Recursive formulas for the overlaps between Bethe states and product states in XXZ Heisenberg chains

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Abstract
We consider the problem of computing the overlaps between the Bethe states of the XXZ spin-1/2 chain and generic states. We derive recursive formulas for the overlaps between some simple product states and off-shell Bethe states within the framework of the algebraic Bethe ansatz. These recursive formulas can be used to prove in a simple and straightforward way the recently obtained results for the overlaps of the Bethe states with the Néel state, the dimer state, and the $q$-deformed dimer state. However, these recursive formulas are derived for a broader class of states and represent a concrete starting point for the computation of rather general overlaps. Our approach can be easily extended to other one-dimensional Bethe ansatz integrable models.

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1. Introduction
The last decade has witnessed an increasing theoretical and experimental effort in the study of the out-of-equilibrium dynamics of isolated many-body quantum systems. In particular, the time evolution following a sudden change in one of the parameters of the Hamiltonian (quantum quench) has received a lot of attention [1]. A number of theoretical and experimental investigations have unambiguously shown that for large times after a quantum quench and in the thermodynamic limit, the expectation values of the local observables relax to stationary values, although the dynamics governing the evolution are unitary. For a generic system, it has been argued and shown in a series of numerical and experimental works that these stationary values are described by a Gibbs distribution in which the (effective) temperature is fixed by the energy of the initial state [2–5]. Conversely, integrable systems keep memory of many details of the initial state also for infinite time [6–9], as a
consequence of the constrained dynamics with an infinite number of (local) conservation laws. It has been conjectured that, for an integrable system, these stationary values can be calculated using a generalized Gibbs ensemble (GGE), a statistical ensemble determined by all local conserved charges [7] (the importance and the role of the locality of the integrals of motion have been highlighted, mainly in [10, 11]). A small perturbation close to integrability leads to interesting pre-thermalization effects that are captured by a (perturbed) GGE [12, 13].

Many analytical works have focused on providing exact results to test the GGE predictions in specific many-body integrable models. The predictions based on GGE resisted all tests in many models both having a free-particle representation [10, 11, 14–24] and being genuinely interacting [25–29], until very recently when it has been found that for the XXZ spin chain, after a quench from the (symmetrized) Néel and dimer states, the obtained stationary values [30–32] disagree with the predictions of the GGE built with all the known local charges [33, 34] (see also [35–37]). It is worth stressing that, besides representing a test for the validity of the GGE, exact results for the time evolution of local observables are also extremely useful to gain insight into the relaxation dynamics.

Let us briefly recall the building blocks needed to study the quench dynamics in a generic situation. The first problem one faces is to write the initial state \( |\Phi_0\rangle \) in terms of the eigenstates of the Hamiltonian \( H \) governing the time evolution. Let us for the moment generically denote the normalized eigenstates as \( |n\rangle \), in such way that the initial state can be written as

\[
|\Phi_0\rangle = \sum_n a_n |n\rangle ,
\]

where \( a_n \) are the overlaps \( a_n \equiv \langle n | \Phi_0 \rangle \) between the initial state and the eigenstates. Consequently, the time-evolved state is

\[
|\Phi(t)\rangle = \sum_n a_n e^{-iE_n t} |n\rangle ,
\]

where \( E_n \) is the energy of the state \( |n\rangle \). This provides the time-dependent expectation values of an arbitrary observable \( O \), in terms of the form factors \( \langle n | O | m \rangle \), as

\[
\langle \Phi(t) | O | \Phi(t) \rangle = \sum_{mn} a_m a_n^* e^{-i(E_m - E_n) t} \langle n | O | m \rangle .
\]

In summary, in order to characterize the quench dynamics, the needed starting elements are (i) a complete characterization of all eigenstates \( |n\rangle \) of a Hamiltonian and their energies; (ii) the norms of the eigenstates and the form factors of relevant operators in this basis; (iii) the overlaps between the initial states and the eigenstates.

For integrable models, the Bethe ansatz is a very efficient tool to obtain most of these ingredients. Indeed, it provides a full set of eigenstates with their energies [38]. The norms and the form factors of the most relevant local operators are the main objectives of the algebraic Bethe ansatz and quantum-inverse scattering program [39]. What is not (yet) known in general is how to obtain the overlaps between Bethe states and generic initial states. Until now, very few exact results exist for these overlaps in integrable models [40–47]. Clearly, finding compact and tractable expressions for the overlaps between Bethe states and the initial state in a generic quantum quench would allow exact calculations for a variety of potentially interesting situations and experiments.

However, the ingredients listed above are only the starting point for the description of quench dynamics because the sum (3) is still to be performed, which this is a very difficult
Indeed, the same problem is also present in the calculation of the equilibrium correlation functions for which the knowledge of the form factors [48, 49] allows analytical calculations only in a few instances/limits (see e.g. [50–53] for the XXZ chain; however, this list is far from being exhaustive). Accurate determinations of the equilibrium correlation functions can be obtained by summing the form factor expansion numerically for finite systems, as is done for the XXZ chain [54] and for the Lieb–Liniger model [55].

Concerning the non-equilibrium quench dynamics, the summation problem is still present even after the overlaps have been discovered. Fortunately, a recently proposed method (termed either ‘representative state approach’ or ‘quench action’) gives an exact analytical description of the post-quench steady state in the thermodynamic limit [9]. The essential building blocks of this method are, once again, the overlaps. Thus, the main obstacle to tackle quite generally the quench dynamics is to find compact and manageable expressions for the overlaps that could subsequently be used for both numerical and analytical calculations (for the sake of completeness, we must mention that there are also some approaches for studying quench dynamics in integrable models partially bypassing the calculations of the overlaps, such as imaginary time formalism [56–60], Yudson representation [61, 62] and others [63–66]).

In this work, we derive recursive formulas for the overlaps between Bethe states in the XXZ spin-1/2 chain and a class of product states. The structure of the paper is as follows. In section 2, we review the XXZ model and the algebraic Bethe ansatz tools that will be used in the rest of this work. In section 3, we introduce a certain class of product states and we derive recursive formulas for the overlaps between these states and the Bethe states. The class we consider includes the Néel state, the dimer state, and the $q$-deformed dimer state, for which overlap formulas were recently derived by B. Pozsgay using boundary Bethe ansatz techniques [43]. In section 4, we show that our recursive formulas can be used to prove in a simple way the overlaps of [43]. Finally, conclusions are presented in section 5.

