XXZ chain with a boundary

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To the memory of Mr. Toyosaburo Taniguchi

Abstract

The XXZ spin chain with a boundary magnetic field $h$ is considered, using the vertex operator approach to diagonalize the Hamiltonian. We find explicit bosonic formulas for the two vacuum vectors with zero particle content. There are three distinct regions when $h \geq 0$, in which the structure of the vacuum states is different. Excited states are given by the action of vertex operators on the vacuum states. We derive the boundary $S$-matrix and present an integral formula for the correlation functions. The boundary magnetization exhibits boundary hysteresis. We also discuss the rational limit, the XXX model.

1 Introduction

In the standard treatment of quantum integrable systems, one starts with a finite size system and imposes periodic boundary conditions, in order to ensure the commutativity of the transfer matrix. Recently, there has been increasing interest in exploring other possible boundary conditions compatible with integrability.

For lattice models with non-periodic boundary conditions, the works on the Ising model are perhaps among the earliest (see McCoy-Wu [1, 2], Bariev [3]). One should also mention Gaudin’s work [4] concerning the Bose gas with a delta-function interaction and the XXZ model (see also [5]). A systematic approach to this problem was initiated by Sklyanin [6] in the framework of the algebraic Bethe ansatz. It is well known that, in the periodic case, one can construct a

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commuting family of transfer matrices from a solution $R(\zeta)$ of the Yang-Baxter equation (YBE). Sklyanin showed that a similar construction is possible with the aid of a solution $K(\zeta)$ to the boundary YBE (also known as the reflection equation)

$$K_2(\zeta_2) R_{21}(\zeta_1 \zeta_2) K_1(\zeta_1) R_{12}(\zeta_1 / \zeta_2) = R_{21}(\zeta_1 / \zeta_2) K_1(\zeta_1) R_{12}(\zeta_1 \zeta_2) K_2(\zeta_2).$$

(1.1)

Several groups have investigated the solutions of (1.1) along with the Bethe ansatz equations for the models associated with them [7,8,9,10,11,12,13]. For a recent review and further references, see [14].

The boundary YBE (1.1) was originally formulated by Cherednik [15], as a factorization condition for scattering at a boundary wall. In massive integrable field theories, Ghoshal and Zamolodchikov [16] discussed integrable massive deformations of conformal field theories in the presence of boundaries [17], and developed a bootstrap approach to them (see also [18,19,20] for related works).

One model treated by Sklyanin’s method is the XXZ spin chain with a boundary magnetic field:

$$H_{\text{bare}}^B = -\frac{1}{2} \sum_{k=1}^{\infty} \left( \sigma_{k+1}^x \sigma_k^x + \sigma_{k+1}^y \sigma_k^y + \Delta \sigma_{k+1}^z \sigma_k^z \right) + h \sigma_1^z. \quad (1.2)$$

Here, we consider the model in the limit of the semi-infinite chain, in the ferromagnetic regime, $\Delta \leq -1$. In this paper, we present an alternative approach to the solution of this model, applying the diagonalization scheme developed in [21,22] for the ‘bulk’ Hamiltonian

$$H_{\text{bare}} = -\frac{1}{2} \sum_{k=-\infty}^{\infty} \left( \sigma_{k+1}^x \sigma_k^x + \sigma_{k+1}^y \sigma_k^y + \Delta \sigma_{k+1}^z \sigma_k^z \right). \quad (1.3)$$

For a systematic account of this method, see [23].

The ground state energy of the bare Hamiltonian (1.2) is a divergent scalar, $c(\Delta, h)$, which we subtract. We subsequently consider the spectrum of the ‘renormalized Hamiltonian,’

$$H_B = H_{\text{bare}}^B - c(\Delta, h), \quad (1.4)$$

which has a ground state energy equal to 0.

The starting point in the bulk theory is to identify the space of eigenvectors of the Hamiltonian (1.4) ‘space of states’ with the tensor product $\mathcal{H} \otimes \mathcal{H}^*$, where $\mathcal{H} = \mathcal{H}^{(0)} \oplus \mathcal{H}^{(1)}$ is the direct sum of level one integrable modules of $U_q(\mathfrak{sl}_2)$, and $\mathcal{H}^*$ its dual. Here,

$$\Delta = \frac{q + q^{-1}}{2}, \quad (1.5)$$

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and $-1 < q < 0$.

In contrast, we relate the space of states of the boundary Hamiltonian (1.2) to the half space $\mathcal{H}$. Accordingly, we rewrite Sklyanin’s transfer matrix $T_B(\zeta)$, on the semi-infinite lattice, in terms of the type I vertex operators $\Phi_\varepsilon(\zeta)$ (see (2.13) below). The renormalized Hamiltonian (1.4) is defined as the derivative of $T_B(\zeta)$ at $\zeta = 1$.

It should be emphasized that, unlike in the bulk theory, the algebra $U_q(\widehat{sl}_2)$ does not commute with the boundary Hamiltonian (1.2), and hence is not a symmetry algebra of this model. Nevertheless, we will show that one can use $\mathcal{H}$ and $\Phi_\varepsilon(\zeta)$ to describe the space of states. A simple bosonization formula is available for the spaces $\mathcal{H}^{(i)}$ and the vertex operators [22,24]. Our basic result here is that, in the bosonization language, the vacuum vectors in each sector $\mathcal{H}^{(i)}$ have the remarkably simple form:

$$|i\rangle_B = e^{F_i} |i\rangle,$$

(1.6)

where $|i\rangle$ is the highest weight vector of $\mathcal{H}^{(i)}$, and $F_i$ is quadratic in the bosonic operators (see (3.4)). This fact allows us to compute the spectrum of (1.4), and the spin correlation functions. We subsequently find the following features.

In the presence of the boundary term, the Hamiltonian (1.2) lacks spin-reversal symmetry, and the two vacuum vectors, $|i\rangle_B$, carry different energies. This energy difference (see (2.28)) corresponds to the binding energy of the boundary bound state of [16].

Although the expression (1.6) makes sense in the bosonic Fock space, there is no a priori guarantee that $|i\rangle_B$ are well defined for all values of $h$. We surmise that they exist as long as they are regular at $q = 0$. According to this criterion, $|1\rangle_B$ exists if and only if $h < h_c^{(1)}$ or $h > h_c^{(2)}$, and $|0\rangle_B$ exists if and only if $h > -h_c^{(1)}$ or $h < -h_c^{(2)}$. Here, the critical fields are

$$h_c^{(1)} = \frac{(1 + q)^2}{-4q} = -\frac{\Delta + 1}{2}, \quad h_c^{(2)} = \frac{(1 - q)^2}{-4q} = -\frac{\Delta - 1}{2}.$$  

(1.7)

We will show, in Section 3, that our criterion for existence agrees with the singularity structure of the boundary $S$-matrix.

As in the bulk theory, excited states are created by action of type II vertex operators $\Psi_\mu^*(\xi)$ on $|i\rangle_B$. Using our expression for the vacuum states (1.6), we deduce that single-particle states obey the relations

$$\Psi_\mu^*(\xi)|i\rangle_B = M_{\mu}^{(i)\mu}(\xi) \Psi_\mu^*(\xi^{-1}) |i\rangle_B, \quad (\mu = \pm).$$

The matrix $M^{(i)}(\xi)$ is therefore the boundary $S$-matrix, analogous to that formulated in [16] for integrable field theories.
The bosonic expression for the vacuum vectors enables us to derive integral formulas for the spin correlation functions. The boundary magnetization is an especially simple case of these correlation functions (see (4.19)). For example,

$$\left. -\frac{B\langle 0\rvert \sigma^z_1 \rvert 0 \rangle_B}{B\langle 0\rvert 0 \rangle_B} \right|_{\theta_B} = 1 + 2 \sum_{i=1}^{\infty} \frac{(-q^2)^i (1-r)^2}{(1-q^{2i}r)^2},$$

where

$$h = \frac{1 - q^2 1 + r}{-4q 1 - r}.$$

The values of $h$ where both vacuum states $\rvert i \rangle_B$ coexist are those where boundary hysteresis, or wetting, occurs [1,2,25].

The text is organized as follows. In Section 2, we briefly review Sklyanin’s theory, and formulate the vertex operator approach to the boundary theory. We calculate the energy difference between the two vacuum vectors $\rvert i \rangle_B$. In Section 3, we find explicit expressions for these vectors, by using the bosonization formulas for vertex operators. We then calculate the boundary $S$-matrix. Section 4 is devoted to finding integral formulas for the spin correlation functions in general, and the boundary magnetization in particular. The rational limit, which corresponds to the XXX model, is discussed in Section 5. In Section 6 we discuss our results and note some open questions.

## 2 Eigenvalues of the transfer matrix

### 2.1 Sklyanin’s formulation

In this section we recall Sklyanin’s results in the context of the XXZ chain on the finite lattice,

$$H_{\text{fin}}^B = -\frac{1}{2} \sum_{k=1}^{N-1} \left( \sigma^x_{k+1} \sigma^x_k + \sigma^y_{k+1} \sigma^y_k + \Delta \sigma^z_{k+1} \sigma^z_k \right) + h_+ \sigma^z_1 + h_+ \sigma^z_N. \quad (2.1)$$

This will motivate our construction of the transfer matrix for the semi-infinite lattice below.

The transfer matrix is constructed as follows. Below, the reader is referred to Appendix A for notation. Let $R(\zeta)$ be the $R$-matrix [A.1] of the six–vertex model, where $\zeta$ is the multiplicative spectral parameter. We also specify a matrix $K(\zeta)$, corresponding to an interaction at the boundary, which satisfies the boundary YBE
Here, we consider only the diagonal solution
\[ K(\zeta) = K(\zeta; r) = \frac{1}{f(\zeta; r)} \begin{pmatrix} 1 - r \zeta^2 & 0 \\ \zeta^2 - r & 1 \end{pmatrix}. \] (2.2)

Nondiagonal solutions correspond to fields coupled to the other spin components.

The scalar \( f(\zeta; r) \) in (2.2) is
\[ f(\zeta; r) = \frac{\varphi(\zeta^2; r)}{\varphi(\zeta^2; r)}, \quad \varphi(z; r) = \frac{(q^4 rz; q^4)_\infty (q^2 z^2; q^8)_\infty}{(q^2rz; q^4)_\infty (q^8z^2; q^8)_\infty}, \] (2.3)
and is chosen so that the \( K \)-matrix obeys the relations
\[ K(\zeta)K(\zeta^{-1}) = 1, \quad \text{(Boundary unitarity)}, \] (2.4)
\[ K_a^b (-q^{-1}\zeta^{-1}) = \sum_{a', b'} R_{a' - b'} (-q\zeta^2) K_{a'}^b(\zeta), \quad \text{(Boundary crossing)}. \] (2.5)

These ensure that the transfer matrix (2.13) satisfies the unitarity and crossing relations (2.16), (2.17).

