Overlaps between eigenstates of the XXZ spin-1/2 chain and a class of simple product states

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Abstract. We consider a class of quantum quenches in the spin-1/2 XXZ chain, where the initial state is of a simple product form. Specific examples are the Néel state, the dimer state and the $q$-deformed dimer state. We compute determinant formulas for finite volume overlaps between the initial state and arbitrary eigenstates of the spin chain Hamiltonian. These results could serve as a basis for calculating the time dependence of correlation functions following the quantum quench.

Keywords: integrable spin chains (vertex models), quantum integrability (Bethe ansatz), exact results, quantum quenches

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1. Introduction

One-dimensional exactly solvable quantum-mechanical models, and in particular integrable spin chains, have attracted a lot of interest since Bethe’s famous solution of the spin-1/2 XXX Heisenberg model in 1931 [1]. A common property of these theories is that the spectrum of the Hamiltonian can be computed with exact methods [2] and even thermodynamic quantities can be obtained in the infinite volume limit [3, 4]. While it was believed for a long time that the Bethe Ansatz is not effective in calculating correlation functions, this situation has drastically changed over the last 25 years. The discovery of determinant formulas for certain overlaps between Bethe states [5] and the solution of the so-called inverse problem of the Algebraic Bethe Ansatz [6, 7] lead to multiple integral formulas for short-range correlations in the ground state of the anti-ferromagnetic XXZ model [8, 9], which were later extended to the finite temperature case using the so-called Quantum Transfer Matrix method [10]. Subsequently it was discovered that the multiple integral formulas can be factorized: it is possible to express them as sums of products of simple integrals (see [11] and references therein).

This tremendous progress concerns correlation functions in thermal equilibrium. On the other hand, in recent years non-equilibrium problems such as quantum quenches and the questions of thermalization stood in the forefront of research of both integrable and non-integrable models [12]. This motivates the development of exact methods for correlation functions of integrable models in non-equilibrium situations.

While there have been recent advances on quantum quenches in the 1D Bose-gas [13–17] there are practically no exact results available for the interacting XXZ spin chain. The long-time limit of local observables was considered in the papers [18, 19].
but these works bypass the derivation of the actual time dependence of the correlation functions and give predictions based on the so-called Generalized Gibbs Ensemble (GGE) hypothesis [20]. This hypothesis states that, in integrable models the long-time limit of observables follows from a statistical physical ensemble incorporating all local conserved charges with appropriate Lagrange-multipliers, which are fixed by the expectation values of the charges in the initial state. Whereas the GGE was shown to be valid for models equivalent to free-fermions [21, 22], there are no actual proofs available for the interacting case and the predictions of [18, 19] have not yet been confirmed by independent methods. A recent exact result for quantum quenches in the XXZ chain also includes a non-linear integral equation for the so-called dynamical free energy (the Loschmidt echo at imaginary times) [23]. While this quantity is not directly relevant to the correlation functions, the paper [23] showed that the techniques of the Boundary Algebraic Bethe Ansatz can be used in quench problems. We should note that the dynamical free energy was considered also in [24] with independent methods based on the GGE hypothesis.

One route towards time dependent observables after a quantum quench is through the form factor expansion. Assuming that at $t = 0$ the system is in a state $|\Psi_0\rangle$, and for $t > 0$ the time evolution is governed by a Hamiltonian $H$, inserting two complete sets of normalized states leads to

$$\mathcal{O}(t) = \sum_{n,m} \langle \Psi_0 | n \rangle \langle n | \mathcal{O} | m \rangle \langle m | \Psi_0 \rangle e^{i(tE_n - E_m)}. \tag{1}$$

The ingredients in the formula above are the energy eigenvalues, the matrix elements of the operator (the form factors) and the exact overlaps between the eigenstates and the initial state. Although the Bethe Ansatz provides the exact spectrum and there are results available for the form factors too [6, 8], the overlaps are typically very hard to compute. If the state $|\Psi_0\rangle$ is of a sufficiently simple form, then the scalar product with a Bethe state can be written down as a sum over permutations, but such formulas are inconvenient for further analytical or numerical calculations.

In the present work we compute determinant formulas for the overlaps between Bethe states and a restricted class of initial states which are products of simple two-site vectors. The specific examples are the Néel state, the dimer and $q$-deformed dimer states (the definitions are given below). Our results could serve as a basis for the evaluation of the expansion (1) with either analytical or numerical methods [25].

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The structure of the paper is as follows. In section 2, we review the Bethe Ansatz solution of the XXZ chain and provide the necessary definitions. In section 3 we compute the overlaps for generic anisotropy $\Delta$. Section 4 includes numerical results for the overlaps between the Néel state and the ground states in the anti-ferromagnetic regime $\Delta > -1$. Also we present a comparison to the exact result of [23] for the infinite volume limit of the ground state overlap with the Néel. Section 5 concerns the XXX limit. Finally we conclude in section 6.
2. The quench problem and the Bethe Ansatz

Consider the anti-ferromagnetic spin-1/2 XXZ Heisenberg model on a chain of length $2M$ with periodic boundary conditions. The Hamiltonian reads

$$H_{XXZ} = \sum_{j=1}^{2M} (\sigma^x_j \sigma^x_{j+1} + \sigma^y_j \sigma^y_{j+1} + \Delta (\sigma^z_j \sigma^z_{j+1} - 1)) . \quad (2)$$

Here $\Delta$ is the anisotropy parameter; we will consider both the massive ($\Delta > 1$) and massless ($-1 < \Delta \leq 1$) regimes.