## 2. The XXZ spin chain and the algebraic Bethe ansatz

We consider the XXZ spin-1/2 chain with Hamiltonian

$$H_{XXZ}^N = \sum_{j=1}^{N} \left[ \sigma_j^+ \sigma_{j+1}^- + \sigma_j^- \sigma_{j+1}^+ + \Delta (\sigma_j^z \sigma_{j+1}^z - 1) \right], \quad (4)$$

where $\sigma_j^\alpha$ are the Pauli matrices at the site $j$ and we impose periodic boundary conditions $\sigma_{N+1}^\alpha = \sigma_1^\alpha$. The hamiltonian (4) is defined in the Hilbert space $H_{N+1} = h_N \otimes \ldots \otimes h_1$, where $h_i \simeq \mathbb{C}_2$ is associated with site $i$ of the chain.

The hamiltonian (4) commutes with the $z$-component of the total spin so that the Hilbert space $H_{N+1}$ can be decomposed into sectors with a well-defined number $P$ of flipped spins with respect to the reference state with all spins up

$$|0\rangle_{N+1} = |\uparrow\rangle_N \otimes \ldots \otimes |\uparrow\rangle_1. \quad (5)$$

The wave function in the spin basis and in the sector with $P$ spins down is given by the ansatz [38]
where \( s_j \) denotes the position of the down spins (we assumed, without loss of generality, \( s_j < s_k \) for \( j < k \)), and we introduced \( \eta = \text{arccosh} \Delta \) and the function

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

The sum runs over the permutations \( Q \) of \( P \) elements. The wave function (6) is an eigenstate of the Hamiltonian (4) with periodic boundary conditions if the rapidities \( \lambda_j \) satisfy the Bethe equations [38]

\[
\prod_{j=1}^N \frac{\sinh(\lambda_j - \eta/2)}{\sinh(\lambda_j + \eta/2)} = \prod_{j \neq j'} \sinh(\lambda_j - \lambda_j' - \eta) \sinh(\lambda_j - \lambda_j' + \eta),
\]

and the corresponding energies are

\[
E\left(\{\lambda_j\}\right) = \sum_{j=1}^P \frac{4 \sinh^2(\eta)}{\cosh(2\lambda_j) - \cosh(\eta)}.
\]

In the thermodynamic limit \( N, P \to \infty \) with \( P/N \) constant, the properties of the XXZ spin-chain can be obtained by means of the thermodynamic Bethe ansatz [67]. In particular, it turns out that the model is gapped for \( \Delta > 1 \) and gapless in the opposite regime.

The wave function (6) already gives an explicit form for the overlaps with product states as a sum over the permutations of the \( P \) elements. However, as stressed elsewhere [43], since the number of permutations grows like \( P! \), these expressions for the overlaps are not useful for any practical numerical or analytic evaluation.

A powerful alternative for the study of the XXZ chain (and in general of Bethe Anstaz solvable models) is the algebraic Bethe ansatz that we are going to briefly review now, remanding for a more detailed treatment to the standard textbook on the subject [39]. The central object of the algebraic Bethe ansatz is the \( R \)-matrix that, for the XXZ model, is (here and below all the non-written elements of matrices are equal to zero)

\[
R(\lambda, \mu) = \begin{pmatrix}
f(\mu, \lambda) & 0 & 0 & \ldots \\
g(\mu, \lambda) & 1 & 0 & \ldots \\
0 & g(\mu, \lambda) & 1 & \ldots \\
0 & 0 & 0 & \ldots
\end{pmatrix},
\]

where

\[
f(\mu, \lambda) = \frac{\sinh(\lambda - \mu + \eta)}{\sinh(\lambda - \mu)}, \quad g(\mu, \lambda) = \frac{\sinh(\eta)}{\sinh(\lambda - \mu)}.
\]

An auxiliary space \( h_0 \approx \mathbb{C}_2 \) is introduced together with the \( L \)-operator acting on the four-dimensional space \( h_0 \otimes h_n \).
\[ L_{0,\eta}(\lambda) = \begin{pmatrix} \sinh \left( \frac{\lambda}{2} + \frac{\eta}{2} \right) & & & \\
 & \sinh \left( \frac{\lambda}{2} - \frac{\eta}{2} \right) & \sinh (\eta) & \\
 & \sinh (\eta) & \sinh \left( \frac{\lambda}{2} - \frac{\eta}{2} \right) & \\
 & & & \sinh \left( \frac{\lambda}{2} + \frac{\eta}{2} \right) \end{pmatrix} \]  

(12)

A second fundamental object of the algebraic Bethe ansatz, the monodromy matrix, is then defined as the product of \( L \)-matrices along the chain

\[ T_{N\ldots 1}(\lambda) = L_N(\lambda) \ldots L_1(\lambda) = \begin{pmatrix} A_{N\ldots 1}(\lambda) & B_{N\ldots 1}(\lambda) \\ C_{N\ldots 1}(\lambda) & D_{N\ldots 1}(\lambda) \end{pmatrix} \]  

(13)

where we have dropped the index corresponding to the auxiliary space. The entries of the monodromy matrix are operators acting on \( H_{N\ldots 1} \). The \( R \)-matrix (10) and the monodromy matrix (13) fulfill the following fundamental relation

\[ R(\lambda, \mu) \left( T_{N\ldots 1}(\lambda) \otimes T_{N\ldots 1}(\mu) \right) = \left( T_{N\ldots 1}(\mu) \otimes T_{N\ldots 1}(\lambda) \right) R(\lambda, \mu). \]  

(14)

Explicitly writing down equation (14) results in a number of quadratic relations for the entries of the monodromy matrix (see [39] for the details).

