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Nuclear Physics B 967 (2021) 115390

NUCLEAR PHYSICS B

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On factorized overlaps: Algebraic Bethe Ansatz, twists, and separation of variables

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Received 10 February 2021; received in revised form 22 March 2021; accepted 1 April 2021
Available online 6 April 2021
Editor: Hubert Saleur

Abstract

We investigate the exact overlaps between eigenstates of integrable spin chains and a special class of states called "integrable initial/final states". These states satisfy a special integrability constraint, and they are closely related to integrable boundary conditions. We derive new algebraic relations for the integrable states, which lead to a set of recursion relations for the exact overlaps. We solve these recursion relations and thus we derive new overlap formulas, valid in the XXX Heisenberg chain and its integrable higher spin generalizations. Afterwards we generalize the integrability condition to twisted boundary conditions, and derive the corresponding exact overlaps. Finally, we embed the integrable states into the "Separation of Variables" framework, and derive an alternative representation for the exact overlaps of the XXX chain. Our derivations and proofs are rigorous, and they can form the basis of future investigations involving more complicated models such as nested or long-range deformed systems.
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1. Introduction

One dimensional quantum integrable models are very special systems, where the exact wave functions can be computed using analytic methods, even in the presence of interactions. However,

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https://doi.org/10.1016/j.nuclphysb.2021.115390
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the computation of composite objects such as correlation functions is a notoriously difficult task even in these systems. In the last couple of years considerable effort was spent to study a special class of objects: the exact overlaps between the eigenstates of the model and a distinguished set of states, which are now called *integrable initial states* [1,2]. These overlaps display very special features and they are important for a number of reasons.

First of all we mention the context of non-equilibrium dynamics of integrable models, where the overlaps play a central role in the study of quantum quenches. In a quench one prepares the system in an initial state, which is not an eigenstate of the Hamiltonian, and the goal is to study the non-equilibrium dynamics, the emergence of steady states, and their properties [3]. The overlaps with the initial state are intermediate objects for the exact computations, and they serve as an input to the so-called Quench Action method, one of the main methods for the study of the steady states [4]. Thus it was crucial to find initial states where exact overlaps could be derived. The first exact results appeared for the Lieb-Liniger model in [5] and the Heisenberg spin chains in [6,7]. The exact overlap formulas played a central role in the early studies of the Generalized Gibbs Ensemble (GGE) in interacting integrable models, see [8,9].

It was found in these early studies that the overlaps are non-zero only if the eigenstate in question is an eigenvector of the space reflection operator. Furthermore the overlaps were found to possess a remarkable factorized form. It was later understood in [1] (see also [10,2]), that these properties are tied to special integrable structures behind the initial states. Namely, the solvable cases can be understood as *integrable boundaries* in time, and they are closely related to integrable boundary conditions. This understanding was inspired by the seminal work of Ghoshal and Zamolodchikov [11], which investigated integrable boundaries in integrable Quantum Field Theories (QFT's).

In QFT the overlaps between the eigenstates and some finite volume integrable boundary state are called "exact g-functions". The name "g-function" originally refers to the overlap between the finite volume ground state and the boundary state, and this quantity has already a rather rich structure [12,13]. Overlaps with excited state are then called excited state g-functions. We note that the factorized structure of the excited state overlaps already appeared in [14], but this work did not influence the later rigorous derivation of [7].

The exact overlaps also appeared in the context of the AdS/CFT duality: it was first found in [15] that they describe one-point functions in defect CFT. To be more precise, in a co-dimension one defect $\mathcal{N} = 4$ SYM the tree-level one-point functions are given by overlaps between Bethe states corresponding to single trace operators and special two-site states or Matrix Product States [16–20]. On the string theory side the surface defect corresponds to a probe brane, where closed strings corresponding to single trace operators can be annihilated. The dual quantity of the one-point function is the annihilation amplitude of the strings. In the 1+1 dimensional sigma model point of view this amplitude is an overlap between and eigenstate and a boundary state, which is thus an excited state g-function. For these reasons the overlaps appear on both the gauge and the string theory sides of the duality.

For the probe D5-brane, which preserves half of the supersymmetry it was showed that the tree level boundary states are integrable in the $SO(6)$ sector, and the corresponding overlaps were also calculated in [18]. In [19] it was also showed that the one-point functions are integrable at one-loop level in the SU(2) sector. Using symmetry considerations the asymptotic all loop boundary state was proposed independently in [21] and [22] and its asymptotic overlaps was proposed for the full spectrum in [22,23]. In [24] the authors took the weak coupling limit of the asymptotic overlap and showed that this formula is covariant under the fermionic dualities and it is compatible with the tree level overlaps in various subsectors [18,20]. This is a strong

consistency check of the assumption that the integrability condition holds at the all loop level. It is worthwhile to mention that integrable boundary states also appear in the investigation of three-point function where two operators are of determinant type and third is of single trace type [25,26].

Let us now discuss the various methods used for the derivation of the exact overlaps. The first work [5] applied coordinate Bethe Ansatz in the Lieb-Liniger model to the overlaps with low particle numbers, and a conjecture was made for the general case. The paper [7] actually proved an exact formula for the Heisenberg spin chains, valid for arbitrary particle numbers. This proof was based on an off-shell overlap formula, originally derived by Tsushiya [27] and adapted to overlaps in [6] (see also [28]). However, this particular proof was valid only for a subclass of states, namely those related to the so-called diagonal K-matrices. Afterwards a number of works simply just assumed the factorized structure of the exact overlap, and determined the pair amplitude of the overlaps using either coordinate Bethe Ansatz [16–20] or the so-called Quantum Transfer Matrix (QTM) method [10,29,30].

A new approach was initiated in [31], where the exact formulas were proven regarding all particle numbers, based on the analytic properties of the coordinate Bethe Ansatz expressions. This method is based on the ideas of Korepin, developed for the derivation of the norm of the Bethe wave function [32]. It was shown in [31] that the method is applicable not only to the Heisenberg chain, but also to spin chains with non-compact local spaces such as the so-called $sl(2,\mathbb{R})$ chain. This method was already used in [33] to give an alternative proof for the overlap formulas between the Lieb-Liniger Bethe states and the Bose-Einstein condensate state, originally derived in [5] and first proven in [34]. However, the drawback of the method of [31] is that it is relatively difficult to apply it to new cases, and it was not clear whether it could be useful for the models solvable by the nested Bethe Ansatz.

It is desirable to develop further methods for the derivation and proof of exact overlap formulas. It is fair to say that none of the existing methods is convenient for actually proving the results in the nested spin chains. Furthermore, it is desirable to find a formulation which would allow an extension to long range deformed models, and in particular to the full AdS/CFT problem.

With this goal in mind we turn to two central methods used in integrability: the Algebraic Bethe Ansatz (ABA) and the Separation of Variables (SoV). Remarkably, up to now neither of these methods have been used for the systematic treatment of integrable initial states and their overlaps. The original work [6] was based on some simple computations with systems with boundaries in ABA, but the applicability of those results is very limited. In integrable QFT the g-functions were considered in connection with SoV in [35], but that work did not treat the integrability condition for the boundary states within SoV. It is worthwhile to recall that the natural language of the AdS/CFT spectral problem is the so-called Q-system, which is a set of relations for the so-called Q-functions [36]. On the other hand, the Q-functions are naturally interpreted as the wave functions in SoV. This gives further motivation to apply the SoV method to the boundary states. Nevertheless, a proper embedding of the integrable states into the SoV framework was missing up to now.

In the present work we initiate a systematic study of the overlaps using the ABA and the SoV approaches. We show that the ABA is capable of deriving new recursion relations for the overlaps, which can complement the methods of [31], leading to a wider applicability. Furthermore we show that the integrable initial states can be represented also in the SoV framework, and we also derive new overlap formulas using this approach.

2. Overlaps and ABA

In this section we review the construction of integrable two-site states for integrable spin chains [1]. We focus on the XXX chain and its integrable higher spin generalizations.

We introduce a new relation (which we call the KT-relation), which is very useful for the derivation of overlap formulas: it leads to a new recursion relation for the off-shell overlaps. This recursion can be solved in certain cases and we obtain the off-shell overlap as a Vandermonde-like determinant. Using the argument of [31] we derive the on-shell formula of general two-site state for inhomogeneous chains with arbitrary quantum space. We close this section by calculating the overlaps for descendant states.

2.1. Integrable states and KT relation

Let us start with the definitions. Let us use the following convention for the R-matrix

$$R(u) = u\mathbf{1} + \mathbf{P} = u\mathbf{1} + e_{ij} \otimes e_{ji}, \tag{2.1}$$

where e_{ij}-s are the 2×2 matrix units and $\mathbf{P}$ is the permutation matrix. Let $E_{ij}^{(r)} \in \mathrm{End}\left(\mathbb{C}^{r+1}\right)$ be the highest weight irrep of $\mathfrak{gl}_2$ with highest weight $(r, 0)$. The basis vectors are $|p, q\rangle^{(r)} \in \mathbb{C}^{r+1}$ for which $p + q = r$, $0 \leq p, q \leq r$ and

$$E_{11}^{(r)} |p, q\rangle^{(r)} = p\, |p, q\rangle^{(r)}, \qquad E_{22}^{(r)} |p, q\rangle^{(r)} = q\, |p, q\rangle^{(r)}. \tag{2.2}$$

Using these representations we define the Lax operators

$$R^{(r)}(u) = u\mathbf{1} + e_{ij} \otimes E_{ji}^{(r)}, \qquad L^{(r)}(u) = R^{(r)}(u - r/2). \tag{2.3}$$

The R- and L-matrices have crossing symmetry:

$$R_{12}(u) = -\sigma_1^y R_{12}^{t_1}(-u-1)\sigma_1^y. \tag{2.4}$$

$$L_{12}^{(r)}(u) = -\sigma_1^y \left[L_{12}^{(r)}(-u)\right]^{t_1} \sigma_1^y = -\Sigma_2 \left[L_{12}^{(r)}(-u)\right]^{t_2} \Sigma_2^{-1}, \tag{2.5}$$

where $\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and the Σ is a matrix for which

$$\begin{aligned} &\Sigma \left(E_{11}^{(r)} - E_{22}^{(r)}\right) \Sigma^{-1} = E_{22}^{(r)} - E_{11}^{(r)}, \\ &\Sigma E_{12}^{(r)} \Sigma^{-1} = -E_{21}^{(r)}, \qquad \Sigma E_{21}^{(r)} \Sigma^{-1} = -E_{12}^{(r)}. \end{aligned} \tag{2.6}$$

Using the Lax operators we can define the monodromy and transfer matrices and their space reflected versions as

$$\begin{aligned} T_0(u) &= L_{0,2L}^{(r_{2L})}(u - \xi_{2L}) L_{0,2L-1}^{(r_{2L-1})}(u - \xi_{2L-1}) \dots L_{0,2}^{(r_2)}(u - \xi_2) L_{0,1}^{(r_1)}(u - \xi_1) \\ T_0^{\pi}(u) &= L_{0,1}^{(r_1)}(u + \xi_1) L_{0,2}^{(r_2)}(u + \xi_2) \dots L_{0,2L-1}^{(r_{2L-1})}(u + \xi_{2L-1}) L_{0,2L}^{(r_{2L})}(u + \xi_{2L}) \end{aligned} \tag{2.7}$$

and

$$t(u) = \mathrm{Tr}_0 T_0(u), \qquad \Pi t(u) \Pi = \mathrm{Tr}_0 T_0^{\pi}(u), \tag{2.8}$$

where Π is the space reflection operator. The matrix entries of the monodromy matrices are

$$T(u) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}, \qquad T^{\pi}(u) = \begin{pmatrix} A^{\pi}(u) & B^{\pi}(u) \\ C^{\pi}(u) & D^{\pi}(u) \end{pmatrix}. \tag{2.9}$$

The T and T^{π} are not independent quantities. We can use the crossing symmetry of Lax matrices to express

$$\sigma_0^y \left(T_0^{\pi}(u)\right)^{t_0} \sigma_0^y = L_{0,2L}(-u-\xi_{2L}) \dots L_{0,1}(-u-\xi_1) = T_0(-u). \tag{2.10}$$

Therefore

$$T^{\pi}(u) = \begin{pmatrix} D(-u) & -B(-u) \\ -C(-u) & A(-u) \end{pmatrix}. \tag{2.11}$$

We can construct the eigenvalues and eigenvectors of the transfer matrix using the algebraic Bethe Ansatz. The eigenvectors can be built form the B-operators as

$$|\mathbf{u}\rangle = B(u_1) \dots B(u_N) |0\rangle , \tag{2.12}$$

where $|0\rangle$ is the reference state:

$$|0\rangle = |r_1, 0\rangle^{(r_1)} \otimes |r_2, 0\rangle^{(r_2)} \otimes \dots \otimes |r_{2L-1}, 0\rangle^{(r_{2L-1})} \otimes |r_{2L}, 0\rangle^{(r_{2L})} . \tag{2.13}$$

Below it is understood that $\mathbf{u}$ is a set of rapidities with N elements, unless otherwise noted.

The action of operators $A(u)$ and $D(u)$ on the pseudovacuum can be written in the usual form

$$A(u) |0\rangle = \lambda^{+}(u) |0\rangle , \qquad D(u) |0\rangle = \lambda^{-}(u) |0\rangle , \tag{2.14}$$

where

$$\lambda^{\pm}(u) = \prod_{k=1}^{2L} (u \pm r_k/2 - \xi_k) . \tag{2.15}$$

The vector $|\mathbf{u}\rangle$ is an eigenvector of the transfer matrix is the Bethe roots u_i satisfy the Bethe Ansatz equations

$$\frac{\lambda^{+}(u_i)}{\lambda^{-}(u_i)} = -\frac{Q_1(u_i+1)}{Q_1(u_i-1)}, \tag{2.16}$$

and the eigenvalue $\Lambda(u)$ reads as

$$\Lambda(u) = \lambda^{+}(u) \frac{Q_1(u-1)}{Q_1(u)} + \lambda^{-}(u) \frac{Q_1(u+1)}{Q_1(u)}, \tag{2.17}$$

where we defined the Q-function

$$Q_1(u) = \prod_{i=1}^{N} (u - u_i). \tag{2.18}$$

We can also construct the left eigenvectors with the same eigenvalue as

$$\langle \mathbf{u}| = \langle 0| C(u_1) \dots C(u_N). \tag{2.19}$$

In this paper we do not use any inner product therefore the quantities like $\langle \mathbf{v}|\mathbf{u}\rangle$ are defined as a natural pairing between a dual vector and a vector, but not as a scalar product.