A commuting family of transfer matrices is constructed from \( R \) and \( K \) as follows [6]:
\[ T_B^{\text{fin}}(\zeta) = \text{tr} V_0 \left( K_+ (\zeta) T(\zeta^{-1})^{-1} K_- (\zeta) T(\zeta) \right). \] (2.6)

Here
\[ T(\zeta) = R_{01}(\zeta) \cdots R_{0N}(\zeta) \in \text{End} \left( V_0 \otimes V_1 \otimes \cdots \otimes V_N \right) \]
denotes the monodromy matrix, \( V_j \) are copies of \( C^2 \), and
\[ K_-(\zeta) = K(\zeta; r_-), \quad K_+(\zeta) = K(-q^{-1}\zeta^{-1}; r_+)^t \in \text{End} \left( V_0 \right), \]
where \( r_{\pm} \) are arbitrary parameters. Graphically, the transfer matrix (2.6) is represented in Figure 1.

With these definitions, the following statements hold [6]:

1. The transfer matrices (2.6) form a commutative family:
\[ [T_B^{\text{fin}}(\zeta), T_B^{\text{fin}}(\zeta')] = 0 \quad \forall \zeta, \zeta'. \]

2. The Hamiltonian (2.1) is obtained as
\[ \left. \frac{d}{d\zeta} T_B^{\text{fin}}(\zeta) \right|_{\zeta=1} = \frac{4q}{1 - q^2} H_B^{\text{fin}} + \text{const}. \] (2.7)
where $\Delta$ is defined by (1.5) and
\[
h_\pm = \mp \frac{1 - q^2}{4q} \frac{1 + r_\pm}{1 - r_\pm}.
\] (2.8)

In [6], an algebraic Bethe ansatz is constructed for the eigenvectors of the transfer matrix (2.6). The Bethe ansatz equations for (2.1) were previously derived in [4,5] using the coordinate Bethe ansatz.

2.2 The semi-infinite spin chain

We now consider the $XXZ$ Hamiltonian in the limit of the semi-infinite chain, (1.4), with $h = h_-$ and $r = r_-$. Since, under conjugation of $H_B$ by the spin-reversal operator $\prod \sigma_j^x$, the sign of the boundary term is reversed, we can restrict our discussion to $h \geq 0$, or

$$-1 \leq r \leq 1.$$  

The free boundary condition, $h = 0$, is $r = -1$, whereas the fixed boundary condition, $h = \infty$, is $r = 1$. When $r = 0$ (or $r = \infty$), the Hamiltonian (1.2) formally enjoys $U_q(sl_2)$–invariance [26].

The transfer matrix $T_B(\zeta)$ corresponding to the limit of (1.2) is depicted in Figure 2. It describes a semi-infinite two dimensional lattice, with alternating spectral parameters.

In the naive tensor product space $\cdots \otimes V \otimes V \otimes V$, the eigenstates of $H_B$ which have finite eigenvalues span a subspace $\mathcal{H}$, which we call the space of states. Much insight about this space can be gained by examining the extreme anisotropic limit, $q \to 0$. In this limit, the Hamiltonian $-2qH_B$ scales to

$$H_{B,0} = \frac{1}{2} \sum_{k=1}^{\infty} (\sigma_{k+1}^z \sigma_k^z + 1) + \frac{1 + r}{2(1 - r)} \sigma_1^z,$$

where a scalar term has been added to ensure that the lowest eigenvalue of $H_{B,0}$ is 0.

When $r = -1$, $H_{B,0}$ has two antiferromagnetic ground states, $|p^{(i)}\rangle$,

$$|p^{(0)}\rangle = \cdots \otimes \nu_+ \otimes \nu_- \otimes \nu_+ \otimes \nu_- \quad |p^{(1)}\rangle = \cdots \otimes \nu_- \otimes \nu_+ \otimes \nu_- \otimes \nu_+.$$ (2.10)

Accordingly, $\mathcal{H}$ splits into two subsectors, $\mathcal{H}^{(0)}$ and $\mathcal{H}^{(1)}$, where $\mathcal{H}^{(i)}$ is the span of vectors $|p\rangle = \otimes_{k=1}^{\infty} v_{p(k)}$, called paths, labeled by maps $p: \mathbb{Z}_{\geq 1} \to \{\pm\}$ satisfying the asymptotic boundary condition

$$p(k) = (-1)^{k+i} \text{ for } k \gg 1.$$ (2.11)
When \( r \neq -1 \), the eigenvalues of \( H_{B,0} \) corresponding to \( |p^{(0)}\rangle \) and \( |p^{(1)}\rangle \) differ:

\[
H_{B,0}|p^{(0)}\rangle = -\frac{1 + r}{2(1 - r)}|p^{(0)}\rangle, \quad H_{B,0}|p^{(1)}\rangle = \frac{1 + r}{2(1 - r)}|p^{(1)}\rangle.
\]

Therefore, \( |p^{(1)}\rangle \) is no longer a ground state.

The splitting into two sectors \( \mathcal{H}^{(i)} (i = 0, 1) \) described above persists for general values of \( r \), and \(-1 < q < 0 \). For \( q \neq 0 \), an eigenvector of \( H_B \) is an “infinite linear combination” of the paths with one of the boundary conditions (2.11), with \( i = 0, 1 \). Near \( r = -1 \), each sector contains a state \( |i\rangle_B \), unique up to a scalar multiple, which has the lowest energy in that sector. We call \( |i\rangle_B \) the vacuum vectors, and extend the definition to all values of \( r \) by analytic continuation. We remark that these analytic continuations are not necessarily physical states for all values of the parameters \( r, q \).

### 2.3 Vertex operators

In order to diagonalize (1.4) for general values of \( q \), with \(-1 < q < 0 \), we follow the strategy proposed in [21]. Figure 2 suggests (see chapter 4 of [23]) that we identify \( \mathcal{H}^{(i)} \) with the integrable highest weight module \( V(\Lambda_i) \) of \( U_q(\hat{sl}_2) \), \( i = 0, 1 \), and the horizontal lines with the components \( \Phi^{(1-i,i)}(\zeta) \) of the vertex operator of type I:

\[
\Phi^{(1-i,i)}(\zeta) : \mathcal{H}^{(1-i)} \to \mathcal{H}^{(1-i)} \otimes V, \quad \Phi^{(1-i,i)}(\zeta) = \sum_\varepsilon \Phi^{(1-i,i)}_{\varepsilon}(\zeta) \otimes v_\varepsilon. \tag{2.12}
\]

In the present case, the algebra \( U_q(\hat{sl}_2) \) does not play the role of a symmetry algebra, as it does not commute with the Hamiltonian. Accordingly we shall treat \( \mathcal{H}^{(i)} \) and \( \Phi^{(1-i,i)}_{\varepsilon}(\zeta) \) simply as objects which enjoy the properties summarized in Appendix A, and disregard their representation theoretical meaning.

The point of using the vertex operators is that they are well defined objects, free from the difficulty of divergence. We define the ‘renormalized’ transfer matrix

\[
T^{(i)}_B(\zeta) = g \sum_{\varepsilon, \varepsilon'} \Phi^{(i,1-i),(1-i)}_{\varepsilon}(\zeta^{-1}) K_{\varepsilon'}(\zeta) \Phi^{(1-i,i)}_{\varepsilon'}(\zeta), \tag{2.13}
\]

(cf. (2.6)). Here,

\[
\Phi^{(i,1-i)}(\zeta) = \Phi^{(i,1-i)}_{(-1)}(q^{-1} \zeta), \quad g = \frac{(q^2; q^4)_\infty}{(q^4; q^4)_\infty}.
\]
Henceforth we shall suppress the label \(i\) for the sectors when there is no fear of confusion. The renormalized Hamiltonian \(H_B\) is then defined through the formula (cf. (2.7))

\[
\frac{d}{d\zeta} T_B(\zeta) \bigg|_{\zeta=1} = \frac{4q}{1-q^2} H_B .
\]

(2.14)

Using the commutation relations of type I vertex operators (A.6), along with the invertibility (A.10), one can show the following properties of the transfer matrix (2.13):

\[
[T_B(\zeta), T_B(\zeta')] = 0 \quad (\forall \zeta, \zeta'),
\]

(2.15)

\[
T_B(1) = \text{id}, \quad T_B(\zeta)T_B(\zeta^{-1}) = \text{id},
\]

(2.16)

\[
T_B(-q^{-1}\zeta^{-1}) = T_B(\zeta).
\]

(2.17)

These relations reduce, respectively, to the boundary YBE (1.1), and the boundary unitarity and crossing relations (2.4), (2.5) for the \(K\)-matrix.

### 2.4 Energy levels

Consider now the eigenvalues of the transfer matrix,

\[
T_B(\zeta)|v\rangle = t(\zeta) |v\rangle ,
\]

(2.18)

where \(|v\rangle\) is some eigenvector of the transfer matrix. The relations (2.15)–(2.17) imply

\[
t(1) = 1, \quad t(\zeta)t(\zeta^{-1}) = 1, \quad t(-q^{-1}\zeta^{-1}) = t(\zeta).
\]

(2.19)

Multiplying \(\Phi_\varepsilon(\zeta^{-1})\) to (2.18) from the left, and using the inversion relation (A.10) and the definition of the transfer matrix (2.13), we see that the eigenvalue problem (2.18) is equivalent to

\[
\sum_{\varepsilon'} K^{\varepsilon'}_\varepsilon(\zeta) \Phi_\varepsilon'(\zeta)|v\rangle = t(\zeta) \Phi_\varepsilon(\zeta^{-1})|v\rangle , \quad (\varepsilon = \pm) .
\]

(2.20)

Consider the region of the parameters where

\[
1 < \zeta < 1 + \varepsilon, \quad -\varepsilon < q < 0, \quad -1 < r < -1 + \varepsilon,
\]

(2.21)

where \(\varepsilon > 0\) is sufficiently small. Since \(\zeta > 1\), the lowest eigenvalue of the Hamiltonian \(H_B\) corresponds to the largest eigenvalue of the transfer matrix \(T_B(\zeta)\) (see (2.14), and note that \(q < 0\)). In view of the study of \(H_{B,0}\) in Section 2.2, we assume that 1) the largest eigenvalue of \(T_B^{(i)}(\zeta)\) has multiplicity one, and 2) the corresponding eigenvector has an expansion at \(q = 0\), starting from \(|p^{(i)}\rangle\).
Let $\Lambda^{(i)}(\zeta)$ denote the eigenvalue corresponding to the vacuum vectors $|i\rangle_B$ of Section 2.2. Then in the region (2.21), $\Lambda^{(0)}(\zeta) > \Lambda^{(1)}(\zeta)$, and $\Lambda^{(0)}(\zeta)$ is the largest eigenvalue within $\mathcal{H}^{(0)}$. These statements are not necessarily true throughout the region

$$1 < \zeta, \quad -1 < q < 0, \quad -1 < r < 1.$$  

(2.22)

We infer that

$$\Lambda^{(0)}(\zeta) = 1.$$  

(2.23)

The reason is as follows. In the region (2.21), this is the largest eigenvalue of the transfer matrix. We assume $\Lambda^{(0)}(\zeta)$ is analytic when $1 \leq |\zeta^2| \leq |q^{-1}|$. Then the solution to (2.19) is unique, and it is (2.23).

As supporting evidence, we use (2.23) to construct $|0\rangle_B$ in Section 3. We then use the result to calculate, in Appendix B, the $q$-expansion of $|0\rangle_B$ for $r = -1$, up to the order $q^3$. We find that this agrees with the $q$-expansion of the unique eigenvector of $H_B$ of the form $|p(0)\rangle + O(q)$, as required in Section 2.3. Therefore we conclude that (2.23) is the correct lowest eigenvalue.