This Hamiltonian can be diagonalized by the Bethe Ansatz \[1\], \[26–28\]. As usual we choose the ferromagnetic state $|F+\rangle$ with all spins up as the reference state and construct interacting spin waves above this state. The explicit coordinate space wave function for a state with $M$ down spins is

$$\tilde{\Psi}_{2M}(\lambda_1, \ldots, \lambda_M | s_1, \ldots, s_M) = \sum_{\mathcal{P} \in \mathcal{O}_M} \prod_j F(\lambda_{P_j}, s_j) \prod_{j<k} \frac{\sinh(\lambda_{P_j} - \lambda_{P_k} - \eta)}{\sinh(\lambda_{P_j} - \lambda_{P_k})} \quad (3)$$

with

$$F(\lambda, s) = \sinh(\eta) \sinh^{s-1}(\lambda + \eta/2) \sinh^{2N-s}(\lambda - \eta/2) . \quad (4)$$

Here $s_j$ denote the positions of the down spins, and we assume $s_j < s_k$ for $j < k$. The parameter $\eta$ is given by the relation $\Delta = \cosh \eta$ and the rapidities $\{\lambda_j\}$ characterize the spin waves. The state (3) is an eigenstate if the Bethe equations hold:

$$\left( \frac{\sinh(\lambda_j - \eta/2)}{\sinh(\lambda_j + \eta/2)} \right)^{2M} \prod_{k \neq j} \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)} = 1. \quad (5)$$

In this case the energy is given by

$$E = \sum_j e(\lambda_j) , \quad \text{where} \quad e(u) = \frac{4\sinh^2 \eta}{\cosh(2u) - \cosh \eta} . \quad (6)$$

In the regime $\Delta > 1$ the typical one-string solutions to the Bethe equations lie on the imaginary axis, while for $\Delta < 1$ they are on the real axis. The $\Delta = 1$ case has to be treated separately, see section 4.

Consider a non-equilibrium situation where at $t = 0$ the system is prepared in a state $|\Psi_0\rangle$ and for $t > 0$ it evolves according to the Hamiltonian (2). The time evolution of a physical observable $O$ can be computed by inserting two complete sets of (not normalized) states:

$$O(t) = \sum_{\{\lambda\}, \{\mu\}} \frac{\langle \Psi_0 | \{\lambda\}_M \rangle \langle \{\lambda\}_M | O(\{\mu\}_M \{\mu\}_M \Psi_0) \exp \left\{ it \sum_j (e(\lambda_j) - e(\mu_j)) \right\}}{\langle \{\lambda\}_M | \{\lambda\}_M \rangle \langle \{\mu\}_M | \{\mu\}_M \rangle} . \quad (7)$$

Here we assumed for simplicity that $|\Psi_0\rangle$ has fixed magnetization equal to 0. The essential ingredients in the formula above are the energy eigenvalues, the form factors and the normalized overlaps. While the Bethe Ansatz is very efficient in computing the
energies through (5)–(6), and there are determinant formulas available for form factors too [6, 8], there are practically no results available for the overlaps.

In this work we consider three specific choices for $|\Psi_0\rangle$ and compute determinant formulas for the overlap with the Bethe states. In all three cases there exists a local Hamiltonian with a gapped spectrum and a twofold degenerate ground state level, which is spanned by $|\Psi_0\rangle$ and $P|\Psi_0\rangle$ with $P$ being the translation operator by one site. The three vectors and the corresponding Hamiltonians are:

- The Néel state:
  $$|\Psi_0\rangle = |N\rangle \equiv \otimes^M |+ -\rangle,$$
  which is a ground state of the XXZ Hamiltonian in the $\Delta \to \infty$ limit.

- The dimer state:
  $$|\Psi_0\rangle = |D\rangle \equiv \otimes^M \frac{|+ -\rangle - |- +\rangle}{\sqrt{2}},$$
  which is a ground state of the Majumdar–Ghosh Hamiltonian [29].

- The $q$-deformed dimer state:
  $$|\Psi_0\rangle = |qD\rangle \equiv \otimes^M \frac{q^{1/2} |+ -\rangle - q^{-1/2} |+ +\rangle}{\sqrt{|q| + 1 / |q|}},$$
  where $q$ is given by the relation $\Delta = (q + 1 / q)/2$. This vector is a ground state of the $q$-deformed Majumdar–Ghosh Hamiltonian [30].

The overlaps are in principle known because the coordinate Bethe Ansatz provides the exact wave functions. For example, in the case of the Néel state we have

$$\langle N| \{ \lambda \}_M \rangle = \sum_{P \in \sigma_M} \prod_j F(\lambda_{P_j}, 2j) \prod_{j > k} \frac{\sinh(\lambda_{P_j} - \lambda_{P_k} - \eta)}{\sinh(\lambda_{P_j} - \lambda_{P_k})}$$

(8)

with $F(u, s)$ given by (4). However, such representations are not convenient for either analytical or numerical treatment, because the number of terms grows as $M!$ and there are no evident ways to sum them up. On the other hand, formulas like (8) can be used to check the determinant formulas calculated below. We wish to note that simple relations can be established between the overlaps with the different initial states based on the coordinate Bethe Ansatz wave function. For example,

$$\langle D| \{ \lambda \}_M \rangle = \langle N| \{ \lambda \}_M \rangle \times \prod_{j=1}^{M} \frac{1}{\sqrt{2}} \left[ 1 - \frac{\sinh(\lambda_j - \eta / 2)}{\sinh(\lambda_j + \eta / 2)} \right].$$

(9)

Such relations can also be used as a check of the formulas presented below.

In the next section we will make use of the Algebraic Bethe Ansatz, which is an alternative method for the diagonalization of the XXZ Hamiltonian. Its basic object is the monodromy matrix which is defined as

$$T(u) = L_1(u) \ldots L_{2M}(u),$$

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where \( L_j(u) \) are local Lax-operators given by
\[
L_j(u) = R_{0j}(u - \eta / 2),
\]
and the \( R \)-matrix is
\[
R(u) = \begin{pmatrix}
\sinh(u + \eta) & \sinh(u) \\
\sinh(\eta) & \sinh(u) \\
\sinh(\eta) & \sinh(u + \eta)
\end{pmatrix}.
\]
In (10) the index \( j \) refers to the spin on site \( j \) whereas 0 refers to the auxiliary space. The monodromy matrix is written in auxiliary space as
\[
T(u) = \begin{pmatrix}
A(u) & B(u) \\
C(u) & D(u)
\end{pmatrix}.
\]
Eigenstates with a total number of \( M \) down spins are then constructed as
\[
|\{\lambda\}_M\rangle = \prod_{j=1}^{M} B(\lambda_j) |F_+\rangle.
\]
It can be shown that with the present normalizations these states are exactly identical to those given by the expression (3).