It is well known that the Bethe states with N magnons are highest weight states and their descendants are also eigenvectors of the transfer matrix with the same eigenvalue. Let us define spin operators as

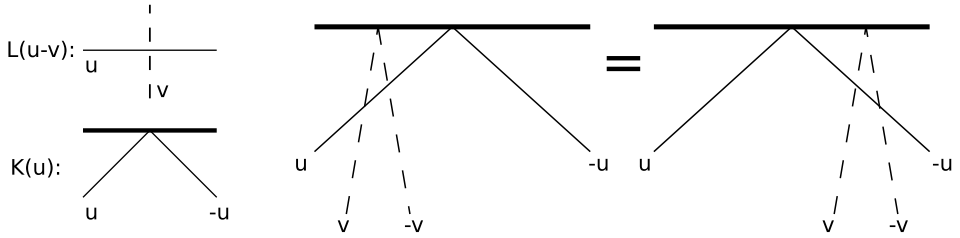

Fig. 1. Pictorial representation of the KYB equation (2.27), see on the right. The action of the Lax operator is represented by the crossing of the straight and dashed lines, which correspond to two (potentially different) auxiliary spaces. The thick horizontal line represents for the integrable final state (boundary in the time direction). The K-matrix connects the physical spaces to the integrable boundary, and its two "legs" carry rapidity parameters (inhomogeneities) opposite to each other.

$$S^+ = e_{21}, \qquad S^- = e_{12}, \qquad S_3 = \frac{1}{2}\left(e_{11} - e_{22}\right), \tag{2.20}$$

for which

$$\left[S^+, S^-\right] = 2S_3, \qquad \left[S_3, S^\pm\right] = \pm S^\pm. \tag{2.21}$$

The asymptotic limit of the operator B is the spin lowering operator

$$\lim_{u\to\infty} \frac{1}{u^{2L-1}} B(u) = \Delta(S^-), \tag{2.22}$$

where Δ is the usual co-product. Let us define the descendant states as

$$|\mathbf{u}, M\rangle := \Delta(S^-)^M |\mathbf{u}\rangle\,. \tag{2.23}$$

Below we will construct integrable two-site states. The construction requires that the sites of the spin chain are "paired" which means that for a pair of sites $(2a-1, 2a)$ the inhomogeneities are opposite to each other i.e.

$$\xi_{2a-1} = \theta_a, \qquad \xi_{2a} = -\theta_a \tag{2.24}$$

and the representations are the same i.e.

$$r_{2a-1} = r_{2a} = s_a. \tag{2.25}$$

Two-site states can be built from K-matrices $K^{(s)}(u)$. The K-matrices are given by their components k_{ij}, which can be arranged into a matrix or into a co-vector as

$$\mathbf{K}_1(u) = \sum_{i,j} k_{ij}(u) e_{ij}, \qquad \vec{K}_{12}(u) = \sum_{i,j} k_{ij}(u) e_i^* \otimes e_j^*. \tag{2.26}$$

These are two representations of the same quantity and we for simplicity we call them both K-matrix.

The defining equation of the K-matrices is the following equation [1,2,22,23]

$$\vec{K}_{12}(u)\vec{K}^{(s)}_{34}(v)L^{(s)}_{14}(u+v)L^{(s)}_{13}(u-v) = \vec{K}_{12}(u)\vec{K}^{(s)}_{34}(v)L^{(s)}_{23}(u+v)L^{(s)}_{24}(u-v). \tag{2.27}$$

Following [22,23] we call it the KYB equation. We will see below that it is very closely related to the Boundary Yang-Baxter (BYB) equation. A graphical interpretation of the KYB equation is given in Fig. 1.

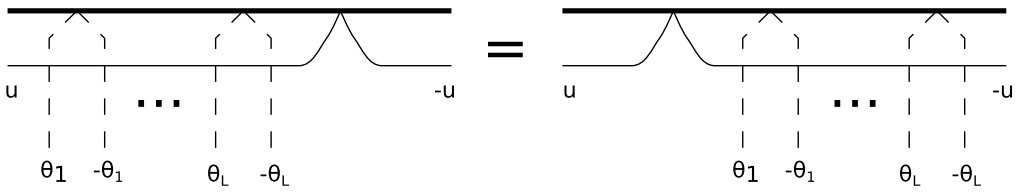

Fig. 2. Graphical interpretation of the KT relation (2.29). The dashed vertical lines stand for the physical spaces of the spin chain, and the horizontal line is the auxiliary space of the monodromy matrix. We assume that this space carries the spin-1/2 representation, but the physical spaces can be higher dimensional. The main idea is to insert one more K-matrix which acts on the auxiliary space, and then to use the KYB relations consecutively, to shift the action of the extra K from the right hand side to the left hand side. Working out the details we obtain (2.29). It is important that the indices at the left and right are free, thus we actually have a collection of 4 algebraic relations. The integrability condition (2.30) is found by multiplying with the inverse of one of the K-matrices, and taking the trace in auxiliary space.

We can now define two-site states as

$$\langle\Psi| = \vec{K}^{(s_1)}(\theta_1) \otimes \cdots \otimes \vec{K}^{(s_L)}(\theta_L). \tag{2.28}$$

We call such a state an *integrable final state*. We use the expression "final state", because in our conventions it is actually a co-vector which acts on the eigenstates of the model.

It follows directly from the KYB equation that such a two-site state satisfies the following relation (see 2 for the graphical derivation)

$$\langle\Psi|\,\vec{K}_{12}(u)T_1(u) = \langle\Psi|\,\vec{K}_{12}(u)T_2^{\pi}(u) \quad \Longleftrightarrow \quad \langle\Psi|\,\sigma^y\mathbf{K}^t(u)T(u) = \langle\Psi|\,T(-u)\sigma^y\mathbf{K}^t(u). \tag{2.29}$$

We call (2.29) the KT-relation; it can be understood as the "time"-boundary analog of the usual RTT-relation[1]. Note that it is actually a collection of 4 equations due to the free indices in the auxiliary space; specific components will be given below. Also, it is shown below that the KT-relation allows us to embed the overlap computations into the framework of algebraic Bethe Ansatz.

Let us assume that the K-matrix is invertible. In this case we can take the trace of the KT relation in auxiliary space after multiplying with the inverse of the K-matrix on either side. This leads to the integrability condition

$$\langle\Psi|\,t(u) = \langle\Psi|\,\Pi t(u)\Pi. \tag{2.30}$$

This condition was introduced in [1], and the equation (2.29) appears there as an intermediate step in the derivation (2.30). In this paper we point out that the equation (2.29) contains more information than the integrability condition (2.30), and we use this extra information in the derivation of the overlaps. We note that (2.30) is formally a relation for co-vectors.

It is known that the KYB equation is equivalent to the reflection equation [1,2,22,23]

$$\begin{aligned} &L_{12}^{(s)}(u-v)\left(\Sigma_1\mathbf{K}_1^{(s)}(-u)\right)L_{12}^{(s)}(u+v)\left(\sigma_2^y\mathbf{K}_2(-v)\right) \\ &\quad = \left(\sigma_2^y\mathbf{K}_2(-v)\right)L_{12}^{(s)}(u+v)\left(\Sigma_1\mathbf{K}_1^{(s)}(-u)\right)L_{12}^{(s)}(u-v). \end{aligned} \tag{2.31}$$

For $s = 1$ the reflection equation can be written as

[1] The KT relation looks very similar as the twisted Yangian invariance of Baxter lattice with boundary, see (24) in [37].

$$R_{12}(u-v-1/2)\left(\sigma_1^y \mathbf{K}_1^{(1)}(-u)\right) R_{12}(u+v-1/2)\left(\sigma_2^y \mathbf{K}_2(-v)\right) = \left(\sigma_2^y \mathbf{K}_2(-v)\right) R_{12}(u+v-1/2)\left(\sigma_1^y \mathbf{K}_1^{(1)}(-u)\right) R_{12}(u-v-1/2). \quad (2.32)$$

Using the definitions

$$\vec{K}^{(1)}(u) := \frac{1}{u+1/2}\vec{K}(u+1/2), \qquad \mathcal{K}_1(u) := \sigma_1^y \mathbf{K}_1(-u) \quad (2.33)$$

we obtain the usual reflection equation of XXX spin chain

$$R_{12}(u-v)\mathcal{K}_1(u)R_{12}(u+v)\mathcal{K}_2(v) = \mathcal{K}_2(v)R_{12}(u+v)\mathcal{K}_1(u)R_{12}(u-v). \quad (2.34)$$

The solutions of this equation are well known. We use the following parametrization

$$k_{11}(u) = au \qquad k_{12}(u) = -b+cu \quad (2.35)$$

$$k_{21}(u) = b+cu \qquad k_{22}(u) = du. \quad (2.36)$$

We will also use normalized matrix entries

$$\kappa(u) := \frac{k_{21}(u)}{k_{11}(u)} = \frac{b+cu}{au}, \quad \frac{k_{12}(u)}{k_{11}(u)} = \frac{-b+cu}{au} = \kappa(-u), \quad \delta := \frac{k_{22}(u)}{k_{11}(u)} = \frac{d}{a}. \quad (2.37)$$

Using this matrix we can obtain the K-matrices for the higher representations by the fusion procedure. It is more convenient to use the reflection equation (2.31) with the R-matrices. We use the $s=1$ equation

$$\vec{K}_{12}^{(1)}(u)\vec{K}_{34}^{(1)}(v)R_{14}(u+v)R_{13}(u-v) = \vec{K}_{12}^{(1)}(u)\vec{K}_{34}^{(1)}(v)R_{23}(u+v)R_{24}(u-v) \quad (2.38)$$

to construct the solution of the general KYB equation

$$\vec{K}_{12}^{(1)}(u)\vec{K}_{34}^{(s)}(v)L_{14}^{(s)}(u+v+1/2)L_{13}^{(s)}(u-v+1/2) = \vec{K}_{12}^{(1)}(u)\vec{K}_{34}^{(s)}(v)L_{23}^{(s)}(u+v+1/2)L_{24}^{(s)}(u-v+1/2). \quad (2.39)$$

The $L_{14}^{(s)}(u \mp v + 1/2)$ can be obtained from the original R-matrix using fusion [38]. We obtain

$$L_{ab}^{(s)}(u \mp v + 1/2) \propto \left[\mathcal{P}_b^{(1,2,\dots,s)}\right]\left[\prod_{k=1}^{s} R_{a,k}(u \mp (v - \frac{s-2k+1}{2}))\right]\left[\mathcal{P}_b^{(1,2,\dots,s)}\right]^T, \quad (2.40)$$

where $\mathcal{P}^{(1,\dots,s)} : \left(\mathbb{C}^2\right)^{\otimes s} \to \mathbb{C}^{s+1}$ is the projection operator to the symmetric subspace of $\left(\mathbb{C}^2\right)^{\otimes s}$. The $K^{(s)}(v)$ can be obtained in an analogous way [39]

$$\vec{K}_{a,b}^{(s)}(v) = \left[\prod_{k=1}^{s} \vec{K}_{2k-1,2k}^{(1)}(v - \frac{s-2k+1}{2})\right] \times \left[\prod_{l=1}^{s-1}\prod_{k=1}^{s-l} \bar{R}_{2k+2l-1,2k}(2v-s+2k+l-1)\right]\left[\mathcal{P}_a^{(1,3,\dots,2s-1)}\right]^T\left[\mathcal{P}_b^{(2,4,\dots,2s)}\right]^T, \quad (2.41)$$

where

$$\bar{R}(u) = \frac{1}{u+1}R(u). \quad (2.42)$$

In Fig. 3 we present a graphical interpretation of the fusion, taking the example of $\vec{K}_{a,b}^{(4)}(v)$.

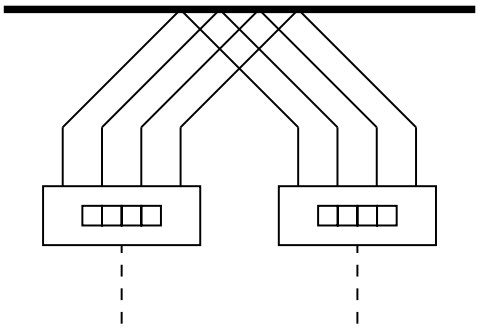

Fig. 3. Graphical illustration of the fusion rule (2.41) for the K-matrices. Here we present the example $K^{(4)}(v)$. The fused K-matrix is obtained by taking 4 copies of the original K-matrices with shifted rapidity parameters. Afterwards we apply a projection, which is symbolized by the boxes.

Using this convention for the K-matrices the overlap between $\langle\Psi|$ and the pseudovacuum is

$$\langle\Psi|0\rangle = a^{\mathcal{L}}, \tag{2.43}$$

where

$$\mathcal{L} = \sum_{k=1}^{L} s_k. \tag{2.44}$$

In this section our goal is finding and proving overlap formulas as

$$\langle\Psi|\mathbf{u}\rangle, \tag{2.45}$$

where $|\mathbf{u}\rangle$ is an on-shell vector i.e. an eigenstate of the transfer matrices. However, quantities like (2.45) are not physical since they depend on our normalization conventions. Of course, for physical system the Hamiltonian is hermitian and we have a well-defined norm on the Hilbert space and we can divide (2.45) by the norm of the state. In this paper we do not introduce any metric but we have an option to define normalized quantities as

$$\frac{\langle\Psi|\mathbf{u}\rangle\langle\mathbf{u}|\Psi^*\rangle}{\langle\mathbf{u}|\mathbf{u}\rangle}, \tag{2.46}$$

where $|\mathbf{u}\rangle$ and $\langle\mathbf{u}|$ are the right and left eigenvectors with the same eigenvalue (and spin). The advantage of this expression is that it does not depend on the normalization of the left/right eigenvectors. The disadvantage is that we have to define a new initial two-site state $|\Psi^*\rangle$ which is independent from the final two-site state $\langle\Psi|$ (because of the absence of the metric). With the asterisk we suggest that it would be a complex conjugated state in a physical situation.

In the general case we can also define the initial two-site states. We can use the vector rearrangement of the previously defined K-matrices

$$\vec{K}_{12}(u)^T = \sum_{i,j} k_{ij}(u) e_i \otimes e_j. \tag{2.47}$$

We saw that they satisfy the reflection equation (2.31)

$$L_{12}^{(s)}(u-v)\left(\Sigma_1\mathbf{K}_1^{(s)}(-u)\right)L_{12}^{(s)}(u+v)\left(\sigma_2^y\mathbf{K}_2(-v)\right)$$
$$=\left(\sigma_2^y\mathbf{K}_2(-v)\right)L_{12}^{(s)}(u+v)\left(\Sigma_1\mathbf{K}_1^{(s)}(-u)\right)L_{12}^{(s)}(u-v). \tag{2.48}$$

This equation can be written as

$$L_{13}^{(s)}(v-u)L_{14}^{(s)}(-u-v)\vec{K}_{12}(-u)^T\vec{K}_{34}^{(s)}(-v)^T$$
$$=L_{24}^{(s)}(v-u)L_{23}^{(s)}(-u-v)\vec{K}_{12}(-u)^T\vec{K}_{34}^{(s)}(-v)^T, \tag{2.49}$$

which will be called KYB equation for right vectors. The initial two-site state is

$$\left|\Psi\right\rangle=\vec{K}^{(s_1)}(-\theta_1)^T\otimes\cdots\otimes\vec{K}^{(s_L)}(-\theta_L)^T, \tag{2.50}$$

for which the corresponding KT-relation can be written as

$$T_2(u)\vec{K}_{12}(u)^T\left|\Psi\right\rangle=T_1^{\pi}(u)\vec{K}_{12}(u)^T\left|\Psi\right\rangle \quad\Longleftrightarrow$$
$$T(u)\mathbf{K}^{*t}(u)\sigma^y\left|\Psi\right\rangle=\mathbf{K}^{*t}(u)\sigma^yT(-u)\left|\Psi\right\rangle. \tag{2.51}$$

In the following we concentrate overlaps with the final two site states but we emphasize that the calculation for the initial two-site state is completely analogous.

2.2. The KT relation and the overlaps

In the following we will use the KT relation to calculate overlaps between the above defined two-site states $\langle\Psi|$ and the off-shell Bethe states. The main advantage of this method is that it can be applied even for inhomogeneous chains and it gives the overlap formula for all representations of the quantum space simultaneously. This is remarkable, because in the higher spin cases it is not necessary to know the explicit form of the K-matrices, it is enough to know they exists e.g. given by fusion(2.41) [2]. Nevertheless it is possible to derive the exact overlaps.