Next we determine $\Lambda^{(1)}(\zeta)$. Set

$$\Lambda(\zeta; r) = \frac{K^+_\zeta(\zeta; r)}{K^-_{\zeta}(\zeta; r^{-1})} = \frac{1}{\zeta^2} \frac{\Theta_{q^4}(r\zeta^2)}{\Theta_{q^4}(q^2r\zeta^{-2})} \frac{\Theta_{q^4}(q^2r\zeta^2)}{\Theta_{q^4}(q^2r\zeta^{-2})},$$  

(2.24)

where $\Theta_p(z)$ is given in (A.9). We now show that

$$\Lambda^{(1)}(\zeta; r) = \Lambda(\zeta; r).$$  

(2.25)

We exploit the spin-reversal symmetry to reduce the calculation of $|1\rangle_B$ to that of $|0\rangle_B$. Let $\nu : \mathcal{H}^{(0)} \to \mathcal{H}^{(1)}$ be the vector space isomorphism corresponding to the Dynkin diagram symmetry (see [23]). Then

$$\nu \Phi^{(0,1)}(\zeta) \nu = \Phi^{(1,0)}_{-\zeta}(\zeta).$$  

(2.26)

Noting the relation

$$\sigma^x K(\zeta; r) \sigma^x = \Lambda(\zeta; r) K(\zeta; r^{-1}),$$

we find that

$$\nu^{-1} T_B^{(1)}(\zeta; r) \nu = \Lambda(\zeta; r) T_B^{(0)}(\zeta; r^{-1}).$$  

(2.27)

If $r$ is close to $-1$, the eigenvalue $1$ of $T_B^{(0)}(\zeta; r^{-1})$ is the largest. Hence the largest eigenvalue of $T_B^{(1)}(\zeta; r)$ is given by (2.25).
Now, let us compare the two energy levels $e^{(0)}(r)$ and $e^{(1)}(r)$ of $H_B$, corresponding to $|0\rangle_B$ and $|1\rangle_B$, respectively. Parameterize $r$ as

$$ r = \begin{cases} -(q^2)^\alpha & \text{if } -1 < r < 0; \\ (q^2)^\alpha & \text{if } 0 < r < 1, \end{cases} $$

where $\alpha$ is real and positive. From (2.23) and (2.14), we have clearly $e^{(0)}(r) = 0$. Hence the energy difference is simply

$$ \Delta e(r) = e^{(1)}(r) - e^{(0)}(r) = e^{(1)}(r). $$

From (2.24) and (2.14), we find

$$ \Delta e(r) = \begin{cases} \frac{\epsilon(1)\text{sn}(2K'\alpha,k')}{} & \text{if } -1 \leq r < 0; \\ \frac{\epsilon(1)}{} & \text{if } 0 < r < 1, \end{cases} $$

(2.28)

where the Jacobi elliptic functions refer to the nome $-q = e^{-\pi K'/K}$ (see 7.5 in [23]), and

$$ \epsilon(\xi) = \frac{2K}{\pi} \text{sh} \frac{\pi K'}{K} \text{dn} \left( \frac{2K}{\pi} \theta, k \right), \quad \xi = -ie^{i\theta}, $$

(2.29)

$$ \epsilon(1) = \frac{2Kk'}{\pi} \text{sh} \frac{\pi K'}{K}. $$

(2.30)

In Figure 3 the energy difference $\Delta e(r)$ is plotted as a function of $h$. The energy increases monotonically from 0 to $\epsilon(1)$ (which is the mass gap, see below) when $0 \leq h < h_c^{(1)}$, and from $\epsilon(1)/k'$ to $\infty$ when $h_c^{(2)} < h \leq \infty$. In the latter region, the energy of $|1\rangle_B$ is greater than the mass gap. The possible existence of such a situation, where the boundary bound state energy is greater than the single particle energy, was mentioned in [16], although it does not occur in the Ising model. When $h_c^{(1)} < h < h_c^{(2)}$, the state $|1\rangle_B$ is well defined, as we shall argue in Section 3.1.

In the next section we shall find the vacuum vectors $|0\rangle_B$ and $|1\rangle_B$ explicitly by using the bosonization formulas for the vertex operators. Once the vacuum vectors are found, it is possible to create the excited states by application of the vertex operators of type $\Pi$, $\Psi^*_\mu(\xi) (\mu = \pm)$, in much the same way as in the bulk theory (see [23]). The commutation relations (A.8) imply that

$$ \Psi^*_\mu(\xi_1) \cdots \Psi^*_\mu(\xi_m)|i\rangle_B$$
is an eigenstate of $T_B(\zeta)$ with eigenvalue $\Lambda^{(i)}(\zeta) \times \prod_{j=1}^{m} \tau_B(\zeta, \xi_j)$, where

$$
\tau_B(\zeta, \xi) = \tau(\zeta/\xi)\tau(\zeta\xi) \quad \text{(2.31)}
$$

and $\tau(\zeta)$ is given in (A.9). The single particle energy is therefore given by $e^{(i)}(r) + \epsilon(\xi)$, with its minimum value being $e^{(i)}(r) + \epsilon(1)$. Therefore the mass gap is $\epsilon(1)$.

3 Vacuum vectors and the boundary S-matrix

3.1 Vacuum vectors

The perturbative calculation of Appendix B suggests that the vacuum vector $|i\rangle_B$ is uniquely determined by the relation

$$
T_B^{(i)}(\zeta)|i\rangle_B = \Lambda^{(i)}(\zeta)|i\rangle_B. \quad \text{(3.1)}
$$

In this section we invoke the bosonization method to find the explicit formulas for them, assuming uniqueness.

First consider the case $|0\rangle_B$. Since the total spin is conserved, it should be a (possibly infinite) linear combination of the states created by the oscillators $a_{-n}$ ($n > 0$) over the highest weight vector $|0\rangle$. We make the ansatz that it has the form (2.20), with

$$
|0\rangle_B = e^{F_0}|0\rangle, \quad F_0 = \frac{1}{2} \sum_{n=1}^{\infty} \frac{n \alpha_n}{[2n][n]} a_{-n}^2 + \sum_{n=1}^{\infty} \beta_n^{(0)} a_{-n}.
$$

Note that the coefficients $\alpha_n, \beta_n^{(0)}$ cannot depend on $\zeta$ due to the commutativity of the transfer matrices. Using the bosonization formula (A.13), equation (2.20), with $t(\zeta) = \Lambda^{(0)}(\zeta) = 1$ and $\epsilon = -$, becomes

$$
\varphi(z;r)e^{P(z)}e^{Q(z)}e^{F_0}|0\rangle = (z \leftrightarrow z^{-1}).
$$

The presence of $e^{F_0}$ has the effect of a Bogoliubov transformation

$$
e^{-F_0}a_n e^{F_0} = a_n + \alpha_n a_{-n} + \frac{[2n][n]}{n} \beta_n^{(0)}, \quad e^{-F_0}a_{-n} e^{F_0} = a_{-n}. \quad \text{(3.2)}
$$

By a straightforward calculation, the coefficients $\alpha_n$ and $\beta_n^{(0)}$ are found to be

$$
\alpha_n = -q^{\delta_n}, \quad \beta_n^{(0)} = -\frac{q^{\delta_n/2}r^n}{[2n]} - \theta_n \frac{q^{\delta_n/2}(1 - q^n)}{[2n]},
$$

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where

\[ \theta_n = \begin{cases} 1 & \text{if } n \text{ is even;} \\ 0 & \text{if } n \text{ is odd.} \end{cases} \]

We must verify that the state \(|0\>_B\) found in this manner satisfies also the relation (2.20) with \(\varepsilon = +\). Using

\[ e^{Q(z)}|0\>_B = \varphi(z^{-1}; r)e^{P(z^{-1})}|0\>_B, \]
\[ e^{S^{-}(w)}|0\>_B = (1 - q^6 w^{-2})(1 - q^4 r w^{-1})e^{R^{-}(q^6 w^{-1})}|0\>_B, \]

the verification is reduced to showing that

\[ \oint \frac{dw}{2\pi i w} (1 - rz)(w^2 - q^6)(w - q r^6) e^{R^{-}(w)+R^{-}(q^6 w^{-1})}|0\>_B = (z \leftrightarrow z^{-1}). \]

Here the contour encircles \(w = 0, q^4 z^\pm 1\) but not \(q^2 z^\pm 1\). The desired equality can be shown by the change of variable \(w \rightarrow q^6 w^4\).

Similar calculations give the other vacuum vector \(|1\>_B\), as well as the vacuum vectors in the dual space, \(\mathcal{H}^*(i)\), defined by

\[ B\langle i|T_B(\zeta) = \Lambda^*(i)|\zeta\rangle B\langle i|. \]

The analog of (2.20) is

\[ \sum_{\varepsilon} B\langle i|\Phi^*_\varepsilon(\zeta^{-1})K^\varepsilon(\zeta) = \Lambda^*(i)|\zeta\rangle B\langle i|\Phi^*_\varepsilon(\zeta), \quad (\varepsilon' = \pm). \quad (3.3) \]

The results are summarized as follows:

\[ |i\rangle_B = e^{F_i}|i\rangle, \quad F_i = \frac{1}{2} \sum_{n=1}^{\infty} \frac{n\alpha_n}{[2n][n]} a_{2n} + \sum_{n=1}^{\infty} \beta_n^{(i)} a_{-n}, \quad (3.4) \]
\[ B\langle i| = \langle i|e^{G_i}, \quad G_i = \frac{1}{2} \sum_{n=1}^{\infty} \frac{n\gamma_n}{[2n][n]} a_{2n} + \sum_{n=1}^{\infty} \delta_n^{(i)} a_{-n}, \quad (3.5) \]

where

\[ \alpha_n = -q^{6n}, \quad \gamma_n = -q^{-2n}, \quad (3.6) \]
\[ \beta_n^{(i)} = -\theta_n q^{5n/2} (1 - q^n) + \begin{cases} -q^{7n/2} & (i = 0) \\ q^{3n/2} & (i = 1) \end{cases}, \quad (3.7) \]
\[ \delta_n^{(i)} = \theta_n q^{-3n/2} (1 - q^n) + \begin{cases} -q^{5n/2} & (i = 0) \\ q^{-n/2} & (i = 1) \end{cases}, \quad (3.8) \]
The relation (2.27) suggests that the two vacuum vectors should be related by
\[ \nu (|0\rangle_B) |_{r \to r^{-1}} = |1\rangle_B. \] (3.9)

However, since the spin-reversal symmetry is obscured in the bosonization, we do not know how to verify this directly from the explicit formulas (3.4).