The reference state (5) is an eigenstate of the diagonal entries of the monodromy matrix; indeed, it holds

\[ A_{N\ldots 1}(\lambda) |0\rangle_{N\ldots 1} = a_{N\ldots 1}(\lambda) |0\rangle_{N\ldots 1} = \sinh^{N} \left( \frac{\lambda}{2} + \frac{\eta}{2} \right) |0\rangle_{N\ldots 1}, \]  

(15)

\[ D_{N\ldots 1}(\lambda) |0\rangle_{N\ldots 1} = d_{N\ldots 1}(\lambda) |0\rangle_{N\ldots 1} = \sinh^{N} \left( \frac{\lambda}{2} - \frac{\eta}{2} \right) |0\rangle_{N\ldots 1}. \]  

(16)

In this algebraic formalism, the eigenstates of Hamiltonian (4) (lying in the \( P \)-sector) are then written in terms of the entries of the monodromy matrix as

\[ \left\{ \lambda_j \right\}_{j=1}^{p} = B(\lambda_P) \ldots B(\lambda_1) |0\rangle_{N\ldots 1}, \]  

(17)

where, once again, the rapidities \( \{ \lambda_j \}_{j=1}^{p} \) fulfill the Bethe equations (8) showing that coordinate and algebraic Bethe ansatz are indeed equivalent.

A crucial property of this algebraic construction is that the state (17) is well defined even if the parameters \( \{ \lambda_j \}_{j=1}^{p} \) do not fulfill the Bethe equations (8) (but obviously it is not an eigenstate of the Hamiltonian (4)). Among the most remarkable results obtained from the algebraic Bethe ansatz, we must mention the proof of the Gaudin formula for the norm of a Bethe state [68]; the Slavnov formula [69], which is a general expression for the scalar product between two Bethe states of the form (17), in which only one of the two sets of rapidities satisfies the Bethe equations; and the determination of the form factors of the most relevant operators [48, 49, 51].

3. Derivation of recursive formulas

In this section, we derive recursive formulas for the overlaps between Bethe states and a class of product states. Our approach uses a two-site generalized model [39, 70] and is based on a
particular representation of the Bethe states in this model. In subsection 3.1, we introduce the class of product states considered in this work and the two-site generalized model representation for Bethe states. General recursive formulas are then derived. In subsection 3.2, we give explicit examples for a number of physically relevant states.

3.1. Two-site generalized model

Suppose the number of sites of the chain \( N \) is divisible by the integer \( G \). In this work, we consider product states of the following form

\[
\psi_{G, N-1, \ldots, N-G+1} = \otimes \psi_{N-G, N-G-1, \ldots, N-2G+1} \otimes \cdots \otimes \psi_{G, G-1, \ldots, 1}.
\]  

(18)

where the state \( \psi_{G, r-1, \ldots, r-G+1} \) belongs to the Hilbert space \( \otimes \psi_{N-2G+1} \). These states include and generalize those considered in [43] for \( G = 2 \) and those in [34] for \( G = 1, 2 \).

We are interested in deriving recursive formulas for the overlaps between states of the form (18) and Bethe states (17). We start considering a chain with \( N + G = G(M + 1) \) sites. The scalar product we are interested in is

\[
S_{M+1} = \langle \psi | B(\lambda_1) \cdots B(\lambda_R) | 0 \rangle_{G(M+1)}.
\]  

(19)

The two-site generalized model of [39] allows us to write the monodromy matrix as follows

\[
T_{G+N-1} = L_{G+N} (\lambda) \cdots L_{N+1} (\lambda) T_{N-1} (\lambda)
\]

\[
= \begin{pmatrix}
A_{G+N-1} (\lambda) & B_{G+N-1} (\lambda) \\
C_{G+N-1} (\lambda) & D_{G+N-1} (\lambda)
\end{pmatrix}
\]

(20)

where the operators \( A_{G+N-1} (\lambda) \), \( B_{G+N-1} (\lambda) \), \( C_{G+N-1} (\lambda) \) and \( D_{G+N-1} (\lambda) \) act on the Hilbert space \( h_{G+N} \otimes h_{N+1} \). For convenience, we introduce the following notations for the operators and the reference states

\[
\overline{X} (\lambda) \equiv X_{G+N-1} (\lambda),
\]

(21)

\[
X (\lambda) \equiv X_{N-1} (\lambda),
\]

(22)

\[
\overline{\psi} \equiv | \uparrow \rangle_{G} \otimes | \uparrow \rangle_{G-1} \otimes \cdots \otimes | \uparrow \rangle_{1},
\]

(23)

\[
| 0 \rangle \equiv | 0 \rangle_{N-1} = | \uparrow \rangle_{N} \otimes \cdots \otimes | \uparrow \rangle_{1}.
\]

(24)

Note that the reference state of the whole chain is the product of two reference states, \( | 0 \rangle_{G+N-1} = \overline{\psi} \). From equation (20) we have

\[
B_{G+N-1} (\lambda) = \overline{X} (\lambda) B (\lambda) + \overline{B} (\lambda) D (\lambda),
\]

(25)

and, using equations (15) and (16), the following relations hold

\[
\overline{X} (\lambda) | \overline{\psi} \rangle = a (\lambda) | \overline{\psi} \rangle = \sinh^2 \left( \lambda + \frac{G}{2} \right) | \overline{\psi} \rangle.
\]

(26)
\[
D(\lambda)|0\rangle = d(\lambda)|0\rangle = \sinh^N\left(\frac{\lambda - \eta}{2}\right)|0\rangle = \sinh^{GM}\left(\frac{\lambda - \eta}{2}\right)|0\rangle.
\] (27)

We can now write the Bethe state in equation (19) as
\[
B(\lambda_P)\ldots B(\lambda_1)|0\rangle_{N+G-1} = \left[ (\tilde{A}(\lambda_P)B(\lambda_P) + \tilde{B}(\lambda_P)D(\lambda_P))\right] \times \left[ (\tilde{A}(\lambda_1)B(\lambda_1) + \tilde{B}(\lambda_1)D(\lambda_1))\right] |\tilde{0}\rangle \otimes |0\rangle.
\] (28)

