Smirnov-type integral formulae for correlation functions of the bulk/boundary XXZ model in the anti-ferromagnetic regime

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Abstract

Presented are the integral solutions to the quantum Knizhnik-Zamolodchikov equations for the correlation functions of both the bulk and boundary XXZ models in the anti-ferromagnetic regime. The difference equations can be derived from Smirnov-type master equations for correlation functions on the basis of the CTM bootstrap. Our integral solutions with an appropriate choice of the integral kernel reproduce the formulae previously obtained by using the bosonization of the vertex operators of the quantum affine algebra $U_q(\widehat{\mathfrak{sl}_2})$.

1 Introduction

In this paper we address both the bulk and boundary XXZ models in the anti-ferromagnetic regime on the basis of Smirnov's axiomatic treatment of massive integrable models [1]. Smirnov found three axioms that the form factors of the sine-Gordon model should satisfy [1]. The said three axioms consist of *the S-matrix symmetry*, *the cyclicity condition*, and *the annihilation pole condition*. Smirnov also pointed out in [2] that the first two axioms imply the quantum KZ equations [3] of level 0 for form factors.

We have a similar story for correlation functions under the scenario based on the CTM (corner transfer matrix) bootstrap approach [4]. As was shown in [5] that correlation functions of bulk massive integrable models such as the XYZ model should satisfy the three relations: *the R-matrix symmetry*, *the cyclicity condition* and *the normalization of correlation functions*. Let us call those three relations *Smirnov-type master equations*. The first two relations imply the quantum Knizhnik-Zamolodchikov (KZ) equations [3] of level -4. The boundary analogue of Smirnov-type master equations were also obtained in [6] for the boundary XYZ model. In the boundary model case, the second cyclicity condition should be replaced by *reflection properties*.

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We start from Smirnov-type master equations for correlation functions of the bulk/boundary XXZ model in the antiferromagnetic regime. We will make the Ansatz in the subsequent sections that the correlation functions are expressed in terms of integral transform of certain rational functions with appropriate integral kernels. We determine the said rational functions such that the R-matrix symmetry holds. We also find the transformation properties and recursion relations for the integral kernels by imposing the cyclicity conditions (resp. reflection properties) and the normalization conditions for the bulk (resp. boundary) XXZ model.

The above mentioned Ansatz was already made in [7, 8, 9], where we constructed the form factors of the anti-ferromagnetic XXZ model by solving Smirnov's three axioms. We will see below that the integral formulae for correlation functions and those for form factors have the very similar structure. The difference between those formulae mainly results from the choice of rational functions, while the integral kernels are essentially the same. For the case of form factors, the freedom of solutions to the quantum KZ equation corresponds to that of local operators of the XXZ model.

In the framework of the representation theory of the affine quantum algebra [10] the space of states of the anti-ferromagnetic XXZ model can be identified with the tensor product of irreducible infinite dimensional modules, one is level 1 highest and the other is level -1 lowest modules of $U_q(\widehat{\mathfrak{sl}_2})$ with $0 < -q < 1$. Here the restriction $0 < -q < 1$ is required by the anti-ferromagnetic condition. The correlation functions of the anti-ferromagnetic XXZ model are given by the trace of the product of the type I vertex operators on the space of physical states [10]. Furthermore, the integral formulae for the correlation functions of the XXZ model was also obtained in [11] by using the bosonization of vertex operators of $U_q(\widehat{\mathfrak{sl}_2})$. The vertex operator approach were also applied to obtain the integral formulae for correlation functions of the anti-ferromagnetic XXZ model with a boundary [12].

One of advantages of the vertex operator approach is that correlation functions in this framework naturally satisfy the quantum KZ equations by the construction. Another advantage is that it is also relevant to massless models. In [13] the integral formulae were conjectured by solving the quantum KZ equations of level -4 for correlation functions of the massless XXZ model, which has $U_q(\widehat{\mathfrak{sl}_2})$-symmetry with $|q| = 1$. This was based on the CTM bootstrap approach [4], which is not directly applicable to the massless regime. In [14] those conjectured formulae were reproduced by using the bosonized vertex operators. The same bosonization method was used to obtain the corresponding formulae for the massless XXZ model with a boundary in [15].

From the view point of solving the quantum KZ equations, the trace construction allows us to chose the level arbitrarily, but gives only a canonical solution. On the other hand, Smirnov-type integral formulae based on the form factor bootstrap approach have the freedom of solutions but only solve the level 0 quantum KZ equations. As for correlation functions, Smirnov-type integral formulae give solutions to the level -4 equations. The relations among those different type integral formulae were discussed by Nakayashiki et al [16]. Furthermore, Nakayashiki proved that the trace functions of type I and type II vertex operators associated with the $U_q(\widehat{\mathfrak{sl}_n})$-symmetric model give a basis of the solution space of the quantum KZ equation at arbitrary level [17]. The CTM bootstrap approach was developed for $A^{(1)}_{n-1}$-symmetric elliptic models without and with a boundary, in order to derive the quantum KZ equations of level $-2n$ [18, 19, 20].

The rest of the present paper is organized as follows. In section 2 we formulate the bulk XXZ model in the anti-ferromagnetic regime, and present Smirnov-type integral formulae for correlation functions. In section 3 we prove that the formulae given in section 2 actually solve the quantum KZ equations. In section 4 we further present Smirnov-type integral formulae for correlation functions of the boundary XXZ model. In section 5 we give some concluding remarks. In Appendix A we give a simple proof of Proposition 2.

2 Integral formulae for the bulk XXZ model

2.1 The Hamiltonian and the R-matrix

In this section we consider the XXZ spin chain in an infinite lattice

$$H_{XXZ}=-\frac{1}{2}\sum_{j\in\mathbb{Z}}(\sigma_{j+1}^x\sigma_j^x+\sigma_{j+1}^y\sigma_j^y+\Delta\sigma_{j+1}^z\sigma_j^z). \tag{2.1}$$

Here σ_j^x, σ_j^y and σ_j^z denote the standard Pauli matrices acting on j-th site, and we restrict ourselves to the anti-ferromagnetic regime: $\Delta<-1$. The XXZ Hamiltonian H_{XXZ} commutes with $U_q(\widehat{\mathfrak{sl}_2})$, where $\Delta=(q+q^{-1})/2$ and $-1<q<0$. For lator convenience we also introduce the positive parameter $x=-q$ such that $0<x<1$. Let $V=\mathbb{C}v_+ +\mathbb{C}v_-$ be a vector representation of $U_q(\widehat{\mathfrak{sl}_2})$. Then the Hamiltonian (2.1) formally acts on $V^{\otimes\infty}=\cdots\otimes V\otimes V\otimes\cdots$. In [10] the space of states $V^{\otimes\infty}$ was identified with the tensor product of level 1 highest and level -1 lowest representations of $U_q(\widehat{\mathfrak{sl}_2})$.

Let us introduce the R-matrix of the six vertex model, where $R(\zeta)\in\mathrm{End}(V\otimes V)$:

$$R(\zeta)v_{\varepsilon_1}\otimes v_{\varepsilon_2}=\sum_{\varepsilon_1',\varepsilon_2'=\pm}v_{\varepsilon_1'}\otimes v_{\varepsilon_2'}R(\zeta)_{\varepsilon_1\varepsilon_2}^{\varepsilon_1'\varepsilon_2'},\qquad R(\zeta)=\frac{1}{\kappa(\zeta)}\overline{R}(\zeta), \tag{2.2}$$

where

$$\kappa(\zeta)=\zeta\frac{(x^4z;x^4)_\infty(x^2z^{-1};x^4)_\infty}{(x^4z^{-1};x^4)_\infty(x^2z;x^4)_\infty},\qquad (a;p_1,\cdots,p_n)_\infty=\prod_{k_i\geq 0}(1-ap_1^{k_1}\cdots p_n^{k_n}), \tag{2.3}$$

and $z=\zeta^2$. The nonzero entries are given by

$$\begin{aligned}
&\overline{R}(\zeta)_{++}^{++}=\overline{R}(\zeta)_{--}^{--}=1,\\
&\overline{R}(\zeta)_{+-}^{+-}=\overline{R}(\zeta)_{-+}^{-+}=b(\zeta)=\frac{x(\zeta^2-1)}{1-x^2\zeta^2},\\
&\overline{R}(\zeta)_{-+}^{+-}=\overline{R}(\zeta)_{+-}^{-+}=c(\zeta)=\frac{(1-x^2)\zeta}{1-x^2\zeta^2}.
\end{aligned} \tag{2.4}$$

Assume that the spectral parameter ζ and the constant x lie in the principal regime: $0<x<\zeta^{-1}<1$. As is well known, the XXZ Hamiltonian in the anti-ferromagnetic regime can be obtained from the transfer matrix for the six vertex model in the principal regime, by taking logalithmic derivative with respect to the spectral parameter ζ.

The main properties of the R-matrix are the Yang-Baxter equation

$$R_{12}(\zeta_1/\zeta_2)R_{13}(\zeta_1/\zeta_3)R_{23}(\zeta_2/\zeta_3)=R_{23}(\zeta_2/\zeta_3)R_{13}(\zeta_1/\zeta_3)R_{12}(\zeta_1/\zeta_2), \tag{2.5}$$

where the subscript of the R-matrix denotes the spaces on which R nontrivially acts; the initial condition

$$R(1) = P; \tag{2.6}$$

the unitarity relation

$$R_{12}(\zeta_1/\zeta_2)R_{21}(\zeta_2/\zeta_1) = 1; \tag{2.7}$$

the $\mathbb{Z}_2$-parity

$$R_{12}(-\zeta) = -\sigma_1^x R_{12}(\zeta)\sigma_1^z; \tag{2.8}$$

and the crossing symmetries

$$R_{21}^{t_1}(\zeta_2/\zeta_1) = \sigma_1^x R_{12}(x^{-1}\zeta_1/\zeta_2)\sigma_1^x, \quad R_{21}^{t_1}(\zeta_2/\zeta_1) = (i\sigma_1^y)R_{12}(-x^{-1}\zeta_1/\zeta_2)(i\sigma_1^y). \tag{2.9}$$

The properties (2.6–2.9) hold if the normalization factor of the R-matrix satisfies the following relations:

$$\kappa(\zeta)\kappa(\zeta^{-1}) = 1, \quad \kappa(\zeta)\kappa(\epsilon x\zeta) = \epsilon b(\zeta), \tag{2.10}$$

where $\epsilon = \pm$. Under this normalization the partition function per lattice site is equal to unity in the thermodynamic limit [4, 10].