**Remark.** It is useful to generalize (2.13) slightly and consider
\[ T_B^{(i)} (\zeta; t) = g \sum_{\varepsilon, \varepsilon'} \Phi^{(i, \varepsilon)} (t\zeta^{-1}) K_{\varepsilon'} (\zeta) \Phi^{(1, \varepsilon')} (t\zeta), \] (3.10)

which corresponds to changing the spectral parameters for the vertical lines from 1 to \( t \). The properties (2.15)–(2.17) are unaffected by this change. The vacuum vectors for (3.10) are obtained by replacing
\[ a_n \to t^{-2n} a_n, \quad a_{-n} \to t^{2n} a_{-n} \quad (n > 0) \]
in (3.4), (3.5). Doing so and specializing \( r = \zeta^{-2} \) (\( i = 0 \)) or \( r = \zeta^2 \) (\( i = 1 \)) we can drop one of the terms in (3.10), to obtain
\[
\begin{align*}
B(0| \Phi^{(i)} (t\zeta^{-1}) \phi (t\zeta) = \lambda (z) B(0|, & \quad \Phi^{(i)} (t\zeta^{-1}) \phi (t\zeta) |0\rangle_B = \lambda (z) |0\rangle_B, \\
B(1| \Phi^{(i)} (t\zeta^{-1}) \phi (t\zeta) = \lambda (z) B(1|, & \quad \Phi^{(i)} (t\zeta^{-1}) \phi (t\zeta) |1\rangle_B = \lambda (z) |1\rangle_B,
\end{align*}
\]
with
\[ \lambda (z) = \frac{(q^8 z^2 q^8)_{\infty} (q^4 z^{-2} q^8)_{\infty}}{(q^8 z^2 q^8)_{\infty} (q^4 z^{-2} q^8)_{\infty}}. \]

These formulas play a role in determining the asymptotic behavior of the iteration of the vertex operators, conjectured in [21] and proved recently in [27].

Next, consider the small \( q \) expansion of the vectors \( |i\rangle_B \) (\( i = 0, 1 \)). As stated in Section 1, we examine whether they exist or not in the sense they are regular at \( q = 0 \). Here, we say a vector is regular if it belongs to the upper crystal lattice of Kashiwara (see (B.6)).

The expression (3.4) for \( |i\rangle_B \) is not suitable for this purpose, since we do not know a simple criterion as to whether a vector expressed in terms of bosons belongs to the crystal lattice. In Appendix B, we rewrite \( |0\rangle_B \) in terms of the global base vectors. Although we have no proof to all orders, the expansion suggests that \( |0\rangle_B \) is well defined when \( h \geq 0 \), but not when \( |r| \geq 1/|q| \), i.e., \(-h_c^{(2)} \leq h \leq -h_c^{(1)} \). The expansion of \( |1\rangle_B \) is obtained by the replacement of \( r \) to \( r^{-1} \) in (B.6). Thus, we observe three regions for \( h \geq 0 \):

(i) \( 0 \leq h < h_c^{(1)} \): Both \( |0\rangle_B \) and \( |1\rangle_B \) are well defined;
(ii) \( h_c^{(1)} \leq h \leq h_c^{(2)} \): \( |0\rangle_B \) is well defined, but \( |1\rangle_B \) is not well defined;
(iii) \( h_c^{(2)} < h \leq \infty \): Both \( |0\rangle_B \) and \( |1\rangle_B \) are again well defined.
3.2 Boundary $S$-matrix

The two particle $S$-matrix is unchanged from the bulk theory:

$$\Psi_{\mu_1}^*(\xi_1)\Psi_{\mu_2}^*(\xi_2)|i\rangle_B = \sum_{\mu_1',\mu_2'} S_{\mu_1\mu_2}^{\mu_1'\mu_2'}(\xi_1/\xi_2) \Psi_{\mu_2'}^*(\xi_2) \Psi_{\mu_1'}^*(\xi_1)|i\rangle_B,$$

$$S(\xi) = -R(\xi)^{t_1t_2} = -R(\xi).$$

The formula (2.31) shows that the eigenvalues corresponding to the states $\Psi_\mu(\xi)|i\rangle_B$ and $\Psi_\mu(\xi^{-1})|i\rangle_B$ are equal. In fact, these states are proportional to each other. Using the bosonic expressions for the states $B|\xi\rangle$ and $\Psi_\mu(\xi^{-1})|i\rangle_B$, we find

$$\Psi_\mu(\xi)|i\rangle_B = M_\mu^{(i)}(\xi)|\Psi_\mu(\xi^{-1})\rangle_B,$$

$$B|\xi\rangle = B|\Psi_\mu(\xi^{-1})\rangle M_\mu^{(i)}(\xi).$$

We therefore interpret $M_\mu^{(i)}(\xi)$ as the boundary $S$-matrix. It is computed as in the previous subsection, where we now use (A.15) and (A.16). We find

$$M_\mu^{(0)}(\xi) = M_\mu^{(1)}(\xi; r), \quad M_\mu^{(1)}(\xi) = M_\mu^{-1}(\xi; r^{-1}),$$

where

$$M(\xi; r) = \frac{1}{f(\xi; r)} \begin{pmatrix} 1 - rq^{-1}\xi^2 & 0 \\ \xi^2 - rq^{-1} & 1 \end{pmatrix}$$

and

$$f(\xi; r) = -\xi^2 \frac{\varphi(\xi^{-2}; r)}{\varphi(\xi; r)}, \quad \varphi(z; r) = \frac{(q^2z; q^4)_\infty (q^2z^2; q^8)_\infty (qrz; q^4)_\infty (q^2r; q^8)_\infty}{(qr; q^4)_\infty (q^2r; q^8)_\infty}. $$

Notice that, up to a scalar factor, the $M$-matrix is of the same form as the $K$-matrix (2.2), except for the shift $r \rightarrow rq^{-1}$. The $M$-matrix has properties similar to those of the $K$-matrix:

$$M_2(\xi_2) S_{12}(\xi_2\xi_1) M_1(\xi_1) S_{21}(\xi_1/\xi_2) = S_{12}(\xi_1/\xi_2) M_1(\xi_1) S_{21}(\xi_1\xi_2) M_2(\xi_2),$$

$$M(\xi) M(\xi^{-1}) = 1,$$

$$M^b_a(-q^{-1}\xi^{-1}) = \sum_{a',b'} S_{a'b}^{b'a}(-q\xi^2) M_{a'}^b(\xi).$$

These formulas can be obtained either directly, or by using (3.11), (3.12). For instance, the last relation follows if we multiply (3.11) by $\Psi_\nu(\xi')$ from the left and take the residue at $\xi' = \xi$ using the property (A.12).
In [16], similar equations to (3.15) were proposed, as the bootstrap conditions for boundary field theories. Here, these equations are derived, in the context of the lattice model.

We now consider the analyticity properties of the boundary S-matrix, whose singularity structure determines the existence of the boundary bound states. First, recall the discussion of the Ising model (in the continuum limit) in [16]. The boundary S-matrix is given by

$$R_h(\theta) = i \tanh(\frac{\pi i}{4} - \frac{\theta}{2}) \kappa - i \sinh \theta \kappa + i \sinh \theta$$

(3.16)

where $\theta$ is the rapidity of the particle with mass $m$, and $\kappa = 1 - h^2/2m$, $h$ being the boundary magnetic field. The result is as follows: If $0 \leq h < \sqrt{2m}$, the pole of $R_h(\theta)$ at $\theta = \frac{\pi i}{2} - iv$, where $\kappa = \cos v$, stays in the physical strip, $0 < \text{Im} \theta \leq \pi$.

When $h \geq \sqrt{2m}$, the pole moves away from the physical strip.

In our case, the pole at $\xi^2 = rq^{-1}$ is in the physical strip, $1 < |\xi^2| \leq |q|^{-2}$, when $-1 \leq r < q$ ($0 \leq h < h^{(1)}_c$), but also when $-q < r \leq 1$ ($h^{(2)}_c < h \leq \infty$). Here, we considered only the region $-1 \leq r \leq 1$ ($h \geq 0$). These two regions are the regions (i) and (iii) discussed in Section 3.1.

We recognize that $|1\rangle_B$ is the bound state corresponding to the above mentioned pole, by using the bosonic expressions for the vacuum and single-particle vectors. The single-particle state $\Psi^+_+(\xi)|0\rangle_B$ has a series of simple poles at

$$\xi^2 = q^{-1}r; \, q^{-1}r^{-1}, \, q^{-5}r^{-1}, \, \cdots; \, q^3r, \, q^7r, \, \cdots.$$

By explicit computation, we find that the state $|1\rangle_B$ can be obtained as the residue at the first pole:

$$\text{Res}_{\xi^2=q^{-1}r} \left( B(0|\Psi^+_+(\xi^{-1}) \frac{d\xi^2}{\xi^2} \right) = g \, c(r^{-1}) \, B(1|, \quad (3.17)$$

$$\text{Res}_{\xi^2=q^{-1}r} \left( \Psi^+_+(\xi)|0\rangle_B \frac{d\xi^2}{\xi^2} \right) = g \, c(r^{-1}) \, |1\rangle_B, \quad (3.18)$$

where $c(z) = (q^2z^2;q^8)_\infty/(q^4z^2;q^8)_\infty$. The equations (3.17), (3.18) are also valid if we replace $B(0|\Psi^+_+(\xi^{-1}) \rightarrow B(1|\Psi^-_-(\xi^{-1})$, $\Psi^+_+(\xi)|0\rangle_B \rightarrow \Psi^+_-(\xi)|1\rangle_B$ and $r \rightarrow r^{-1}$.

The formulas above allow us to interpret $|i\rangle_B$ as the ‘boundary bound states’ in the regions (i), (iii) mentioned above.
4 Correlation functions

4.1 $N$-point function

In this section we calculate the vacuum expectation values of products of type I vertex operators, and obtain them as integrals of meromorphic functions involving infinite products. Upon specialization of the spectral parameters, they give multi-point correlation functions of the local spin operators of the XXZ chain with a boundary interaction.

We will consider the following $N$-point function with $N$ even:

$$P^{(i)}_{\varepsilon_1, \ldots, \varepsilon_N}(\zeta_1, \ldots, \zeta_N) = \frac{B\langle i | \Phi^{(i,1-i)}(\zeta_1) \Phi^{(1-i,i)}(\zeta_2) \cdots \Phi^{(1-i,i)}(\zeta_N) | i \rangle_B}{B\langle i | i \rangle_B}.$$  \hspace{1cm} (4.1)

Fixing $\{\varepsilon_1, \ldots, \varepsilon_N\}$, let us denote by $A$ the index set

$$A = \{ j \mid 1 \leq j \leq N, \varepsilon_j = +1 \}.$$

Since the total spin is conserved, (4.1) is non-trivial only if $\sum_{j=1}^{N} \varepsilon_j = 0$, in which case $A$ has $N/2$ elements.