Besides the overlaps it is also essential to know the norms of Bethe states [31, 32]. It was derived in [32] that if the rapidities satisfy the Bethe equations then the norm is given by the determinant formula
\[
\langle \lambda_1, ..., \lambda_M | \lambda_1, ..., \lambda_M \rangle = \sinh^M(\eta) \prod_j \left( \sinh(\lambda_j + \eta / 2) \sinh(\lambda_j - \eta / 2) \right)^{2M}
\times \prod_{j \neq k} f(\lambda_j, \lambda_k) \times \det G,
\]
where
\[
f(u) = \frac{\sinh(u + \eta)}{\sinh(u)},
\]
and \( G \) is the Gaudin matrix:
\[
G_{jk} = \delta_{j,k} \left( 2M \varphi(\lambda_j, \eta / 2) - \sum_l \varphi(\lambda_j - \lambda_l, \eta) \right) + \varphi(\lambda_j - \lambda_k, \eta)
\]
with
\[
\varphi(a, b) = \frac{\sinh(2b)}{\sinh(a-b) \sinh(a+b)}.
\]
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\[ + \quad + \quad \sinh(u + \eta) \quad + \quad + \quad \sinh(u) \quad + \quad + \quad \sinh(\eta) \]

**Figure 1.** The 6–vertex model weights as given by the trigonometric $R$–matrix (11). Here $u$ is attached to the horizontal line and $0$ to the vertical one.

Consider the boundary transfer matrix of a spin chain of length $M$:

\[ R(u) = \text{Tr}_0 \{ K^+(u) \ T_1(u) \ K^-(u) \ T_2(u) \} . \]  

Here

\[ T_1(u) = \bar{L}_M(u) \ldots \bar{L}_1(u) , \]  

where $\bar{L}_j(u)$ are given by

\[ \bar{L}_j(u) = R_{0j}(u - \xi_j) \]  

and

\[ T_2(u) = \gamma(u) \sigma^y \ T_1^{iu}(u) \]  

The parameters $\xi_j$ are inhomogeneities which will be specified below. The function $\gamma(u)$ is related to the crossing properties of the $R$-matrix; in the present normalization $\gamma(u) = (-1)^M$. For simplicity we assume that $M$ is even and we will use the relation

\[ (-1)^M = 1 \]

throughout this work. The operator in (15) is depicted in figure 2.

**3. Boundary algebraic Bethe ansatz for the overlaps**

In this section we derive determinant formulas for the overlaps between arbitrary Bethe states and the three initial states specified above. The method we apply is the Boundary Algebraic Bethe Ansatz, which was originally devised to diagonalize open spin chains with boundary magnetic fields and to compute correlation functions in these models [33, 34]. For a thorough explanation of the Boundary Algebraic Bethe Ansatz we refer the reader to [34]; here we only use the relevant results of [34].

Consider the boundary transfer matrix of a spin chain of length $M$:

\[ R(u) = \text{Tr}_0 \{ K^+(u) \ T_1(u) \ K^-(u) \ T_2(u) \} . \]  

Here

\[ T_1(u) = \bar{L}_M(u) \ldots \bar{L}_1(u) , \]  

where $\bar{L}_j(u)$ are given by

\[ \bar{L}_j(u) = R_{0j}(u - \xi_j) \]  

and

\[ T_2(u) = \gamma(u) \sigma^y \ T_1^{iu}(u) \]  

The parameters $\xi_j$ are inhomogeneities which will be specified below. The function $\gamma(u)$ is related to the crossing properties of the $R$-matrix; in the present normalization $\gamma(u) = (-1)^M$. For simplicity we assume that $M$ is even and we will use the relation

\[ (-1)^M = 1 \]

throughout this work. The operator in (15) is depicted in figure 2.
The matrices $K^\pm$ in (14) are the diagonal solutions to the reflection equation [33, 34]:

$$K^\pm(u) = K(u \pm \eta / 2, \xi_\pm) \quad \text{with} \quad K(u, \xi) = \begin{pmatrix} \sinh(\xi + u) & 0 \\ 0 & \sinh(\xi - u) \end{pmatrix}. $$

In the original problem of the boundary spin chain the parameters $\xi_\pm$ are related to the boundary magnetic fields. Here we leave them unspecified for the moment.

The common eigenstates of the operators $R(u)$ can be created from the ferromagnetic reference state $|F_+\rangle = |++\cdots\rangle$ as

$$|\{\lambda\}_n\rangle = \prod_{j=1}^n B_+(\lambda_j) |F_+\rangle, $$

where the $B_+(u)$ operators are defined through

$$T^u_{11}(\lambda) K^u_+(\lambda) T^u_{22}(\lambda) = \begin{pmatrix} A_+(u) & C_+(u) \\ B_+(u) & D_+(u) \end{pmatrix}. $$

Writing out the components we obtain

$$B_+(u) = B_1(u) D_1(-u) k_1(u) - D_1(u) B_1(-u) k_2(u) $$

with

$$k_1(u) = \sinh(\xi_+ + u + \eta / 2) \quad k_2(u) = \sinh(\xi_- - u - \eta / 2). $$