2.2 Correlation functions and difference equations

Let us introduce the $V^{\otimes 2n}$-valued correlation functions

$$G_\sigma^{(n)}(\zeta_1, \cdots, \zeta_{2n}) = \sum_{\substack{\varepsilon_j = \pm \\ \varepsilon_1 + \cdots + \varepsilon_{2n} = 0}} v_{\varepsilon_1} \otimes \cdots \otimes v_{\varepsilon_{2n}} G_\sigma^{(n)}(\zeta_1, \cdots, \zeta_{2n})^{\varepsilon_1 \cdots \varepsilon_{2n}}, \quad (\sigma = \pm). \tag{2.11}$$

Here, we restrict $G_\sigma^{(n)}(\zeta)$ to the 'total spin-0' subspace of $V^{\otimes 2n}$. In the framework of the representation theory of $U_q(\widehat{\mathfrak{sl}_2})$, the correlation function (2.11) gives the expectation value of the local operator of the form

$$\mathcal{O} = E^{(1)}_{\varepsilon_1 \varepsilon_1'} \cdots E^{(n)}_{\varepsilon_n \varepsilon_n'},$$

where $E^{(j)}_{\varepsilon_j \varepsilon_j'}$ is the matrix unit on the j-th site, by specializing the spectral parameters as follows:

$$\langle \mathcal{O} \rangle_\sigma = G_\sigma^{(n)}(\overbrace{x^{-1}\zeta, \cdots, x^{-1}\zeta}^{n}, \overbrace{\zeta, \cdots, \zeta}^{n})^{-\varepsilon_n \cdots -\varepsilon_1 \varepsilon_1' \cdots \varepsilon_n'}. \tag{2.12}$$

In what follows we often use the abbreviations: $(\zeta) = (\zeta_1, \cdots, \zeta_{2n})$, $(\zeta') = (\zeta_1, \cdots, \zeta_{2n-1})$, $(\zeta'') = (\zeta_1, \cdots, \zeta_{2n-2})$, $(z) = (z_1, \cdots z_{2n})$, $(z') = (z_1, \cdots z_{2n-1})$; and $(\varepsilon) = (\varepsilon_1 \cdots \varepsilon_{2n})$, $(\varepsilon') = (\varepsilon_1 \cdots \varepsilon_{2n-1})$, $(\varepsilon'') = (\varepsilon_1 \cdots \varepsilon_{2n-2})$. On the basis of the CTM (corner transfer matrix) bootstrap approach, the correlation functions satisfy the following three conditions [5]:

1. R-matrix symmetry

$$P_{j\,j+1} G_\sigma^{(n)}(\cdots, \zeta_{j+1}, \zeta_j, \cdots) = R_{j\,j+1}(\zeta_j/\zeta_{j+1}) G_\sigma^{(n)}(\cdots, \zeta_j, \zeta_{j+1}, \cdots) \quad (1 \leqslant j \leqslant 2n-1), \tag{2.13}$$

where $P(x \otimes y) = y \otimes x$.

2. Cyclicity

$$P_{12}\cdots P_{2n-12n}G^{(n)}_{\sigma}(\zeta', x^2\zeta_{2n}) = \sigma G^{(n)}_{\sigma}(\zeta_{2n}, \zeta'). \tag{2.14}$$

3. Normalization

$$G^{(n)}_{\sigma}(\zeta'', \zeta_{2n-1}, \zeta_{2n})|_{\zeta_{2n}=\epsilon x^{-1}\zeta_{2n-1}} \quad = \quad G^{(n-1)}_{\epsilon\sigma}(\zeta'') \otimes u_{\epsilon} \qquad (\epsilon = \pm), \tag{2.15}$$

where $u_{\epsilon} = v_+ \otimes v_- + \epsilon v_- \otimes v_+$.

These three conditions can be componentwisely recast as follows:

$$\begin{aligned} & G^{(n)}_{\sigma}(\cdots, \zeta_{j+1}, \zeta_j, \cdots)^{\cdots\varepsilon_{j+1}\varepsilon_j\cdots} \\ = & \sum_{\varepsilon'_j, \varepsilon'_{j+1}=\pm} R(\zeta_j/\zeta_{j+1})^{\varepsilon_j\varepsilon_{j+1}}_{\varepsilon'_j\varepsilon'_{j+1}} G^{(n)}_{\sigma}(\cdots, \zeta_j, \zeta_{j+1}, \cdots)^{\cdots\varepsilon'_j\varepsilon'_{j+1}\cdots}. \end{aligned} \tag{2.16}$$

$$G^{(n)}_{\sigma}(\zeta', x^2\zeta_{2n})^{\varepsilon'\varepsilon_{2n}} = \sigma G^{(n)}_{\sigma}(\zeta_{2n}, \zeta')^{\varepsilon_{2n}\varepsilon'}. \tag{2.17}$$

$$G^{(n)}_{\sigma}(\zeta'', \zeta_{2n-1}, \epsilon x^{-1}\zeta_{2n-1})^{\varepsilon'' ss'} \quad = \quad s^{(1-\epsilon)/2}\delta_{s+s',0}G^{(n-1)}_{\epsilon\sigma}(\zeta'')^{\varepsilon''} \qquad (s, s' = \pm). \tag{2.18}$$

Combining (2.16) and (2.18) we obtain another expression of the normalization condition:

$$\sum_{s=\pm} s^{(1-\epsilon)/2} G^{(n)}_{\sigma}(\zeta'', \zeta_{2n-1}, \epsilon x\zeta_{2n-1})^{\varepsilon''\, s\, -s} = G^{(n-1)}_{\epsilon\sigma}(\zeta'')^{\varepsilon''},$$

where we also use

$$R(\epsilon x^{-1}) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \epsilon & 1 & 0 \\ 0 & 1 & \epsilon & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Since the R-matrix preserves the 'total spin' of the correlation function, we can restrict $G^{(n)}_{\sigma}(\zeta)$ to an element of the 'total spin-0' subspace, when we consider the equations (2.13–2.15). Note that the first two conditions imply the difference equation of the quantum KZ type [3] of level -4:

$$\begin{aligned} T_j G^{(n)}_{\sigma}(\zeta) = & R_{j\,j-1}(x^{-2}\zeta_j/\zeta_{j-1}) \cdots R_{j\,1}(x^{-2}\zeta_j/\zeta_1) \\ & \times R_{j\,2n}(\zeta_j/\zeta_{2n}) \cdots R_{j\,j+1}(\zeta_j/\zeta_{j+1}) G^{(n)}_{\sigma}(\zeta), \end{aligned} \tag{2.19}$$

where T_j is the shift operator such that

$$T_j F(\zeta) = F(\zeta_1, \cdots, x^{-2}\zeta_j, \cdots, \zeta_{2n}), \tag{2.20}$$

for any $2n$-variate function F. When the definition of T_j is replaced by

$$T_j F(\zeta) = F(\zeta_1, \cdots, x^{l+2}\zeta_j, \cdots, \zeta_{2n}),$$

and all the arguments $x^{-2}\zeta_j/\zeta_k$ in the first line of the RHS of (2.19) are also replaced by $x^{l+2}\zeta_j/\zeta_k$, the difference equation (2.19) is called the quantum KZ equations of level l.

Remark. As a result of $\mathbb{Z}_2$-symmetry of R-matrix, there are two ground states for the anti-ferromagnetic XXZ model. Let us specify the two ground states by $i = 0, 1$, and denote the correlation function on the i-th ground state by $G_i^{(n)}(\zeta)$. The CTM bootstrap approach suggest that both $G_0^{(n)}(\zeta)$ and $G_1^{(n)}(\zeta)$ will appear in the cyclicity condition as follows:

$$P_{12}\cdots P_{2n-12n}G_i^{(n)}(\zeta_1,\cdots,\zeta_{2n-1},x^2\zeta_{2n})=G_{1-i}^{(n)}(\zeta_{2n},\zeta_1,\cdots,\zeta_{2n-1}).$$

Thus we introduce $G_\sigma^{(n)}(\zeta)=G_0^{(n)}(\zeta)+\sigma G_1^{(n)}(\zeta)$ such that the second equation (2.14) involves only $G_\sigma^{(n)}(\zeta)$.

2.3 Integral formulae

Set

$$G_\sigma^{(n)}(\zeta)=c_n\prod_{1\leqslant j<k\leqslant 2n}\zeta_j g(z_j/z_k)\times\overline{G}_\sigma^{(n)}(\zeta). \tag{2.21}$$

Here c_n is a constant which will be determined below, and the function $g(z)$ has the properties

$$g(z)=g(x^{-4}z^{-1}),\qquad \kappa(\zeta)=\zeta\frac{g(z)}{g(z^{-1})}. \tag{2.22}$$

The explicit form of $g(z)$ is as follows:

$$g(z)=\frac{(x^6z;x^4,x^4)_\infty(x^2z^{-1};x^4,x^4)_\infty}{(x^8z;x^4,x^4)_\infty(x^4z^{-1};x^4,x^4)_\infty}. \tag{2.23}$$

Thanks to (2.22) the first two equations (2.16–2.17) are rephrased in terms of $\overline{G}_\sigma^{(n)}(\zeta)$ and $\overline{R}(\zeta)$ as follows

$$\overline{G}_\sigma^{(n)}(\cdots,\zeta_{j+1},\zeta_j,\cdots)^{\cdots\varepsilon_{j+1}\varepsilon_j\cdots}=\sum_{\varepsilon_j',\varepsilon_{j+1}'=\pm}\overline{R}(\zeta_j/\zeta_{j+1})_{\varepsilon_j',\varepsilon_{j+1}'}^{\varepsilon_j,\varepsilon_{j+1}}\overline{G}_\sigma^{(n)}(\cdots,\zeta_j,\zeta_{j+1},\cdots)^{\varepsilon_j',\varepsilon_{j+1}'}, \tag{2.24}$$

$$\overline{G}_\sigma^{(n)}(\zeta',x^2\zeta_{2n})^{\varepsilon'\,\varepsilon_{2n}}=\overline{G}_\sigma^{(n)}(\zeta_{2n},\zeta')^{\varepsilon_{2n}\,\varepsilon'}\prod_{j=1}^{2n-1}\frac{\zeta_{2n}}{\zeta_j}. \tag{2.25}$$