We remark that, as a consequence of the relation of the two vacuum vectors (3.9) and the one for the vertex operators (2.26), one obtains

$$P^{(1)}_{\varepsilon_1, \ldots, \varepsilon_N}(\zeta_1, \ldots, \zeta_N) = P^{(0)}_{-\varepsilon_1, \ldots, -\varepsilon_N}(\zeta_1, \ldots, \zeta_N) \big|_{r \rightarrow r-1}.$$  \hspace{1cm} (4.2)

In order to evaluate the expectation values (4.1) we invoke the bosonization formulas (A.13), (A.14), (A.18), (A.19). By normal-ordering the product of vertex operators, we have

$$P^{(i)}_{\varepsilon_1, \ldots, \varepsilon_N}(\zeta_1, \ldots, \zeta_N) = \left( -q^3 \right)^{N^2/4 + \frac{N^2}{2} - \sum_{a \in A} a} \prod_{j=1}^{N} \zeta_j^{1+\varepsilon_j-j+N+1} \prod_{j<k} (q^2 z_k/z_j;q^4)_\infty \prod_{a \in A} \frac{dw_a}{2\pi\sqrt{-1}} \prod_{a<b} \left( w_a - w_b \right) \prod_{a \leq j} \left( z_j - q^{-2} w_a \right) \prod_{a \leq j} \left( w_a - q^4 z_j \right) \times I^{(i)}(\{z_j\}, \{w_a\}),$$  \hspace{1cm} (4.3)

where each contour $C_a$ is the same one defined in (A.14) as $C_1$. Here, $z_j = \zeta_j^2$ and

$$I^{(i)}(\{z_j\}, \{w_a\}) = \frac{B\langle i | \exp \left( \sum_{n=1}^{\infty} a_{n,n} X_n \right) \exp \left( -\sum_{n=1}^{\infty} a_{n,n} Y_n \right) | i \rangle_B}{B\langle i | i \rangle_B},$$
\[ X_n = \frac{q^{7n/2}}{[2n]} \sum_{j=1}^{N} z_j^n - \frac{q^{n/2}}{[n]} \sum_{a} w_a^n, \quad Y_n = \frac{q^{-5n/2}}{[2n]} \sum_{j=1}^{N} z_j^{-n} - \frac{q^{n/2}}{[n]} \sum_{a} w_a^{-n}. \]

Next let us calculate the expectation value \( I^{(i)}(\{z_j\}, \{w_a\}) \). By using the Bogoliubov transformation \((3.2)\), we obtain
\[
I^{(i)}(\{z_j\}, \{w_a\}) = \frac{\langle i | e^{G} e^{F} \exp \left( \sum_{n=1}^{\infty} a_{-n}(X_n - \alpha_n Y_n) \right) | i \rangle}{B \langle i | i \rangle B} \times \exp \left( - \sum_{n=1}^{\infty} \frac{[2n][n]}{n} \beta_n^{(i)} \gamma_n Y_n \right) \exp \left( \frac{1}{2} \sum_{n=1}^{\infty} \frac{[2n][n]}{n} \alpha_n \gamma_n X_n Y_n \right).
\]

We then insert between \( e^{G} i \) and \( e^{F} \) the completeness relation of the coherent states \((\ref{eq:4})\) and use the integration formula \((\ref{eq:3})\). As a result we find
\[
I^{(i)}(\{z_j\}, \{w_a\}) \times \prod_{n=1}^{\infty} (1 - \alpha_n \gamma_n)^{1/2} = \
\exp \left( \sum_{n=1}^{\infty} \frac{[2n][n]}{n} \frac{1}{1 - \alpha_n \gamma_n} \left\{ \gamma_n \beta_n^{(i)} X_n - \alpha_n \gamma_n \gamma_n^{(i)} Y_n \right\} \right.
+ \left. \frac{1}{2} \alpha_n \gamma_n^{(i)} Y_n + \left( \delta_n^{(i)} + \gamma_n \beta_n^{(i)} \right) X_n - \left( \beta_n^{(i)} + \alpha_n \delta_n^{(i)} \right) Y_n \right) \right), \quad (4.4)
\]
\[
B \langle i | i \rangle B \times \prod_{n=1}^{\infty} (1 - \alpha_n \gamma_n)^{1/2} = \
\exp \left( \frac{1}{2} \sum_{n=1}^{\infty} \frac{[2n][n]}{n} \frac{1}{1 - \alpha_n \gamma_n} \left\{ 2 \gamma_n \beta_n^{(i)} + \alpha_n \gamma_n^{(i)} + 2 \beta_n^{(i)} \delta_n^{(i)} \right\} \right). \quad (4.5)
\]

The sums in the right hand sides are evaluated by making use of the following formulas.
\[
\exp \left( \sum_{n=1}^{\infty} \frac{[n]}{n} q^{5n/2} q^{-5n/2} z_n \beta_n^{(i)} \right) = \left( \frac{q^{4z^2}; q^4}{q^{2z^2}; q^4} \right)^{-1/2} \left\{ \varphi(z; r)^{-1}, \left(1 - r^{-1} z\right) \varphi(z; r^{-1})^{-1} \right\},
\]
\[
\exp \left( \sum_{n=1}^{\infty} \frac{[2n]}{n} q^{n^2} w_n \beta_n^{(i)} \right) = \left( \frac{1 - q^{2a+5} w^2}{1 - q^{2a+5} w^2} \right)^{1/2} \left\{ 1 - q^{a+7/2} w, \left(1 - q^{a+3/2} w^{-1} \right)^{-1} \right\},
\]
\[
\exp \left( \sum_{n=1}^{\infty} \frac{[n]}{n} q^{3n/2} z_n \delta_n^{(i)} \right) = \left( \frac{q^{4z^2}; q^4}{q^{2z^2}; q^4} \right)^{-1/2} \left\{ (1 - rz) \varphi(z; r), \varphi(z; r^{-1}) \right\}. \]
\[
\exp \left( \sum_{n=1}^{\infty} \frac{[2n]}{n} q^{an} w^n \delta_n^{(i)} \right) = \left( \frac{1 - q^{2a-1} w^2}{1 - q^{2a-3} w^2} \right)^{1/2} \left\{ \frac{1 - q^{a-5/2} r w}{1 - q^{a-1/2} r^{-1} w} \right\}.
\]

In the above, the upper line applies to the case \( i = 0 \) and the lower to \( i = 1 \). Let us summarize below the results of computation.

The norm of the vacuum vectors:

\[
E^0(0) = \frac{(q^4 r^2; q^8)_{\infty}}{(q^4; q^8)_{\infty}(q^2 r^2; q^8)_{\infty}} \quad (4.6)
\]

\[
E^1(1) = \frac{(q^4/r^2; q^8)_{\infty}}{(q^4; q^8)_{\infty}(q^2/r^2; q^8)_{\infty}} \quad (4.7)
\]

The \( N \)-point function:

\[
P_{\epsilon_1, \ldots, \epsilon_N}^{(i)}(\zeta_1, \ldots, \zeta_N) = \left( -q^3 \right)^{N^2/4 - \sum_{a \in A} a} \left( \frac{\{q_6 \}^{\infty}}{\{q_8 \}^{\infty}} \right)^N \left( q^2; q^8 \right)^{N/2} \prod_{j=1}^{N} \left( q^{2j} \right)^{1 + \epsilon_j - j + N}
\]

\[
\times \prod_{j<k} \left\{ q^6 z_j z_k \right\}_{\infty} \left\{ q^6 z_j / z_k \right\}_{\infty} \left\{ q^6 z_k / z_j \right\}_{\infty} \left\{ q^2 z_j z_k \right\}_{\infty} \left\{ q^2 z_j / z_k \right\}_{\infty} \left\{ q^2 z_k / z_j \right\}_{\infty} \\
\times \prod_{j=1}^{N} \left[ q^{10 z_j^2} \right]_{\infty} \left[ q^{4 z_j^2} \right]_{\infty} \left[ q^{6 z_j^2} \right]_{\infty} \left[ q^{6 z_j^2} \right]_{\infty} \\
\times \prod_{a \in A} \int_{C_a^{(i)}} \frac{dw_a}{2\pi \sqrt{-1}} \prod_{j \leq a} \left( z_j - q^{-2} w_a \right) \prod_{a \leq j} \left( w_a - q^4 z_j \right) \\
\times \prod_{a < b} \left( q^{2} w_a w_b ; q^{2} \right)_{\infty} \left( q^{4} w_a / w_b ; q^{2} \right)_{\infty} \left( w_b / w_a ; q^{2} \right)_{\infty} \left( q^{6} / w_a w_b ; q^{2} \right)_{\infty} \\
\times \prod_{a \leq j} \left( q^{2} z_j w_a ; q^{2} \right)_{\infty} \left( q^{4} z_j / w_a ; q^{2} \right)_{\infty} \left( q^{2} w_a / z_j ; q^{2} \right)_{\infty} \left( q^{4} / z_j w_a ; q^{2} \right)_{\infty} \\
\times \prod_{j=1}^{N} \left( q^{2} r z_j ; q^{4} \right)_{\infty} \prod_{a \leq j} \frac{w_a}{1 - q^{-2} r w_a} \left( \text{for } i = 0 \right) \\
\times \left( -q^3 \right)^{N/2} \prod_{j=1}^{N} \zeta_j \left( q^{2} r^{-1} z_j ; q^{4} \right)_{\infty} \prod_{a \leq j} \frac{1}{1 - q^{2} r^{-1} w_a} \left( \text{for } i = 1 \right) \quad (4.8)
\]

Here, the contour \( C_a^{(0)} \) encircles the points \( q^{4 l} z_j^{-1} \) (for all \( j \)), \( q^{4 j} z_j \) (\( a \leq j \)) and \( q^{4 + 4l} z_j \) (\( a > j \)), \( l = 1, 2, 3, \ldots \) but not the point \( q^{2} r^{-1} \), whereas the contour \( C_a^{(1)} \).
encircles the point $q^{2r-1}$ in addition to the same points as $C_a^{(0)}$ does. We have also set

$$\{z\}_\infty = (z; q^4, q^4)_\infty, \quad [z]_\infty = (z; q^8, q^8)_\infty$$

with $(z; p, q)_\infty = \prod_{j,k \geq 0}(1 - zp^j q^k)$.

### 4.2 Boundary magnetization

We now specialize the formula (4.8) to obtain the correlation functions of local operators. In particular, we obtain the boundary magnetization $\langle \sigma^i \rangle$.

Let $L$ be a linear operator on the $n$-fold tensor product of the two dimensional space $V \otimes \cdots \otimes V$. The corresponding local operator $\mathcal{L}$ acting on our space of states $\mathcal{H}$ can be defined in terms of the type I vertex operators, in exactly the same way as in the bulk theory $\mathcal{P}_2 [23]$. Explicitly, if $L$ is the spin operator at the $n$-th site

$$\sigma_n^\alpha = \sigma^\alpha \otimes \mathbf{id} \otimes \cdots \otimes \mathbf{id}$$

the corresponding local operator $\mathcal{L}_n^{(i)\alpha}$ is given by

\begin{align*}
\mathcal{L}_n^{(i)\pm} &= E_n^{(i)}(1, \ldots, 1), \\
\mathcal{L}_n^{(i)z} &= E_n^{(i)}(1, \ldots, 1) - E_n^{(i)}(1, \ldots, 1),
\end{align*}

(4.9) (4.10)

where

$$E_n^{(i)}(\zeta_1, \ldots, \zeta_n) = g^n \sum_{\epsilon_1, \ldots, \epsilon_{n-1}} \Phi_{\epsilon_1}^{(i,1-i)}(\zeta_1) \cdots \Phi_{\epsilon_{n-1}}^{(i,1-i)}(\zeta_{n-1}) \Phi_{\epsilon_n}^{(1-i,1)}(\zeta_n) \times \Phi_{\epsilon_n}^{(1-i,1)}(\zeta_n) \cdots \Phi_{\epsilon_1}^{(1-i,1)}(\zeta_1)$$

(4.11)

with $i = i$ for even $n$ and $i = 1 - i$ for odd $n$.