Alternatively, eigenstates could be created from the spin-reversed reference state $|F_-\rangle = |--\cdots\rangle$ by the action of the operators $C_+(u)$ for which we have

$$C_+(u) = -A_1(u) C_1(-u) k_1(u) + C_1(u) A_1(-u) k_2(u). $$

Consider the scalar product

$$Z(\mu, \xi, \xi_+) = \langle F_+| C_+(\mu_1) \cdots C_+(\mu_M) |F_-\rangle. $$

Using (20) it can be interpreted as a partition function of a 6-vertex model with boundary conditions and inhomogeneities defined in figure 3. The two-site states $|\nu(u)\rangle$ which serve as the boundary condition on the left hand side follow from (19) and (20):

$$\langle \nu(u) | = -\sinh(\xi_+ + u + \eta / 2) \langle + + | + \sinh(\xi_- - u - \eta / 2) \langle - + |. $$

The six-vertex model vertex weights are invariant under the reflection along the NW diagonal and a simultaneous sign change of the rapidities. Performing these operations we obtain the partition function represented in figure 4. Here the horizontal lines can be interpreted as the $B$-operators of a spin chain of length $2M$ with alternating inhomogeneities given by $\{\mu_j, -\mu_j\}$. In the homogeneous limit $\mu_j \rightarrow 0$ we have

$$\lim_{\mu_j \rightarrow 0} Z(\mu, \xi, \xi_+) = \langle \Psi(\xi_+) | B(-\xi_1 + \eta / 2) B(-\xi_2 + \eta / 2) \cdots B(-\xi_M + \eta / 2) |F_+\rangle, $$

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\[
\langle v(\mu_M) | = | + \mu_M + -\mu_M + + - + - + \\
\vdots \quad \vdots \\
\langle v(\mu_1) | = | + \mu_1 + -\mu_1 + + - + - + \\
\xi_M \quad \cdots \quad \xi_1
\]

**Figure 3.** The 6–vertex model configuration whose partition function gives the scalar product defined in (21).

\[
|v(\mu_1) \rangle |v(\mu_2) \rangle \cdots |v(\mu_M) \rangle \\
+ + + + + - - - - - - \\
\vdots \quad \vdots \\
+ + + + + - - - - - - \\
-\mu_M \mu_M -\mu_2 \mu_1
\]

**Figure 4.** The 6–vertex model configuration obtained from the one in figure 3 after a reflection along the NW diagonal. Here the horizontal lines can be interpreted as \(B\)-operators acting on the ferromagnetic reference state of an inhomogeneous spin chain. The two–site states \(|v(\mu_j)\rangle\) create a boundary condition at the top, which in the \(\mu_j \to 0\) limit generates the desired overlaps between Bethe states and the initial states \(|\Psi_0\rangle\).

\[
\langle \Psi(\xi_\pm) | = \bigotimes M \langle v | \langle v | = -\sinh (\xi_+ + \eta / 2) \langle + + | + \sinh (\xi_+ - \eta / 2) \langle - + |,
\]

and the \(B\)-operators are defined by the monodromy matrix of the original periodic problem (12). The shift of \(\eta/2\) in the rapidities in (23) follows from the definition (10).
In the construction above the parameter $\xi_+$ can be chosen arbitrarily. The Néel, the dimer and the q-dimer states are obtained as

$$
\langle N \rangle = \frac{\langle \Psi(\eta / 2) \rangle}{\sinh(\eta)^M} \quad \langle D \rangle = \frac{\langle \Psi(i\pi / 2) \rangle}{\cosh(\eta / 2)^M} \quad \langle qD \rangle = \lim_{\xi \to \infty} \langle \Psi(\xi) \rangle \frac{|\sinh(\xi - \eta / 2)|^2 + |\sinh(\xi + \eta / 2)|^2}{M/2}.
$$

In the last relation the parameter $q$ is recovered as $q = e^{\eta}$.

In [35] Tsuchiya derived a determinant formula for the partition function (21). In the present conventions it reads

$$
\langle F_+ | C_+(\mu_1) \ldots C_+(\mu_M) | F_- \rangle = \prod_j a(\mu_j) a(-\mu_j) \prod_{j,k} \sinh(\mu_j + \xi_k) \sinh(\mu_j - \xi_k) \prod_{j<k} \sinh(\mu_j - \mu_k) \sinh(\mu_j + \mu_k) \prod_{j<k} \sinh(\xi_j - \xi_k) \sinh(\xi_j + \xi_k - \eta) \det I,
$$

where

$$
I_{jk} = \frac{\sinh(\eta) \sinh(-2\mu_j - \eta) \sinh(-\xi_+ + \xi_k - \eta / 2)}{\sinh(\mu_j + \xi_k - \eta) \sinh(\mu_j - \xi_k + \eta) \sinh(-\mu_j + \xi_k) \sinh(\mu_j + \xi_k)},
$$

and

$$
a(u) = \prod_j \sinh(u - \xi_j + \eta).
$$

Performing a simple factorization, substituting $\xi_j = -\lambda_j + \eta / 2$ and using the relations (24) we find

$$
\langle \Psi_0 | \lambda_1, \ldots, \lambda_M \rangle = \langle \Psi_0 | \prod_{j=1}^M B(\lambda_j) | F_- \rangle \sinh(\eta)^{2M} \prod_k \left( \sinh(\lambda_k + \eta / 2) \sinh(\lambda_k - \eta / 2) \right)^{2M} \mathcal{D} \prod_{j<k} \sinh(\lambda_j - \lambda_k) \sinh(\lambda_j + \lambda_k),
$$

where

$$
\mathcal{D} = \lim_{\mu_j \to 0} \frac{1}{\prod_{j<k} \sinh(\mu_j - \mu_k) \sinh(\mu_j + \mu_k)} \det I.
$$
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\[ I_{jk} = \frac{1} {\sinh(\mu_j + \lambda_k + \eta/2) \sinh(\mu_j - \lambda_k - \eta/2) \sinh(\mu_j + \lambda_k - \eta/2) \sinh(\mu_j - \lambda_k + \eta/2)} \]

and the factor \( \mathcal{P} \) includes all information about the initial state:

- For the Néel state:
  \[ \mathcal{P}_N = \prod_k \frac{\sinh(\eta/2 + \lambda_k)}{\sinh(\eta)^M} \]

- For the dimer state:
  \[ \mathcal{P}_D = \prod_k \frac{\cosh(\lambda_k)}{2^{M/2} \cosh(\eta/2)^M} \]

- For the \( q \)-deformed dimer:
  \[ \mathcal{P}_{qD} = \prod_k e^{\lambda_k} (2 \cosh(\eta))^{M/2}, \quad \text{for } \Delta > 1 \]
  \[ \mathcal{P}_{qD} = \frac{\prod_k e^{\lambda_k}}{2^{M/2}}, \quad \text{for } \Delta < 1. \]

The delicate limit (28) can be performed in at least two ways. One possibility is to ‘pull out’ a Cauchy determinant from the matrix \( I \) as it was done for a closely related matrix in [36] (see equation 2.19); the \( \mu \to 0 \) limit is trivial afterwards. However, this representation is plagued by a singularity if \( \lambda_j = -\lambda_k \) for some \( j, k \), which is difficult to resolve. Therefore here we take the limit by explicitly calculating the derivatives of the matrix elements of \( I \). Using the deformed binomial formula \( \sinh(a+b) \sinh(a-b) = \sinh^2(a) - \sinh^2(b) \) and partial fraction expansion it follows that

\[ I_{jk} = \frac{1} {\sinh(2\lambda_j) \sinh(\eta)} \left[ \frac{1} {\sinh^2(\lambda_j - \eta/2) - x_k} - \frac{1} {\sinh^2(\lambda_j + \eta/2) - x_k} \right] \]

with \( x_k = \sinh^2(\mu_k) \). The \( x_j \to x_k \) limit of the determinant can be performed using the method of [37] and after some simple manipulations we arrive at

\[ D = \prod_k \frac{1} {\sinh\eta \sinh(2\lambda_k)} \times \det L \]

where

\[ L_{jk} = q_{2j}(\lambda_k), \quad q_a(u) = \coth^a(u - \eta/2) - \coth^a(u + \eta/2), \]

Our final formula for the overlap with the Néel state reads

\[ \langle N|\lambda_1, \ldots, \lambda_M \rangle = \frac{\prod_j \sinh^{2M}(\lambda_j - \eta/2) \sinh^{2M+1}(\lambda_j + \eta/2)} {\prod_j \sinh(2\lambda_j) \prod_{j<k} \sinh(\lambda_j - \lambda_k) \sinh(\lambda_j + \lambda_k)} \times \det L \]
with $L$ given by (30). Similarly, for the overlap with the dimer and $q$-dimer state we obtain
\[
\langle D| \lambda_1, \ldots, \lambda_M \rangle = \frac{\sinh(\eta)^M}{2^{M/2}\cosh(\eta/2)^M} \times \prod_j \sinh^2(M(\lambda_j-\eta/2) \sinh^2(M(\lambda_j+\eta/2) \cosh(\lambda_j) \prod_j \sinh(2\lambda_j) \prod_{j<k} \sinh(\lambda_j-\lambda_k) \sinh(\lambda_j+\lambda_k) \times \det L \tag{32}
\]
and
\[
\langle qD| \lambda_1, \ldots, \lambda_M \rangle = \frac{\sinh(\eta)^M}{(2\Gamma)^{M/2}} \prod_j \sinh(2\lambda_j) \prod_{j<k} \sinh(\lambda_j-\lambda_k) \sinh(\lambda_j+\lambda_k) \times \det L, \tag{33}
\]
where
\[
\Gamma = \begin{cases} \Delta & \text{if } \Delta > 1 \\ 1 & \text{if } \Delta < 1. \end{cases}
\]
Equations (31)–(33) are the main results of this work. They are off-shell formulas valid for an arbitrary set of rapidities provided $\lambda_j + \lambda_k \neq 0$ for any $j$, $k$.

The formula (31) was checked analytically by comparing it to (8) for $M = 1, 2, 3$ using the computer program Mathematica. Also, it is easy to see that the relation (9) holds, together with a similar formula for the $q$-dimer state.

### 3.1. Pairs of rapidities

The above determinant formulas are plagued by singularities whenever $\lambda_j + \lambda_k = 0$, in which case further derivatives of the matrix elements of $L$ need to be taken. Due to the non-linear nature of the Bethe equations two rapidities with opposite signs only appear in very special cases. For an even number of roots there are two types of such states, which will be discussed in the following.

One special configuration is when all rapidities appear in pairs:
\[
\{ \lambda \}_M = \{ (\lambda_1, -\lambda_1), (\lambda_2, -\lambda_2) \ldots (\lambda_{M/2}, -\lambda_{M/2}) \}, \quad \lambda_j \neq 0. \tag{34}
\]
The ground states of the XXZ Hamiltonian are of this form for arbitrary $\Delta$. For such a configuration let $\{ \lambda^+ \}_{M/2}$ denote the set $\{ \lambda_1, \ldots, \lambda_{M/2} \}$. For the overlap with the Néel state we find
\[
\langle N| \lambda_1, \ldots, \lambda_M \rangle = (-1)^{M(M-1)/4} \prod_j \sinh(\lambda_j^- - \eta/2) \sinh(\lambda_j^+ + \eta/2) \right)^{M+1} \prod_j \sinh^3(2\lambda_j^+) \prod_{j<k} \sinh^4(\lambda_j^+ - \lambda_k^+) \sinh^4(\lambda_j^+ + \lambda_k^+) \times \det \bar{L}, \tag{35}
\]
where
\[
\bar{L}_{jk} = q_{2j}(\lambda_k^+) \quad k = 1 \ldots M/2
\]
\[
\bar{L}_{j,M/2+k} = 2j(q_{2j+1}(\lambda_k^+) - q_{2j-1}(\lambda_k^+)) \quad k = 1 \ldots M/2
\]
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with \( q_d(u) \) given by (30). Similar formulas can be written down for the overlap with the dimer and \( q \)-dimer states.