The key representation for Bethe states is obtained expanding the product in (28) and collecting together all terms with the same number of \(\tilde{B}\) operators, arriving finally to
\[
B(\lambda_P)\ldots B(\lambda_1)|0\rangle_{N+G-1} = \sum_{J=0}^{P} |I_J\rangle,
\] (29)
where \(|I_J\rangle\) contains all the terms with a number \(J\) of \(\tilde{B}\) operators that result from expanding the product in equation (28). The explicit expression for \(|I_J\rangle\) can be found in [39]:
\[
|I_J\rangle = \sum_{\{\lambda\}_{J}} \prod_{l=1}^{P} \prod_{m=1}^{J} \tilde{a}(\lambda_m^H) d(\lambda_l^I) f(\lambda_m^H, \lambda_l^I)\]
\[
\times \prod_{r=1}^{J} \tilde{B}(\lambda_r^I) |\tilde{0}\rangle \otimes \prod_{l=1}^{P} B(\lambda_l^H)|0\rangle.
\] (30)

where the summation is over all decomposition of \(\{\lambda_j\}_{J=1}^{P}\) into two disjoint subsets \(\{\lambda_j^I\}\) and \(\{\lambda_j^H\}\), such that the cardinality of the set \(\{\lambda_j^I\}\) is equal to \(J\). As an example, we give the explicit expression of \(|I_J\rangle\) for \(J = 0, 1, 2\)
\[
|I_0\rangle = \prod_{j=1}^{P} \tilde{a}(\lambda_j^I)|\tilde{0}\rangle \otimes \prod_{l=1}^{P} B(\lambda_l^H)|0\rangle.
\] (31)
\[
|I_1\rangle = \sum_{j=1}^{P} d(\lambda_j) \prod_{l=1}^{P} \tilde{a}(\lambda_l^I) f(\lambda_k^I, \lambda_j^I) \tilde{B}(\lambda_j^I) |\tilde{0}\rangle \otimes \prod_{l=1}^{P} B(\lambda_l^H)|0\rangle.
\] (32)
\[
|I_2\rangle = \sum_{l<j} \prod_{k \neq l,j} d(\lambda_l) d(\lambda_j) \prod_{k \neq l,j} \tilde{a}(\lambda_k^I) f(\lambda_k^I, \lambda_l^I) f(\lambda_k^I, \lambda_j^I)
\times \tilde{B}(\lambda_j^I) \tilde{B}(\lambda_j^I) |\tilde{0}\rangle \otimes \prod_{r=1}^{P} B(\lambda_r^H)|0\rangle.
\] (33)

We now take the scalar product between the Bethe state (29) and the product state
\[
|\psi\rangle_{N+G-1} = |\psi\rangle_{N+G-1} \otimes |\psi\rangle_{N-1}.
\] (34)

Using the same notation as in equation (19) for the scalar product, from equations (29), (30) and (34), we finally arrive at the recursive formula
The quantity \( \langle \psi | \prod_{j=1}^{J} \tilde{B}(\lambda_j^f) | 0 \rangle \) can be computed using equation (23) and the definition of the \( \tilde{B} \) operator given in equation (20). In order to derive the general expression (35), we have considered all the terms \( |I_J^f \rangle \) in the sum in equation (29). On the other hand, for specific examples of states of the form (18), only a few terms in the sum in equation (29) have to be considered, because most of the vectors \( |I_J^f \rangle \) have zero overlap with them.

Specifically, the number of vectors \( |I_J^f \rangle \) in equation (29) having non-zero overlap with the product state (18) is related to the number of down spins of \( |\psi\rangle \) in equation (18). This occurs because \( |I_J^f \rangle \) is the sum of terms containing a number \( J \) of \( \tilde{B} \) operators and thus lies in the \( J \)-sector of the Hilbert space \( h_{N+G} \otimes \cdots \otimes h_{N+1} \). For example, if \( |\psi\rangle \) lies in the one-sector of the corresponding Hilbert space, the only term in the sum (29) with non-zero overlap is \( |I_1^f \rangle \). Accordingly, when specific states are considered, equation (35) can be greatly simplified to obtain tractable expressions.

Note that given the integer \( G \) in equation (18), the \( \tilde{B} \) operator is obtained as the entry of the product of \( G \) consecutive \( L \)-matrices, according to equation (20). For increasing values of \( G \), more lengthy calculations are thus needed for the computation of \( \langle \psi | \prod_{j=1}^{J} \tilde{B}(\lambda_j^f) | 0 \rangle \), which is necessary for deriving explicit expressions for the recursive formulas of specific states.

In the next subsection, we consider a number of physically relevant states and present the corresponding recursive formulas for the overlaps with Bethe states.

3.2. Recursive formulas for specific states

We now write explicitly the general recursive formula (35) for the following specific, physically relevant states of the form (18).

1. The ferromagnet along the \( x \)-direction, \( |xF\rangle = 1 \rightarrow \cdots \rightarrow \). The state \( |xF\rangle \) is of the form (18) with \( G = 1 \) and \( |\psi\rangle = |1 \uparrow\rangle = (|1 \uparrow\rangle + |1 \downarrow\rangle)/\sqrt{2} \). In this case, we only have to consider \( |I_0^f \rangle \) and \( |I_1^f \rangle \) in the expansion (29), the other terms having zero overlap as discussed in the previous subsection. Since \( G = 1 \), the definition of \( \tilde{B} \) involves only one \( L \)-matrix. From equation (12) we have directly

\[
\tilde{B}(\lambda_j^f) = \begin{pmatrix} 0 & 0 \\ \sinh(\eta) & 0 \end{pmatrix},
\]

so that

\[
| \rightarrow | \tilde{B}(\lambda_j^f) | \uparrow \rangle = \left( \frac{1}{\sqrt{2}} \quad \frac{1}{\sqrt{2}} \right) \times \begin{pmatrix} 0 & 0 \\ \sinh(\eta) & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\sinh(\eta)}{\sqrt{2}}.
\]

The recursive formula (35) can thus be simplified as follows...
\[ S_{N+1}[xF](\lambda_1, \ldots, \lambda_P) = \frac{1}{\sqrt{2}} \left[ \prod_{k=1}^{P} \sinh \left( \lambda_k + \frac{\eta}{2} \right) \right] S_N[xF](\lambda_1, \ldots, \lambda_P) \]
\[ + \frac{\sinh(\eta)}{\sqrt{2}} \sum_{j=1}^{P} \sinh^N \left( \lambda_j - \frac{\eta}{2} \right) \left[ \prod_{k=1 \atop k \neq j}^{P} \sinh \left( \lambda_k + \frac{\eta}{2} \right) f \left( \lambda_k, \lambda_j \right) \right] \]
\[ \times S_N[xF](\lambda_1, \ldots, \hat{\lambda}_j, \ldots, \lambda_P). \] (38)

where the notation \( \hat{\lambda}_j \) means, as usual, that the rapidity \( \lambda_j \) is removed from the set \( \{\lambda_1, \ldots, \lambda_P\} \) and \( f(\mu, \nu) \) is given in equation (11).