We start with the following component of the KT relations:

$$\langle\Psi|\left(k_{11}(u)B(u)+k_{21}(u)D(u)\right)=\langle\Psi|\left(k_{21}(u)A^{\pi}(u)+k_{22}(u)C^{\pi}(u)\right). \tag{2.52}$$

Using the crossing relation for the space reflected monodromy matrix (2.11) we obtain

$$\langle\Psi|\left(k_{11}(u)B(u)+k_{21}(u)D(u)\right)=\langle\Psi|\left(k_{21}(u)D(-u)-k_{22}(u)C(-u)\right). \tag{2.53}$$

We can see that this equation can be used to replace B-operators with D- and C-operators, therefore we can decrease the number of magnons iteratively. Using the normalized matrix entries $\kappa(u)$ and δ the equation (2.53) can be written as

$$\langle\Psi|B(u)=\kappa(u)\langle\Psi|\left(D(-u)-D(u)\right)-\delta\langle\Psi|C(-u). \tag{2.54}$$

This will lead to a recursion relation for the overlaps, as we show below. We note that a different type of recursion was earlier used in [41], where the recursion also involved changing the length of the spin chain in each step. In contrast, the relation (2.54) does not change the volume, thus it leads to a different recursion procedure.

Now we demonstrate the usefulness of the KT-relation by very simple and instructive calculations which give the off-shell overlaps for one and two magnons.

[2] A closed form expression can be found in [40]. It is for the non-compact chain but should work for the compact case too.

N=1

We calculate the one magnon overlap as

$$\begin{aligned}\langle\Psi|\, B(u)\,|0\rangle =&\kappa(u)\,\langle\Psi|\,(D(-u)-D(u))\,|0\rangle - A\,\langle\Psi|\,C(-u)\,|0\rangle\\ =&a^{\mathcal{L}}\kappa(u)\left(\lambda^{+}(u)-\lambda^{-}(u)\right),\end{aligned}\tag{2.55}$$

where we used the identities

$$\lambda^{\pm}(-u)=\lambda^{\mp}(u).\tag{2.56}$$

N=2

Let us calculate the two magnon overlap

$$\langle\Psi|\, B(u_1)B(u_2)\,|0\rangle = \kappa(u_1)\,\langle\Psi|\,(D(-u_1)-D(u_1))\,B(u_2)\,|0\rangle - \delta\,\langle\Psi|\,C(-u_1)B(u_2)\,|0\rangle\,.\tag{2.57}$$

Using the commutation relations

$$D(u)B(v)=\frac{u-v+1}{u-v}B(v)D(u)-\frac{1}{u-v}B(u)D(v)\tag{2.58}$$

$$C(u)B(v)=B(v)C(u)+\frac{1}{u-v}\left(A(v)D(u)-A(u)D(v)\right)\tag{2.59}$$

we obtain the following expressions

$$\begin{aligned}\langle\Psi|\, D(u_1)B(u_2)\,|0\rangle =&\frac{u_1-u_2+1}{u_1-u_2}\lambda^{-}(u_1)\,\langle\Psi|\,B(u_2)\,|0\rangle\\ &-\frac{1}{u_1-u_2}\lambda^{-}(u_2)\,\langle\Psi|\,B(u_1)\,|0\rangle\\ =&a^{\mathcal{L}}\Bigg[\kappa(u_2)\frac{u_1-u_2+1}{u_1-u_2}\lambda^{-}(u_1)\left(\lambda^{+}(u_2)-\lambda^{-}(u_2)\right)\\ &-\kappa(u_1)\frac{1}{u_1-u_2}\lambda^{-}(u_2)\left(\lambda^{+}(u_1)-\lambda^{-}(u_1)\right)\Bigg]\end{aligned}\tag{2.60}$$

and

$$\langle\Psi|\, C(-u_1)B(u_2)\,|0\rangle = -a^{\mathcal{L}}\frac{1}{u_1+u_2}\left(\lambda^{+}(u_1)\lambda^{+}(u_2)-\lambda^{-}(u_1)\lambda^{-}(u_2)\right).\tag{2.61}$$

Therefore the two magnon overlap can be written as

$$\begin{aligned}\langle\Psi|\, B(u_1)B(u_2)\,|0\rangle = a^{\mathcal{L}}\Bigg[&\left(\kappa(u_1)\kappa(u_2)\frac{u_1+u_2-1}{u_1+u_2}+\delta\frac{1}{u_1+u_2}\right)\lambda^{+}(u_1)\lambda^{+}(u_2)-\\ &-\kappa(u_1)\kappa(u_2)\frac{u_1-u_2+1}{u_1-u_2}\lambda^{-}(u_1)\lambda^{+}(u_2)-\\ &-\kappa(u_1)\kappa(u_2)\frac{u_1-u_2-1}{u_1-u_2}\lambda^{+}(u_1)\lambda^{-}(u_2)+\\ &+\left(\kappa(u_1)\kappa(u_2)\frac{u_1+u_2+1}{u_1+u_2}-\delta\frac{1}{u_1+u_2}\right)\lambda^{-}(u_1)\lambda^{-}(u_2)\Bigg].\end{aligned}\tag{2.62}$$

2.3. Global rotation

The previous examples showed that the term in the KT-relation proportional to δ causes significant difficulty. This arises from the appearance of the C-operators, whose commutation relations with the B-operators are more involved.

However, we can use a global rotation to eliminate the δ-terms. Applying the following rotation

$$\vec{K}'_{12}(u) = \vec{K}_{12}(u) \exp\left(\frac{\gamma - c}{a} S^+\right), \tag{2.63}$$

where

$$\gamma^2 = c^2 - ad \tag{2.64}$$

the components of the rotated K matrix are

$$k'_{11}(u) = au \qquad k'_{12}(u) = -b + \gamma u \tag{2.65}$$

$$k'_{21}(u) = b + \gamma u \qquad k'_{22}(u) = 0. \tag{2.66}$$

At the end of the day we want to obtain on-shell overlap formulas and we know that the on-shell Bethe vectors are highest weight states i.e.

$$S^+ |\mathbf{u}\rangle = 0, \tag{2.67}$$

therefore

$$\langle \Psi | \mathbf{u} \rangle = \langle \Psi' | \exp\left(\frac{c - \gamma}{a} S^+\right) | \mathbf{u} \rangle = \langle \Psi' | \mathbf{u} \rangle, \tag{2.68}$$

where the two-site state $\langle \Psi |$ is built from the K-matrix $\vec{K}'_{12}$. The last equation shows that we can work with this rotated K-matrix for which

$$\kappa'(u) = \frac{b + \gamma u}{au}, \qquad \delta' = 0. \tag{2.69}$$

2.4. Recursion relation for the overlap

Let us continue with the derivation of a recursion formula for the off-shell formula

$$\mathcal{S}_N(u_1, \dots, u_N) = \langle \Psi' | u_1, \dots, u_N \rangle. \tag{2.70}$$

We only need the following commutation relations [42]

$$\begin{aligned} D(u_1)B(u_2)\dots B(u_N) = &\prod_{k=2}^{N} \frac{u_1 - u_k + 1}{u_1 - u_k} B(u_2)\dots B(u_N)D(u_1) - \\ &- \sum_{l=2}^{N} \frac{1}{u_1 - u_l} \prod_{k=2 \neq l}^{N} \frac{u_l - u_k + 1}{u_l - u_k} B(u_1)\dots \widehat{B(u_l)} \dots B(u_N)D(u_l). \end{aligned} \tag{2.71}$$

Let us start with the KT relation

$$\begin{aligned}\mathcal{S}_N(u_1,\dots,u_N) =& \left\langle \Psi' \right| B(u_1)B(u_2)\dots B(u_N)\left|0\right\rangle \\ =& \kappa'(u_1)\left\langle \Psi' \right| \left(D(-u_1)-D(u_1)\right)B(u_2)\dots B(u_N)\left|0\right\rangle . \end{aligned} \tag{2.72}$$

Substituting the commutation relations we can obtain the recursion relation:

$$\begin{aligned}\mathcal{S}_N(u_1,\dots,u_N) =& \\ \kappa'(u_1)\Bigg(& \prod_{k=2}^{N}\frac{u_1+u_k-1}{u_1+u_k}\lambda^+(u_1)\mathcal{S}_{N-1}(u_2,\dots,u_N)- \\ & -\prod_{k=2}^{N}\frac{u_1-u_k+1}{u_1-u_k}\lambda^-(u_1)\mathcal{S}_{N-1}(u_2,\dots,u_N)+ \\ & +\sum_{l=2}^{N}\frac{1}{u_1+u_l}\prod_{k=2\neq l}^{N}\frac{u_l-u_k+1}{u_l-u_k}\lambda^-(u_l)\mathcal{S}_{N-1}(-u_1,u_2\dots\widehat{u_l}\dots u_N)+ \\ & +\sum_{l=2}^{N}\frac{1}{u_1-u_l}\prod_{k=2\neq l}^{N}\frac{u_l-u_k+1}{u_l-u_k}\lambda^-(u_l)\mathcal{S}_{N-1}(u_1,u_2\dots\widehat{u_l}\dots u_N)\Bigg). \end{aligned} \tag{2.73}$$

We saw that the two magnon overlap is simplified as

$$\begin{aligned}\mathcal{S}_2(u_1,u_2) =& a^{\mathcal{L}}\kappa'(u_1)\kappa'(u_2)\Bigg(\frac{u_1+u_2-1}{u_1+u_2}\lambda^+(u_1)\lambda^+(u_2)-\frac{u_1-u_2+1}{u_1-u_2}\lambda^-(u_1)\lambda^+(u_2)- \\ & -\frac{u_1-u_2-1}{u_1-u_2}\lambda^+(u_1)\lambda^-(u_2)+\frac{u_1+u_2+1}{u_1+u_2}\lambda^-(u_1)\lambda^-(u_2)\Bigg). \end{aligned} \tag{2.74}$$

Seeing this formula we may assume that the N magnon overlap reads as

$$\begin{aligned}\mathcal{S}_N(u_1\dots u_N) =& a^{\mathcal{L}}\left[\prod_{k=1}^{N}\kappa'(u_k)\right] \\ & \times\left[\sum_{\{\sigma_1,\dots,\sigma_N\}=\{\pm,\dots,\pm\}}\prod_{1\leq k<l\leq N}\frac{\sigma_k u_k+\sigma_l u_l-1}{\sigma_k u_k+\sigma_l u_l}\prod_{k=1}^{N}\sigma_k\lambda^{\sigma_k}(u_k)\right]. \end{aligned} \tag{2.75}$$

It turns out that this assumption is true: the formula above can be proved using the recursion relation (2.73). We present the derivation in Appendix A.

The overlap formula (2.75) can be also written in a determinant form. After a simple rearrangement we obtain that

$$\begin{aligned}\mathcal{S}_N(u_1\dots u_N) =& a^{\mathcal{L}}\frac{\left[\prod_{k=1}^{N}\kappa'(u_k)\right]}{\prod_{1\leq k<l\leq N}\left[u_l^2-u_k^2\right]} \\ & \times\left[\sum_{\sigma_1,\dots,\sigma_N}\prod_{k<l}\left[\left(u_l-\frac{\sigma_l}{2}\right)^2-\left(u_k-\frac{\sigma_k}{2}\right)^2\right]\prod_{k=1}^{N}\sigma_k\lambda^{\sigma_k}(u_k)\right], \end{aligned} \tag{2.76}$$

which can be written as

$$\mathcal{S}_N(u_1 \dots u_N) = a^{\mathcal{L}} \left[\prod_{k=1}^{N} \kappa'(u_k) \right] \frac{\det V_N^+(u_1, \dots, u_N)}{\prod_{1 \le k < l \le N} \left[u_l^2 - u_k^2 \right]}, \tag{2.77}$$

where we defined a Vandermonde-like determinant

$$\left[V_N^+(u_1, \dots, u_N) \right]_{kl} = (u_k - 1/2)^{2l-2} \lambda^+(u_k) - (u_k + 1/2)^{2l-2} \lambda^-(u_k). \tag{2.78}$$

This result is reminiscent of the determinant formula found by Tsushiya in [27], which describes the off-shell overlaps the diagonal K-matrices in the spin-1/2 chain [6]. However, the matrix elements are different already in the spin-1/2 chain, with no direct connection to the formulas of Tsushiya. Thus (2.77) seems to be a completely new result. We stress that it is valid not only in the spin-1/2 XXX chain, but also in the higher spin integrable generalizations.

2.5. On-shell overlaps

In this subsection we review the connection between the integrability condition and the pair structure of Bethe roots. Furthermore, we also derive the on-shell overlap formulas, which are new in the higher spin cases.

We remind that the first derivation of exact on-shell overlaps of the Heisenberg spin chains was presented in [7]. In that work the on-shell limit of the off-shell formulas of [6,28] was taken, and the factorized structure was found. The only work after [7,43] which actually proved overlap formulas was [31]. In [31] a new method was introduced, which derived the on-shell overlaps based on the analytic properties of the of-shell cases. Below we review this method, and we use it to derive new on-shell overlaps.

Let us first discuss the implications of the integrability condition on Bethe roots. Applying on-shell Bethe vectors on the integrability condition (2.30) we obtain that

$$\langle \Psi | \, t(u) \, | \mathbf{u} \rangle = \langle \Psi | \, \Pi t(u) \Pi \, | \mathbf{u} \rangle \quad \longrightarrow \quad (\Lambda(u) - \Lambda(-u)) \langle \Psi | \mathbf{u} \rangle = 0, \tag{2.79}$$

where $\Lambda(u)$ is the eigenvalue of the transfer matrix

$$t(u) \, | \mathbf{u} \rangle = \Lambda(u) \, | \mathbf{u} \rangle \, , \qquad \Pi t(u) \Pi \, | \mathbf{u} \rangle = t(-u) \, | \mathbf{u} \rangle = \Lambda(-u) \, | \mathbf{u} \rangle \, . \tag{2.80}$$

We just obtained that non-vanishing overlaps can be found only if

$$\Lambda(u) = \Lambda(-u) \tag{2.81}$$

The explicit form of the eigenvalue is

$$\Lambda(u) = \lambda^+(u) \frac{Q_1(u-1)}{Q_1(u)} + \lambda^-(u) \frac{Q_1(u+1)}{Q_1(u)}. \tag{2.82}$$

Using the formula for $\Lambda(u)$ (2.17) we can convince ourselves that the condition (2.81) is equivalent to

$$Q_1(-u) = (-1)^N Q_1(u) \tag{2.83}$$

This implies that the set of (finite) Bethe roots is parity symmetric. Generally the two possibilities are

$$\begin{aligned} &\mathbf{u} = \left\{ u_1, -u_1, u_2, -u_2, \dots, u_{N/2}, -u_{N/2} \right\} \quad \text{or} \\ &\mathbf{u} = \left\{ u_1, -u_1, u_2, -u_2, \dots, u_{(N-1)/2}, -u_{(N-1)/2}, 0 \right\}. \end{aligned} \tag{2.84}$$

Let us now turn to the method of [31] for the derivation of on-shell overlaps. For simplicity we focus on the case when all rapidities come in pairs. We also use the following notation for the two halves of the set of Bethe roots:

$$\mathbf{u}^{+}_{N/2} = \left\{u_1, u_2, \ldots, u_{N/2}\right\}, \tag{2.85}$$

$$\mathbf{u}^{-}_{N/2} = \left\{u_{N/2+1}, u_{N/2+2}, \ldots, u_N\right\}. \tag{2.86}$$

The key observation of [31] was that the non-zero terms in the on-shell overlaps are obtained from apparent poles of the off-shell overlaps associated with the pair structure. The paper [31] concentrated on homogeneous spin chains. Let us introduce the notation

$$w(u) = e^{iLp(u)} \tag{2.87}$$

where $p(u)$ is the lattice momentum in the model under consideration. In [31] $w(u)$ was denoted as $a(u)$, but we chose to change the notation to avoid confusion with the parameter a of the K-matrix.