In order to present our integral formulae for $\overline{G}_\sigma^{(n)}(\zeta)$ let us prepare some notation. Let

$$A:=\{a|\varepsilon_a>0,\ 1\leqslant a\leqslant 2n\}. \tag{2.26}$$

Then the number of elements of A is equal to n, because we consider only the 'total-spin-0' case. We often use the abbreviations $(w)=(w_{a_1},\cdots,w_{a_n})$, $(w')=(w_{a_1},\cdots,w_{a_{n-1}})$ and $(w'')=(w_{a_1},\cdots,w_{a_{n-2}})$ for $a_j\in A$ such that $a_1<\cdots<a_n$. Let us define the following $V^{\otimes 2n}$-valued meromorphic function

$$Q^{(n)}(w|\zeta)=\sum_{\substack{\varepsilon_j=\pm\\ \varepsilon_1+\cdots+\varepsilon_{2n}=0}}v_{\varepsilon_1}\otimes\cdots\otimes v_{\varepsilon_{2n}}Q^{(n)}(w|\zeta)^\varepsilon, \tag{2.27}$$

where

$$Q^{(n)}(w|\zeta)^\varepsilon=\prod_{a\in A}\zeta_a\left(\prod_{j=1}^{a-1}(xz_j-w_a)\prod_{j=a+1}^{2n}(xw_a-z_j)\right)\Bigg/\prod_{\substack{a,b\in A\\ a<b}}(x^{-1}w_b-xw_a). \tag{2.28}$$

Note that the $Q_n(\alpha|\beta)^\varepsilon$ in [13], the massless analogue of $Q^{(n)}(w|\zeta)^\varepsilon$, can be obtained by substituting $\zeta_j=e^{-\nu\beta_j}$, $x=e^{\pi i\nu}$, and $w_a=e^{-2\nu\alpha_a}$ into (2.28), up to a trivial factor.

We wish to find integral formulae of the form

$$\overline{G}_\sigma^{(n)}(\zeta) = \prod_{a\in A} \oint_{C_a} \frac{dw_a}{2\pi i w_a} \Psi_\sigma^{(n)}(w|\zeta) Q^{(n)}(w|\zeta). \tag{2.29}$$

Here, the kernel has the form

$$\Psi_\sigma^{(n)}(w|\zeta) = \vartheta_\sigma^{(n)}(w|\zeta) \prod_{a\in A} \prod_{j=1}^{2n} \psi\Big(\frac{w_a}{z_j}\Big), \tag{2.30}$$

where

$$\psi(z) = \frac{1}{(xz;x^4)_\infty (xz^{-1};x^4)_\infty}. \tag{2.31}$$

For the function $\vartheta_\sigma^{(n)}(w|\zeta)$ we assume that

- it is anti-symmetric and holomorphic in the $w_a \in \mathbb{C}\backslash\{0\}$,
- it is symmetric and meromorphic in the $\zeta_j \in \mathbb{C}\backslash\{0\}$,
- it has the two transformation properties

$$\frac{\vartheta_\sigma^{(n)}(w|\zeta', x^2\zeta_{2n})}{\vartheta_\sigma^{(n)}(w|\zeta)} = \sigma \prod_{a\in A} \frac{w_a}{x^4 z_{2n}} \prod_{j=1}^{2n-1} \frac{\zeta_{2n}}{\zeta_j} = \sigma x^{-4n} \prod_{a\in A} w_a \prod_{j=1}^{2n} \zeta_j^{-1}, \tag{2.32}$$

$$\frac{\vartheta_\sigma^{(n)}(w', x^4 w_{a_n}|\zeta)}{\vartheta_\sigma^{(n)}(w|\zeta)} = x^{2n} \prod_{j=1}^{2n} \frac{z_j}{x^4 w_{a_n}} = x^{-6n} \prod_{j=1}^{2n} \frac{z_j}{w_{a_n}}. \tag{2.33}$$

- it satisfies the following recursion relation

$$\frac{\vartheta_\sigma^{(n)}(w', x^{-1}z_{2n-1}|\zeta'', \zeta_{2n-1}, \epsilon x^{-1}\zeta_{2n-1})}{\vartheta_{\epsilon\sigma}^{(n-1)}(w'|\zeta'')} = x^{2n} z_{2n-1}^{-2n} \prod_{j=1}^{2n-2} z_j^{-1} \prod_{\substack{a\in A\\ a\neq a_{2n}}} w_a^{-1} \Theta_{x^2}(xw_a/z_{2n-1}). \tag{2.34}$$

  Here

$$\Theta_p(z) := (z;p)_\infty (pz^{-1};p)_\infty (p,p)_\infty = \sum_{m\in\mathbb{Z}} p^{m(m-1)}(-z)^m,$$

  and we also fix the constant c_n as follows:

$$c_n = \frac{(-1)^{n(n+1)/2}}{x^{n(n-1)/2}(x^2;x^2)_\infty^{n(n-1)/2}} \frac{(x^2;x^4,x^4)_\infty^{2n}}{(x^8;x^4,x^4)_\infty^{2n}}. \tag{2.35}$$

The function $\vartheta_\sigma^{(n)}(w|\zeta)$ is otherwise arbitrary, and the choice of $\vartheta_\sigma^{(n)}(w|\zeta)$ corresponds to that of solutions to (2.13–2.15). The transformation property of $\vartheta_\sigma^{(n)}(w|\zeta)$ implies

$$\frac{\Psi_\sigma^{(n)}(w|\zeta', x^2\zeta_{2n})}{\Psi_\sigma^{(n)}(w|\zeta)} = \sigma \prod_{a\in A} \frac{w_a - xz_{2n}}{x^4 z_{2n} - xw_a} \prod_{j=1}^{2n} \frac{\zeta_{2n}}{\zeta_j}, \tag{2.36}$$

$$\frac{\Psi_\sigma^{(n)}(w', x^4 w_{a_n}|\zeta)}{\Psi_\sigma^{(n)}(w|\zeta)} = \prod_{j=1}^{2n} \frac{z_j - xw_{a_n}}{x^3 w_{a_n} - z_j}. \tag{2.37}$$

The integrand may have poles at

$$w_a = \begin{cases} x^{\pm(1+4k)} z_j & (1 \leqslant j \leqslant 2n, k \in \mathbb{Z}_{\geqslant 0}), \\ x^2 w_b & (b < a), \\ x^{-2} w_b & (b > a). \end{cases}$$

We choose the integration contour C_a with respect to w_a ($a \in A$) such that C_a is along a simple closed curve oriented anti-clockwise, and encircles the points $x^{1+4k}z_j (1 \leqslant j \leqslant 2n, k \in \mathbb{Z}_{\geqslant 0})$ and $x^2 w_b$ ($b < a$) but not $x^{-1-4k}z_j (1 \leqslant j \leqslant 2n, k \in \mathbb{Z}_{\geqslant 0})$ nor $x^{-2}w_b$ ($b > a$). Thus the contour C_a actually depends on z_j's besides a, so that it precisely should be denoted by $C_a(z) = C_a(z_1, \cdots, z_{2n})$. The LHS of (2.14) refers to the analytic continuation with respect to ζ_{2n}. Nevertheless, once we restrict ourselves to the principal regime $0 < x < \zeta_j^{-1} < 1$, we can tune all C_a's to be the common integration contour $C : |w_a| = x^{-1}$ because of the inequality $xz_j < x^{-1} < x^{-1}z_j$.

3 Main proposition

In this section we prove the following proposition in the bulk anti-ferromagnetic XXZ model case:

Proposition 1 *Assume the properties of the function $\vartheta^{(n)}_\sigma$ below (2.31) and the integration contour C_a below (2.35). Then the integral formulae (2.11, 2.21, 2.29) with (2.23, 2.27, 2.28, 2.30, 2.31) solves the three equations (2.13–2.15).*

3.1 Proof of the R-matrix symmetry

Let us first prove (2.13), or equivalently (2.24), in a componentwise way.

Suppose that $j, j+1 \notin A$. Then the relation (2.24) holds, because the integrand $\overline{G}^{(n)}_\sigma(\zeta)$ is symmetric with respect to ζ_j and ζ_{j+1}.

When $j \notin A$ and $j+1 \in A$ the relation (2.24) reduces to

$$\begin{aligned} & \overline{G}^{(n)}_\sigma(\cdots, \zeta_{j+1}, \zeta_j, \cdots)^{\cdots+-\cdots} \\ = \ & b(\zeta_j/\zeta_{j+1})\overline{G}^{(n)}_\sigma(\cdots, \zeta_j, \zeta_{j+1}, \cdots)^{\cdots-+\cdots} + c(\zeta_j/\zeta_{j+1})\overline{G}^{(n)}_\sigma(\cdots, \zeta_j, \zeta_{j+1}, \cdots)^{\cdots+-\cdots}. \end{aligned} \tag{3.1}$$

Note that the set of the integration variables in the second term of the RHS is different from the other terms. Since w_a's are integration variables, we can replace w_j in the second term of the RHS by w_{j+1}. After that, the relation (3.1) follows from the equality of the integrands. In this step we use

$$xw_{j+1} - z_j = \frac{x(z_j - z_{j+1})}{z_{j+1} - x^2 z_j}(xz_j - w_{j+1}) + \frac{(1-x^2)z_j}{z_{j+1} - x^2 z_j}(xw_{j+1} - z_{j+1}).$$

The case $j \in A$ and $j+1 \notin A$ can be proved in a similar way to the previous case. Here we use

$$xz_{j+1} - w_j = \frac{x(z_j - z_{j+1})}{z_{j+1} - x^2 z_j}(xw_j - z_{j+1}) + \frac{(1-x^2)z_{j+1}}{z_{j+1} - x^2 z_j}(xz_j - w_j).$$

Finally consider the case $j, j+1 \in A$. Since $\Psi^{(n)}_\sigma(w|\zeta)$ is antisymmetric with respect to w_a's, only the antisymmetric part of $Q^{(n)}(w|\zeta)^{\cdots++\cdots}$ with respect to w_j and w_{j+1} gives non-zero contribution for the integral. Thus the relation (2.24) in this case follows from the fact that the following combination

$$\frac{(xw_j - z_{j+1})(xz_j - w_{j+1})}{x^{-1}w_{j+1} - xw_j} - \frac{(xw_{j+1} - z_{j+1})(xz_j - w_j)}{x^{-1}w_j - xw_{j+1}}$$

is symmetric with respect to z_j and z_{j+1}.