The other special root configuration is when
\[
\{ \lambda \}_M = \{ (\lambda_1, -\lambda_1), (\lambda_2, -\lambda_2) \ldots (\lambda_{M/2-1}, -\lambda_{M/2-1}) \}, \quad 0, i\pi / 2 \}
\] (37)
Such states appear in the spectrum for both \( \Delta > 1 \) and \( \Delta < 1 \). In the massive regime \( \Delta > 1 \) the first excited state (which becomes degenerate with the ground state in the infinite volume limit) is of this form with all rapidities being purely imaginary. In the \( \Delta < 1 \) regime the rapidity \( i\pi / 2 \) is a so-called ‘negative parity one-string’ [3], and the remaining rapidities are either real, or have fixed imaginary part \( i\pi / 2 \), or they form strings centered on the real axis.

Let \( \{ \lambda^+ \}_{M/2-1} \) denote the set \( \{ \lambda_1, \ldots, \lambda_{M/2-1} \} \). Then the overlap with the Néel state reads
\[
\langle N | \lambda_1, \ldots, \lambda_M \rangle = (-1)^{2-2M-5} (\sinh(\eta))^2 \prod_j (\sinh(\lambda_j^+ - \eta / 2) \sinh(\lambda_j^+ + \eta / 2))^2 \times \det \hat{L},
\]
(38)
where
\[
\begin{align*}
\hat{L}_{jk} &= q_{2j}(\lambda_j^+) \quad \text{for } k = 1 \ldots M / 2 - 1 \\
\hat{L}_{j,M/2+k-1} &= 2j(q_{2j+1}(\lambda_j^+) - q_{2j-1}(\lambda_j^+)) \quad \text{for } k = 1 \ldots M / 2 - 1 \\
\hat{L}_{j,M-1} &= 2j(\coth^{2j+1}(\eta / 2) - \coth^{2j-1}(\eta / 2)) \\
\hat{L}_{j,M} &= 2j(\tanh^{2j+1}(\eta / 2) - \tanh^{2j-1}(\eta / 2)).
\end{align*}
\]
(39)
A similar formula holds for the overlap with the \( q \)-dimer state, but for the dimer state formula (32) gives
\[
\langle D | \lambda_1, \ldots, \lambda_M \rangle = 0.
\]
(40)
This can be understood by noting that
\[
\langle D | B(i\pi / 2) = 0,
\]
(41)
which can be easily checked by an explicit calculation using the definition of the \( B \)-operators.

4. Numerical results

In this section we present numerical results for the normalized overlaps between the three initial states and the ground states of the XXZ Hamiltonian for different \( \Delta \). Let us denote
\[
S_0^A(\Delta, 2M) = \frac{|\langle A | GS \rangle|}{\sqrt{\langle GS | GS \rangle}},
\]
where \( A = N, D, qD \) and \( |GS\rangle = |\lambda_1, \ldots, \lambda_M\rangle \) is the ground state of the form (34) with the rapidities being the unique solution of the Bethe equations such that all of them
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are purely imaginary (real) for $\Delta > 1$ ($\Delta < 1$), respectively. In the $\Delta > 1$ case we also considered the first excited state which is of the form (37); the corresponding overlaps will be denoted by $S^A_1(\Delta, 2M)$.

We solved the Bethe equations for different values of $\Delta$ and $M$ and computed the overlaps together with the norm (13). In order to check the numerical results we also performed an exact diagonalization of the XXZ Hamiltonian up to length $2M = 16$ and computed the required overlaps. In all cases we found perfect numerical agreement.

Numerical results for the overlaps in the case $2M = 12$ are shown in figure 5. It can be seen that for large $\Delta$ the q-dimer and Néel states are closer to the ground state, but for smaller $\Delta$ the overlap with the dimer state is bigger. This is expected because the $z-z$ term in the Hamiltonian tends to ‘freeze’ the anti-ferromagnetic order, whereas the kinetic $x-x$ and $y-y$ terms make the positions of the down spins more dispersed. The cusp in the overlap with the q-dimer is due to the non-analyticity in its overall normalization; at $\Delta = 1$ the overlap with the dimer and the q-dimer is the same, as expected. Note that the overlap with the dimer state is largest at the $SU(2)$-symmetric point $\Delta = 1$.

The limiting values of the overlaps are as follows. In the large $\Delta$ limit the ground state turns into the linear combination

$$\lim_{\Delta \to \infty} S^N_0(\Delta, 2M) = \frac{|N\rangle + |AN\rangle}{\sqrt{2}},$$

where $|AN\rangle$ is the anti-Néel state. Therefore

$$\lim_{\Delta \to \infty} S^N_0(\Delta, 2M) = \lim_{\Delta \to \infty} S^{qD}_0(\Delta, 2M) = \frac{1}{\sqrt{2}} \lim_{\Delta \to \infty} S^D_0(\Delta, 2M) = (\sqrt{2})^{(1-M)},$$

where we made use of the fact that $M$ is assumed to be even.