It was observed in [31] that the off-shell overlap has apparent poles of the type

$$\frac{w(u_1)w(u_2) - 1}{u_1 + u_2} \tag{2.88}$$

where we selected for simplicity a concrete pair (u_1, u_2). In the on-shell limit such factors will acquire some finite value (depending on L) if $u_1 + u_2 \to 0$. However, it was also shown in [31] that the regular terms all add up to zero, and the finite on-shell overlap consists only of these pole contributions. Thus it is necessary to understand the precise pole structure of the off-shell overlaps.

Let us now turn to our new off-shell formulas. It is our goal to use the arguments of [31] to derive new on-shell overlaps. In our case the w-variables are replaced by

$$w_k = \frac{\lambda^{+}(u_k)}{\lambda^{-}(u_k)}, \tag{2.89}$$

because we also treat the inhomogeneous cases. In the homogeneous case the original functions are reproduced. In the on-shell limit the Bethe Ansatz equations

$$w_k \prod_{j=1}^{N} \frac{f(u_k - u_j)}{f(u_j - u_k)} = -1 \tag{2.90}$$

are satisfied where

$$f(u) = \frac{u-1}{u}. \tag{2.91}$$

Returning to the representation (2.75) of the off-shell overlaps we see the occurrence of the formal poles of the type $(u_1 + u_2)^{-1}$. However, our normalization is different from that of [31]. Let us therefore introduce the new normalization

$$S_N(u_1, \ldots, u_N) = \prod_{k=1}^{N} \frac{1}{\lambda^{-}(u_k)} \mathcal{S}_N(u_1, \ldots, u_N) \tag{2.92}$$

with the exact result given by

$$S_N(u_1\dots u_N) = a^{\mathcal{L}}\left[\prod_{k=1}^{N}\kappa'(u_k)\right] \times \left[\sum_{\{\sigma_1,\dots,\sigma_N\}=\{\pm,\dots,\pm\}}\prod_{1\le k<l\le N}\frac{\sigma_k u_k+\sigma_l u_l-1}{\sigma_k u_k+\sigma_l u_l}\prod_{k=1}^{N}\sigma_k w_k^{\sigma_k+1/2}\right]. \quad (2.93)$$

We can see that this overlap function depends only on the w_i parameters, and the separate dependence on $\lambda^{\pm}(u_i)$ disappeared.

Let us regard the off-shell overlap as a function of the u-variables and w-variables, which are treated as formally independent variables. Taking the $u_1+u_2\to 0$ limit we obtain the singular piece

$$\begin{aligned} S_N(u_1\dots u_N) =& \frac{1-w_1w_2}{u_1+u_2}\kappa'(u_1)\kappa'(-u_1) \\ &\times\left[\prod_{k=3}^{N}\kappa(u_k)\right]\left[\prod_{k=3}^{N}\frac{u_1-u_k-1}{u_1-u_k}\frac{u_1+u_k+1}{u_1+u_k}\right] \\ &\times a^{\mathcal{L}}\left[\sum_{\{\sigma_3,\dots,\sigma_N\}}\prod_{3\le k<l\le N}\frac{\sigma_k u_k+\sigma_l u_l-1}{\sigma_k u_k+\sigma_l u_l}\right. \\ &\left.\times\prod_{k=3}^{N}\sigma_k\left(\frac{u_k+u_1-1}{u_k+u_1+1}\frac{u_k-u_1-1}{u_k-u_1+1}\right)^{\sigma_k+1/2}w_k^{\sigma_k+1/2}\right] \\ &+\text{reg.} \end{aligned} \quad (2.94)$$

Therefore the residue can be written as

$$S_N(u_1\dots u_N|w_1,\dots,w_N) = \frac{w_1w_2-1}{u_1+u_2}F(u_1)\times\left[\prod_{k=3}^{N}f(u_1-u_k)f(-u_1-u_k)\right]\times S_{N-2}(u_3\dots u_N|\tilde{w}_3,\dots,\tilde{w}_N)+\text{reg.} \quad (2.95)$$

where S_{N-2} contains the modified w_k parameters

$$\tilde{w}_k = \frac{f(u_k+u_1)}{f(-u_k-u_1)}\frac{f(u_k-u_1)}{f(u_1-u_k)}w_k. \quad (2.96)$$

Above $F(u)$ is a rational function which carries the dependence on the initial state:

$$F(u) = -\kappa'(u)\kappa'(-u) = -\frac{\gamma^2}{a^2}\frac{u^2-b^2/\gamma^2}{u^2}. \quad (2.97)$$

The structure of the residue in (2.95) agrees with Proposition 1 of [31]. Repeating the derivation of [31] one can show that if the above residue property holds, then the un-normalized on-shell overlap is equal to

$$S_N \to a^{\mathcal{L}}\prod_{j=1}^{N/2}F(u_j^+)\prod_{1\le j<k\le N/2}\bar{f}(u_j^+,u_k^+)\times\det G^+_{N/2}, \quad (2.98)$$

where $G^{\pm}$ are the so-called Gaudin-like matrices of size $\frac{N}{2}\times\frac{N}{2}$, with matrix elements

$$G^{\pm}_{jk} = \left(\frac{\partial}{\partial u^+_j} \phi(u^+_k) \pm \frac{\partial}{\partial u^+_j} \phi(u^-_k) \right) \Bigg|_{u^-_i = -u^+_i}, \tag{2.99}$$

with

$$\phi(u) = \log \left[\frac{\lambda^+(u)}{\lambda^-(u)} \prod_{j=1}^{N} \frac{f(u-u_j)}{f(u_j-u)} \right] \tag{2.100}$$

and

$$\bar{f}(\lambda,\mu) = f(\lambda-\mu) f(\lambda+\mu) f(-\lambda-\mu) f(-\lambda+\mu). \tag{2.101}$$

Therefore we just proved that the overlap function has the following on-shell limit

$$\langle \Psi | \mathbf{u}^+_{N/2} \rangle = a^{\mathcal{L}} \prod_{j=1}^{N/2} F(u^+_j) \prod_{j=1}^{N/2} \lambda^+(u^+_j) \lambda^-(u^+_j) \prod_{1 \le j < k \le N/2} \bar{f}(u^+_j, u^+_k) \times \det G^+_{N/2}. \tag{2.102}$$

To calculate the normalized overlap we need the pairing between left and right eigenstates

$$\langle \mathbf{u} | \mathbf{u} \rangle = \prod_{j=1}^{N} \lambda^+(u_j) \lambda^-(u_j) \prod_{1 \le j < k \le N} f(u_j - u_k) f(u_k - u_j) \times \det G_N, \tag{2.103}$$

where G is the Gaudin matrix

$$G_{jk} = \frac{\partial}{\partial u_j} \phi(u_k). \tag{2.104}$$

For the pair structure the Gaudin determinant is factorized

$$\det G_N = \det G^+_{N/2} \det G^-_{N/2}. \tag{2.105}$$

We can then obtain the normalized overlap as

$$\frac{\langle \Psi | \boldsymbol{u}^+_{N/2} \rangle \langle \boldsymbol{u}^+_{N/2} | \Psi \rangle}{\langle \boldsymbol{u}^+_{N/2} | \boldsymbol{u}^+_{N/2} \rangle} = a^{2\mathcal{L}} \prod_{j=1}^{N/2} \nu(u^+_j) \frac{\det G^+_{N/2}}{\det G^-_{N/2}}, \tag{2.106}$$

where the one particle overlap function is

$$\nu(u) = \frac{(F(u))^2}{f(2u) f(-2u)} = \frac{\gamma^4}{a^4} \frac{(u^2 - b^2/\gamma^2)^2}{u^2(u^2 - 1/4)}. \tag{2.107}$$

We observe the remarkable factorized form of the on-shell overlap. It is important that the formula (2.106) is valid also in the integrable higher spin chains with $SU(2)$-symmetry. The dependence on the spin representation is carried only through the Gaudin-like matrices, because their entries depend on the functions $\lambda^{\pm}(u)$, which on the other hand depend on the spin, see (2.15). In contrast, the pair amplitude $\nu(u)$ is completely independent of the spin. The algebraic reason behind this remarkable separation and factorization is that in the higher spin cases the K-matrices are constructed using the fusion relation (2.41), and they are completely determined by the K-matrices of the defining representation.

An alternative interpretation of the factorized formula (including the higher spin cases) can be given using the Quantum Transfer Matrix (QTM) method, see [1,2,30]. We do not pursue that method here, nevertheless let us give a few comments. In the QTM method the fused K-matrices

describe the fusion of boundary transfer matrices, which belong to the same commuting hierarchy. It can then be argued using the methods of [10], that the pair amplitude $\nu(u)$ has to be the same for all spins. The argument using the QTM method can be applied only in the infinite volume limit, but our computations here reach the same conclusions, using rigorous computations in arbitrary finite volume.

2.6. Descendant states

We close this section by calculating the overlaps for the descendant states

$$\langle \Psi | \mathbf{u}, M \rangle. \tag{2.108}$$

Overlaps with $\langle \Psi' |$

Let us start with the two-site state $\langle \Psi' |$, which is obtained from the rotated K-matrix (2.63) and for which the off-shell formula is available. For an off-shell state we can continuously change the rapidities, which means that we can obtain the descendant overlaps from a simple limit

$$\langle \Psi' | u_1 \dots, u_N, M \rangle = \lim_{u_{N+1},\dots,u_{N+M}\to\infty} \prod_{i=1}^{M} \frac{1}{u_{N+i}^{2L-1}} S_{N+M}(u_1, \dots, u_{N+M}). \tag{2.109}$$

Let us start with the case $M = 1$. Now

$$S_{N+1}(u_1, \dots, u_{N+1}) = a^{\mathcal{L}} \left[\prod_{k=1}^{N+1} \kappa'(u_k) \right] \left[\sum_{\{\sigma_1,\dots,\sigma_{N+1}\}=\{\pm,\dots,\pm\}} f_{N+1}(\sigma_1 \dots, \sigma_{N+1}) \right], \tag{2.110}$$

where

$$f_{N+1}(\sigma_1 \dots, \sigma_{N+1}) = \prod_{1\le k<l\le N+1} \frac{\sigma_k u_k + \sigma_l u_l - 1}{\sigma_k u_k + \sigma_l u_l} \prod_{k=1}^{N+1} \sigma_k \lambda^{\sigma_k}(u_k). \tag{2.111}$$

We can pair the terms as

$$f_{N+1}(\sigma_1 \dots, \sigma_N, +) + f_{N+1}(\sigma_1 \dots, \sigma_N, -) = \prod_{1\le k<l\le N} \frac{\sigma_k u_k + \sigma_l u_l - 1}{\sigma_k u_k + \sigma_l u_l} \prod_{k=1}^{N} \sigma_k \lambda^{\sigma_k}(u_k) \times$$
$$\left[\prod_{1\le k\le N} \left(1 - \frac{1}{u_{N+1} + \sigma_k u_k}\right) \lambda^{+}(u_{N+1}) - \prod_{k=1}^{N} \left(1 + \frac{1}{u_{N+1} - \sigma_k u_k}\right) \lambda^{-}(u_{N+1}) \right] =$$
$$f_N(\sigma_1 \dots, \sigma_N) u_{N+1}^{2L-1} \left[2(\mathcal{L} - N) + \mathcal{O}(u_{N+1}^{-1}) \right], \tag{2.112}$$

where we used the following asymptotic expansions

$$u^{-2L} \lambda^{-}(u) = 1 + \pm \mathcal{L} u^{-1} + \mathcal{O}(u^{-2}), \tag{2.113}$$

$$\prod_{k=1}^{N} \left(1 \mp \frac{1}{u \pm \sigma_k u_k}\right) = 1 \mp N u^{-1} + \mathcal{O}(u^{-2}). \tag{2.114}$$

Substituting (2.112) to (2.110) we obtain that

$$\lim_{u_{N+1}\to\infty} \frac{1}{u_{N+1}^{2L-1}} S_{N+1}(u_1,\dots,u_{N+1}) = 2\,(\mathcal{L}-N)\,\frac{\gamma}{a} S_N(u_1,\dots,u_N). \tag{2.115}$$

Using this formula we get the following off-shell result

$$\langle \Psi' | u_1 \dots, u_N, M\rangle = \left(\frac{2\gamma}{a}\right)^M \prod_{i=0}^{M-1} (\mathcal{L}-N-i)\, S_N(u_1,\dots,u_N). \tag{2.116}$$

Therefore the ratio of off-shell formulas can be written as

$$\frac{\langle \Psi' | \mathbf{u}, M\rangle}{\langle \Psi' | \mathbf{u}\rangle} = \left(\frac{2\gamma}{a}\right)^M \prod_{i=0}^{M-1} (\mathcal{L}-N-i) = \left(\frac{2\gamma}{a}\right)^M \frac{(\mathcal{L}-N)!}{(\mathcal{L}-N-M)!}. \tag{2.117}$$

This result holds also in the on-shell limit.