2. The tilted ferromagnet \( |\theta F\rangle = |\theta; \nearrow, \ldots, \nearrow\rangle = e^{i\theta/2} \sum_{\sigma} |\uparrow \ldots \uparrow\rangle \). As before, we have \( G = 1 \), but in this case \( |\varphi\rangle = \cos \left( \theta/2 \right) \uparrow \rangle - \sin \left( \theta/2 \right) \downarrow \rangle \). Thus, analogously to equation (37), we simply have
\[ \langle \theta; \nearrow | \tilde{B}(\lambda) | \uparrow \rangle = -\sin \left( \theta/2 \right) \sinh(\eta), \] (39)
so that the corresponding recursive formula reads
\[ S_{N+1}[\theta F](\lambda_1, \ldots, \lambda_P) = \cos \left( \frac{\theta}{2} \right) \times \left[ \prod_{k=1}^{P} \sinh \left( \lambda_k + \frac{\eta}{2} \right) \right] S_N[\theta F](\lambda_1, \ldots, \lambda_P) \]
\[ - \sin \left( \frac{\theta}{2} \right) \sinh(\eta) \sum_{j=1}^{P} \sinh^N \left( \lambda_j - \frac{\eta}{2} \right) \]
\[ \times \left[ \prod_{k=1 \atop k \neq j}^{P} \sinh \left( \lambda_k + \frac{\eta}{2} \right) f \left( \lambda_k, \lambda_j \right) \right] S_N[\theta F](\lambda_1, \ldots, \hat{\lambda}_j, \ldots, \lambda_P). \] (40)

3. The Néel state \( |N\rangle \), the dimer state \( |D\rangle \) and the \( q \)-deformed dimer state \( |qD\rangle \) (considered in [43])
\[ |N\rangle = |\uparrow \downarrow \uparrow \downarrow \ldots \uparrow \downarrow \rangle = \otimes^{N/2} |\uparrow \downarrow \rangle. \] (41)
\[ |D\rangle = \otimes^{N/2} \left[ \frac{|\uparrow \downarrow \rangle - |\downarrow \uparrow \rangle}{\sqrt{2}} \right], \] (42)
\[ |qD\rangle = \otimes^{N/2} \frac{q^{1/2} |\uparrow \downarrow \rangle - q^{-1/2} |\downarrow \uparrow \rangle}{\sqrt{|q| + 1/|q|}} \right), \Delta = (q + 1/q)/2. \] (43)

The dimer state and the \( q \)-deformed dimer state are, respectively, the ground states of the Majumdar–Ghosh Hamiltonian [71] and the \( q \)-deformed Majumdar–Ghosh Hamiltonian [72].

We now assume the number of sites \( N \) to be even: \( N = 2 M \). The states (41), (42) and (43) are of the form (18) with \( G = 2 \). The overlap between these states for \( N = 2 M \) and a Bethe state is non-zero only if the number of rapidities corresponding to the Bethe state is \( M \). Furthermore, in the computation of recursive formulas for these states, we only have
to consider \( U_1 \) in the expansion (29), the other terms having zero overlap. The recursive formulas for the three states (41), (42) and (43) thus read

\[
S_{M+1}(\lambda_1, \ldots, \lambda_{M+1}) = \sum_{j=1}^{M+1} \sinh^2 M \left( \lambda_j - \frac{\eta}{2} \right) \langle \phi | B(\lambda_j) | \uparrow \uparrow \rangle 
\times \prod_{k=1, k \neq j}^{M+1} \sinh^2 \left( \lambda_k + \frac{\eta}{2} \right) f \left( \lambda_k, \lambda_j \right) S_M(\lambda_1, \ldots, \lambda_j, \ldots, \lambda_{M+1}).
\]  

(44)

The element \( \langle \phi | B(\lambda_j) | \uparrow \uparrow \rangle \) can be simply obtained from the product of two \( L \)-matrices because in this case \( G = 2 \). Using again equation (12) we have

\[
B(\lambda_j) = \begin{pmatrix} \sinh (\lambda_j + \eta/2) & 0 \\ 0 & \sinh (\lambda_j - \eta/2) \end{pmatrix}
\]

\[
\otimes \left( \begin{pmatrix} 0 & 0 \\ \sinh (\eta) & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \sinh (\eta) & 0 \end{pmatrix} \right)
\]

\[
= \begin{pmatrix} \sinh (\lambda_j - \eta/2) & 0 \\ 0 & \sinh (\lambda_j + \eta/2) \end{pmatrix}.
\]

(45)

so that for the Néel state

\[
\langle \uparrow \downarrow | B(\lambda_j) | \uparrow \uparrow \rangle = (1 \ 0) \otimes (0 \ 1) \begin{pmatrix} \sinh (\lambda_j + \eta/2) & 0 \\ 0 & \sinh (\lambda_j - \eta/2) \end{pmatrix} 
\otimes \begin{pmatrix} 0 & 0 \\ \sinh (\eta) & 0 \end{pmatrix} = \sinh (\eta) \sinh (\lambda_j + \eta/2).
\]  

(46)

Analogously for the dimer state and the \( q \)-dimer state, we obtain

\[
\left( \frac{\uparrow \downarrow - \downarrow \uparrow}{\sqrt{2}} \right) B(\lambda_j) \left( \uparrow \uparrow \right) = \sqrt{2} \sinh (\eta) \sinh (\eta/2) \cosh (\lambda_j),
\]

(47)

\[
\frac{1}{\sqrt{|q|} + 1/|q|} \left( q^{1/2} \langle \uparrow \downarrow | - q^{-1/2} \downarrow \uparrow | \right) B(\lambda_j) | \uparrow \uparrow \rangle = \frac{\sinh^2(\eta)e^{\lambda_j}}{\sqrt{|q|} + 1/|q|}.
\]

(48)

where in equation (48) we have used \( q = e^{\eta} \).