3.2 Proof of the cyclicity

Let $2n \notin A$. When the integral (2.29) is analytically continued from ζ_{2n} to $x^2\zeta_{2n}$, the points

$$\cdots\cdots, x^9 z_{2n}, x^5 z_{2n}, xz_{2n}, x^{-1}z_{2n}, x^{-5}z_{2n}, x^{-9}z_{2n}, \cdots\cdots$$

move to the points

$$\cdots\cdots, x^{13}z_{2n}, x^9 z_{2n}, x^5 z_{2n}, x^3 z_{2n}, x^{-1}z_{2n}, x^{-5}z_{2n}, \cdots\cdots.$$

In the LHS of (2.25) the point $x^3 z_{2n}$ and consequently xz_{2n} are outside the integral contour $C'_a = C_a(z', x^4 z_{2n})$. Nevertheless, we can deform C'_a to the original one $C_a = C_a(z)$ without crossing any poles. That is because the factor

$$\prod_{a\in A}(xw_a - x^4 z_{2n}),$$

contained in $Q^{(n)}(w|\zeta', x^2\zeta_{2n})^{\varepsilon' -}$ cancels the singularity at $w_a = x^3 z_{2n}$. Thus the integral contours for both sides of (2.25) coincide.

Furthermore, by using (2.36) we obtain

$$\Psi^{(n)}_\sigma(w|\zeta', x^2\zeta_{2n})\prod_{a\in A}(xw_a - x^4 z_{2n}) = \sigma\Psi^{(n)}_\sigma(w|\zeta)\prod_{a\in A}(xz_{2n} - w_a)\prod_{j=1}^{2n}\frac{\zeta_{2n}}{\zeta_j},$$

which implies that the integrands of both sides of (2.25) coincide and therefore the relation (2.25) holds when $\varepsilon_{2n} < 0$.

Next let $2n \in A$. In this case we also make the rescale of variable $w_{2n} \mapsto x^4 w_{2n}$ in the LHS of (2.25). Then the integral contur with respect to w_a ($a \in A\backslash\{2n\}$) will be $C'_a = C_a(z', x^4 z_{2n})$, and the other one will be $\widetilde{C} = C_{2n}(x^{-4}z', z_{2n})$. For $a \in A\backslash\{2n\}$, we can deform the contour C'_a to the original C_a without crossing any poles, as the same reason as before. The integral contour $\widetilde{C}$ encircles $x^{-3+4k}z_j$ ($1 \leqslant j \leqslant 2n-1$, $k \in \mathbb{Z}_{\geqslant 0}$) and $x^{1+4k}z_{2n}$ ($k \in \mathbb{Z}_{\geqslant 0}$), but not $x^{-5-4k}z_j$ ($1 \leqslant j \leqslant 2n-1$, $k \in \mathbb{Z}_{\geqslant 0}$) nor $x^{-1-4k}z_{2n}$ ($k \in \mathbb{Z}_{\geqslant 0}$). Since $Q^{(n)}(w|\zeta', x^2\zeta_{2n})^{\varepsilon' +}$ contains the factor

$$x^2\zeta_{2n}\prod_{j=1}^{2n-1}(xz_j - x^4 w_{2n})\prod_{\substack{a\in A\\ a\neq 2n}}\frac{xw_a - x^4 z_{2n}}{x^{-1}x^4 w_{2n} - xw_a}, \tag{3.2}$$

the pole at $w_{2n} = x^{-3}z_{2n}$ ($1 \leqslant j \leqslant 2n-1$) disappears. Thus we can deform the contour $\widetilde{C}$ to the original one $C_{2n} = C_{2n}(z)$ without crossing any poles. Thus the integral contours in both sides of (2.25) coincide.

Replace the integral variables such that $(w', w_{2n}) \mapsto (w_{2n}, w')$ in the RHS of (2.25), and compare the integrands of both sides. From (2.36, 2.37) and the antisymmetric property of $\Psi_\sigma^{(n)}$ with respect to w_a's, we have

$$\frac{\Psi_\sigma^{(n)}(w', x^4 w_{2n}|\zeta', x^2\zeta_{2n})}{\Psi_\sigma^{(n)}(w_{2n}, w'|\zeta)} = (-1)^{n-1} x^{-3} \prod_{\substack{a\in A\\ a\neq 2n}} \frac{w_a - x z_{2n}}{x^4 z_{2n} - x w_a} \prod_{j=1}^{2n-1} \frac{\zeta_{2n}}{\zeta_j} \frac{z_j - x w_{2n}}{x^3 w_{2n} - z_j}. \tag{3.3}$$

Note that (3.2) describes all w_{2n}- and z_{2n}-dependence of $Q^{(n)}(w|\zeta', x^2\zeta_{2n})^{\varepsilon +}$. The product of (3.2) and (3.3) is equal to

$$\zeta_{2n} \prod_{j=1}^{2n-1} \frac{\zeta_{2n}}{\zeta_j}(x w_{2n} - z_j) \prod_{\substack{a\in A\\ a\neq 2n}} \frac{x z_{2n} - w_a}{x^{-1} w_a - x w_{2n}},$$

which implies that the integrands of both sides of (2.25) coincide and therefore the relation (2.25) holds when $\varepsilon_{2n} > 0$.

3.3 Proof of the normalization condition

Let us prove (2.15), or equivalently (2.18). The factor $g(z_{2n-1}/z_{2n})$ hase a zero at $\zeta_{2n} = \epsilon x^{-1}\zeta_{2n-1}$. On the other hand, the two points $x z_{2n}$ and $x^{-1} z_{2n-1}$ are required to locate opposite sides of the integral contour C_a, so that a pinching may occur as $\zeta_{2n} \to \epsilon x^{-1}\zeta_{2n-1}$. If there is no pinching the correlation function $G_\sigma^{(n)}(\zeta)$ vanishes at $\zeta_{2n} = \epsilon x^{-1}\zeta_{2n-1}$.

Suppose $2n-1, 2n \notin A$. In this case the factor $(x w_a - z_{2n-1})$ contained in $Q^{(n)}(w|\zeta)^{\varepsilon'' --}$ cancel the poles of $\psi(w_a/z_{2n-1})$ at $w_a = x^{-1} z_{2n-1}$, and therefore no pinching occurs as $\zeta_{2n} \to x^{-1}\zeta_{2n-1}$. Thus the condition (2.18) holds if $2n-1, 2n \notin A$.

When $2n-1, 2n \in A$, no pinching occurs for the integral contour for C_a ($a \in A\backslash\{2n-1, 2n\}$), as the same reason as before. Concerning the integral with respect to w_{2n-1} and w_{2n}, there is no singularities at $w_{2n-1} = x z_{2n}$ and $w_{2n} = x z_{2n}$ and consequently no pinching occurs actually. In order to see such vanishing singularities, let us first evaluate the residue at $w_{2n} = x z_{2n}$. Because of the antisymmetric property of $\vartheta_\sigma^{(n)}$ with respect to w_a's, the zero of $\vartheta_\sigma^{(n)}(w'', w_{2n-1}, x z_{2n}|\zeta)$ at $w_{2n-1} = x z_{2n}$ cancels the poles of $\psi(w_{2n-1}/z_{2n})$ at the same point. Furthermore, the poles of $\psi(w_{2n}/z_{2n})$ and $\psi(w_{2n}/z_{2n-1})$ at $w_{2n} = x z_{2n}$ and $z_{2n} = x^{-2} z_{2n-1}$ are canceled by the zeros of $g(z_{2n-1}/z_{2n})$ and $Q^{(n)}(w'', w_{2n-1}, x z_{2n}|\zeta)^{\varepsilon'' ++}$ at the same points. The latter cancellation can be shown as follows. Note that the integral is invariant as we replace $Q^{(n)}(w'', w_{2n-1}, x z_{2n}|\zeta)^{\varepsilon'' ++}$ by its antisymmetric part with respect to w_{2n-1} and $x z_{2n}$. When $z_{2n} = x^{-2} z_{2n-1}$ the antisymmetric part contains the following vanishing factor:

$$\frac{(x w_{2n-1} - z_{2n})(x z_{2n-1} - x z_{2n})}{x^{-1} x z_{2n} - x w_{2n-1}} - \frac{(x x z_{2n} - z_{2n})(x z_{2n-1} - w_{2n-1})}{x^{-1} w_{2n-1} - x x z_{2n}}.$$

Thus there is no singularity at $w_{2n} = x z_{2n}$ as $\zeta_{2n} \to \epsilon x^{-1}\zeta_{2n-1}$. The same thing at $w_{2n-1} = x z_{2n}$ can be easily shown in the same way. Hence the condition (2.18) is verified when $2n-1, 2n \in A$.

Next let $2n-1 \notin A$ and $2n \in A$. In this case there is no pinching for the integrals with respect to w_a ($a \in A\backslash\{2n\}$). Let $\widehat{C}$ denote the integral contour with respect to w_{2n} such that $\widehat{C}$ encircles the same points as C_{2n} does but xz_{2n}. Note that no pinching occurs with respect to the integral along $\widehat{C}$ because both the two points $x^{-1}z_{2n-1}$ and xz_{2n} lie outside the contour $\widehat{C}$. Thus the integral with respect to w_{2n} along the contour C_{2n} can be replaced by the residue at $w_{2n} = xz_{2n}$.