Overlaps with $\langle\Psi|$

Let us continue with the general case. Since we have no off–shell formula we have to do something different as in the previous case. We can only use the on-shell formula

$$\langle \Psi | \mathbf{u}\rangle = a^{\mathcal{L}} \prod_{i=1}^{N/2} F(u_i^+) \times \mathcal{G}_{N/2}, \tag{2.118}$$

where $\mathcal{G}_N$ is independent form the two-site state

$$\mathcal{G}_{N/2} = \prod_{j=1}^{N/2} \lambda^+(u_j^+)\lambda^-(u_j^+) \prod_{1\le j<k\le N/2} \bar{f}(u_j^+,u_k^+) \times \det G^+_{N/2}, \tag{2.119}$$

and

$$F(u) = -\kappa'(u)\kappa'(-u) = -\frac{\gamma^2}{a^2}\frac{u^2-b^2/\gamma^2}{u^2} = \frac{\gamma^2}{a^2} h(u), \tag{2.120}$$

where

$$h(u) = -\frac{u^2-b^2/\gamma^2}{u^2}. \tag{2.121}$$

Using these notations the overlap can be written as

$$\langle \Psi | \mathbf{u}\rangle = a^{\mathcal{L}-N}\gamma^N \prod_{i=1}^{N/2} h(u_i^+) \times \mathcal{G}_{N/2}. \tag{2.122}$$

Let us use the following expression for the descendant states

$$|\mathbf{u}, M\rangle := \frac{d^M}{d\alpha^M} \exp\left(\alpha\Delta(S^-)\right)\Big|_{\alpha=0} |\mathbf{u}\rangle\,. \tag{2.123}$$

Applying it to the overlap

$$\langle \Psi | \mathbf{u}, M\rangle = \frac{d^M}{d\alpha^M} \langle \Psi | \exp\left(\alpha\Delta(S^-)\right) | \mathbf{u}\rangle \Big|_{\alpha=0} = \frac{d^M}{d\alpha^M} \langle \Psi_\alpha | \mathbf{u}\rangle \Big|_{\alpha=0}. \tag{2.124}$$

The rotated two-site state can be built from the rotated K-matrix

$$K_{12}(u|\alpha) = K_{12}(u)\left[\exp\left(\alpha S^-\right) \otimes \exp\left(\alpha S^-\right)\right] = \begin{pmatrix} a_\alpha u & -b_\alpha + c_\alpha u \\ b_\alpha + c_\alpha u & d_\alpha u \end{pmatrix}, \tag{2.125}$$

where

$$a_\alpha = a + 2c\alpha + d\alpha^2 \qquad b_\alpha = b \tag{2.126}$$

$$c_\alpha = c + d\alpha \qquad d_\alpha = d. \tag{2.127}$$

From this rotated K-matrix we can build a two-site state $\langle\Psi_\alpha|$. We observe that

$$\gamma_\alpha^2 = c_\alpha^2 - a_\alpha d_\alpha = c^2 - ad = \gamma^2, \tag{2.128}$$

therefore γ and the function $h(u)$ are invariant quantities w.r.t rotations. The rotated overlap can be written as

$$\frac{d^M}{d\alpha^M}\langle\Psi_\alpha|\mathbf{u}\rangle\Big|_{\alpha=0} = \frac{d^M}{d\alpha^M}\left[a_\alpha^{\mathcal{L}-N}\right]_{\alpha=0}\gamma^N\prod_{i=1}^{N/2}h(u_i^+)\times\mathcal{G}_{N/2}. \tag{2.129}$$

Using the expansion

$$\begin{aligned} a_\alpha^{\mathcal{L}-N} =& (a + 2c\alpha + d\alpha^2)^{\mathcal{L}-N} \\ =& \sum_{M=0}^{\mathcal{L}-N}\alpha^M\sum_{i=0}^{\lfloor M/2\rfloor}\binom{\mathcal{L}-N}{i}\binom{\mathcal{L}-N-i}{M-2i}d^i(2c)^{M-2i}a^{\mathcal{L}-N-M+i} \end{aligned} \tag{2.130}$$

we obtain

$$\frac{d^M}{d\alpha^M}\left[a_\alpha^{\mathcal{L}-N}\right]_{\alpha=0} = a^{\mathcal{L}-N}A(N,M), \tag{2.131}$$

where

$$A(N,M) = M!\sum_{i=0}^{\lfloor M/2\rfloor}\binom{\mathcal{L}-N}{i}\binom{\mathcal{L}-N-i}{M-2i}d^i(2c)^{M-2i}a^{i-M}. \tag{2.132}$$

Therefore the overlaps for descendant states are

$$\langle\Psi|\mathbf{u},M\rangle = A(N,M)a^{\mathcal{L}-N}\gamma^N\prod_{i=1}^{N/2}h(u_i^+)\times\mathcal{G}_{N/2}. \tag{2.133}$$

We can see that the overlaps with the Bethe state and its descendant states are the same up to a numerical prefactor[3]:

$$\frac{\langle\Psi|\mathbf{u},M\rangle}{\langle\Psi|\mathbf{u}\rangle} = A(N,M). \tag{2.134}$$

This is consistent with the previous result, since

$$A(N,M)\Big|_{\delta=0} = M!\binom{\mathcal{L}-N}{M}(2c)^M a^{-M} = \left(\frac{2c}{a}\right)^M\frac{(\mathcal{L}-N)!}{(\mathcal{L}-N-M)!}. \tag{2.135}$$

[3] For a special matrix product state it was already observed that the overlaps with the Bethe and their descendant states are the same up to a combinatorical prefactor [44].

3. Integrable final states for twisted spin chains

So far the integrable initial states and the exact overlaps have not yet been considered in spin chains with twisted boundary conditions. The main reason for this is that the observed properties of the integrable states, such as the "pair structure" for the overlaps seemed to be tied to the periodic boundary conditions. Here we show that there is a natural generalization to twisted cases, given that the twist is compatible with the K-matrix. Furthermore, we also derive new overlap formulas. The computations in this Section will form the basis of the SoV treatment in Section 4.

3.1. Twisted spin chains

The transfer matrix for the twisted case can be written as

$$t(u) = \mathrm{Tr}_0 \left[T_0(u) G_0 \right], \tag{3.1}$$

where G is the twist matrix. For the simplicity we use a diagonal twist

$$G = \begin{pmatrix} z_1 & 0 \\ 0 & z_2 \end{pmatrix}. \tag{3.2}$$

The off-shell Bethe vectors have the same form as the untwisted ones

$$|\mathbf{u}\rangle = B(u_1) \dots B(u_N) |0\rangle . \tag{3.3}$$

The only difference is that now the eigenvalue of the transfer matrix is

$$\Lambda(u) = z_1 \lambda^+(u) \frac{Q_1(u-1)}{Q_1(u)} + z_2 \lambda^-(u) \frac{Q_1(u+1)}{Q_1(u)}. \tag{3.4}$$

There is an alternative way to build the eigenstates

$$|\mathbf{v}\rangle = C(v_1) \dots C(v_{2\mathcal{L}-N}) \left|0'\right\rangle, \tag{3.5}$$

where $\left|0'\right\rangle$ is the lowest weight reference state

$$\left|0'\right\rangle = |0, s_1\rangle^{(s_1)} \otimes |0, s_1\rangle^{(s_1)} \otimes \dots \otimes |0, s_L\rangle^{(s_L)} \otimes |0, s_L\rangle^{(s_L)} . \tag{3.6}$$

The new vector $|\mathbf{v}\rangle$ is an eigenvector of $t(u)$ with the same eigenvalue as $|\mathbf{u}\rangle$ when the QQ-relation is satisfied

$$z_2 Q_1\left(u+\frac{1}{2}\right) Q_2\left(u-\frac{1}{2}\right) - z_1 Q_1\left(u-\frac{1}{2}\right) Q_2\left(u+\frac{1}{2}\right) = (z_2 - z_1) Q_{12}(u), \tag{3.7}$$

where

$$Q_{12}(u) = \prod_{k=1}^{L} \left(u^2 - \left(\theta_k + \frac{s_k - 1}{2}\right)^2\right)\left(u^2 - \left(\theta_k + \frac{s_k - 3}{2}\right)^2\right) \times \cdots$$
$$\cdots \times \left(u^2 - \left(\theta_k + \frac{-s_k + 3}{2}\right)^2\right)\left(u^2 - \left(\theta_k + \frac{-s_k + 1}{2}\right)^2\right). \tag{3.8}$$

In summary, the eigenvalues can be expressed in two formally different ways

$$\Lambda(u) = z_1\lambda^+(u)\frac{Q_1(u-1)}{Q_1(u)} + z_2\lambda^-(u)\frac{Q_1(u+1)}{Q_1(u)} \tag{3.9}$$

$$= z_2\lambda^+(u)\frac{Q_2(u-1)}{Q_2(u)} + z_1\lambda^-(u)\frac{Q_2(u+1)}{Q_2(u)}, \tag{3.10}$$

which are however equivalent if the QQ-relation is satisfied.

Let us continue with the integrable states. In the untwisted case the intuition of the integrability condition was that the action of the conserved charges and the space reflected conserved charges on the integrable state must be equal. However, this argument implicitly assumed that the space reflection is a symmetry of the system, or equivalently that the transfer matrix and the space reflected transfer matrix are commuting. This is generally not true for twisted models.

On the other hand, we saw that we can also use $t(-u)$ in the integrability definition instead of the space reflected transfer matrix (these are equal for the untwisted case but not in the twisted one) and the $t(-u)$ generate the same set of conserved charges as $t(u)$. Therefore the natural generalization of the integrability condition is

$$\langle\Psi|\, t(u) = \langle\Psi|\, t(-u). \tag{3.11}$$

Importantly, $t(u)$ is now the twisted transfer matrix. The natural question is: What is the implication of this definition on the Q-functions or the Bethe roots?

Applying the Bethe state $|\mathbf{u}\rangle$ on the integrability condition we obtain that

$$(\Lambda(u) - \Lambda(-u))\langle\Psi|\mathbf{u}\rangle = 0, \tag{3.12}$$

therefore the non-vanishing overlaps require that

$$\Lambda(u) = \Lambda(-u). \tag{3.13}$$

Using (3.9)-(3.10) the left and right hand side can be written as

$$\Lambda(u) = z_1\lambda^+(u)\frac{Q_1(u-1)}{Q_1(u)} + z_2\lambda^-(u)\frac{Q_1(u+1)}{Q_1(u)} \tag{3.14}$$

$$\Lambda(-u) = z_1\lambda^+(u)\frac{Q_2(-u+1)}{Q_2(-u)} + z_2\lambda^-(u)\frac{Q_2(-u-1)}{Q_2(-u)}. \tag{3.15}$$

We can see that the condition (3.13) is equivalent to

$$Q_2(-u) = (-1)^N Q_1(u). \tag{3.16}$$

This condition obviously requires that there is a selection rule for the number of magnons

$$N = \mathcal{L}, \tag{3.17}$$

and the set of $\mathbf{u}$ is the same as $\mathbf{v}$ but with opposite signs

$$\{u_1, u_2, \ldots, u_N\} = \{-v_1, -v_2, \ldots, -v_N\}. \tag{3.18}$$

This is the natural generalization of the pair structure to the twisted cases. In the original untwisted case the rapidities are paired with each other; here the rapidities from two different representations of the same state are paired. Going back to the un-twisted case we get $-\mathbf{v} = \mathbf{u}$ iff the pair structure for $\mathbf{u}$ also holds, thus the different integrability conditions are indeed equivalent. We stress that (3.18) is very restrictive and it does not hold for an arbitrary on-shell configuration.

Let us continue with the two site states which are solutions of the integrability condition (3.11). For the two-site state

$$\langle\Psi| = \vec{K}^{(s_1)}(\theta_1) \otimes \cdots \otimes \vec{K}^{(s_L)}(\theta_L) \tag{3.19}$$

we saw that it satisfies the KT-relation

$$\langle\Psi|\, \vec{K}_{12}(u) T_1(u) = \langle\Psi|\, \vec{K}_{12}(u) T_2^{\pi}(u), \tag{3.20}$$

or equivalently

$$\langle\Psi|\, \sigma^y \mathbf{K}^t(u) T(u) = \langle\Psi|\, T(-u) \sigma^y \mathbf{K}^t(u). \tag{3.21}$$

Using this equation the action of the twisted transfer matrix can be written as

$$\langle\Psi|\, t(u) = \langle\Psi|\, \mathrm{Tr}\Big[T(-u) \sigma^y \mathbf{K}^t(u) G \left(\sigma^y \mathbf{K}^t(u)\right)^{-1} \Big], \tag{3.22}$$

which means that the integrability condition is satisfied if

$$\sigma^y \mathbf{K}^t(u) G = G \sigma^y \mathbf{K}^t(u). \tag{3.23}$$

This is an important compatibility condition between the twist and the K-matrix.

Solutions of the KYB equation also satisfying this condition can be written as

$$k_{11}(u) = 0 \qquad k_{12}(u) = -b + cu \tag{3.24}$$

$$k_{21}(u) = b + cu \qquad k_{22}(u) = 0. \tag{3.25}$$

Let us continue with the determination of the off-shell overlap formula. Since the off-shell Bethe vectors are completely independent from the twist we can apply the previous off-shell overlap formula (2.77) for the twisted chain. Due to the compatibility condition we have to take the limit $a \to 0$. In this limit the reflection factor $\kappa(u)$ goes to ∞. Taking the proper limit we obtain that non-vanishing overlaps require that

$$N = \mathcal{L}, \tag{3.26}$$

and the final formula is

$$\mathcal{S}_{\mathcal{L}}(u_1 \dots u_{\mathcal{L}}) = \left[\prod_{k=1}^{\mathcal{L}} \tilde{\kappa}(u_k) \right] \frac{\det V_{\mathcal{L}}^{+}(u_1, \dots, u_{\mathcal{L}})}{\prod_{1 \le k < l \le \mathcal{L}} \left[u_l^2 - u_k^2\right]}, \tag{3.27}$$

where the Vandermonde-like determinant is given by (2.78) and

$$\tilde{\kappa}(u) = \frac{b + cu}{u}. \tag{3.28}$$

The overlap formula (3.27) is also well-defined for on-shell states. Potential problems could only appear from the poles, but in the twisted case the pair structure does generally not hold and therefore generally $u_k^2 - u_l^2 \neq 0$.

We can also see that ratio of overlaps with different integrable states only depends on the $\tilde{\kappa}$ functions, namely

$$\frac{\langle\Psi|\mathbf{u}\rangle}{\langle\Psi'|\mathbf{u}\rangle} = \prod_{k=1}^{\mathcal{L}} \frac{\tilde{\kappa}(u_k)}{\tilde{\kappa}'(u_k)}. \tag{3.29}$$

Let $\langle\Psi_0|$ be the two-site state corresponding to $b = 1, c = 0$. The state $\langle\Psi_0|$ is the generalization of the Dimer state to arbitrary spins. Using this state as reference state we can obtain the general overlap as

$$\langle\Psi|\mathbf{u}\rangle = \prod_{k=1}^{\mathcal{L}} (cu_k + b)\langle\Psi_0|\mathbf{u}\rangle = (-c)^{\mathcal{L}} Q_1(-b/c)\langle\Psi_0|\mathbf{u}\rangle. \tag{3.30}$$

3.2. Untwisted limit

Here we investigate the limit when the model is tuned back the original untwisted case.

The twisted boundary condition restricts the possible two-site states radically, because the components a and d are fixed to zero by the compatibility with the twist. Therefore one might think that the integrability definition is too restrictive, as we loose a number of states which were integrable for the untwisted model. It might appear that we have not found the proper generalization of the integrability condition to the twisted case, and that the twisted case is not very useful to study the original untwisted problem.

However, it turns out that the twisted overlap formula (3.27) already contains all the information which is needed to reconstruct the most general untwisted on-shell overlap formula. This happens because the general two-site state can be obtained from the restricted one by a rotation and the twisted overlap formula gives all the non-vanishing untwisted overlaps for the Bethe states, as well as their descendants.