Thanks to the inversion property (A.10), the $n$-point function of the product of successively ordered operators of the form (4.11) becomes particularly simple:

$$B\langle i | E_n^{(i)}(\zeta_1, \ldots, \zeta_n) E_{n-1}^{(i)}(\zeta_1, \ldots, \zeta_{n-1}) \cdots E_1^{(i)}(\zeta_1) | i \rangle_B = g^n B\langle i | \Phi_{\epsilon_1}^{(i,1-i)}(\zeta_1) \cdots \Phi_{\epsilon_n}^{(1-i,1)}(\zeta_n) \Phi_{\epsilon_1}^{(i,1-i)}(\zeta_1) \cdots \Phi_{\epsilon_1}^{(1-i,1)}(\zeta_1) | i \rangle_B.$$

The integral formula for this function is obtained from (4.8) by the specialization

$$\epsilon_1, \epsilon_2, \ldots, \epsilon_N \rightarrow -\epsilon_1, \ldots, -\epsilon_n, \epsilon'_n, \ldots, \epsilon'_1$$

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\[ \zeta_1, \zeta_2, \ldots, \zeta_N \rightarrow -q^{-1}\zeta_1, \ldots, -q^{-1}\zeta_n, \zeta_n, \ldots, \zeta_1. \]

In the rest of this subsection we will examine in detail the one-point function,

\[ M(i)(\zeta; r) = B(i) \left( E^{(i)}(\zeta) - E^{(i)}_{-}(\zeta) \right) |i\rangle_B \]

\[ = g\left( p^{(i)}_{\pm}(q^{-1}\zeta, \zeta) - p^{(i)}_{-\pm}(q^{-1}\zeta, \zeta) \right). \]

By virtue of the formulas (2.20), (3.3) and (2.4), \( M(i)(\zeta; r) \) has the symmetry

\[ M(i)_{\pm}(\zeta^{-1}; r) = M(i)(\zeta; r). \] (4.12)

From (4.2) we have in addition

\[ M^{(1)}(\zeta; r) = -M^{(0)}(\zeta; r^{-1}), \] (4.13)

which we shall check directly (see (4.15) below).

Specializing the integral formula (4.8) to \( N = 2, \ z_1 = -q^{-1}\zeta \) and \( z_2 = \zeta \), we obtain

\[ g P^{(i)}_{\pm}(q^{-1}\zeta, \zeta) = \mp g(z) p^{(i)}_{\pm}(z, r) \] (4.14)

where

\[ g(z) = \frac{(q^2; q^2)^{\infty}_s \Theta_{q^4}(z^2)}{(q^4; q^4)^{\infty}_s 1 - z^2} = g(z^{-1}), \]

\[ p^{(i)}_{\pm}(z, r) = \oint_{C^{(i)}_{\pm \pm}} \frac{dw}{2\pi \sqrt{-1}} F(w, z, r), \]

\[ F(w, z, r) = \frac{(1 - rz)(1 - q^{-2} wz)}{z(1 - q^{-2} wr)} \Theta_{q^2}(q^2 w^2) \Theta_{q^2}(w z) \Theta_{q^2}(w/z). \]

The contour \( C^{(0)}_{\pm \pm} \) encircles the points \( q^{2l}z, q^{2l}z^{-1} \) with \( l = 1, 2, \ldots, \) but not the point \( q^2r^{-1}. \) The contour \( C^{(0)}_{\pm +} \) encircles \( q^{2l}z, q^{2l}z^{-1} \) with \( l = 2, 3, \ldots, \) but not \( q^2r^{-1}. \) (There is no pole at \( w = q^2z^{-1}. \) The contour \( C^{(1)}_{\pm \pm} \) encircles the point \( q^2r^{-1} \) in addition to the same points as \( C^{(0)}_{\pm \pm} \) does. With the change of variables \( w \rightarrow q^4/w \) we find

\[ P^{(1)}_{\pm \pm}(q^{-1}\zeta, \zeta) = P^{(0)}_{\pm \pm}(q^{-1}\zeta, \zeta) |_{r \rightarrow r^{-1}}, \] (4.15)

\[ p^{(0)}_{\pm}(z, r) = -p^{(0)}_{\pm}(z^{-1}, r^{-1}) + G(z, r), \] (4.16)
where

\[ G(z, r) = -\text{Res}_{w=q^2} F(w, z^{-1}, r^{-1}) \]
\[ = (1 - rz)(1 - r/z) \frac{\Theta_{q^2}(q^2 r^2)}{\Theta_{q^2}(q^2 z) \Theta_{q^2}(q^2/r)} \]

Using (4.16), (4.12), and noting that \( G(z, r) = G(z^{-1}, r) \), we have

\[ -\left( \mathcal{M}^{(0)}(\zeta; r) + \mathcal{M}^{(0)}(\zeta; r^{-1}) \right) \]
\[ = g(z) \left( p_+(0)^0(z, r) + p_-(0)^0(z, r) + p_+(0)^0(z, r^{-1}) + p_-(0)^0(z, r^{-1}) \right) \]
\[ = 2g(z)G(z, r). \quad (4.17) \]

The integral for \( p_\pm(0)(z, r) \) can be evaluated explicitly by the calculus of residues, making use of the quasi-periodicity property \( \Theta_{p}(pz) = -z^{-1} \Theta_{p}(z) \). We find

\[ -\mathcal{M}^{(0)}(\zeta; r) = g(z) \left( p_+(0)^0(z, r) + p_-(0)^0(z, r) \right) \]
\[ = 1 + 2 \sum_{l=1}^{\infty} \frac{(-q^2)^l(1 - rz)(1 - r/z)}{(1 - q^2 rz)(1 - q^2/r z)}. \quad (4.18) \]

The symmetry (4.12) is now manifest in the expression.

The boundary magnetization \( \mathcal{M}^{(i)}(r) \) in the sector \( i \) is

\[ \mathcal{M}^{(i)}(r) = \frac{B^{(i)|\bar{\sigma}^z|i}B}{B^{(i)|i}B} = \mathcal{M}^{(i)}(1; r). \]

Noting (4.13), we have

\[ -\mathcal{M}^{(0)}(r) = \mathcal{M}^{(1)}(r^{-1}) = 1 + 2 \sum_{l=1}^{\infty} \frac{(-q^2)^l(1 - r)^2}{(1 - q^2 r^2)^2}, \quad (4.19) \]
\[ \mathcal{M}^{(1)}(r) - \mathcal{M}^{(0)}(r) = 2\frac{(q^2; q^4)^2_{\infty}}{(q^2; q^2)^2_{\infty}} \frac{(q^2 r^2; q^4)^2_{\infty}}{(q^2 r; q^2)^2_{\infty}} \frac{(q^2/r^2; q^4)^2_{\infty}}{(q^2/r; q^2)^2_{\infty}}. \quad (4.20) \]

When \( r \) takes the values \( r_c^{(1)} = -q \) and \( r_c^{(2)} = q \), corresponding to the critical fields \( h_c^{(1)} \) and \( h_c^{(2)} \), the difference (4.20) is 0, as it should be \[25\]. At these points, the two boundary magnetizations are equal (at the edge of the hysteresis loop).

Since the ground state is \( |0\rangle_B \) for \( h \geq 0 \) and \( |1\rangle_B \) for \( h \leq 0 \), the boundary magnetization of the ground state is

\[ \mathcal{M}(r) = \begin{cases} \mathcal{M}^{(0)}(r) & \text{for } |r| < 1, \\ \mathcal{M}^{(1)}(r) & \text{for } |r| > 1. \end{cases} \]
We see that at $h = 0 (r = -1)$ the spontaneous magnetization $\mathcal{M}^{(0)}(-1) = -\mathcal{M}^{(1)}(-1)$ is nonvanishing. Specializing (4.20) to $r = -1$, we find

$$\mathcal{M}^{(0)}(-1) = -\frac{(q^2; q^2)_\infty^4}{(-q^2; q^2)_\infty^4}. \quad \text{(4.21)}$$

Note that $-\mathcal{M}^{(0)}(-1)$ is the square of the bulk magnetization [28].

One can check the formula (4.18) by comparing (4.20) with the derivative of the energy difference $\Delta e(r) = e^{(1)}(r) - e^{(0)}(r)$ with respect to the field $h$. One can verify directly, by differentiating (2.28), that the following relation holds:

$$\frac{\partial \Delta e(r)}{\partial h} = \mathcal{M}^{(1)}(r) - \mathcal{M}^{(0)}(r). \quad \text{(4.22)}$$

5 Rational limit

Grisaru et al. [10] calculated the boundary $S$-matrix for the XXX chain using the Bethe ansatz method. To make comparison, let us consider the limit $q \to -1$. In order to get a non-trivial boundary term, it is necessary to scale $r$ near the point $r = 1$. Setting $r = (q^2)^\alpha$ the Hamiltonian (1.2) scales to

$$H^\text{bare}_B = \frac{1}{2} \sum_{k=1}^{\infty} \left(-\sigma^x_{k+1} \sigma^x_k - \sigma^y_{k+1} \sigma^y_k + \sigma^z_{k+1} \sigma^z_k\right) + \hbar \sigma^z_1,$$

where $\hbar = 1/2\alpha$. It turns out that we should also scale the parameter $\xi$ in (3.14) as it approaches $\xi = \sqrt{-1}$. If we set

$$\xi = \sqrt{-1}(q^2)^{\sqrt{-1}\lambda/2},$$

the formula (3.14) for $M(\xi; r)$ can be expressed in terms of the $q$-gamma function. For example,

$$M^-(\xi; r) = (q^2)^{-\sqrt{-1}\lambda} \times$$

$$\Gamma_{q^4} \left(\frac{1}{4} + \frac{a+\sqrt{-1}\lambda}{2}\right) \Gamma_{q^4} \left(\frac{3}{4} + \frac{a-\sqrt{-1}\lambda}{2}\right) \Gamma_{q^8} \left(\frac{1}{4} + \frac{\sqrt{-1}\lambda}{2}\right) \Gamma_{q^8} \left(\frac{1}{4} - \frac{\sqrt{-1}\lambda}{2}\right) \Gamma_{q^8} \left(\frac{3}{4} + \frac{\sqrt{-1}\lambda}{2}\right) \Gamma_{q^8} \left(\frac{3}{4} - \frac{\sqrt{-1}\lambda}{2}\right).$$

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In the limit $q \to -1$, the $q$-gamma function is the ordinary gamma function, and
\[
\frac{M_+^q (\lambda; \alpha)}{M_-^q (\lambda; \alpha)} = \sqrt{-1} \lambda + \alpha - \frac{1}{2}, \\
\frac{M_-^q (\lambda; \alpha)}{M_+^q (\lambda; \alpha)} = \sqrt{-1} \lambda - \alpha + \frac{1}{2}.
\]
Denoting by $\mathcal{R}(\lambda)$ and $\mathcal{K}(\lambda; \alpha)$ the $R$- and $K$-matrices in [10] (see eq. (5.17), (5.19), (5.30) and (5.36) in [10]),
\[
\lim S_{12}(\xi_1/\xi_2) = -\sigma^x_1 \mathcal{R}(\lambda_1 - \lambda_2) \sigma^z_2, \\
\lim M(\xi; r) = -\sigma^z \mathcal{K}(\lambda; \alpha).
\]
Following [29], p.99, let us modify the signs and define the limiting states by
\[
|\lambda_n, \ldots, \lambda_1\rangle_{\mu_n, \ldots, \mu_1;i_B} = \prod_{j: \text{odd}} (-\mu_j) \lim \Psi_{\mu_n}(\xi_n) \cdots \Psi_{\mu_1}(\xi_1) |i\rangle_B
\]
where $\xi_j = \sqrt{-1}(q^2)\sqrt{-1}\lambda_j/2$. Notice that
\[
| -\lambda_1\rangle_{\mu_1;i_B} = \lim \Psi^*_{\mu_1}(-\xi_1^{-1}) |i\rangle_B = (-1)^{i+(1-\mu)/2} \lim \Psi^*_{\mu_1}(\xi_1^{-1}) |i\rangle_B.
\]
Taking into account the signs properly, we find that in the basis (5.1) our bulk and boundary $S$-matrices become in the limit $-\mathcal{R}(\lambda_1 - \lambda_2)$ and $-\mathcal{K}(\lambda; \alpha)$, respectively.