In order to evaluate the residue, the following formulae are useful:

$$\lim_{z_{2n}\to x^{-2}z_{2n-1}} g\left(\frac{z_{2n-1}}{z_{2n}}\right)\psi\left(\frac{xz_{2n}}{z_{2n-1}}\right) = \frac{(x^6;x^4)_\infty}{(x^4;x^4)_\infty}\frac{(x^4;x^4,x^4)^2_\infty}{(x^2;x^4,x^4)^2_\infty}, \tag{3.4}$$

$$\mathrm{Res}_{w_{2n}=xz_{2n}}\frac{dw_{2n}}{w_{2n}}\psi\left(\frac{w_{2n}}{z_{2n}}\right) = \frac{1}{(x^2;x^2)_\infty}. \tag{3.5}$$

$$g(z)g(x^2z)\psi(xz) = \frac{1}{1-x^2z}. \tag{3.6}$$

$$\psi\left(\frac{w}{z}\right)\psi\left(\frac{x^2w}{z}\right)(z-xw) = \frac{-xw}{(xw/z;x^2)_\infty(xz/w;x^2)_\infty}. \tag{3.7}$$

Using these the condition (2.18) with $\varepsilon_{2n-1}<0$ and $\varepsilon_{2n}>0$ reduces to

$$\begin{aligned} c_{n-1}\vartheta^{(n-1)}_{\epsilon\sigma}(w'|\zeta'') &= c_n\vartheta^{(n)}_\sigma(w',x^{-1}z_{2n-1}|\zeta'',\zeta_{2n-1},\epsilon x^{-1}\zeta_{2n-1}) \\ &\times (-1)^n x^{-n-1}\frac{(x^8;x^4,x^4)^2_\infty}{(x^2;x^4,x^4)^2_\infty}z^{2n}_{2n-1}\prod_{j=1}^{2n-2}z_j\prod_{\substack{a\in A\\ a\neq 2n}}\frac{w_a(x^2;x^2)_\infty}{\Theta_{x^2}(xw_a/z_{2n-1})}, \end{aligned}$$

which is valid under the assumption of (2.34) and (2.35).

When $2n-1\in A$ and $2n\notin A$, the only difference from the previous case is that the rational function $Q^{(n)}(w|\zeta)^\varepsilon$ contains the factor

$$\zeta_{2n-1}(xw_{2n-1}-z_{2n})|_{w_{2n-1}=xz_{2n}} = (x^2-1)\zeta_{2n-1}z_{2n}, \tag{3.8}$$

in the present case, while the corresponding factor in the previous case is

$$\zeta_{2n}(xz_{2n-1}-w_{2n})|_{w_{2n}=xz_{2n}} = x\zeta_{2n}(z_{2n-1}-z_{2n}). \tag{3.9}$$

Since (3.8) is equal to ϵ times (3.9) as $\zeta_{2n}=\epsilon x^{-1}\zeta_{2n-1}$, the condition (2.18) with $\varepsilon_{2n-1}>0$ and $\varepsilon_{2n}<0$ follows from the previous case. After all, the condition (2.18) was componentwisely proved.

3.4 Non-trivial theta function

In subsections 3.1–3.3 we proved Proposition 1. The key point in proving (2.16) was the $\overline{R}$-matrix symmetry of the rational function $Q^{(n)}(w|\zeta)^\varepsilon$. We observed that the other two conditions (2.17) and (2.18) hold under the assumption of the transformation properties and the recursion relation of $\vartheta^{(n)}_\sigma$. But actually, you can easily find (2.32), (2.33) and (2.34) by imposing (2.25) for $\varepsilon_{2n}<0$, (2.25) for $\varepsilon_{2n}>0$ and (2.17), respectively.

In this way we obtained the integral solutions to Smirnov-type master equations for correlation functions of the anti-ferromagnetic XXZ model, with the freedom of the choice of $\vartheta^{(n)}_\sigma$. Now we wish to present an example of $\vartheta^{(n)}_\sigma$ satisfying all the properties given below (2.31).

$$\vartheta^{(n)}_\sigma(w|\zeta) = \Theta_{x^2}\left(-\sigma\prod_{a\in A}w_a^{-1}\prod_{j=1}^{2n}\zeta_j\right)\prod_{j=1}^{2n}z_j^{-n}\prod_{\substack{a,b\in A\\ a<b}}w_a^{-1}\Theta_{x^2}(w_a/w_b). \tag{3.10}$$

You can easily see that (3.10) satisfies all the properties of symmetry with respect to ζ_j's, antisymmetry with respect to w_a's, (2.32), (2.33) and (2.34). Note that this example of the function $\vartheta^{(n)}_\sigma(w|\zeta)\prod_{j=1}^{2n} z_j^n$ coincides with the theta function for the anti-ferromagnetic XXZ model form factors [8] in the 'total spin-0' sector, up to a constant. We therefore conclude that Smirnov-type integral solutions for both form factors and correlation functions hold the essentially common integral kernel, and that the only difference among both formulae results from the choice of the rational functions.

Taking into account that $x = q^2$ in [10] while we set $x = -q$, you can easily confirm that our integral formulae with the choice of the function $\vartheta^{(n)}_\sigma$ (3.10) reproduce the ones obtained in the trace construction [10], up to a trivial constant. Here, the following formulae are useful in order to compare eq. (8.21) in [10] with our solutions:

$$\prod_{a\in A}\zeta_a = \prod_{j=1}^{2n}\zeta^{(1+\varepsilon_j)/2},$$

and

$$\frac{1}{2}\left(\Theta_{x^2}(-u)\pm\Theta_{x^2}(u)\right) = \begin{cases}\Theta_{x^8}(-x^2u^2),\\ u\Theta_{x^8}(-x^6u^2).\end{cases}$$

We also notice that there is actually no poles at $w_a = x^2 w_b$ ($b < a$) and $w_a = x^{-2}w_b$ ($b > a$) when we fix $\vartheta^{(n)}_\sigma$ to (3.10) because of the factor $\Theta_{x^2}(w_a/w_b)$.

4 Integral formulae for the boundary XXZ model

4.1 The Hamiltoninan and the K-matrix

In this section we consider the XXZ spin chain in a half-infinite lattice

$$H_{bXXZ} = -\frac{1}{2}\sum_{j=1}^{\infty}(\sigma^x_{j+1}\sigma^x_j + \sigma^y_{j+1}\sigma^y_j + \Delta\sigma^z_{j+1}\sigma^z_j) + h\sigma^z_1, \tag{4.1}$$

where

$$\Delta = -\frac{x+x^{-1}}{2}, \qquad h = \frac{1-x^2}{4x}\frac{1+r}{1-r}. \tag{4.2}$$

We again restrict ourselves to the anti-ferromagnetic regime: $0 < x < 1$. We also restrict the discussion below to the case $0 < x^2 < |r| < z^{-1} < 1$ such that $h > 0$. Since the quantity h denotes the magnegic field at the boundary site, the $\mathbb{Z}_2$-symmetry is broken by the boundary term. In what follows we assume that there is only one ground state for the anti-ferromagnetic XXZ model with a boundary. In the presence of the positive magnetic field at the boundary, we should fix the unique ground state to $|0\rangle_B$, in the terminology of Ref. [12].

As done in the bulk case, the Hamiltonian (4.1) can be obtained from the transfer matrix for the six vertex model on a half-infinite lattice, by taking logarithmic derivative with respect to the spectral parameter ζ. The boundary interaction in the boundary six vertex model is specified by the following diagonal reflection matrix [21, 22]

$$K(\zeta)v_\varepsilon = \sum_{\varepsilon'=\pm} v_{\varepsilon'}K(\zeta)^{\varepsilon'}_{\varepsilon}, \qquad K(\zeta) = \frac{1}{f(z;r)}\overline{K}(\zeta). \tag{4.3}$$

Here the scalar function $f(z;r)$ is given by

$$f(z;r)=f_1(z;r)f_2(z), \qquad f_1(z;r)=\frac{\varphi_1(z;r)}{\varphi_1(z^{-1};r)}, \qquad f_2(z)=\frac{\varphi_2(z^2)}{\varphi_2(z^{-2})},$$

and

$$\varphi_1(z;r)=\frac{(x^2rz;x^4)_\infty}{(x^4rz;x^4)_\infty}, \qquad \varphi_2(z^2)=\frac{(x^8z^2;x^8)_\infty}{(x^6z^2;x^8)_\infty}. \tag{4.4}$$

The non-zero entries are

$$\overline{K}(\zeta)_+^+=k_+(z)=\frac{1-rz}{z-r}, \qquad \overline{K}(\zeta)_-^-=k_-(z)=1. \tag{4.5}$$

We also introduce another K-matrix $K'(\zeta)$:

$$K'(\zeta)v_\varepsilon=\sum_{\varepsilon'=\pm}v_{\varepsilon'}K(x^{-1}\zeta)_{-\varepsilon}^{-\varepsilon'}.$$

The explicit form of $K'(\zeta)$ is given as follows:

$$K'(\zeta)=\frac{1}{f'(z;r)}\overline{K'}(\zeta), \qquad f'(z;r)=x^{-2}z\frac{\varphi_1(z^{-1};r)}{\varphi_1(x^{-4}z;r)}\frac{\varphi_2(x^2z^{-1};r)}{\varphi_2(x^{-2}z;r)}, \tag{4.6}$$

and the non-zero entries are

$$\overline{K'}(\zeta)_+^+=k'_+(z)=\frac{1}{k_+(x^{-2}z)}, \qquad \overline{K'}(\zeta)_-^-=k'_-(z)=1. \tag{4.7}$$

The main properties of the K-matrix are the reflection (boundary Yang-Baxter) equation

$$K_2(z_2)R_{21}(z_1+z_2)K_1(z_1)R_{12}(z_1-z_2)=R_{21}(z_1-z_2)K_1(z_1)R_{12}(z_1+z_2)K_2(z_2). \tag{4.8}$$

the initial condition

$$K(1)=I; \tag{4.9}$$

and the unitarity relation

$$K(\zeta)K(\zeta^{-1})=1; \tag{4.10}$$

the $\mathbb{Z}_2$-parity

$$K(-\zeta)=K(\zeta); \tag{4.11}$$

and the boundary crossing symmetry

$$K(\zeta)_{\varepsilon_1}^{\varepsilon'_1}=\sum_{\varepsilon_2,\varepsilon'_2=\pm}R(\zeta^2)_{\varepsilon'_2-\varepsilon'_1}^{-\varepsilon_1\varepsilon_2}K(\epsilon x^{-1}\zeta)_{\varepsilon_2}^{\varepsilon'_2} \qquad (\epsilon=\pm). \tag{4.12}$$

Under this normalization the partition function per boundary lattice site is equal to unity in the thermodynamic limit [12].