Let us start with the behavior of the Bethe roots in the untwisted limit. It is common knowledge that as the twist is tuned back to zero, the Bethe roots go either to the solutions of the untwisted Bethe equations, or they approach infinity. We know that the non-vanishing overlap requires the pair structure of the Bethe roots for periodic boundary conditions. This means that for $z_1, z_2 \to 1$ the Bethe roots have the following limit

$$u_{2a+1} + u_{2a} \to 0, \qquad \text{for } a = 1, \dots, N/2, \tag{3.31}$$

$$u_k \to \infty, \qquad \text{for } k = N+1, \dots, \mathcal{L}, \tag{3.32}$$

and the limit of the Bethe vectors reads as

$$\lim_{z_1,z_2\to 1} \prod_{i=1}^{\mathcal{L}-N} \frac{1}{u_{N+i}^{2L-1}} \mathcal{S}_{\mathcal{L}}(u_1 \dots u_{\mathcal{L}}) = \lim_{z_1,z_2\to 1} \prod_{i=1}^{\mathcal{L}-N} \frac{1}{u_{N+i}^{2L-1}} \langle\bar{\Psi}|u_1, \dots, u_{\mathcal{L}}\rangle = \langle\bar{\Psi}|\mathbf{u}, \mathcal{L}-N\rangle, \tag{3.33}$$

where $\langle\bar{\Psi}|$ is the two-site state which can be built from the K-matrix $\bar{K}(u)$ for which

$$\bar{k}_{11}(u) = 0 \qquad \bar{k}_{12}(u) = -b + \gamma u \tag{3.34}$$

$$\bar{k}_{21}(u) = b + \gamma u \qquad \bar{k}_{22}(u) = 0. \tag{3.35}$$

Taking the untwisted limit of the twisted formula we obtain that

$$\lim_{z_1,z_2\to 1} \prod_{i=1}^{\mathcal{L}-N} \frac{1}{u_{N+i}^{2L-1}} \mathcal{S}_{\mathcal{L}}(u_1 \dots u_{\mathcal{L}}) = (2\gamma)^{\mathcal{L}-N} (\mathcal{L}-N)! \mathcal{S}_N(u_1, \dots, u_N) =$$

$$= 2^{\mathcal{L}-N} (\mathcal{L}-N)! \gamma^{\mathcal{L}} \prod_{i=1}^{N/2} h(u_i) \times \mathcal{G}_N(\mathbf{u}), \tag{3.36}$$

where we used the $\kappa' = \bar{\kappa}$ and $M = \mathcal{L} - N$ limit of the equations (2.116) and (2.122) in the first and the second rows. From (3.33) and (3.36) we obtained the on-shell untwisted overlaps for the special state $\langle\bar{\Psi}|$

$$\left\langle \bar{\Psi} \middle| \mathbf{u}, \mathcal{L}-N \right\rangle = 2^{\mathcal{L}-N}\,(\mathcal{L}-N)!\gamma^{\mathcal{L}} \prod_{i=1}^{N/2} h(u_i) \times \mathcal{G}_N(\mathbf{u}). \tag{3.37}$$

The general K-matrix (2.35)-(2.36) can obtained from $\bar{K}$ as

$$K_{12}(u) = \bar{K}_{12}(u)\left(\exp(\alpha S^-) \otimes \exp(\alpha S^-)\right)\left(\exp(\beta S^+) \otimes \exp(\beta S^+)\right), \tag{3.38}$$

where

$$\alpha = \frac{a}{2\gamma}, \qquad \beta = \frac{c-\gamma}{a}. \tag{3.39}$$

Therefore the general two-site state can be obtained by a rotation as

$$\left\langle \Psi \right| = \left\langle \bar{\Psi} \right| \exp(\alpha \Delta(S^-)) \exp(\beta \Delta(S^+)), \tag{3.40}$$

which means that the general on-shell untwisted overlap can be written as

$$\left\langle \Psi \middle| \mathbf{u} \right\rangle = \left\langle \bar{\Psi} \right| \exp(\alpha \Delta(S^-)) \exp(\beta \Delta(S^+)) \left| \mathbf{u} \right\rangle. \tag{3.41}$$

The highest weight property of the Bethe state implies that S^+ acts trivially, and we can use simply the expansion of the exponential of S^- to obtain

$$\left\langle \Psi \middle| \mathbf{u} \right\rangle = \frac{\alpha^{\mathcal{L}-N}}{(\mathcal{L}-N)!} \left\langle \bar{\Psi} \middle| \mathbf{u}, \mathcal{L}-N \right\rangle, \tag{3.42}$$

where it was used that the states with non-zero spin have vanishing overlap with $\left\langle \bar{\Psi} \right|$.

Substituting (3.37) we obtain that

$$\left\langle \Psi \middle| \mathbf{u} \right\rangle = \frac{\alpha^{\mathcal{L}-N}}{(\mathcal{L}-N)!} 2^{\mathcal{L}-N}\,(\mathcal{L}-N)!\gamma^{\mathcal{L}} \prod_{i=1}^{N/2} h(u_i) \times \mathcal{G}_N(\mathbf{u}) = a^{\mathcal{L}-N}\gamma^N \prod_{i=1}^{N/2} h(u_i) \times \mathcal{G}_N(\mathbf{u}), \tag{3.43}$$

which agrees with the result of the previous section.

4. Overlaps and SoV

In this section we embed the integrable initial states into the framework of Separation of Variables. We investigate the overlaps between the SoV basis and the integrable two-site states. We will see that the SoV techniques can be used to derive the overlaps in question, but interestingly we obtain a formula which is different from the previous result (3.27).

The SoV approach was pioneered by Sklyanin [45]. The idea of the SoV is to find a basis in which the eigenvectors of the transfer matrix factorize into one particle blocks. It turns out that the SoV basis can be found by diagonalizing the B-operator. However, in the periodic case the B-operator is nilpotent, therefore one usually introduces a twist. For a diagonal twist the B-operator is still nilpotent, therefore a non-diagonal twist is required. In the SoV construction it is advantageous if the spectrum of the B operator is non-degenerate and this is the situation in the XXX spin chain if the inhomogeneities are in a generic position.

There exist a number of equivalent realizations of the SoV construction, depending on the conventions for the twists. For our purposes the most convenient choice is the set of conventions of [46] which uses a rotated version of the transfer matrix. Following [46] we call it the "good" transfer matrix.

For simplicity we concentrate here on the case when the quantum space is in the defining representation i.e. $s_k = 1$ for $k = 1, \dots, L$. At first we review of the construction of the SoV basis following [46]. This basis diagonalizes the "good" B-operator. Let us define the "good" monodromy matrix

$$\mathbb{T}(u) = U^{-1} T(u) G U \tag{4.1}$$

and "good" B-operator

$$\mathbb{B}(u) = \mathbb{T}_{12}(u), \qquad \bar{\mathbb{B}}(u) = \frac{z}{z^2-1}\mathbb{B}(u), \tag{4.2}$$

where we use the following conventions for the twist and U:

$$G = \begin{pmatrix} z & 0 \\ 0 & 1/z \end{pmatrix}, \qquad U = \begin{pmatrix} \alpha & \alpha \\ 0 & 1/\alpha \end{pmatrix}. \tag{4.3}$$

The operator $T(u)$ in (4.1) is the original monodromy matrix defined in (2.7).

The left/right eigenvectors of $\mathbb{B}$ form the left/right SoV basis:

$$\begin{aligned} \langle h_1 \dots h_{2L} | \bar{\mathbb{B}}(u) &= \prod_{i=1}^{2L} (u - \xi_i + h_i) \langle h_1 \dots h_{2L} |, \\ \bar{\mathbb{B}}(u) | h_1 \dots h_{2L} \rangle &= \prod_{i=1}^{2L} (u - \xi_i + h_i) | h_1 \dots h_{2L} \rangle, \end{aligned} \tag{4.4}$$

where $h_i = \pm\frac{1}{2}$. We choose the normalization as

$$\langle \mathbf{h} | 0 \rangle = 1, \qquad \langle 0' | \mathbf{h} \rangle = 1. \tag{4.5}$$

These vectors and co-vectors are orthogonal and their "norm" is [46]

$$\mu(\mathbf{h}) = \frac{1}{\langle \mathbf{h} | \mathbf{h} \rangle} = \frac{1}{\alpha^{4L}(z^2-1)^{2L}} \prod_{i=1}^{2L} (2h_i) \prod_{i<j} \frac{\xi_i - \xi_j + h_i - h_j}{\xi_i - \xi_j}. \tag{4.6}$$

The off-shell Bethe vectors can be written as

$$| \mathbf{u} \rangle = \prod_{i=1}^{N} \bar{\mathbb{B}}(u_i) | 0 \rangle, \qquad \langle \mathbf{v} | = \prod_{i=1}^{2L-N} \langle 0' | \bar{\mathbb{B}}(v_i). \tag{4.7}$$

The overlaps are

$$\langle \mathbf{h} | \mathbf{u} \rangle = \prod_{i=1}^{2L} Q_1(\xi_i - h_i), \qquad \langle \mathbf{v} | \mathbf{h} \rangle = \prod_{i=1}^{2L} Q_2(\xi_i - h_i). \tag{4.8}$$

When the vector $|\mathbf{u}\rangle$ and co-vector $\langle \mathbf{v}|$ are right and left eigenvectors of the transfer matrix with the same eigenvalue then the Q-functions satisfy the QQ-relation:

$$z^2 Q_1(u - 1/2) Q_2(u + 1/2) - Q_1(u + 1/2) Q_2(u - 1/2) = (z^2 - 1) Q_{12}(u), \tag{4.9}$$

where

$$Q_{12}(u) = \prod_{i=1}^{2L} (u - \xi_i). \tag{4.10}$$

The overlap between off-shell Bethe states can be written as

$$\langle \mathbf{v}|\mathbf{u}\rangle = \sum_{\mathbf{h}} \mu(\mathbf{h})\langle \mathbf{v}|\mathbf{h}\rangle\langle \mathbf{h}|\mathbf{u}\rangle = \frac{1}{\alpha^{4L}(z^2-1)^{2L}} \sum_{\mathbf{h}} \prod_{i<j} \frac{\xi_i - \xi_j + h_i - h_j}{\xi_i - \xi_j} \times$$
$$\times \prod_{i=1}^{2L} 2h_i Q_1(\xi_i - h_i) Q_2(\xi_i - h_i) = \frac{1}{\alpha^{4L}(z^2-1)^{2L}} \prod_{i<j} \frac{1}{\xi_j - \xi_i} \det W_{2L}, \quad (4.11)$$

where the matrix W is

$$[W_{2L}]_{ij} = (\xi_i + 1/2)^{j-1} Q_1^-(\xi_i) Q_2^-(\xi_i) - (\xi_i - 1/2)^{j-1} Q_1^+(\xi_i) Q_2^+(\xi_i),$$
$$\text{for } 1 \le a, b \le 2L. \quad (4.12)$$

We are interested in overlaps with integrable final states. In accordance with the previous Sections we require that the inhomogeneities are in pairs:

$$\xi_{2i-1} = \theta_i, \qquad \xi_{2i} = -\theta_i. \quad (4.13)$$

Similarly as before, non-vanishing overlaps can be found if the Q-functions satisfy the integrability condition

$$Q_1(u) = (-1)^L Q_2(-u). \quad (4.14)$$

Let us use these restrictions to simplify the Vandermonde-like determinants. The rows with odd and even indices can be written as

$$[W_{2L}]_{2i-1,b} = \Big[(\theta_i + 1/2)^{b-1} Q_1^-(\theta_i) Q_2^-(\theta_i) - (\theta_i - 1/2)^{b-1} Q_1^+(\theta_i) Q_2^+(\theta_i)\Big] \quad (4.15)$$
$$[W_{2L}]_{2i,b} = (-1)^b \Big[(\theta_i + 1/2)^{b-1} Q_1^-(\theta_i) Q_2^-(\theta_i) - (\theta_i - 1/2)^{b-1} Q_1^+(\theta_i) Q_2^+(\theta_i)\Big]. \quad (4.16)$$

Subtracting the rows $W_{2i-1,b}$ from $W_{2i,b}$ we obtain that the determinant is factorized as

$$\det W_{2L} = \begin{vmatrix} W_{1,1} & W_{1,2} & W_{1,3} & W_{1,4} & \dots \\ -W_{1,1} & W_{1,2} & -W_{1,3} & W_{1,4} & \dots \\ W_{3,1} & W_{3,2} & W_{3,3} & W_{3,4} & \dots \\ -W_{3,1} & W_{3,2} & -W_{3,3} & W_{3,4} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix}_{2L\times 2L}$$
$$= \begin{vmatrix} W_{1,1} & W_{1,2} & W_{1,3} & W_{1,4} & \dots \\ 0 & 2W_{1,2} & 0 & 2W_{1,4} & \dots \\ W_{3,1} & W_{3,2} & W_{3,3} & W_{3,4} & \dots \\ 0 & 2W_{3,2} & 0 & 2W_{3,4} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix}_{2L\times 2L}$$
$$= 2^L \begin{vmatrix} W_{1,1} & W_{3,3} & \dots \\ W_{3,1} & W_{3,3} & \dots \\ \vdots & \vdots & \ddots \end{vmatrix}_{L\times L} \times \begin{vmatrix} W_{1,2} & W_{1,4} & \dots \\ W_{3,2} & W_{3,4} & \dots \\ \vdots & \vdots & \ddots \end{vmatrix}_{L\times L}. \quad (4.17)$$

Thus we find

$$\det W_{2L} = 2^L \det W_L^+ \det W_L^-, \tag{4.18}$$

where

$$\left[W_L^+\right]_{ab} = (\theta_a + 1/2)^{2b-2} Q_1^-(\theta_a) Q_2^-(\theta_a) - (\theta_a - 1/2)^{2b-2} Q_1^+(\theta_a) Q_2^+(\theta_a), \tag{4.19}$$

$$\left[W_L^-\right]_{ab} = (\theta_a + 1/2)^{2b-1} Q_1^-(\theta_a) Q_2^-(\theta_a) - (\theta_a - 1/2)^{2b-1} Q_1^+(\theta_a) Q_2^+(\theta_a), \tag{4.20}$$

for $1 \leq a, b \leq L$. Using the condition (4.14) we can express the matrices using only the Q_1 function as

$$\left[W_L^+\right]_{ab} = (-1)^L \left[(\theta_a + 1/2)^{2b-2} Q_1^-(\theta_a) Q_1^+(-\theta_a) - (\theta_a - 1/2)^{2b-2} Q_1^+(\theta_a) Q_1^-(-\theta_a)\right], \tag{4.21}$$

$$\left[W_L^-\right]_{ab} = (-1)^L \left[(\theta_a + 1/2)^{2b-1} Q_1^-(\theta_a) Q_1^+(-\theta_a) - (\theta_a - 1/2)^{2b-1} Q_1^+(\theta_a) Q_1^-(-\theta_a)\right]. \tag{4.22}$$

Substituting this to the overlap between two off-shell Bethe states (4.11) we obtain that

$$\langle \mathbf{v} | \mathbf{u} \rangle = \frac{(-1)^L}{\alpha^{4L}(z^2-1)^{2L}} \left[\prod_{a=1}^{L} \frac{1}{\theta_a}\right] \left[\prod_{a<b} \frac{1}{(\theta_a^2 - \theta_b^2)^2}\right] \det W_L^+ \det W_L^-. \tag{4.23}$$

4.1. Overlap formulas

Now we want to calculate the overlaps with the previously defined boundary state. For $s_i = 1$ this is the Dimer which can be written as

$$\mathbf{K}^{(1)} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{4.24}$$

and

$$\langle \Psi_0 | = \vec{K}^{(1)} \otimes \cdots \otimes \vec{K}^{(1)}, \qquad |\Psi_0\rangle = \vec{K}^{(1)T} \otimes \cdots \otimes \vec{K}^{(1)T}. \tag{4.25}$$

For the non-vanishing overlaps with on-shell Bethe states the Q-function have to satisfy the integrability condition (4.14). Using the KT-relation (2.29) we can also check that the operator $\mathbb{B}$ acts on the Dimer state as

$$\langle \Psi_0 | \mathbb{B}(u) = \langle \Psi_0 | \mathbb{B}(-u), \qquad \mathbb{B}(u) | \Psi_0 \rangle = \mathbb{B}(-u) | \Psi_0 \rangle, \tag{4.26}$$

which means the overlaps $\langle \Psi_0 | \mathbf{h} \rangle$ and $\langle \mathbf{h} | \Psi_0 \rangle$ are not zero iff

$$h_{2i-1} = -h_{2i}, \qquad \text{for } i = 1, \ldots, L. \tag{4.27}$$

We can see that the local degrees of freedom is halved, because for each pair (h_{2i-1}, h_{2i}) only two possibilities give non-zero overlap. The vectors with $h_{2i-1} = h_{2i}$ lead to zero overlap for all $i = 1, \ldots, L$. This halving of the degrees of freedom in this particular case is the analogous to the "pair structure" on the level of the Bethe roots.