4. The tilted Néel state \( \theta N \rangle = \{0; \uparrow \downarrow \ldots \uparrow \downarrow \} = e^{i\theta/2} \sum_i \sigma_i^z | \uparrow \downarrow \ldots \uparrow \downarrow \rangle \). This state is of the form (18) with \( G = 2 \). The vector |\( \phi \rangle \) is given by
\[ |\theta_; \mathcal{A}| \rangle = \sin \left( \frac{\theta}{2} \right) \cos \left( \frac{\theta}{2} \right) |\uparrow \uparrow \rangle - |\downarrow \downarrow \rangle + \cos^2 \left( \frac{\theta}{2} \right) |\uparrow \downarrow \rangle - \sin^2 \left( \frac{\theta}{2} \right) |\downarrow \uparrow \rangle. \]  

(49)

From equation (49), we see that in order to write down the recursive formula (35) for the tilted Néel state, in the expansion (29) we have to keep the terms \(|I_0\rangle, |I_1\rangle \) and \(|I_2\rangle\), written explicitly in equations (31), (32) and (33). We then need the following expressions, which are easily computed:

\[ \langle \theta; \mathcal{A} | \tilde{B}(\lambda_j)| \uparrow \uparrow \rangle = \sinh(\eta) \left[ \cosh(\eta/2) \sinh \left( \lambda_j - \eta/2 \right) - \sin(\theta/2) \sinh \left( \lambda_j - \eta/2 \right) \right], \]  

(50)

\[ \langle \theta; \mathcal{A} | \tilde{B}(\lambda_j)\tilde{B}(\lambda_i)| \uparrow \uparrow \rangle = -\sin(\theta/2) \cos(\theta/2) \sinh^2(\eta) \times \left[ \cosh(\eta) \cosh(\lambda_j + \lambda_i) - \cosh(\lambda_j - \lambda_i) \right]. \]  

(51)

The recursive formula (35) for the tilted Néel can thus be written as

\[
S_{M+1}[\theta N](\lambda_1, \ldots, \lambda_p) = \sin(\theta/2) \cos(\theta/2) \left[ \prod_{k=1}^p \sinh^2 \left( \lambda_k + \frac{\eta}{2} \right) \right] S_M[\theta N](\lambda_1, \ldots, \lambda_p) \\
+ \sum_{j=1}^p \sinh^2 M \left( \lambda_j - \frac{\eta}{2} \right) \langle \theta; \mathcal{A} | \tilde{B}(\lambda_j)| \uparrow \uparrow \rangle \\
\times \left[ \prod_{k=1}^p \sinh^2 \left( \lambda_k + \frac{\eta}{2} \right) f(\lambda_k, \lambda_j) \right] S_M[\theta N](\lambda_1, \ldots, \lambda_j, \ldots, \lambda_p) \\
+ \sum_{j<l} \sinh^2 M \left( \lambda_j - \frac{\eta}{2} \right) \sinh^2 M \left( \lambda_l - \frac{\eta}{2} \right) \\
\times \left[ \prod_{k=1}^p \sinh^2 \left( \lambda_k + \frac{\eta}{2} \right) f(\lambda_k, \lambda_l)f(\lambda_k, \lambda_j) \right] \\
\times \langle \theta; \mathcal{A} | \tilde{B}(\lambda_j)\tilde{B}(\lambda_l)| \uparrow \downarrow \rangle S_M[\theta N](\lambda_1, \ldots, \lambda_j, \ldots, \lambda_l, \ldots, \lambda_p). \]  

(52)

where \( \langle \theta; \mathcal{A} | \tilde{B}(\lambda_j)| \uparrow \uparrow \rangle \) and \( \langle \theta; \mathcal{A} | \tilde{B}(\lambda_j)\tilde{B}(\lambda_l)| \uparrow \downarrow \rangle \) are given in equations (50) and (51).

5. Finally, as an example of a product state of the form (18) with \( G > 2 \), we consider the ferromagnetic domain state with \( G = 4 \):

\[ |FD_4\rangle = |\uparrow \uparrow \downarrow \downarrow \rangle. \]  

(53)

We now have \( N = 4 M \). The only Bethe states with non-zero overlap with the
ferromagnetic domain state are those parametrized by sets of rapidities with the cardinality of $M^2$. Furthermore, in the expansion (29), the only term we have to consider is $\Gamma_{\uparrow \uparrow \downarrow \downarrow} | \upsilon \rangle^2$, the other terms having zero overlap with (53). As usual, we have to compute a matrix element which is easily worked out as

$$\langle \uparrow \uparrow \downarrow \downarrow | \tilde{B}(\lambda_j) \tilde{B}(\lambda_i) | \uparrow \uparrow \uparrow \uparrow \rangle = \sinh^2(\lambda_j + \eta/2) \sinh^2(\lambda_i + \eta/2) \sinh^2(\eta) \times \left[ \cosh(\eta) \cosh(\lambda_j + \lambda_i) - \cosh(\lambda_j - \lambda_i) \right].$$

(54)

The recursive formula for the overlap between Bethe states and the ferromagnetic domain state with $G = 4$ thus reads

$$S_{M+1}[FD_4](\lambda_1, \ldots, \lambda_{2(M+1)}) = \sum_{l<j} \sinh^4\left(\lambda_j - \frac{\eta}{2}\right) \sinh^4\left(\lambda_j - \frac{\eta}{2}\right) \times \left( \prod_{k \neq l,j} \sinh^4\left(\lambda_k + \frac{\eta}{2}\right) \right) \times \langle \uparrow \uparrow \downarrow \downarrow | \tilde{B}(\lambda_j) \tilde{B}(\lambda_i) | \uparrow \uparrow \uparrow \uparrow \rangle S_M[FD_4](\lambda_1, \ldots, \lambda_i, \ldots, \lambda_j, \ldots, \lambda_{2(M+1)}),$$

(55)

where $\langle \uparrow \uparrow \downarrow \downarrow | \tilde{B}(\lambda_j) \tilde{B}(\lambda_i) | \uparrow \uparrow \uparrow \uparrow \rangle$ is given by equation (54).