The $\Delta \to -1$ limit can be understood by the well-known transformation

$$U \ H_{XXZ}(\Delta = -1) \ U = -\sum_{j=1}^{2M} (\sigma^x_j \sigma^x_{j+1} + \sigma^y_j \sigma^y_{j+1} + \sigma^z_j \sigma^z_{j+1} - 1),$$

where $U$ is a unitary operator that diagonalizes the Hamiltonian at $\Delta = -1$. The resulting Hamiltonian is

$$H_{XXZ}^{\Delta = -1} = \sum_{j=1}^{2M} (\sigma^x_j \sigma^x_{j+1} + \sigma^y_j \sigma^y_{j+1} + \sigma^z_j \sigma^z_{j+1}).$$

Figure 5. The normalized overlaps with the ground state of the XXZ Hamiltonian as a function of $\Delta$ for a spin chain of length $2M = 12$. The solid line correspond to the Néel state, the dashed to the dimer state and the dotted to the q-dimer state.
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Table 1. Numerical results for the logarithm of the normalized overlaps with the Neel state. Here \( S_0 \) denoted the scalar product with the ground state, whereas for \( S_1 \) represents the overlap with the first excited state.

| \( 2M \) | 4     | 8     | 12    | 16    | 20    | 24    |
|--------|-------|-------|-------|-------|-------|-------|
| \( \log(S_0(\Delta = 1.5)) \) | -0.50102 | -0.74718 | -0.97158 | -1.18790 | -1.40000 | -1.60930 |
| \( \log(S_1(\Delta = 1.5)) \) | -0.34657 | -0.53730 | -0.75873 | -0.98233 | -1.20450 | -1.42470 |
| \( \log(S_0(\Delta = 0.5)) \) | -0.61291 | -1.13460 | -1.65560 | -2.17700 | -2.69880 | -3.22100 |

where

\[
U = \sum_{j=1}^{M} \sigma_{j}^{z}.
\]

The isotropic ferromagnetic Hamiltonian on the r.h.s. of (42) has an \( 2M + 1 \)-fold degenerate ground state, and the \( \Delta \to -1 \) limit selects the state with zero total magnetization. Therefore

\[
\lim_{\Delta \to -1} \frac{|GS\rangle}{\sqrt{(GS|GS\rangle)}} = U^{-\frac{(S_{-})^{M}}{\sqrt{(2M)!}}} |F_{+}\rangle,
\]

where \( S_{-} \) is the global spin lowering operator. This leads to

\[
\lim_{\Delta \to -1} S_{0}^{N}(\Delta, 2M) = \frac{1}{\sqrt{2M}} \lim_{\Delta \to -1} S_{0}^{P}(\Delta, 2M) = \frac{(\sqrt{2})^{M}}{\sqrt{2M}} \lim_{\Delta \to -1} S_{0}^{P}(\Delta, 2M) = 0.
\]

All three results agree with the numerical data obtained from the determinant formulas.

We also investigated the \( M \)-dependence of the overlaps for fixed \( \Delta \); for simplicity, here we have only considered the case of the Neel state. Numerical results for the logarithm of the scalar product are given in table 1 for chain lengths \( 2M = 4 \cdot 24 \). For \( \Delta > 1 \) we also give the overlap with the first excited state.

In the large \( M \) limit we expect an exponential decay of the overlap:

\[
\log(S_{0}(\Delta, 2M)) = 2M\alpha_{0}(\Delta) + \beta_{0}(\Delta) + \ldots, \quad \alpha_{0}(\Delta) < 0. \tag{43}
\]

In the recent article [23] an analytic result was derived for the linear coefficient \( \alpha_{0} \) using a non-linear integral equation (NLIE) for the so-called dynamical free energy (the Loschmidt echo at imaginary times). Moreover, it was conjectured that in the \( \Delta > 1 \) regime the overlap with the first excited state is of the form (43) with the same linear term:

\[
\log(S_{1}(\Delta, 2M)) = 2M\alpha_{0}(\Delta) + \beta_{1}(\Delta) + \ldots. \tag{44}
\]

Here we attempt to check the exact results and the latter conjecture of [23] by comparing them to the finite volume data.

We evaluated the corresponding equations of [23] (equations (5.23) and (5.24)) for three values of \( \Delta \). Also, we performed a linear fit of the data in table 1. The results are shown in table 2. It can be seen that the numerical results are close to each other, but the deviation between the NLIE and finite volume results is in all cases larger than the

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error of the linear fit. This discrepancy might be attributed to additional finite volume effects, for which there is no estimate available. Numerical data from larger spin chains might give a better fit; we leave this question for further work. On the other hand, we note that the two results agree very well in the massless case \( \Delta = 0.5 \). The derivation in [23] only applies to the massive case, but based on this finite volume analysis we conclude that the corresponding integral equation is valid also in the massless regime.

5. The XXX limit

In this section we consider the special case of the \( SU(2) \)-symmetric chain with \( \Delta = 1 \). All relevant formulas for the normalized overlaps can be obtained by setting \( \eta = i \varepsilon \) and performing the limit

\[
\varepsilon \to 0, \quad \frac{\lambda}{\eta} \text{ fixed.}
\]

Alternatively the construction of section 3 can be repeated using the rational R-matrix

\[
\tilde{R}(u) = \begin{pmatrix} u + i & u & u & u \\ u & i & u & u \\ i & u & u & u \\ u + i & u & u & u \end{pmatrix}.
\] (45)

Bethe states are then created as

\[
|\{\lambda\}_{n}\rangle = \prod_{j=1}^{n} \tilde{B}(\lambda_{j}) |F\rangle,
\] (46)

where are the appropriate creation operators obtained from the monodromy matrix

\[
\tilde{T}(u) = \tilde{L}_{1}(u) \ldots \tilde{L}_{2M}(u),
\]

with

\[
\tilde{L}_{j}(u) = \tilde{R}_{0j}(u - i/2).
\]

The Bethe equations become

\[
\left( \frac{\lambda_{j} - i/2}{\lambda_{j} + i/2} \right)^{2M} \prod_{k \neq j} \frac{\lambda_{j} - \lambda_{k} + i}{\lambda_{j} - \lambda_{k} - i} = 1,
\] (47)
and the energy is given by
\[ E = \sum_j e(\lambda_j) \quad e(u) = \frac{4}{u^2 + 1}. \]