It is now convenient to define a new notation for the independent degrees of freedom as

$$\langle f_1 \ldots f_L | = \langle h_1 h_2 \ldots h_{2L-1} h_{2L} |, \qquad | f_1 \ldots f_L \rangle = | h_1 h_2 \ldots h_{2L-1} h_{2L} \rangle, \tag{4.28}$$

where

$$(h_{2i-1} = +\frac{1}{2}, h_{2i} = -\frac{1}{2}) \longleftrightarrow f_i = +1 \tag{4.29}$$

$$(h_{2i-1} = -\frac{1}{2}, h_{2i} = +\frac{1}{2}) \longleftrightarrow f_i = -1. \tag{4.30}$$

Our goal is to calculate the overlap

$$\langle \Psi_0 | \mathbf{u} \rangle = \sum_{\mathbf{h}} \mu(\mathbf{h}) \langle \Psi_0 | \mathbf{h} \rangle \langle \mathbf{h} | \mathbf{u} \rangle = \sum_{\mathbf{f}} \mu(\mathbf{f}) \langle \Psi_0 | \mathbf{f} \rangle \langle \mathbf{f} | \mathbf{u} \rangle. \tag{4.31}$$

In the formula we already know the norm and the overlap $\langle \mathbf{f} | \mathbf{u} \rangle$:

$$\mu(\mathbf{f}) = \frac{1}{\alpha^{4L}(z^2-1)^{2L}} \prod_{a=1}^{L} \frac{2\theta_a + f_a}{2\theta_a} \prod_{a<b} \left(\frac{f_a\theta_a + f_b\theta_b + 1}{f_a\theta_a + f_b\theta_b} \right)^2, \tag{4.32}$$

$$\langle \mathbf{f} | \mathbf{u} \rangle = (-1)^L \prod_{a=1}^{L} Q_1(\theta_a - f_a/2) Q_2(\theta_a - f_a/2), \tag{4.33}$$

$$\langle \mathbf{v} | \mathbf{f} \rangle = (-1)^L \prod_{a=1}^{L} Q_1(\theta_a - f_a/2) Q_2(\theta_a - f_a/2). \tag{4.34}$$

In the formulas above we used the integrability condition for the Q-functions (4.14). In the Appendix B we derive that the overlap $\langle \Psi_0 | \mathbf{f} \rangle$ can be written as

$$\langle \Psi_0 | \mathbf{f} \rangle = C_r \prod_{a=1}^{L} \frac{f_a 2\theta_a}{2\theta_a + f_a} \prod_{a<b} \frac{f_a\theta_a + f_b\theta_b}{f_a\theta_a + f_b\theta_b + 1}, \tag{4.35}$$

$$\langle \mathbf{f} | \Psi_0 \rangle = C_l \prod_{a=1}^{L} \frac{f_a 2\theta_a}{2\theta_a + f_a} \prod_{a<b} \frac{f_a\theta_a + f_b\theta_b}{f_a\theta_a + f_b\theta_b + 1}, \tag{4.36}$$

where the product of the normalization factors is

$$C_l C_r = \alpha^{4L}(z^2-1)^{2L} \prod_{a=1}^{L} \frac{(\theta_a + 1/2)(\theta_a - 1/2)}{\theta_a^2}. \tag{4.37}$$

Substituting (4.32), (4.33) and (4.35) to the overlap formula we obtain that

$$\begin{aligned} \langle \Psi_0 | \mathbf{u} \rangle &= \frac{C_r(-1)^L}{\alpha^{4L}(z^2-1)^{2L}} \sum_{\mathbf{f}} \prod_{a<b} \frac{f_a\theta_a + f_b\theta_b + 1}{f_a\theta_a + f_b\theta_b} \prod_{a=1}^{L} f_a Q_1(\theta_a - f_a/2) Q_2(\theta_a - f_a/2) \\ &= \frac{C_r(-1)^L}{\alpha^{4L}(z^2-1)^{2L}} \prod_{a<b} \frac{1}{\theta_b^2 - \theta_a^2} \sum_{\mathbf{f}} \prod_{a<b} \left((\theta_b + f_b/2)^2 - (\theta_a + f_a/2)^2 \right) \\ &\quad \times \prod_{a=1}^{L} f_a Q_1(\theta_a - f_a/2) Q_2(\theta_a - f_a/2). \end{aligned} \tag{4.38}$$

We can see that this formula can be written in a compact form using the Vandermonde-like determinant W_L^+:

$$\langle \Psi_0 | \mathbf{u} \rangle = \frac{C_r(-1)^L}{\alpha^{4L}(z^2-1)^{2L}} \prod_{a<b} \frac{1}{\theta_b^2 - \theta_a^2} \det W_L^+. \tag{4.39}$$

Similarly we can derive the overlap for the co-vectors:

$$\langle \mathbf{v}|\Psi_0\rangle = \frac{C_l(-1)^L}{\alpha^{4L}(z^2-1)^{2L}} \prod_{a<b} \frac{1}{\theta_b^2-\theta_a^2} \det W_L^+. \tag{4.40}$$

Using these formulas the normalized overlap reads as

$$\frac{\langle \Psi_0|\mathbf{u}\rangle\langle \mathbf{v}|\Psi_0\rangle}{\langle \mathbf{v}|\mathbf{u}\rangle} = (-1)^L \prod_{a=1}^{L} \frac{(\theta_a+q/2)(\theta_a-q/2)}{\theta_a} \frac{\det W_L^+}{\det W_L^-}. \tag{4.41}$$

We used the "generalized pair" structure (or integrability condition) $Q_1(u) = (-1)^L Q_2(-u)$ in the derivation of the factorization of $\det W$ (4.18) and in (4.33)-(4.34), but we did not use the Bethe Ansatz or the QQ-relations. This means that the above formula holds for both *off-shell and on-shell states*.

In the previous Section we saw that the on-shell overlap of general two-site state can be obtained from the overlap of the reference state $\langle\Psi_0|$ as

$$\frac{\langle \Psi|\mathbf{u}\rangle}{\langle \Psi_0|\mathbf{u}\rangle} = \frac{\langle \mathbf{v}|\Psi\rangle}{\langle \mathbf{v}|\Psi_0\rangle} = (-c)^L Q_1(-b/c) = (c)^L Q_2(b/c). \tag{4.42}$$

Therefore the general normalized overlap can be written as

$$\frac{\langle \Psi|\mathbf{u}\rangle\langle \mathbf{v}|\Psi\rangle}{\langle \mathbf{v}|\mathbf{u}\rangle} = (-c^2)^L Q_1^2(b/c) \prod_{i=1}^{L} \frac{(\theta_i+q/2)(\theta_i-q/2)}{\theta_i} \frac{\det W_L^+}{\det W_L^-}. \tag{4.43}$$

We emphasize that this formula is different from the previous result (3.27), even though some of the ingredients might look similar. At this point the connection between these two results is not clear, and it deserves further study.

Also, it would be important to compute the homogeneous limit of the final formula (4.43). It is known that in SoV the computation of the homogeneous limit is often very challenging, and usually it requires a separate study.[4] Thus we leave this task to a future work.

5. Conclusion

In this paper we investigated integrable initial/final states and their overlaps using the Algebraic Bethe Ansatz and the Separation of Variables method. We obtained a number of results, and we feel it is worthwhile to give here a list of them:

Our main results are *a)* the KT-relation (2.30) which leads to the recursion relations for the overlap, *b)* the off-shell overlap formula (2.78) valid for all integrable final states of the higher spin models, *c)* the corresponding on-shell formula (2.102)-(2.106), *d)* a generalization of the integrability condition to twisted spin chains, see (3.16)-(3.18), *e)* the corresponding overlap formula (3.27), valid on-shell and off-shell, *f)* the SoV representation (4.27) of the integrability condition for the Dimer state, and *g)* the final overlap formula (4.43) within SoV, valid for arbitrary integrable states of the spin-1/2 chain.

[4] An interesting computation was presented in Appendix R of [26], where a known overlap formula was expressed in a form that is reminiscent of the SoV results, for example it involves only the Q-functions. Connections to our results are not yet clear.

In our view the most important results are the KT relation, the generalization of the integrability condition to the twisted chains and also to the SoV method. This opens the way to study nested systems using Algebraic Bethe Ansatz (ABA) and SoV. Combining the KT-relation with the techniques of [47] used in ABA one could get recursive equations and sum rules for the overlaps, similar to those obtained for the scalar products of the Bethe vectors in the models with $\mathfrak{gl}(m|n)$ symmetry [48,49]. Focusing on SoV, our present results are expressed using the Q-functions, which are the natural building blocks to treat the exact operator spectrum of the $\mathcal{N}=4$ SYM theory. The extension of our methods to nested systems and long range spin chains is a promising direction. Thus our present results constitute an important step towards the exact one-point functions in the defect CFT.

One of the interesting open questions is to what extent the present methods are helpful for the overlaps in those cases, when the initial/final states are given by integrable MPS [16–20,2]. We believe that the KT-relation could be established also in those cases, but it would lead to considerably more complicated recursion relations. At present it is not clear whether the methods could be useful in practical computations.

CRediT authorship contribution statement

Tamás Gombor: Conceptualization, Methodology, Writing (original and revision)
Balázs Pozsgay: Conceptualization, Writing (original and revision), Funding acquisition

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

We acknowledge collaboration with Yunfeng Jiang and Deliang Zhong on early stages of this project. We also thank Rouven Frassek for valuable comments. T.G. was supported by NKFIH grant K134946.

Appendix A. Derivation of the off-shell overlap formula (2.75)

In this section we prove the off-shell overlap formula (2.75). In the derivation the following expression will appear

$$E_M(v|u_1,\dots,u_M)=\prod_{k=1}^{M}\frac{v+u_k-1}{v+u_k}\frac{v-u_k}{v-u_k-1}+$$
$$\sum_{l=1}^{M}\left(\frac{\kappa(-v)}{\kappa(u_l)}\frac{1}{v+u_l}-\frac{\kappa(v)}{\kappa(u_l)}\frac{1}{v-u_l}\right)\frac{v-u_l}{v-u_l-1}\prod_{k=1\neq l}^{M}\frac{u_l-u_k+1}{u_l-u_k}\frac{u_l+u_k}{u_l+u_k+1}, \tag{A.1}$$

where $u_k\neq 0$ and $u_k\neq u_l$ for $k\neq l$ and

$$\kappa(u)=\frac{b+cu}{au}. \tag{A.2}$$

At first, we prove that the following identity holds

$$E_M(v|u_1,\dots,u_M)=1. \tag{A.3}$$

To prove this identity we have to check that the $E_M(v|u_1,\dots,u_M)$ as a meromorphic function of v is equal to 1. In the $v\to\infty$ limit, it is satisfied i.e.

$$\lim_{v\to\infty} E_M(v|u_1,\dots,u_M)=1. \tag{A.4}$$

Therefore the identity (A.3) holds if the meromorphic function $E_M(v)$ has no poles in the v-plane. The formal poles are $v=0,u_n,-u_n,u_n+1$. It is easy to convince ourselves that residues vanish

$$\operatorname*{Res}_{v=u_n} E_M(v|u_1,\dots,u_M)=0 \tag{A.5}$$

$$\begin{aligned}&\operatorname*{Res}_{v=0} E_M(v|u_1,\dots,u_M)\\ &=\sum_{l=1}^{M}\left(\frac{-b/a}{\kappa(u_l)}\frac{1}{u_l}+\frac{b/a}{\kappa(u_l)}\frac{1}{u_l}\right)\frac{u_l}{u_l+1}\prod_{k=1\neq l}^{M}\frac{u_l-u_k+1}{u_l-u_k}\frac{u_l+u_k}{u_l+u_k+1}=0.\end{aligned} \tag{A.6}$$

$$\begin{aligned}\operatorname*{Res}_{v=-u_n} E_M(v|u_1,\dots,u_M)=&-\frac{2u_n}{2u_n+1}\prod_{k=1\neq n}^{M}\frac{-u_n+u_k-1}{-u_n+u_k}\frac{-u_n-u_k}{-u_n-u_k-1}+\\ &+\frac{2u_n}{2u_n+1}\prod_{k=1\neq n}^{M}\frac{u_n-u_k+1}{u_n-u_k}\frac{u_n+u_k}{u_n+u_k+1}=0\end{aligned} \tag{A.7}$$

$$\begin{aligned}\operatorname*{Res}_{v=u_n+1} E_M(v|u_1,\dots,u_M)=&\frac{2u_n}{2u_n+1}\prod_{k=1\neq n}^{M}\frac{u_n+u_k}{u_n+u_k+1}\frac{u_n-u_k+1}{u_n-u_k}+\\ &+\left(\frac{\kappa(-u_n-1)}{\kappa(u_n)}\frac{1}{2u_n+1}-\frac{\kappa(u_n+1)}{\kappa(u_n)}\right)\\ &\times\prod_{k=1\neq l}^{M}\frac{u_n-u_k+1}{u_n-u_k}\frac{u_n+u_k}{u_n+u_k+1}=0,\end{aligned} \tag{A.8}$$

therefore the identity (A.3) is satisfied.

