371i	-1.57080+0.55219i	1.57080-0.73359i
25	-0.17362i	-0.51089i	0.56888i	-1.57080+0.11563i
26	-0.18992i	-0.62127i	0.66947i	
27*	0.39770	-0.39770	-0.44618i	0.44618i
28*	0	-0.39770	0.39770	-1.57080
29	0.02845i	-0.02845i	0.81043	-0.81043
30	-0.07634i	-0.39925+0.36643i	0.39925+0.36643i	1.57080-0.65652i
31	0.11033i	-0.39820+0.29906i	0.39820+0.29906i	-1.57080-0.70845i
32	0.22711i	-0.39770-0.09840i	0.39770-0.09840i	
33	-0.06572i	0.43479+0.65780i	-0.43479+0.65780i	
34	-0.33388i	0.33388i		
35	0.11339i	-0.42937+0.61132i	0.42937+0.61132i	
36	0.05033i	0.96789i		
37	0.30501i	-0.30501i	-1.57080	
38	0.03844i	0.70050i	1.57080-0.30395i	
39	0.03543i	0.59541i	1.57080+0.23043i	-1.57080-0.86128i
40	0.20450i	0.39770-0.07752i	-0.39770-0.07752i	-1.57080-0.04947i
41	-0.12135i	0.99398i		
42	0			

Table 5: Bethe root content in the first few states at $\Delta = 0.7$, $L = 8$. Note that here the ground state rapidities are all purely imaginary and in the excited states the strings are centered around the imaginary axis; this is simply a result of our intentions to apply the same conventions for both the $\Delta < 1$ and $\Delta > 1$ regimes, as explained in the main text. Whenever degenerate states are connected to each other by space or spin reflection we only kept one of them in the list. States marked with a star include the singular rapidities $\pm i\eta/2$.

	E	N	J	$\langle\sigma_{12}\rangle$	$\langle\sigma_{13}\rangle$	$\langle\sigma_{14}\rangle$
1	-22.60437	4	0	-0.60852	0.26104	-0.25194
2	-20.51368	3	4	-0.52140	0.23367	-0.12039
3*	-18.79851	4	4	-0.44994	-0.06564	0.19466
4	-17.83495	3	1	-0.40979	0.04117	0.12669
5	-16.58059	3	3	-0.35752	0.10082	-0.04167
6	-15.41855	3	2	-0.30911	-0.01099	-0.10432
7	-15.20775	2	0	-0.30032	0.27600	-0.09850
8	-14.82843	4	3	-0.28452	-0.16667	-0.04882
9	-14.47214	4	2	-0.26967	-0.09213	0.02847
10	-13.06814	2	2	-0.21117	0.03583	0.19537
11	-12.80656	3	4	-0.20027	0.00522	-0.05067
12	-12.57649	2	1	-0.19069	0.10541	0.08528
13*	-12.00000	3	0	-0.16667	-0.16667	0
14	-11.43569	3	3	-0.14315	-0.16631	0.01031
15*	-11.04351	4	4	-0.12681	-0.24628	-0.13355
16	-10.90444	4	0	-0.12102	-0.16067	-0.21444
17	-10.51351	3	1	-0.10473	-0.02145	-0.16411
18	-10.38787	3	2	-0.09949	-0.19118	-0.07307
19	-10.05073	3	1	-0.08545	-0.16809	0.03510
20	-9.78017	2	0	-0.07417	-0.07899	0.05466
21	-9.74806	2	3	-0.07284	0.10541	-0.03257
22	-9.17157	4	1	-0.04882	-0.16667	-0.28452
23	-9.03461	2	2	-0.04311	0.08643	-0.02556
24	-8.00000	2	4	0	-0.16667	0.08333
25	-8.00000	1	4	0	0.33333	0
26	-8.00000	3	0	0	-0.16667	-0.08333
27	-6.93819	3	3	0.04424	-0.24910	-0.09301
28	-6.82843	1	3	0.04882	0.16667	0.28452
29	-6.49119	4	0	0.06287	-0.43370	-0.20029
30	-6.25194	2	1	0.07284	-0.10541	0.03257
31	-6.19358	3	2	0.07527	-0.29784	-0.15595
32	-5.52786	4	2	0.10301	-0.24120	-0.19514
33	-4.42923	3	1	0.14878	-0.18496	-0.21317
34*	-4.00000	2	4	0.16667	-0.16667	0
35	-4.00000	1	2	0.16667	0	0.16667
36	-3.42351	2	3	0.19069	-0.10541	-0.08528
37	-3.01208	2	0	0.20783	-0.03034	-0.12283
38	-2.67977	3	4	0.22168	-0.07222	-0.32894
39	-2.21710	3	3	0.24095	-0.01875	-0.32682
40*	-2.15798	4	4	0.24342	-0.02141	-0.39445
41	-1.89725	2	2	0.25428	0.04441	-0.16981
42	-1.17157	1	1	0.28452	0.16667	0.04882