4.2 Correlation functions and difference equations

Let us introduce the $V^{\otimes 2n}$-valued correlation functions

$$G_b^{(n)}(\zeta_1,\cdots,\zeta_{2n}) = \sum_{\substack{\varepsilon_j=\pm \\ \varepsilon_1+\cdots+\varepsilon_{2n}=0}} v_{\varepsilon_1}\otimes\cdots\otimes v_{\varepsilon_{2n}} G_b^{(n)}(\zeta_1,\cdots,\zeta_{2n})^{\varepsilon_1\cdots\varepsilon_{2n}}. \tag{4.13}$$

Here, we restrict $G_b^{(n)}(\zeta)$ to the 'total spin-0' subspace of $V^{\otimes 2n}$. The subscript b refers to quantities in the boundary model. In the bulk model, we considered two correlation functions $G_\pm^{(n)}(\zeta)$ for each n. On the contrary, because of the $\mathbb{Z}_2$-symmetry breakdown, we will consider only one correlation function $G_b^{(n)}(\zeta)$ for each n in the boundary model. As in the bulk model case, by specializing the spectral parameters the correlation function (4.13) gives the expectation value of the local operator as follows:

$$\langle E^{(1)}_{\varepsilon_1\varepsilon'_1}\cdots E^{(n)}_{\varepsilon_n\varepsilon'_n}\rangle_b = G_b^{(n)}(\overbrace{x^{-1}\zeta,\cdots,x^{-1}\zeta}^{n},\overbrace{\zeta,\cdots,\zeta}^{n})^{-\varepsilon_n\cdots-\varepsilon_1\varepsilon'_1\cdots\varepsilon'_n}. \tag{4.14}$$

In this section we often use the abbreviations $(\tilde{\zeta})=(\zeta_2,\cdots,\zeta_{2n})$, and $(\tilde{\varepsilon})=(\varepsilon_2,\cdots,\varepsilon_{2n})$. For fixed indices $a_1,\cdots,a_n$ such that $a_1<\cdots<a_n$, we also use the abbreviation $(\tilde{w})=(w_{a_2},\cdots,w_{a_n})$. On the basis of the boundary CTM bootstrap approach, the correlation functions satisfy the following four conditions [6]:

1. R-matrix symmetry

$$P_{j\,j+1}G_b^{(n)}(\cdots,\zeta_{j+1},\zeta_j,\cdots) \quad = R_{j\,j+1}(\zeta_j/\zeta_{j+1})G_b^{(n)}(\cdots,\zeta_j,\zeta_{j+1},\cdots) \qquad (1\leqslant j\leqslant 2n-1). \tag{4.15}$$

2. Reflection properties

$$K_{2n}(\zeta_{2n})G_b^{(n)}(\zeta',\zeta_{2n}) = G_b^{(n)}(\zeta',\zeta_{2n}^{-1}); \tag{4.16}$$

and

$$K'_1(\zeta_1)G_b^{(n)}(\zeta_1^{-1},\tilde{\zeta}) = G_b^{(n)}(x^{-2}\zeta_1,\tilde{\zeta}). \tag{4.17}$$

3. Normalization

$$G_b^{(n)}(\zeta'',\zeta_{2n-1},\zeta_{2n})|_{\zeta_{2n}=\epsilon x^{-1}\zeta_{2n-1}} \quad = \quad G_b^{(n-1)}(\zeta'')\otimes u_\epsilon \qquad (\epsilon=\pm). \tag{4.18}$$

Since the R-matrix and K-matrix preserves the 'total spin' of the correlation function, we can regard $G_b^{(n)}(\zeta)$ as the element of the 'total spin-0' subspace, when we consider the equations (4.15–4.18). Note that the first three equations imply the boundary analogue of the quantum KZ difference equation:

$$\begin{aligned} T_j G_b^{(n)}(\zeta) &= R_{jj-1}(x^{-2}\zeta_j/\zeta_{j-1})\cdots R_{j1}(x^{-2}\zeta_j/\zeta_1)\hat{K}_j(\zeta_j) \\ &\times R_{1j}(\zeta_1\zeta_j)\cdots R_{j-1j}(\zeta_{j-1}\zeta_j)R_{j+1j}(\zeta_{j+1}\zeta_j)\cdots R_{2nj}(\zeta_{2n}\zeta_j) \\ &\times K_j(\zeta_j)R_{j2n}(\zeta_j/\zeta_{2n})\cdots R_{jj+1}(\zeta_j/\zeta_{j+1})G_b^{(n)}(\zeta), \end{aligned} \tag{4.19}$$

where T_j is the shift operator defined by (2.20).

4.3 Integral formulae

Set

$$G_b^{(n)}(\zeta) = c_n' \prod_{1\leqslant j<k\leqslant 2n} \zeta_j g(z_j/z_k) g(z_j z_k) \prod_{j=1}^{2n} \varphi_1(z_j; r) g_b(z_j) \times \overline{G}_b^{(n)}(\zeta). \tag{4.20}$$

Here c_n' is a constant which will be determined below, and the scalar function $g_b(z)$ has the properties

$$g_b(z) = g_b(x^{-2}z^{-1}), \qquad f_2(z) = \frac{g_b(z)}{g_b(z^{-1})}. \tag{4.21}$$

The explicit form of $g_b(z)$ is as follows:

$$g_b(z) = \frac{(x^{10}z^2; x^4, x^8)_\infty (x^6 z^{-2}; x^4, x^8)_\infty}{(x^{12}z^2; x^4, x^8)_\infty (x^8 z^{-2}; x^4, x^8)_\infty}. \tag{4.22}$$

Thanks to (2.22) and (4.21) the first three equations (4.15–4.17) are rephrased in terms of $\overline{G}_b^{(n)}(\zeta)$ and $\overline{R}(\zeta)$ as follows

$$\overline{G}_b^{(n)}(\cdots, \zeta_{j+1}, \zeta_j, \cdots)^{\cdots \varepsilon_{j+1}\varepsilon_j \cdots} = \sum_{\varepsilon_j', \varepsilon_{j+1}' = \pm} \overline{R}(\zeta_j/\zeta_{j+1})_{\varepsilon_j', \varepsilon_{j+1}'}^{\varepsilon_j, \varepsilon_{j+1}} \overline{G}_b^{(n)}(\cdots, \zeta_j, \zeta_{j+1}, \cdots)^{\varepsilon_j', \varepsilon_{j+1}'}, \tag{4.23}$$

$$k_{\varepsilon_{2n}}(\zeta_{2n}) \overline{G}_b^{(n)}(\zeta', \zeta_{2n})^{\varepsilon' \, \varepsilon_{2n}} = \overline{G}_b^{(n)}(\zeta', \zeta_{2n}^{-1})^{\varepsilon' \, \varepsilon_{2n}}, \tag{4.24}$$

$$(x^2 z_1^{-1})^{2n} k_{\varepsilon_1}'(\zeta_1) \overline{G}_b^{(n)}(\zeta_1^{-1}, \tilde{\zeta})^{\varepsilon_1 \, \tilde{\varepsilon}} = \overline{G}_b^{(n)}(x^{-2}\zeta_1, \tilde{\zeta})^{\varepsilon_1 \, \tilde{\varepsilon}}, \tag{4.25}$$

Let us define the following $V^{\otimes 2n}$-valued meromorphic function

$$Q_b^{(n)}(w|\zeta) = \sum_{\substack{\varepsilon_j = \pm \\ \varepsilon_1 + \cdots + \varepsilon_{2n} = 0}} v_{\varepsilon_1} \otimes \cdots \otimes v_{\varepsilon_{2n}} Q_b^{(n)}(w|\zeta)^{\varepsilon}, \tag{4.26}$$

where

$$Q_b^{(n)}(w|\zeta)^{\varepsilon} = Q^{(n)}(w|\zeta)^{\varepsilon} q_b^{(n)}(w|\zeta), \qquad q_b^{(n)}(w|\zeta) = \prod_{a\in A} \prod_{j=1}^{2n} (x z_j - w_a^{-1}). \tag{4.27}$$

Since the factor $q_b^{(n)}(w|\zeta)$ is symmetric with respect to ζ_j's and w_a's, respectively, the R-matrix symmetry (4.23) is also valid in the boundary case.

We wish to find integral formulae of the form

$$\overline{G}_b^{(n)}(\zeta) = \prod_{a\in A} \oint_{C_a} \frac{dw_a}{2\pi i w_a} \Psi_b^{(n)}(w|\zeta) Q_b^{(n)}(w|\zeta). \tag{4.28}$$

Here, the kernel has the form

$$\Psi_b^{(n)}(w|\zeta) = \vartheta_b^{(n)}(w|\zeta) \prod_{a\in A} \prod_{j=1}^{2n} \psi_b(w_a, z_j), \tag{4.29}$$

where

$$\psi_b(w, z) = \psi\left(\frac{w}{z}\right) \psi(wz) = \frac{1}{(xw/z; x^4)_\infty (xz/w; x^4)_\infty (xwz; x^4)_\infty (x/zw; x^4)_\infty}. \tag{4.30}$$

Note that $\psi_b(w,z) = \psi_b(w, z^{-1}) = \psi_b(w^{-1}, z)$. For the function $\vartheta_b^{(n)}(w|\zeta)$ we assume that

- it is anti-symmetric and holomorphic in the $w_a \in \mathbb{C}\backslash\{x^{-1}r^{-1}\}$,