Thus, in the XXX model, there is only one critical field, which is at $\alpha = 1/2$, and it is the limit of our $h_{c(2)}$. The pole in the boundary $S$-matrix at $\lambda = \sqrt{-1}(1/2 - \alpha)$ is in the physical strip, $0 < \text{Im} \lambda \leq 1$, when $h > h_{c(2)} = 1$. The energy difference and the boundary magnetization in this limit are:
\[
\lim \Delta e(r) = \frac{\pi}{\sin \pi \alpha}, \\
\lim M^{(0)}(r) = -1 - 2 \sum_{l=1}^{\infty} (-1)^l \frac{\alpha^2}{(l + \alpha)^2} = 1 + \frac{\alpha^2}{2} \left( \psi'\left(\frac{\alpha + 1}{2}\right) - \psi'\left(\frac{\alpha}{2}\right) \right)
\]
where $\psi'(x) = (d^2/dx^2) \log \Gamma(x)$.

6 Discussion

In conclusion, we have obtained the following results for the XXZ Hamiltonian on the semi-infinite chain [12]: (i) the space of states and the renormalized transfer
matrix (2.13), (ii) the vacuum vectors (3.4) and the energy difference between them (2.28), (iii) the boundary S-matrix (3.14), and (iv) the correlation functions (4.8) and the boundary magnetization (4.19) in particular. We have also found the critical values of the boundary magnetic field (1.7) at which one of the metastable vacuum states turn to be unphysical. Above the second critical field, one of the vacuum states has an energy higher than the mass gap.

Contrary to the case of the infinite chain, the symmetry algebra corresponding to the boundary problem is not \( U_q(\hat{sl}_2) \), since the boundary Hamiltonian does not commute with it. In this paper, we have bypassed this point to get the results. Sklyanin has suggested to us that the relevant algebra may be the one associated with the boundary YBE as formulated in his paper [6]. In order to discuss highest weight representations for this algebra, we would probably need a central extension, just as was discussed by Reshetikhin and Semenov-Tian-Shansky [30] in the case of the quantum affine algebras.

Our approach allows us to diagonalize the transfer matrix (2.6) on the semi-infinite lattice. However, the corresponding six–vertex model contains alternating spectral parameters (see Figure 2). Therefore the corner transfer matrix is not diagonalized by our vertex operators, since in [21,22,23] a uniform spectral parameter is assumed. In particular, we have not given a method of diagonalizing the transfer matrix acting in the transverse direction. This would involve reformulation of the vertex operators to accommodate nonuniform spectral parameters.

In the field theory limit, there are also two different directions in which we can formulate the Hamiltonians, corresponding to the exchange of the space and time coordinates. Sklyanin’s transfer matrix corresponds to a spatial boundary condition. If the roles of space and time are exchanged, the spatial boundary condition is replaced by some initial condition in time. In [16] this is represented by the ‘boundary state’ \(|B\rangle\). Such a state has also been discussed in the context of conformal field theory [31,32]. Our expression (1.6) for \(|i\rangle_B\) bears some resemblance to the expression for \(|B\rangle\), e.g. (3.38) of [16]. However, the two states exist in different spaces. The states \(|i\rangle_B\) correspond (see (3.18)) to the ‘boundary bound states’ of [16].

Although there exists a Bethe ansatz for the model [4,5,6], the excitation structure have not yet been analyzed using this method. In the case of periodic boundary conditions, only even-number particle states appear in the spectrum of the Hamiltonian, although both even and odd states are found using the vertex operator approach. It is unclear whether all of the states we describe appear in the Bethe ansatz for the boundary problem. The boundary scattering matrix (3.14) should also be obtainable using the Bethe ansatz.

We believe that the case of a non-diagonal \( K \)-matrix, corresponding to a bound-
any magnetic field acting on all three spin components, can be analyzed using a
similar method to the one described in this paper. Finally, one may ask whether
there exist difference equations for correlation functions of the boundary Hamilto-
nian, as for the bulk case.

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A Vertex operators

We summarize here some basic formulas for the $R$-matrix and the vertex operators,
following the Appendix in [23].

A.1 $R$-matrix

The $R$-matrix for the six-vertex model is

$$
R(\zeta) = \frac{1}{\kappa(\zeta)} \begin{pmatrix}
1 & (1 - \zeta^2)q & (1 - q^2)\zeta \\
1 - q^2\zeta^2 & 1 - q^2\zeta^2 & (1 - q^2)q \\
1 - q^2\zeta^2 & (1 - q^2)\zeta & 1 - q^2\zeta^2
\end{pmatrix},
$$

(A.1)

where

$$
\kappa(\zeta) = \zeta \left( \frac{q^4\zeta^2; q^4}{q^4\zeta^{-2}; q^4} \right) \left( q^2\zeta^2; q^2 \right) \infty, \quad (z; p) \infty = \prod_{n=0}^{\infty} (1 - zp^n).
$$

(A.2)

Let $\{v_+, v_-\}$ denote the natural basis of $V = \mathbb{C}^2$. When viewed as an operator on
$V \otimes V$, the matrix elements of $R(\zeta)$ are defined by

$$
R(\zeta) \left(v_{\epsilon_1} \otimes v_{\epsilon_2}\right) = \sum_{\epsilon_1', \epsilon_2'} v_{\epsilon_1'} \otimes v_{\epsilon_2'} R_{\epsilon_1 \epsilon_2}^{\epsilon_1' \epsilon_2'}(\zeta).
$$
As usual, when copies $V_j$ of $V$ are involved, $R_{ij}(\zeta)$ acts as $R(\zeta)$ on the $i$-th and $j$-th components and as the identity elsewhere. The Yang-Baxter equation satisfied by (A.1) is

$$R_{12}(\zeta_1/\zeta_2)R_{13}(\zeta_1/\zeta_3)R_{23}(\zeta_2/\zeta_3) = R_{23}(\zeta_2/\zeta_3)R_{13}(\zeta_1/\zeta_3)R_{12}(\zeta_1/\zeta_2). \quad (A.3)$$

The scalar factor $\kappa(\zeta)$ (A.2) is so chosen that the unitarity and crossing relations are

$$R_{12}(\zeta_1/\zeta_2)R_{21}(\zeta_2/\zeta_1) = 1, \quad (A.4)$$

$$R_{\varepsilon_2\varepsilon_1}(\zeta_2/\zeta_1) = R_{-\varepsilon_1\varepsilon_2}(-q^{-1}\zeta_1/\zeta_2). \quad (A.5)$$

### A.2 Vertex operators

We list here the commutation relations for the vertex operators:

$$\Phi_{\varepsilon_2}(\zeta_2)\Phi_{\varepsilon_1}(\zeta_1) = \sum_{\varepsilon_1',\varepsilon_2'} R_{\varepsilon_1\varepsilon_2'}(\zeta_1/\zeta_2)\Phi_{\varepsilon_1'}(\zeta_1)\Phi_{\varepsilon_2'}(\zeta_2), \quad (A.6)$$

$$\Psi^*_{\mu_1}(\xi_1)\Psi^*_{\mu_2}(\zeta_2) = -\sum_{\mu_1,\mu_2} R_{\mu_1\mu_2}(\xi_1/\zeta_2)\Psi^*_{\mu_2}(\zeta_2)\Psi^*_{\mu_1}(\xi_1), \quad (A.7)$$

$$\Phi_\varepsilon(\zeta)\Psi^*_{\mu}(\xi) = \tau(\zeta/\xi)\Psi^*_{\mu}(\xi)\Phi_\varepsilon(\zeta). \quad (A.8)$$

Here

$$\tau(\zeta) = \zeta^{-1}\frac{\Theta_{q^4}(q\zeta^2)}{\Theta_{q^4}(q\zeta^{-2})}, \quad \Theta_{p}(z) = (z;p)_\infty(pz^{-1};p)_\infty(p;p)_\infty. \quad (A.9)$$

The type I vertex operators satisfy the invertibility

$$g \sum_\varepsilon \Phi^*_\varepsilon(\zeta)\Phi_\varepsilon(\zeta) = id, \quad g \Phi_{\varepsilon_1}(\zeta)\Phi^*_{\varepsilon_2}(\zeta) = \delta_{\varepsilon_1\varepsilon_2}id, \quad (A.10)$$

where $g$ is given by

$$g = \frac{(q^2; q^4)_{\infty}}{(q^4; q^4)_{\infty}}. \quad (A.11)$$

For the type II operators the corresponding property is

$$\Psi^{\mu_1}(\xi_1)\Psi^{\mu_2}(\xi_2) = \frac{g \delta_{\mu_1\mu_2}}{1 - \xi_2/\xi_1} \left( \frac{\xi_2}{\xi_1} \right)^{i+1-\mu_1} + \cdots \quad (\xi_1 \to \pm \xi_2), \quad (A.12)$$

where

$$\Psi^{(i,1-i)}(\xi) = \Psi^{-(i,1-i)}(-q^{-1}\xi)$$

and $\cdots$ means regular terms.
A.3 Bosonization

For $i = 0, 1$, consider the bosonic Fock space

$$\mathcal{H}^{(i)} = \mathbb{C}[a_{-1}, a_{-2}, \cdots] \otimes \left( \bigoplus_{n \in \mathbb{Z}} \mathbb{C} e^{\Lambda_1 \alpha + n\alpha} \right).$$

The commutation relations of $a_n$ are

$$[a_m, a_n] = \delta_{m+n,0} \left[ \frac{m! \cdot 2m}{m} \right], \quad (m, n \neq 0), \quad [n] = \frac{q^n - q^{-n}}{q - q^{-1}}.$$

On the symbols $e^\gamma$, the operators $e^\beta, z^\partial$ act as

$$e^\beta e^\gamma = e^{\beta + \gamma}, \quad z^\partial e^\gamma = z^{[\partial, \gamma]} e^\gamma,$$

where $[\partial, \alpha] = 2$, $[\partial, \Lambda_0] = 0$ and $\Lambda_1 = \Lambda_0 + \alpha/2$. The highest weight vector of $\mathcal{H}^{(i)}$ is given by $|i\rangle = 1 \otimes e^{\Lambda_1 \alpha}$.