4. Proof of overlaps determinant formulas

In this section, we show that the recursive formulas (44) can be used to prove in a simple way determinant formulas for the overlaps between Bethe states and the Néel state, the dimer state and the $q$-deformed dimer state, first derived by B. Pozsgay in [43] using boundary Bethe ansatz techniques [73]. Denoting generically with $\langle \psi \rangle$ the Néel state, the dimer state and the $q$-deformed dimer state (which are two-site shift-invariant states), we want to prove the following determinant formula [43]

$$\langle \psi | \lambda_1, \ldots, \lambda_M \rangle = \prod_{j=1}^M \left( \frac{\sinh^2 M(\lambda_j - \eta/2) \sinh^2 M(\lambda_j + \eta/2)}{\sinh(2\lambda_j) \sinh(\eta)} \right) \times \prod_{j=1}^M \langle \psi | \tilde{B}(\lambda_j) \rangle | \uparrow \uparrow \rangle \prod_{j<k} \frac{1}{\sinh(\lambda_j - \lambda_k) \sinh(\lambda_j + \lambda_k)} \times \det L_M(\lambda_1, \ldots, \lambda_M),$$

(56)

where the elements of the $M \times M$ matrix $L$ (not to be confused with the $L$-matrix of the algebraic Bethe ansatz) are

$$\left[ L(\lambda_1, \ldots, \lambda_M) \right]_{jk} = \coth^2(\lambda_k - \eta/2) - \coth^2(\lambda_k + \eta/2),$$

(57)
and $\langle \phi | \tilde{B}(\lambda_j) | \uparrow \uparrow \rangle$ are given in equations (46), (47) and (48) for the Néel state, the dimer state, and the $q$-deformed dimer state, respectively. Equation (56) is a simple rewriting in our notations of the overlaps formulas in [43] for these states. From the structure of equation (44), it is natural to look for a solution in terms of the determinant of a certain matrix. In fact, recursive formula (44) has the same form of the Laplace’s recursive formula for the determinant of a square matrix. The proof of equation (56) is indeed straightforward from the recursion relation, and it proceeds by induction.

First, we see that the case of $M = 1$ is obvious. Next, we prove that equation (56) fulfills recursive formula (44). Plugging equation (56) into equation (44), we have

\[
det L_{M+1}(\hat{\lambda}_1, \ldots, \hat{\lambda}_{M+1})
\]

\[
= \sinh (\eta) \sum_{j=1}^{M+1} \prod_{k \neq j}^{M+1} f(\lambda_k, \lambda_j) \sinh \left(2\hat{\lambda}_j \right) \prod_{r=1}^{j-1} \sinh (\lambda_r - \hat{\lambda}_j) \prod_{r=j+1}^{M+1} \sinh (\hat{\lambda}_j - \lambda_r) \prod_{r \neq j}^{M+1} \sinh (\hat{\lambda}_j + \lambda_r)
\]

\[
\times \sinh^2 (\hat{\lambda}_j - \eta/2) \sinh^{2M+2} (\lambda + \eta/2) \prod_{k \neq j}^{M+1} \sinh^2 (\lambda_k - \eta/2)
\]

\[
\times \det L_M(\lambda_1, \ldots, \hat{\lambda}_j, \ldots, \lambda_{M+1}),
\]  

(58)

where $f(\mu, \nu)$ is given in equation (11). We now define

\[
a_j \equiv \lambda_j + \eta/2, \quad b_j \equiv \lambda_j - \eta/2,
\]  

(59)

and

\[
\alpha_k \equiv \coth^2(a_k), \quad \beta_k \equiv \coth^2(b_k).
\]  

(60)

Using the identities

\[
\frac{\sinh (\eta) \sinh \left(2\lambda_j \right)}{\sinh^2 (\hat{\lambda}_j - \eta/2) \sinh^2 (\hat{\lambda}_j + \eta/2)} = \coth^2 (b_j) - \coth^2 (a_j) = \beta_j - \alpha_j,
\]  

(61)

\[
\frac{\sinh (\lambda_j - \lambda_k + \eta) \sinh (\lambda_j + \lambda_k)}{\sinh^2 (\hat{\lambda}_j + \eta/2) \sinh^2 (\hat{\lambda}_k - \eta/2)} = \coth^2 (b_k) - \coth^2 (a_j) = \beta_k - \alpha_j,
\]  

(62)

\[
\left( \prod_{k=1}^{j-1} \sinh (\lambda_k - \lambda_j) \right) \left( \prod_{r=j+1}^{M+1} \sinh (\hat{\lambda}_j - \lambda_r) \right)
\]

\[
= (-1)^{j+1} \prod_{k=1}^{M+1} \sinh (\hat{\lambda}_j - \lambda_k).
\]  

(63)
equation (58) can be written as

\[
\det L_{M+1}(\lambda_1, \ldots, \lambda_{M+1}) = \sum_{j=1}^{M+1} (-1)^{j+1} \times \prod_{k=1}^{M+1} (\beta_k - \alpha_j) \det L_M(\lambda_1, \ldots, \lambda_{M+1}).
\]  

(64)

Consider now Laplace’s formula for the determinant of a square matrix \(A\) (with elements \(a_{jk}\)) of size \(N\)

\[
\det A = \sum_{j=1}^{N} (-1)^{N+j} a_{nj} \det \tilde{A}_{nj},
\]