Table 6: List of the correlation functions in the highest weight states of the XXX model for $L = 8$. Whenever degenerate states are connected to each other by space reflection we only kept one of them in the list. In the table N denotes the number of Bethe particles, $J = 0 \ldots (L/2)$ is the overall momentum quantum number. States marked with a star include the singular rapidities $\pm i/2$. The factorized formulas correctly reproduce the correlators in all cases except the singular states.

1	-0.12947	0.12947	0.52501	-0.52501
2	0	-0.26391	0.26391	
3*	-0.14247	0.14247	0.50000i	-0.50000i
4	0.05372	-0.19358	-0.65085	
5	0.02382	0.28883	-0.72050	
6	-0.20971	0.30632	-0.68166	
7	-0.11412	0.11412		
8	0.12119	0.22521+0.50003i	0.22521-0.50003i	-0.57161
9	-0.14701	-0.55707	0.35204-0.50056i	0.35204+0.50056i
10	0.08200	0.35910		
11	0	0.76302	-0.76302	
12	-0.13044	0.37844		
13*	0	-0.50000i	0.50000i	
14	-0.23264	-0.72324	0.79382	
15*	0.50000i	-0.50000i	-0.56383	0.56383
16	-0.04131	0.04131	-1.02571i	1.02571i
17	-0.08884	0.62094-0.51103i	0.62094+0.51103i	
18	0.13981	0.55039-0.50687i	0.55039+0.50687i	
19	0.27866	-0.11627+0.50000i	-0.11627-0.50000i	
20	0.39874	-0.39874		
21	0.05396	0.91480		
22	-0.08379	0.24433	-0.08027+1.00559i	-0.08027-1.00559i
23	-0.15507	0.94957		
24	0.28868	0.86603		
25	0			
26	0.34781	-0.67391-0.51443i	-0.67391+0.51443i	
27	0.31492+0.50018i	0.31492-0.50018i	0.59567	
28	-0.20711			
29	0.46326-0.50229i	-0.46326+0.50229i	-0.46326-0.50229i	0.46326+0.50229i
30	-0.42841	0.98514		
31	-0.21341-0.49999i	-0.21341+0.49999i	0.77127	
32	-0.22056	0.66912	-0.22428+1.00225i	-0.22428-1.00225i
33	0.86575	-0.74066-0.51922i	-0.74066+0.51922i	
34*	0.50000i	-0.50000i		
35	-0.50000			
36	-0.41534+0.49953i	-0.41534-0.49953i		
37	-1.03826	1.03826		
38	0	1.00092i	-1.00092i	
39	-0.63120	-0.61576-0.98815i	-0.61576+0.98815i	
40*	0.50000i	-0.50000i	1.55613i	-1.55613i
41	-0.95114-0.54450i	-0.95114+0.54450i		
42	-1.20711			

Table 7: Bethe root content in the heighest weight states of the XXX model for $L = 8$. Whenever degenerate states are connected to each other by space reflection we only kept one of them in the list. The singular states including rapidities $\pm i/2$ are denoted by a star.