Now, we turn on to prove (2.75). Here we use induction. Let us assume that (2.75) holds for $\mathcal{S}_{N-1}$ i.e.

$$\mathcal{S}_{N-1}(u_1,\dots,u_{N-1})=\sum_{\{\sigma_1,\dots,\sigma_N\}=\{\pm,\dots,\pm\}} f(\sigma_1,\dots,\sigma_{N-1})\prod_{k=1}^{N-1}\sigma_k\lambda^{\sigma_k}(u_k), \tag{A.9}$$

where

$$f(\sigma_1,\dots,\sigma_N)=a^{\mathcal{L}}\left[\prod_{k=1}^{N}\kappa(u_k)\right]\left[\prod_{1\le k<l\le N}\frac{\sigma_k u_k+\sigma_l u_l-1}{\sigma_k u_k+\sigma_l u_l}\right]. \tag{A.10}$$

Using the formula of $\mathcal{S}_{N-1}$ and the recursion relation (2.73) we can obtain an expression for $\mathcal{S}_N$:

$$\begin{aligned}\mathcal{S}_N(u_1\dots u_N) =&\kappa(u_1)\Bigg[\prod_{k=2}^{N}\frac{u_1+u_k-1}{u_1+u_k}\lambda^+(u_1)\mathcal{S}_{N-1}(u_2\dots u_N)-\\&-\prod_{k=2}^{N}\frac{u_1-u_k+1}{u_1-u_k}\lambda^-(u_1)\mathcal{S}_{N-1}(u_2\dots u_N)+\\&+\sum_{l=2}^{N}\frac{1}{u_1+u_l}\prod_{k=2\neq l}^{N}\frac{u_l-u_k+1}{u_l-u_k}\lambda^-(u_l)\mathcal{S}_{N-1}(-u_1,u_2\dots\widehat{u_l}\dots u_N)+\\&+\sum_{l=2}^{N}\frac{1}{u_1-u_l}\prod_{k=2\neq l}^{N}\frac{u_l-u_k+1}{u_l-u_k}\lambda^-(u_l)\mathcal{S}_{N-1}(u_1,u_2\dots\widehat{u_l}\dots u_N)\Bigg]=\\&=\sum_{\{\sigma_1,\dots,\sigma_N\}=\{\pm,\dots,\pm\}}\tilde{f}(\sigma_1,\dots,\sigma_{N-1})\prod_{k=1}^{N-1}\sigma_k\lambda^{\sigma_k}(u_k).\end{aligned}\tag{A.11}$$

The proof is complete if we show that the coefficients f and $\tilde{f}$ are the same. Let us collect the terms $\lambda^+(u_1)\lambda^-(u_2)\dots\lambda^-(u_M)\lambda^+(u_{M+1})\dots\lambda^+(u_N)$. Dividing the coefficients f and $\tilde{f}$ we obtain that

$$\begin{aligned}&\frac{\tilde{f}(+,-,\dots,-,+,\dots,+)}{f(+,-,\dots,-,+,\dots,+)}=\prod_{k=2}^{M}\frac{u_1-u_k}{u_1-u_k-1}\frac{u_1+u_k-1}{u_1+u_k}+\\&+\sum_{l=2}^{M}\left(\frac{\kappa(-u_1)}{\kappa(u_l)}\frac{1}{u_1+u_l}-\frac{\kappa(u_1)}{\kappa(u_l)}\frac{1}{u_1-u_l}\right)\frac{u_1-u_l}{u_1-u_l-1}\prod_{k=2\neq l}^{M}\frac{u_l-u_k+1}{u_l-u_k}\frac{u_l+u_k}{u_l+u_k+1}=\\&=E_{M-1}(u_1|u_2,\dots,u_M)=1,\end{aligned}\tag{A.12}$$

where the last line we used the identity (A.3). Since the recursion relation is symmetry under the permutations of $u_2,\dots,u_N$ we just obtained that

$$\tilde{f}(+,\sigma_2,\dots,\sigma_{N-1})=f(+,\sigma_2,\dots,\sigma_{N-1}).\tag{A.13}$$

Analogously we can handle the coefficients with $\sigma_1=+$:

$$\begin{aligned}&\frac{\tilde{f}(-,-,\dots,-,+,\dots,+)}{f(-,-,\dots,-,+,\dots,+)}=\prod_{k=2}^{M}\frac{u_1+u_k}{u_1+u_k+1}\frac{u_1-u_k+1}{u_1-u_k}+\\&+\sum_{l=2}^{M}\left(\frac{\kappa(-u_1)}{\kappa(u_l)}\frac{1}{u_1+u_l}-\frac{\kappa(u_1)}{\kappa(u_l)}\frac{1}{u_1-u_l}\right)\frac{u_1+u_l}{u_1+u_l+1}\prod_{k=2\neq l}^{M}\frac{u_l-u_k+1}{u_l-u_k}\frac{u_l+u_k}{u_l+u_k+1}=\\&=E_{M-1}(-u_1|u_2,\dots,u_M)=1,\end{aligned}\tag{A.14}$$

and using the permutation symmetry we just obtained that

$$\tilde{f}(-,\sigma_2,\dots,\sigma_{N-1})=f(-,\sigma_2,\dots,\sigma_{N-1}).\tag{A.15}$$

Thus we proved (2.75).

Appendix B. The overlap between the Dimer state and the SoV basis vectors

The calculation of the overlap $\langle\Psi_0|\mathbf{f}\rangle$ is based on the integrability condition

$$\langle\Psi_0|t(u)|\mathbf{f}\rangle = \langle\Psi_0|t(-u)|\mathbf{f}\rangle. \tag{B.1}$$

Therefore we need two to know how the transfer matrix act on the SoV basis. The transfer matrix can be written as

$$t(u) = \mathbb{A}(u) + \mathbb{D}(u), \tag{B.2}$$

where the operators $\mathbb{A}$ and $\mathbb{D}$ are the diagonal elements of the "good" monodromy matrix

$$\mathbb{A}(u) = \mathbb{T}_{11}(u), \qquad \mathbb{D}(u) = \mathbb{T}_{22}(u). \tag{B.3}$$

Since the R-matrix is $\mathfrak{gl}(2)$ invariant "good" monodromy is satisfy the RTT relation

$$R_{12}(u-v)\mathbb{T}_1(u)\mathbb{T}_2(v) = \mathbb{T}_2(v)\mathbb{T}_1(u)R_{12}(u-v), \tag{B.4}$$

therefore

$$(v-u+1)\mathbb{A}(v)\mathbb{B}(u) = (v-u)\mathbb{B}(u)\mathbb{A}(v) + \mathbb{A}(u)\mathbb{B}(v) \tag{B.5}$$

$$(u-v+1)\mathbb{D}(v)\mathbb{B}(u) = (u-v)\mathbb{B}(u)\mathbb{D}(v) + \mathbb{D}(u)\mathbb{B}(v). \tag{B.6}$$

Substituting $v = \xi_i - h_i$ we obtain that

$$\mathbb{B}(u)\mathbb{A}(\xi_i - h_i)|\mathbf{h}\rangle = \frac{u-\xi_i+h_i-1}{u-\xi_i+h_i}\lambda_{\mathbf{h}}(u)\mathbb{A}(\xi_i-h_i)|\mathbf{h}\rangle \tag{B.7}$$

$$\mathbb{B}(u)\mathbb{D}(\xi_i - h_i)|\mathbf{h}\rangle = \frac{u-\xi_i+h_i+1}{u-\xi_i+h_i}\lambda_{\mathbf{h}}(u)\mathbb{D}(\xi_i-h_i)|\mathbf{h}\rangle. \tag{B.8}$$

Therefore the $\mathbb{A}(\xi_i - h_i)$ and $\mathbb{D}(\xi_i - h_i)$ are lowering and raising operator, respectively i.e.

$$\begin{aligned}&\mathbb{A}(\xi_i - 1/2)|\dots, h_i = +1/2, \dots\rangle = F_i^{(+\frac{1}{2})}|\dots, h_i = -1/2, \dots\rangle,\\ &\mathbb{A}(\xi_i + 1/2)|\dots, h_i = -1/2, \dots\rangle = 0,\end{aligned} \tag{B.9}$$

$$\begin{aligned}&\mathbb{D}(\xi_i + 1/2)|\dots, h_i = -1/2, \dots\rangle = F_i^{(-\frac{1}{2})}|\dots, h_i = +1/2, \dots\rangle,\\ &\mathbb{D}(\xi_i - 1/2)|\dots, h_i = +1/2, \dots\rangle = 0,\end{aligned} \tag{B.10}$$

which means that at these special rapidities the transfer matrix acts on the SoV basis as

$$t(\xi_i - h_i)|\dots, h_i, \dots\rangle = F_i^{(h_i)}|\dots, -h_i, \dots\rangle. \tag{B.11}$$

We can easily fix the parameters $F_i^{(h_i)}$. Let us consider the following expression

$$\langle 0'|t(\xi_i - h_i)|\dots, h_i, \dots\rangle = F_i^{(h_i)}. \tag{B.12}$$

We also know the action of the transfer matrix on the pseudovacuum $\langle 0'|$

$$\langle 0'|t(u) = z\,Q_{12}(u-1/2) + \frac{1}{z}Q_{12}(u+1/2), \tag{B.13}$$

therefore

$$\langle 0'|t(\xi_i - h_i)|\dots, h_i, \dots\rangle = z^{2h_i}\,Q_{12}(\xi_i - 2h_i), \tag{B.14}$$

which means

$$F_i^{(h_i)} = z^{2h_i} Q_{12}(\xi_i - 2h_i). \tag{B.15}$$

Since the transfer matrix is a matrix valued polynomial with degree $2L$ we can use the following interpolation

$$t(u) = t_\infty \prod_{i=1}^{2L}(u - \xi_i - h_i) + \sum_{j=1}^{2L} t(\xi_j - h_j) \prod_{i=1\neq j}^{2L} \frac{u - \xi_i + h_i}{\xi_j - h_j - \xi_i + h_i}, \tag{B.16}$$

where t_∞ is proportional to the identity. Using this interpolation formula and (B.12) we obtain that

$$t(u)\big|\mathbf{h}\big\rangle = t_\infty \big|\mathbf{h}\big\rangle \prod_{i=1}^{2L}(u - \xi_i + h_i) + \sum_{j=1}^{2L} F_i^{(h_i)} \big|\dots, -h_i, \dots\big\rangle \prod_{i=1\neq j}^{2L} \frac{u - \xi_i + h_i}{\xi_j - h_j - \xi_i + h_i}. \tag{B.17}$$

Substituting this into the integrability condition

$$\big\langle \Psi_0 \big| t(\theta_1 + 1/2) \big| -\frac{1}{2}, -\frac{1}{2}, \dots \big\rangle = \big\langle \Psi_0 \big| t(-\theta_1 - 1/2) \big| -\frac{1}{2}, -\frac{1}{2}, \dots \big\rangle \tag{B.18}$$

we obtain that

$$\begin{aligned} F_1^{(-\frac{1}{2})} \big\langle \Psi_0 \big| + \frac{1}{2}, -\frac{1}{2}, \dots \big\rangle = -\frac{1}{2\theta_1} F_1^{(-\frac{1}{2})} \big\langle \Psi_0 \big| + \frac{1}{2}, -\frac{1}{2}, \dots \big\rangle \\ + \frac{2\theta_i + 1}{2\theta_1} F_2^{(-\frac{1}{2})} \big\langle \Psi_0 \big| - \frac{1}{2}, +\frac{1}{2}, \dots \big\rangle \prod_{i=3}^{2L} \frac{\theta_1 + \frac{1}{2} + \xi_i - h_i}{\theta_1 - \frac{1}{2} + \xi_i - h_i}. \end{aligned} \tag{B.19}$$

Here we used the selection rules $h_{2b-1} = -h_{2b}$ for the non-vanishing overlaps $\big\langle \Psi_0 \big| \mathbf{h} \big\rangle$, see (4.27). We can see that the quotient of overlaps can be written as

$$\begin{aligned} \frac{\big\langle \Psi_0 \big| + \frac{1}{2}, -\frac{1}{2}, \dots \big\rangle}{\big\langle \Psi_0 \big| - \frac{1}{2}, +\frac{1}{2}, \dots \big\rangle} = \frac{F_2^{(-\frac{1}{2})}}{F_1^{(-\frac{1}{2})}} \prod_{i=3}^{2L} \frac{\theta_1 + \frac{1}{2} + \xi_i - h_i}{\theta_1 - \frac{1}{2} + \xi_i - h_i} = \\ - \frac{2\theta_i - 1}{2\theta_i + 1} \prod_{b=2}^{L} \frac{\theta_1 + \frac{1}{2} + \theta_b - h_{2b-1}}{\theta_1 + \frac{1}{2} + \theta_b + \frac{1}{2}} \frac{\theta_1 - \frac{1}{2} - \theta_b - \frac{1}{2}}{\theta_1 - \frac{1}{2} - \theta_b + h_{2b-1}} \\ \times \frac{\theta_1 + \frac{1}{2} - \theta_b + h_{2b-1}}{\theta_1 + \frac{1}{2} - \theta_b + \frac{1}{2}} \frac{\theta_1 - \frac{1}{2} + \theta_b - \frac{1}{2}}{\theta_1 - \frac{1}{2} + \theta_b - h_{2b-1}}. \end{aligned} \tag{B.20}$$

Using the notation $\big| f_1 \dots, f_L \big\rangle$ this equation is simplified as

$$\frac{\big\langle \Psi_0 \big| + 1, f_2, \dots, f_L \big\rangle}{\big\langle \Psi_0 \big| - 1, f_2, \dots, f_L \big\rangle} = -\frac{2\theta_i - 1}{2\theta_i + 1} \frac{\theta_1 + f_b\theta_b}{\theta_1 + f_b\theta_b + 1} \frac{-\theta_1 + f_b\theta_b + 1}{-\theta_1 + f_b\theta_b}, \tag{B.21}$$

therefore the overlap between the Dimer state and the SoV basis vectors can be written as

$$\big\langle \Psi_0 \big| \mathbf{f} \big\rangle = C_r \prod_{a=1}^{L} \frac{2\theta_a}{2 f_a\theta_a + 1} \prod_{a<b} \frac{f_a\theta_a + f_b\theta_b}{f_a\theta_a + f_b\theta_b + 1}, \tag{B.22}$$

where C_r is independent on the variables f_a.

Analogously way we can calculate the overlap with the co-vector basis $\langle \mathbf{f}|\Psi_0\rangle$. The only difference is the action of the transfer matrix on $\langle \mathbf{h}|$, which is given by

$$\langle \dots, h_i, \dots | t(\xi_i - h_i) = G_i^{(h_i)} \langle \dots, -h_i, \dots |, \tag{B.23}$$

where

$$G_i^{(h_i)} = z^{-2h_i} Q_{12}(\xi_i - 2h_i). \tag{B.24}$$

Repeating the same calculation as above we obtain that

$$\frac{\langle +\frac{1}{2}, -\frac{1}{2}, \dots |\Psi_0\rangle}{\langle -\frac{1}{2}, +\frac{1}{2}, \dots |\Psi_0\rangle} = \frac{G_2^{(-\frac{1}{2})}}{G_1^{(-\frac{1}{2})}} \prod_{i=3}^{2L} \frac{\theta_1 + \frac{1}{2} + \xi_i - h_i}{\theta_1 - \frac{1}{2} + \xi_i - h_i} = \frac{\langle \Psi_0| + \frac{1}{2}, -\frac{1}{2}, \dots \rangle}{\langle \Psi_0| - \frac{1}{2}, +\frac{1}{2}, \dots \rangle}, \tag{B.25}$$

therefore

$$\langle \mathbf{f}|\Psi_0\rangle = C_l \prod_{a=1}^{L} \frac{2\theta_a}{2f_a\theta_a + 1} \prod_{a<b} \frac{f_a\theta_a + f_b\theta_b}{f_a\theta_a + f_b\theta_b + 1}, \tag{B.26}$$

where C_l is independent of f_a-s. We can fix the product $C_l C_r$ by calculating the norm $\langle \Psi_0|\Psi_0\rangle = 2^L$ and inserting the full system

$$\langle \Psi_0|\Psi_0\rangle = \sum_{\mathbf{h}} \mu(\mathbf{h}) \langle \Psi_0|\mathbf{h}\rangle\langle \mathbf{h}|\Psi_0\rangle = \sum_{\mathbf{f}} \mu(\mathbf{f}) \langle \Psi_0|\mathbf{f}\rangle\langle \mathbf{f}|\Psi_0\rangle. \tag{B.27}$$

Substituting (4.32), (B.22) and (B.26) we obtain that

$$\begin{aligned}
\langle \Psi_0|\Psi_0\rangle =& \frac{C_l C_r}{\alpha^{4L}(z^2-1)^{2L}} \sum_{\mathbf{f}} \prod_{a=1}^{L} \frac{2\theta_a}{2\theta_a + f_a} \\
=& \frac{C_l C_r}{\alpha^{4L}(z^2-1)^{2L}} \prod_{a=1}^{L} \frac{2\theta_a}{4\theta_a^2 - 1} \sum_{\mathbf{f}} \prod_{a=1}^{L} (2\theta_a - f_a) \\
=& 2^L \frac{C_l C_r}{\alpha^{4L}(z^2-1)^{2L}} \prod_{a=1}^{L} \frac{4\theta_a^2}{4\theta_a^2 - 1}.
\end{aligned} \tag{B.28}$$

Therefore

$$C_l C_r = \alpha^{4L}(z^2-1)^{2L} \prod_{a=1}^{L} \frac{(\theta_a + 1/2)(\theta_a - 1/2)}{\theta_a^2}. \tag{B.29}$$

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