The norm of the Bethe states defined in (46) is
\[ \langle \lambda_1, \ldots, \lambda_M | \lambda_1, \ldots, \lambda_M \rangle = \prod_j (\lambda_j^2 + 1/4)^{2M} \prod_{j<k} \bar{f}(\lambda_j, \lambda_k) \times \det \bar{G}, \quad (48) \]
where
\[ \bar{f}(u) = \frac{u + i}{u} \]
and
\[ \bar{G}_{jk} = \delta_{j,k} (2M \varphi(\lambda_j, 1/2) - \sum_l \varphi(\lambda_j - \lambda_l, 1) + \varphi(\lambda_j - \lambda_k, 1)) + \varphi(\lambda_j - \lambda_k, 1) \quad (49) \]
with
\[ \varphi(a, b) = \frac{2b}{a^2 + b^2}. \quad (50) \]

The limiting expression for the overlap with the Néel state reads
\[ \langle N | \lambda_1, \ldots, \lambda_M \rangle = \prod_j (\lambda_j - i/2)^{2M} (\lambda_j + i/2)^{2M+1} \prod_j (2\lambda_j) \prod_{j<k} (\lambda_j - \lambda_k) (\lambda_j + \lambda_k) \times \det K \quad (51) \]
with
\[ K_{jk} = \frac{1}{(\lambda_k - i/2)^{2j}} - \frac{1}{(\lambda_k + i/2)^{2j}}. \quad (52) \]

The overlap with the dimer state follows from (32) or (33):
\[ \langle D | \lambda_1, \ldots, \lambda_M \rangle = \prod_j (\lambda_j^2 + 1/4)^{2M} \prod_j (2\lambda_j) \prod_{j<k} (\lambda_j - \lambda_k) (\lambda_j + \lambda_k) \times \det K. \quad (53) \]

In these formulas we assumed that \( \lambda_j \neq \lambda_k \) for any \( j \neq k \). In the XXX case the only special configuration is that of a state consisting of rapidity pairs only, for which a formula analogous to (35) is easily derived.

### 5.1. Overlap with non-highest weight states

It is known that the Bethe states (46) are the highest weight states with respect to global \( SU(2) \) symmetry. Non-highest weight states can be produced by the action of the global spin lowering operator. It is easy to see from the definition of the \( B \)-operators that
\[ S_- = \frac{1}{i} \lim_{u \to \infty} \frac{1}{u^{2N-1}} B(u). \]
This relation provides a way to compute overlaps with non-highest weight states. Consider the vector

\[ (S_-)^m \left| \lambda_{m+1}, \lambda_{m+2}, \ldots, \lambda_M \rightbra_{M-m}. \]

It can be obtained by taking an auxiliary Bethe state with rapidities

\[ (xp_1, xp_2, \ldots, xp_m, \lambda_{m+1}, \lambda_{m+2}, \ldots, \lambda_N), \]

and taking the \( x \to \infty \) limit. The numbers \( \{p_i\}_m \) can be chosen arbitrarily with the only requirement that they all be distinct.

Substituting these rapidities into (51) and taking the \( x \to \infty \) limit results in

\[
\langle N| (S_-)^m \left| \lambda_{m+1}, \lambda_{m+2}, \ldots, \lambda_M \right\rangle_{M-m} = \frac{2^{m-M}(m!) \prod_{j=m+1}^{M} (\lambda_j-i/2)^{2M} (\lambda_j+i/2)^{2M+1}}{\prod_{j=m+1}^{M} \lambda_j \prod_{j<k} (\lambda_j-\lambda_k) (\lambda_j+\lambda_k)} \times \det K
\]

where is a \((M - m) \times (M - m)\) matrix given by the lower-right sub-matrix of the original \( K \).

In the special case of \( m = M \) the overlap is

\[ \langle N| (S_-)^M \left| F \right\rangle = M! \]

This is the expected result.

Concerning the dimer state the same limiting procedure gives

\[ \langle D| (S_-)^m \left| \lambda_{m+1}, \lambda_{m+2}, \ldots, \lambda_M \right\rangle_{M-m} = 0, \]

as expected based on the \( SU(2) \) invariance of the dimer state.

6. Conclusions

In this work we have computed determinant formulas for the overlaps between Bethe states and three special initial states: the Néel, the dimer and the \( q \)-dimer states. We have also considered the special cases when the Bethe roots form pairs with opposite rapidities. We stress that our formulas are valid for arbitrary Bethe states, the rapidities do not need to satisfy the Bethe equations. This makes it possible to consider the special cases with simple limiting procedures.

It is known that most eigenstates of the XXZ spin chain consist of strings with different length. Our formulas do not include any singularities associated with the strings, except when the string center is exactly at \( \lambda = 0 \). In the latter case the formula (38) can be used, whereas for a generic configuration we expect that it is sufficient to substitute the approximate positions of the string rapidities into the determinant, unless the string deviations are large.

It is an important question whether there are more efficient formulas than those presented here. As was noted in section 1 there exists an alternative determinant formula which makes use of the Bethe equations; it can be obtained following the methods...
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of [36]. We did not include that result here, because it is not convenient for the states with opposite rapidities and it is not clear if it is better suited for numerical studies.

Another open question is how to investigate the large volume limit of the determinant formula; in particular, how to extract the leading part in the logarithm of the overlap. First of all, this could lead to an independent derivation of the exact result of [23] for the ‘overlap per site’ between the ground state and the different initial states. On the other hand, this could also help to find the saddle point state of the ‘quench-action’ which determines what configurations are relevant for the long-time behavior following the quantum quench [25]. If the string densities of the saddle point state could be found then that could lead to an independent check (or possibly an actual derivation) of the Generalized Gibbs Ensemble applied to the XXZ chain [18, 19].

Note added: This article was made available as an arXiv e-print in September 2013, but it has not been submitted to a journal until now. In the meantime, two papers by Brockmann et al [38, 39] presented a more efficient determinant formula for the overlaps, building on the results of the present paper; the formula in [36] is cited above.

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