(65)

where \(\tilde{A}_{nj}\) is the square matrix of size \(N-1\) that results from \(A\) by removing the \(N\)th row and the \(j\)th column. Using equation (65) and the induction hypothesis we see that the r.h.s. of equation (64) is equal to

\[
\begin{bmatrix}
\beta_1 - \alpha_1 & \cdots & \beta_{M+1} - \alpha_{M+1} \\
\beta_1^2 - \alpha_1^2 & \cdots & \beta_{M+1}^2 - \alpha_{M+1}^2 \\
\vdots & \ddots & \vdots \\
\beta_1^M - \alpha_1^M & \cdots & \beta_{M+1}^M - \alpha_{M+1}^M \\
\end{bmatrix}
\]

(66)

\[-1]^M \prod_{k=1}^{M+1} (\beta_k - \alpha_1) \ldots (-1)^M \prod_{k=1}^{M+1} (\beta_k - \alpha_{M+1})
\]

To conclude the proof, it is sufficient to show that (66) is equal to

\[
\begin{bmatrix}
\beta_1 - \alpha_1 & \beta_2 - \alpha_2 & \cdots & \beta_{M+1} - \alpha_{M+1} \\
\beta_1^2 - \alpha_1^2 & \beta_2^2 - \alpha_2^2 & \cdots & \beta_{M+1}^2 - \alpha_{M+1}^2 \\
\vdots & \ddots & \vdots \\
\beta_1^M + 1 - \alpha_1^M + 1 & \beta_2^M + 1 - \alpha_2^M + 1 & \cdots & \beta_{M+1}^M + 1 - \alpha_{M+1}^M + 1 \\
\end{bmatrix}
\]

(67)

This can be done as follows. Expand the \(j\)th entry in the last row of equation (66) as

\[
(-1)^M \prod_{k=1}^{M+1} (\beta_k - \alpha_j) = -\alpha_j^M + 1 + \alpha_j^M \left( \sum_{i=1}^{M+1} \beta_i \right) - \alpha_j^{M-1} \left( \sum_{1 \leq i < j \leq M+1} \beta_i \beta_j \right) + \alpha_j^{M-2} \left( \sum_{i<j<k} \beta_i \beta_j \beta_k \right) + \ldots.
\]

(68)

Exploiting the properties of the determinant, we can simplify equation (68) without changing the determinant in equation (66) with the following manipulations

- multiply row \(M\) of (66) by \(\left( \sum_{i=1}^{M+1} \beta_i \right)\) and sum it to the row \(M+1\);
- multiply row \((M-1)\) of (66) by \(\left( \sum_{i<j} \beta_i \beta_j \right)\) and subtract it from the row \(M+1\);
multiply row \((M - 2)\) of \((66)\) by \(\sum_{i<j<k} \beta_i \beta_j \beta_k\) and sum it to the row \(M + 1\).

iterate the steps above for the remaining rows of \((66)\) until the last one.

From equation \((68)\), it is easy to see that, at the end of the procedure described above, the last row of the matrix in equation \((66)\) is written as

\[
\left( \beta_1^{M+1} - \alpha_1^{M+1} \right), \left( \beta_2^{M+1} - \alpha_2^{M+1} \right), \ldots, \left( \beta_M^{M+1} - \alpha_M^{M+1} \right),
\]

and this concludes the proof.

We finish this section considering why a similar proof is not valid for the other initial product states we considered, as, for example, the ferromagnets (with \(G = 1\)) and the ferromagnetic domain state (with \(G = 4\)). In the three cases that we solved above, there is always a down spin in one of the two sites that we add at each step. Therefore, this addition of two sites leads to a recursive formula similar to the Laplace expansion \((65)\). Conversely, for the ferromagnetic states, one has to choose at each step whether to add a down spin or an up spin, an operation which cannot be cast in a simple sum. Indeed, looking at equation \((38)\), we see an additional term compared to equation \((44)\), which makes it more difficult to solve. For the ferromagnetic domain state, at each step, we add two down spins so that instead of a single sum we have a double one in equation \((55)\). Thus, the Laplace expansion in equation \((65)\) cannot be directly used because it involves a single sum.

5. Conclusions

In this work, we derived a very general recursive formula for the overlaps between Bethe states and a broad class of product states in the XXZ spin-1/2 chain (which includes all product states considered so far in analytic and numerical computation). Explicit examples, i.e. for particular initial states of recursive formulas are reported in section 3.2. These recursive formulas are obtained using the algebraic Bethe ansatz and rely exclusively on the lattice structure of the XXZ model. Our approach is straightforwardly generalized to other lattice Bethe ansatz solvable models such as the integrable lattice regularizations of the Lieb–Liniger model \([74, 75]\).

In the case of the Néel state, the dimer state, and the q-deformed dimer state, our recursive formula allows us to prove very easily the recently found overlaps in \([43]\). As a relevant difference, our proof does not use any concept coming from the boundary algebraic Bethe ansatz solution of the classical six-vertex model, and it is genuinely based on the solution of the XXZ chain. It is then highly desirable to find compact (determinant) solutions of all the recursive formulas listed in section 3.2. Of course, a trivial solution of these recursive formulas is given by the formal expression obtained using the coordinate Bethe ansatz wave functions, but such an expression is neither numerically nor analytically tractable. Compact solutions would be very useful for analytical studies of the quench dynamics of the XXZ model based on the representative state approach \([9]\), on the same lines of those presented in \([30, 31]\) for the dimer and Néel states, respectively. This would allow to confront with the GGE solution \([34]\) for a wide class of states.

It is worth stressing that our recursive formulas refer to off-shell scalar products; that is, the rapidities \(\{ \lambda_i \}\) defining the Bethe states do not necessarily fulfill the Bethe equations \((8)\). Provided that compact solutions for recursive formulas can be found, following \([44]\), they could be used as a starting point for obtaining simplified, on-shell formulas suitable for taking the thermodynamic limit. The question remains whether compact formulas exist in the XXZ model for the overlaps between Bethe states and other states besides those discussed in
section 4. We mention that product states of the form (18) can be used as good approximations of the ground states of gapped Hamiltonian with correlation length $\xi \lesssim G$ in a matrix product-state representation, on the same lines of what occurred for the GGE in [34].

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