- it is symmetric and meromorphic in the $\zeta_j \in \mathbb{C}\backslash\{0\}$,
- it has the four transformation properties

$$
\begin{aligned}
\frac{\vartheta_b^{(n)}(w|\zeta',\zeta_{2n}^{-1})}{\vartheta_b^{(n)}(w|\zeta)} &= z_{2n}^{2n}, && (4.31)\\
\frac{\vartheta_b^{(n)}(w',w_{a_n}^{-1}|\zeta)}{\vartheta_b^{(n)}(w|\zeta)} &= -\frac{w_{a_n}^{-1}-rx}{w_{a_n}-rx}\prod_{\substack{a\in A\\ a\neq a_n}}\frac{x^{-1}w_{a_n}^{-1}-xw_a}{x^{-1}w_{a_n}-xw_a}, && (4.32)\\
\frac{\vartheta_b^{(n)}(w|x^{-2}\zeta_1,\tilde{\zeta})}{\vartheta_b^{(n)}(w|\zeta)} &= x^{4n}, && (4.33)\\
\frac{\vartheta_b^{(n)}(x^{-4}w_{a_1},\tilde{w}|\zeta)}{\vartheta_b^{(n)}(w|\zeta)} &= x^{-12n}w_{a_1}^{4n}\frac{1-xrw_{a_1}}{1-x^{-3}rw_{a_1}}\prod_{\substack{a\in A\\ a\neq a_1}}\frac{x^{-1}w_{a_1}^{-1}-xw_a}{x^{-1}w_{a_1}^{-1}-x^{-3}w_a}. && (4.34)
\end{aligned}
$$

- it satisfies the following recursion relation

$$
\begin{aligned}
&\frac{\vartheta_b^{(n)}(w',x^{-1}z_{2n-1}|\zeta'',\zeta_{2n-1},\epsilon x^{-1}\zeta_{2n-1})}{\vartheta_b^{(n-1)}(w'|\zeta'')} = x^{2n}z_{2n-1}^{-2n}\prod_{j=1}^{2n-2}z_j^{-1}\\
&\times\frac{\Theta_{x^4}(x^{-2}z_{2n-1}^2)}{1-rz_{2n-1}}\prod_{\substack{a\in A\\ a\neq a_{2n}}}\frac{\Theta_{x^2}(xw_a/z_{2n-1})\Theta_{x^2}(x^{-1}z_{2n-1}w_a)}{z_{2n-1}^{-1}-xw_a}.
\end{aligned}
\tag{4.35}
$$

Here we also fix the constant c_n' as follows:

$$
c_n' = \frac{x^{2n}(x^2;x^4)_\infty^n(x^2;x^4,x^4)_\infty^{2n}}{(x^2;x^2)_\infty^{n^2}(x^8;x^4,x^4)_\infty^{2n}}. \tag{4.36}
$$

The function $\vartheta_b^{(n)}(w|\zeta)$ is otherwise arbitrary, and the choice of $\vartheta_b^{(n)}(w|\zeta)$ corresponds to that of solutions to (4.15–4.18).

From (4.26, 4.32, 4.34, 4.35), we find that the integrand may have poles at

$$
w_a = \begin{cases}
x^{\pm(1+4k)}z_j & 1\leqslant j\leqslant 2n, k\in\mathbb{Z}_{\geqslant 0},\\
x^{1+4k}z_j^{-1} & 1\leqslant j\leqslant 2n, k\in\mathbb{Z}_{\geqslant 0},\\
x^{-5-4k}z_j^{-1} & 1\leqslant j\leqslant 2n, k\in\mathbb{Z}_{\geqslant 0},\\
x^{-1}r^{-1}.
\end{cases}
$$

We choose the integration contour C_a with respect to w_a ($a\in A$) such that C_a is along a simple closed curve oriented anti-clockwise, and encircles the points $x^{1+4k}z_j^{\pm1}$ ($1\leqslant j\leqslant 2n, k\in\mathbb{Z}_{\geqslant 0}$), but not $x^{-1-4k}z_j$, $x^{-5-4k}z_j^{-1}$ ($1\leqslant j\leqslant 2n, k\in\mathbb{Z}_{\geqslant 0}$) nor $x^{-1}r^{-1}$. We further fix the contour C_a such that $x^{-1}z_j^{-1}$ lie outside C_a, as in the bulk model case.

4.4 Main propositions

We are now in a position to state the proposition in the boundary anti-ferromagnetic XXZ model case:

Proposition 2 *Assume the properties of the function $\vartheta_b^{(n)}$ below (4.30) and the integration contour C_a below (4.36). Then the integral formulae (4.13, 4.20, 4.28) with (4.4, 4.22, 4.26, 2.28, 4.27, 4.29, 4.30) solves the four equations (4.15–4.18).*

A proof will be given in Appendix A.

The following example of $\vartheta_\sigma^{(n)}$ satisfies all the properties given below (4.30):

$$\vartheta_\sigma^{(n)}(w|\zeta) = \prod_{j=1}^{2n} z_j^{-n} \prod_{a\in A} \frac{\Theta_{x^4}(w_a^2)}{1-xrw_a} \prod_{\substack{a,b\in A\\ a<b}} \frac{w_b\Theta_{x^2}(w_a/w_b)\Theta_{x^2}(w_aw_b)}{x^{-1}-xw_aw_b}. \tag{4.37}$$

Taking into account that our integral variables w_a's correspond to q^3w_a in [12], you can easily confirm that our integral formulae with the choice of the function $\vartheta_b^{(n)}$ (4.37) reproduce the ones obtained in the trace construction [12], up to a trivial constant.

5 Concluding remarks

In this paper we have constructed the correlation functions of both the bulk and boundary XXZ model in the antiferromagnetic regime. This was done by directly solving Smirnov-type master equations; i.e., the R-matrix symmetry, cyclicity conditions (resp. reflection properties) and the normalization conditions for the bulk (resp. boundary) case. Precisely speaking, we made the Ansatz that the correlation functions of the bulk (resp. boundary) XXZ model are expressed in terms of integral transform of the rational functions $Q_\sigma^{(n)}(w|\zeta)$ (resp. $Q_b^{(n)}(w|\zeta)$) with the integral kernels $\Psi_\sigma^{(n)}(w|\zeta)$ (resp. $\Psi_b^{(n)}(w|\zeta)$).

The integral solutions to Smirnov-type master equations for the bulk case were given by (2.11, 2.21, 2.29) with (2.23, 2.27, 2.28, 2.30, 2.31), where the function $\vartheta_\sigma^{(n)}(w|\zeta)$ satisfies (2.32–2.34). Those for the boundary case were given by (4.13, 4.20, 4.28) with (4.4, 4.22, 4.26, 2.28, 4.27, 4.29, 4.30), where the function $\vartheta_b^{(n)}(w|\zeta)$ satisfies (4.31–4.35). Our integral formulae with appropriate choice of the functions $\vartheta_\sigma^{(n)}(w|\zeta)$ and $\vartheta_b^{(n)}(w|\zeta)$ reproduce the known results [11, 12]. The explicit choice was given in (3.10) (resp. (4.37)) for the bulk (resp. boundary) case.

In comparison with the form factor integral formulae [7, 8, 9], the corresponding rational function has the determinant structure and consequently different from $Q_\sigma^{(n)}(w|\zeta)$ obtained in the present paper. On the other hand, the integral kernels are essentially the same. Now we have a natural question whether the integral formulae for form factors of the boundary XXZ model can be written by using the integral kernel $\Psi_b^{(n)}(w|\zeta)$. We wish to address this problem in a subsequent paper.

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A Appendix A. A proof of Proposition 2

The R-matrix symmetry (4.15) can be shown by repeating the similar arguments as proving (2.13). Straightforward calculations shows that the normalization condition (4.18) follows from (4.35, 4.36).

Here the formulae (3.4–3.7) are again useful. In order to show the reflection properties (4.16, 4.17), the following observation is very relevant. The recursion relation (4.35) indicates that the function $\vartheta_b^{(n)}$ contains the factor

$$\prod_{a\in A}\frac{\Theta_{x^4}(w_a^2)}{1-xrw_a}.$$

Thus we find that

$$\vartheta_b^{(n)}(w|\zeta) \text{ has zeros at } w_a=x^{2n}\ (n\in\mathbb{Z}), \quad \text{and has a pole at } w_a=x^{-1}r^{-1}. \tag{A.1}$$

Let us prove (4.16) by showing (4.24). First consider the case $\varepsilon_{2n}<0$. By comparing the integrands of both sides, the desired equality follows from (4.31) and the equality

$$\vartheta_b^{(n)}(w|\zeta',\zeta_{2n})\prod_{a\in A}(xw_a-z_{2n})(xz_{2n}-w_a^{-1})=\vartheta_b^{(n)}(w|\zeta',\zeta_{2n}^{-1})\prod_{a\in A}(xw_a-z_{2n}^{-1})(xz_{2n}^{-1}-w_a^{-1}).$$

When $\varepsilon_{2n}>0$ the relation (4.24) is equivalent to

$$\frac{1-rz_{2n}}{z_{2n}-r}\overline{G}_b^{(n)}(\zeta',\zeta_{2n})^{\varepsilon'+}=\overline{G}_b^{(n)}(\zeta',\zeta_{2n}^{-1})^{\varepsilon'+}.$$

The difference between both sides are equal to

$$\frac{1}{z_{2n}}\prod_{a\in A}\oint_{C_a}\frac{dw_a}{2\pi i w_a}\Psi_b^{(n)}(w|\zeta)Q_b^{(n)}(w|\zeta)\left(\frac{1-rz_{2n}}{1-rz_{2n}^{-1}}-\frac{xw_{2n}-z_{2n}}{xw_{2n}-z_{2n}^{-1}}\right). \tag{A.2}$$

Since the integral (A.2) vanishes, the relation (4.24) with $\varepsilon_{2n}>0$ holds. In order to see this, let us consider the change of the integral variable $w_{2n}\mapsto w_{2n}^{-1}$. Under this transform, the integral contour C_{2n} is invariant while the integrand of (A.2) negates the sign. The latter follows from (4.31) and the equality

$$\sum_{s=\pm}\vartheta_b^{(n)}(w',w_{2n}^s|\zeta',\zeta_{2n})(w_{2n}^{-s}-xr)\prod_{\substack{a\in A\\ a\neq 2n}}(x^{-1}w_{2n}^s-xw_a)^{-1}=0.$$

Thus the one of the reflection properties (4.16) is proved.

Finally, let us prove another reflection property (4.17) by showing (4.25). First consider the case $\varepsilon_1<0$. Since the function $Q_b^{(n)}(w|\zeta)$ contains the factor $(xz_1-w_a)(xz_1-w_a^{-1})$ for any $a\in A$, there is no pole at $w_a=(xz_1)^{\pm1}$ in the integrand of $\overline{G}_b^{(n)}(\zeta)^{-\tilde{\varepsilon}}$. When the RHS of (4.25) with $\varepsilon_1<0$ is analytically continued from ζ_1 to $x^{-2}\zeta_1$, the poles of the integrands

$$\cdots\cdots,\ x^{13}z_1^{\pm1},\ x^9z_1^{\pm1},\ x^5z_1^{\pm1},\ xz_1^{-1},\ x^{-1}z_1,\ x^{-5}z_1^{\pm1},\ x^{-9}z_1^{\pm1},\ x^{-13}z_1^{\pm1},\ \cdots\cdots,$$

move to the points

$$\cdots\cdots,\ x^{13}z_1^{\pm1},\ x^9z_1^{\pm1},\ x^5z_1^{\pm1},\ xz_1,\ x^{-1}z_1^{-1},\ x^{-5}z_1^{\pm1},\ x^{-9}z_1^{\pm1},\ x^{-13}z_1^{\pm1},\ \cdots\cdots.$$

Thus the integral contour C_a for any $a\in A$ is invariant even if we make the analytical continuation $\zeta_1\to x^{-2}\zeta_1$. Furthermore, by using (4.33), the desired equality follows from that of the integrands.

When $\varepsilon_1>0$ the LHS of (4.25) times $(x^{-2}z_1)^{2n-1}$ reduces to

$$\prod_{a\in A}\oint_{C_a}\frac{dw_a}{2\pi i w_a}\Psi_b^{(n)}(w|\zeta_1^{-1},\tilde{\zeta})Q_b^{(n)}(w|\zeta_1^{-1},\tilde{\zeta})\frac{1-x^2rz_1^{-1}}{1-x^{-2}rz_1}. \tag{A.3}$$

Concerning the RHS of (4.25), the integral contour C_a for $a \in A\backslash\{1\}$ is again invariant from the same reason as the previous case. As for the the integral with respect to w_1, we have to keep in mind that the integrand of $\overline{G}_b^{(n)}(\zeta)^{+\tilde{\varepsilon}}$ has a pole at $w_1 = xz_1$. Thus the RHS of (4.25) times $(x^{-2}z_1)^{2n-1}$ reduces to

$$\prod_{a\in A\backslash\{1\}} \oint_{C_a} \frac{dw_a}{2\pi i w_a} \left(\oint_{C_1} + 2\pi i \mathrm{Res}_{w_1=x^{-3}z_1} \right) \frac{dw_1}{2\pi i w_1} \Psi_b^{(n)}(w|\zeta_1^{-1},\tilde{\zeta}) Q_b^{(n)}(w|\zeta_1^{-1},\tilde{\zeta}) \frac{xz_1^{-1}-w_1}{x^{-3}z_1-w_1}. \quad (A.4)$$

Let us denote (A.3) by L and (A.4) by R, respectively. Furthermore, we will divide R into the sum of three parts as follows. In (A.4) we denote the integral part with respect to w_1 by R_1; and the residue part by $R_2 - R_3$, the difference of two contour integrals. For that purpose, we introduce the function

$$R(w) = \frac{x^{-3}z_1 - x^{-4}w_1^{-1}}{w_1 - x^{-4}w_1^{-1}} \frac{1-xrw_1}{1-x^{-2}rz_1},$$

as we have done in [7]. The integrand of (A.4) has poles at $w_1 = x^{-3}z_1, xz_1^{-1}, x^{-1}r^{-1}$ in the annulus between the closed lines C_1 and $x^{-4}C_1$. Here, the closed line $x^{-4}C_1$ denotes the one obtained from C_1 by similarity transformation with the ratio being x^{-4}. Since $R(x^{-3}z_1) = 1$ and $R(xz_1^{-1}) = R(x^{-1}r^{-1}) = 0$, the residue at $w_1 = x^{-3}z_1$ can be evaluated as follows:

$$\prod_{a\in A\backslash\{1\}} \oint_{C_a} \frac{dw_a}{2\pi i w_a} \left(\oint_{x^{-4}C_1} - \oint_{C_1} \right) \frac{dw_1}{2\pi i w_1} \Psi_b^{(n)}(w|\zeta_1^{-1},\tilde{\zeta}) Q_b^{(n)}(w|\zeta_1^{-1},\tilde{\zeta}) \frac{xz_1^{-1}-w_1}{x^{-3}z_1-w_1} R(w_1). \quad (A.5)$$

Let us denote the first and the second term of (A.5) by R_2 and $-R_3$, respectively. The function $R(w_1)$ has a pole at $w_1 = x^{-2}$, however, we notice that the integrand of (A.5) is regular at this point because of (A.1). The integral R_2 can be rewritten in terms of the integral along the contour C_1 by changing the integral variable $w_1 \mapsto x^{-4}w_1^{-1}$ as follows:

$$R_2 = \prod_{a\in A\backslash\{1\}} \oint_{C_a} \frac{dw_a}{2\pi i w_a} \oint_{C_1} \frac{dw_1}{2\pi i w_1} \Psi_b^{(n)}(w|\zeta_1^{-1},\tilde{\zeta}) Q_b^{(n)}(w|\zeta_1^{-1},\tilde{\zeta}) \frac{xz_1^{-1} - x^{-4}w_1^{-1}}{w_1 - x^{-4}w_1^{-1}} \frac{1-xrw_1}{1-x^{-2}rz_1}.$$

Thus we obtain

$$L - R_1 = R_2 - R_3 = \prod_{a\in A} \oint_{C_a} \frac{dw_a}{2\pi i w_a} \Psi_b^{(n)}(w|\zeta_1^{-1},\tilde{\zeta}) Q_b^{(n)}(w|\zeta_1^{-1},\tilde{\zeta}) \frac{x^{-3}z_1 - xz_1^{-1}}{x^{-3}z_1 - w_1} \frac{1-xrw_1}{1-x^{-2}rz_1},$$

which implies (4.25) with $\varepsilon_1 > 0$. Thus Proposition 2 was proved.

References

[1] Smirnov F A: *Form factors in completely integrable models of quantum field theory, Advanced Series in Mathematical Physics*, Vol 14, World Scientific, Singapore, 1992.

[2] Smirnov, F A: Dynamical symmetries of massive integrable models 1,2, in *Proceedings of the RIMS Research Project 1991, "Infinite Analysis"*; Int. J. Mod. Phys. **7A, Suppl. 1B** (1992) 813–837, 839–858.

[3] Frenkel I B and Reshetikhin N Y: Quantum affine algebras and holonomic difference equations, Commun. Math. Phys. **146** (1992) 1–60.

[4] Baxter R J: *Exactly Solved Models in Statistical Mechanics, Academic Press, London*, 1982.

[5] Jimbo M, Miwa T and Nakayashiki A: Difference equations for the correlation functions of the eight-vertex model, J. Phys. A: Math. Gen. **26** (1993) 2199–2209.

[6] Jimbo M, Kedem R, Konno K, Miwa T and Weston R: Difference equations in spin chains with a boundary, Nucl. Phys. **B448** [**FS**] (1995) 429–456.

[7] Jimbo M, Kojima T, Miwa T and Quano Y.-H: Smirnov's integral and quantum Knizhnik-Zamolodchikov equation of level 0, J. Phys. A: Math. Gen. **27** (1994) 3267–3283.

[8] Kojima T, Miki K and Quano Y.-H, Annihilation poles of a Smirnov-type integral formula for solutions to quantum Knizhnik–Zamolodchikov equation, *J. Phys. A: Math. Gen.* **28** (1995) 3479–3491.

[9] Quano Y.-H, Form factors of the XXZ model and quantum affine symmetry, *J. Phys. A: Math Gen.* **31** (1998) 1791–1800.

[10] Jimbo M and Miwa T: *Algebraic analysis of solvable lattice models, CBMS Regional Conferences Series in Mathematics*, Vol 85, AMS, Providence, RI, 1994.

[11] Jimbo M, Miki K, Miwa T and Nakayashiki A: Correlation functions of the XXZ model for $\Delta < -1$, *Phys. Lett. A*, **168** 256–263, 1992.

[12] Jimbo M, Kedem R, Kojima T, Konno H and Miwa T: XXZ chain with a boundary, Nucl. Phys. **B441** [**FS**] (1995) 437–470.

[13] Jimbo M and Miwa T: Quantum KZ equation with $|q| = 1$ and correlation functions of the XXZ model in the gapless regime, *J. Phys. A: Math. Gen.* **29** (1996) 2923–2958.

[14] Jimbo M, Konno H and Miwa T: Massless XXZ model and deformation of the elliptic algebra $\mathcal{A}_{Q,P}(\widehat{SL_2})$, in *Deformation Theory and Symplectic Geometry, Eds. Sternheimer D, Rawnsley J and Gutt S, Math. Phys. Studies, Kluwere* **20** pp117–138, 1997.

[15] Kojima T: The massless XXZ chain with a boundary, preprint, nlin.SI/0006026, 2000.

[16] Nakayashiki A, Pakuliak A, Tarasov V: On solutions of the KZ and qKZ equations at level zero, *Ann. Inst. Henri Poincaré*, **71** (1999) 459–496.

[17] Nakayashiki A: Trace construction of a basis for the solution space of sl_N qKZ equation, *Commun. Math. Phys.* **212** (2000) 29–61.

[18] Quano Y.-H: Spontaneous polarization of the $\mathbb{Z}_n$-Baxter model, *Mod. Phys. Lett.* **A8** (1993) 3363–3375.

[19] Quano Y.-H: Difference equations for correlation functions of Belavin's $\mathbb{Z}_n$-symmetric model with boundary reflection, *J. Phys. A: Math Gen.* **33** (2000) 8275–8303.

[20] Quano Y.-H: Difference equations for correlation functions of $A^{(1)}_{n-1}$-face model with boundary reflection, hep-th/0102100, 2001.

[21] Cherednik I V: Factorizing particles on a half-line and root systems, *Theor. Math. Phys.* **61** (1984) 977–983.

[22] Sklyanin E K: Boundary conditions for integrable quantum systems, J. Phys. A: Math. Gen. **21** (1988) 2375–2389.