We have the following bosonic realization for the vertex operators:

$$\Phi_+^{(1-i,i)}(\zeta) = e^{P(\zeta^2)} e^{Q(\zeta^2)} \otimes e^{\alpha/2 (-q^3 \zeta^2)(\partial+i)/2} \zeta^{-i}, \quad \text{(A.13)}$$

$$\Phi_-^{(1-i,i)}(\zeta) = \oint_{C_1} \frac{dw}{2\pi i q(w - q^2 \zeta^2)} \cdot \Phi_-^{(1-i,i)}(\zeta) X^{-}(w) :, \quad \text{(A.14)}$$

$$\Psi_-^{(1-i,i)}(\zeta) = e^{-P(q^{-1} \zeta^2)} e^{-Q(q^2 \zeta^2)} \otimes e^{-\alpha/2 (-q^3 \zeta^2)(\partial-i)/2} \zeta^{-1-i}, \quad \text{(A.15)}$$

$$\Psi_+^{(1-i,i)}(\zeta) = \oint_{C_2} \frac{dw}{2\pi i (w - q^2 \zeta^2)(w - q^4 \zeta^2)} \cdot \Psi_-^{(1-i,i)}(\zeta) X^{+}(w) :, \quad \text{(A.16)}$$

$$X^{\pm}(z) = e^{R^{\pm}(z)} e^{S^{\pm}(z)} \otimes e^{\pm \alpha z^{\pm \partial}}, \quad \text{(A.17)}$$

where

$$P(z) = \sum_{n=1}^{\infty} \frac{a_{-n}}{[2n]} q^{7n/2} z^n, \quad Q(z) = -\sum_{n=1}^{\infty} \frac{a_n}{[2n]} q^{-5n/2} z^{-n}, \quad \text{(A.18)}$$

$$R^{\pm}(z) = \pm \sum_{n=1}^{\infty} \frac{a_{-n}}{[n]} q^{7n/2} z^n, \quad S^{\pm}(z) = \mp \sum_{n=1}^{\infty} \frac{a_n}{[n]} q^{-5n/2} z^{-n}. \quad \text{(A.19)}$$

The integration contours encircle $w = 0$ in such a way that

$$C_1 : \quad q^4 \zeta^2 \text{ is inside and } q^2 \zeta^2 \text{ is outside},$$

$$C_2 : \quad q^4 \zeta^2 \text{ is outside and } q^2 \zeta^2 \text{ is inside}.$$
These operators act also on the dual (right) modules $H^{\ast}(i)$, which are defined analogously by replacing $e^{\Lambda_{i}+\alpha}$ with $e^{-(\Lambda_{i}+\alpha)}$. In particular the highest weight vector is $|i| = 1 \otimes e^{-\Lambda_{i}}$. The right actions of $e^{\beta}$ and $z^{\theta}$ are given by

$$e^{\gamma}.e^{\beta} = e^{\gamma+\beta}, \quad e^{\gamma}.z^{\theta} = e^{\gamma}z^{[\gamma,\theta]}.$$ 

B The $q$-expansion

In this section we calculate the ground state vector $|0\rangle_{B}$ of the Hamiltonian (1.4), as a $q$-series expansion in terms of paths for $r = -1$ [33,21]. Next we develop the vector $|0\rangle_{B}$ written in terms of bosonic operators into a similar $q$-series. We find that the two results agree to the order $q^{3}$.

B.1 The path expansion

In the naïve approach, we can expand the ground state vector $|0\rangle_{B}$ as a linear combination of vectors $|p\rangle$ in the semi-infinite tensor product $\otimes_{k \geq 1} V_{k}$ (see (2.11)):

$$|p\rangle = \otimes_{k \geq 1} v_{p(k)},$$

where

$$p : \mathbb{Z}_{\geq 1} \rightarrow \{\pm\}, \quad p(k) = (-1)^{k} \text{ if } k \gg 1.$$

We call such a map $p$ a path, as well as the vector $|p\rangle$ itself. In what follows, we find it convenient to represent a path $p$ by a sequence of non-negative integers

$$Y = (f_{1}, f_{2}, \cdots, f_{n}), \quad f_{1} > f_{2} > \cdots > f_{n},$$

given via the correspondence

$$p(k) = p(k + 1) \text{ if and only if } k \in Y.$$

We also use the convention that $|f_{1}, \cdots, f_{n}, 0\rangle = |f_{1}, \cdots, f_{n}\rangle$. The degree of $Y$ is $f_{1} + \cdots + f_{n}$. The ‘vacuum path’ $p_{0}$ given by $p_{0}(k) = (-1)^{k}$ is the unique one of degree 0, which we represent by the symbol $Y = \phi$.

Let

$$|0\rangle_{B} = |\phi\rangle + \sum_{j \geq 1} \epsilon^{j}v_{j} \quad \text{(B.1)}$$

be the expansion of the ground state vector for [1,2], where $\epsilon = -1/(2\Delta) = -q/(1 + q^{2})$.

Each $v_{j}$ is a linear combination of paths

$$v_{j} = \sum_{Y \neq \phi} c_{j}(Y)|Y\rangle \quad \text{(B.2)}$$

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Here we demanded that $\phi$ never appears in $v_j$ ($j \geq 1$), by multiplying a scalar to $|0\rangle_B$ as necessary.

We are going to solve the following eigenvalue equation order by order in $\varepsilon$:

$$\left(\sum_{k \geq 1} \frac{1}{2} (\sigma^z_{k+1} \sigma^z_k + 1 + c_k(\varepsilon)) - 2\varepsilon Q\right) |0\rangle_B = 0,$$

where

$$Q = \sum_{k \geq 1} (\sigma^+_{k+1} \sigma^-_k + \sigma^-_{k+1} \sigma^+_k).$$

We have included the $c$-number terms $c_k(\varepsilon) = \sum_{j \geq 1} \varepsilon^j c_{k,j}$ to ensure that the eigenvalue is 0.

Up to the third order, we obtain

$$v_1 = 2|2\rangle + \sum_{k \geq 1} |k + 2, k\rangle,$$

$$v_2 = 6|4\rangle + 2 \sum_{k \geq 1} |k + 4, k\rangle + 2 \sum_{k \geq 3} |k + 2, k, 2\rangle + \sum_{k \geq 1} \sum_{l \geq k+3} |l + 2, l, k + 2, k\rangle,$$

$$v_3 = -4|2\rangle + 20|6\rangle - 3|3, 1\rangle + 2|4, 2\rangle - \sum_{k \geq 3} |k + 2, k\rangle + 5 \sum_{k \geq 1} |k + 6, k\rangle$$

$$+ 4|4, 3, 1\rangle + 4 \sum_{k \geq 3} |k + 4, k, 2\rangle + 6 \sum_{k \geq 5} |k + 2, k, 4\rangle + \sum_{k \geq 1} |k + 4, k + 3, k + 1, k\rangle$$

$$+ 2 \sum_{k \geq 1} \sum_{l \geq k+5} |l + 2, l, k + 4, k\rangle + 2 \sum_{k \geq 1} \sum_{l \geq k+3} |l + 4, l, k + 2, k\rangle$$

$$+ 2 \sum_{k \geq 3} \sum_{l \geq k+3} |l + 2, l, k + 2, k, 2\rangle + \sum_{k \geq 1} \sum_{l \geq k+3} \sum_{m \geq l+3} |m + 2, m, l + 2, l, k + 2, k\rangle.$$

(B.5)

### B.2 Monomials in bosons and the upper global bases

Next, we expand bosonic expression for the vector $|0\rangle_B$ (B.3) in terms of paths. Since $|0\rangle_B$ is written in terms of bosons, there is a difficulty in handling its expansion in the sense of crystal lattice. We expect that each homogeneous component of $|0\rangle_B$ belongs to the upper crystal lattice (see \cite{21}), although we have no proof.

On the other hand, the global basis vectors have a $q$-expansion in terms of paths.
In the following we shall relate the vectors created by bosons to the global base vectors up to degree 6. This will make it possible (to this degree) to develop the homogeneous components of $|0\rangle_B$ into a \( q \)-series, which can be compared to the results of the previous subsection.

For a path \( Y \), denote by \( G(Y) \in \mathcal{H}^{(0)} \) the corresponding upper global base of Kashiwara (see Section 2 of \[21\]). Up to degree 6, the possible paths and monomials in the bosons are as follows.

| degree | path | monomials |
|--------|------|-----------|
| 0      | \( \phi \) | 1         |
| 1      | (1)  | \( e^\alpha \) |
| 2      | (2)  | \( a_{-2} \) |
| 3      | (3), (2, 1) | \( a_{-1} e^\alpha, e^{-\alpha} \) |
| 4      | (4), (3, 1) | \( a_{-2}^2, a_{-1} \) |
| 5      | (5), (4, 1), (3, 2) | \( a_{-1} e^{-\alpha}, a_{-2}^2 e^\alpha, a_{-2} e^{2\alpha} \) |
| 6      | (6), (5, 1), (4, 2), (3, 2, 1) | \( a_{-3}, a_{-1} a_{-2}, a_{-1}^2, e^{2\alpha} \) |

In the second column we abbreviated \( X \otimes e^{\Lambda_0 + \beta} \) to \( X e^\beta \).

The following is the explicit relation between the two bases:

\[
G(\phi) = 1 \otimes e^{\Lambda_0},
\]
\[
G(1) = q^2 \otimes e^{\Lambda_0 + \alpha},
\]
\[
G(2) = -\frac{q^{5/2}}{2} a_{-1} \otimes e^{\Lambda_0},
\]
\[
G(3) = \frac{q^{5/2}}{2} a_{-1} \otimes e^{\Lambda_0 + \alpha},
\]
\[
G(2, 1) = -q^3 \otimes e^{\Lambda_0 - \alpha},
\]
\[
G(4) = \left( \frac{q^5}{2[2]} a_{-1}^2 - \frac{q^5}{4} a_{-2} \right) \otimes e^{\Lambda_0},
\]
\[
G(3, 1) = \left( -\frac{q^3}{2[2]} a_{-1}^2 + \frac{q^4}{4} a_{-2} \right) \otimes e^{\Lambda_0},
\]
\[
G(5) = \left( \frac{q^3}{2[2]} a_{-1}^2 + \frac{q^3}{4} a_{-2} \right) \otimes e^{\Lambda_0 + \alpha},
\]
\begin{align*}
G(4, 1) &= \frac{q^{11/2}}{2} a_{-1} \otimes e^{A_0 - \alpha}, \\
G(3, 2) &= \left( \frac{q^3}{2[2]^2} a_{-1}^2 - \frac{q^3}{4} a_{-2} \right) \otimes e^{A_0 + \alpha}, \\
G(6) &= q^{5/2} \left( \frac{q^5}{6[2]^3} a_{-3} + \frac{q^5}{4[2]} a_{-2} a_{-1} - \frac{q^5}{6[2]} a_{-1}^3 \right) \otimes e^{A_0}, \\
G(5, 1) &= q^{5/2} \left( \frac{q^4 - 1}{6} a_{-3} - \frac{q^2}{2} a_{-2} a_{-1} + \frac{q(q^2 - 1)}{6[2]^2} a_{-1}^3 \right) \otimes e^{A_0}, \\
G(4, 2) &= q^{5/2} \left( - \frac{q(q^2 - 1)}{6} a_{-3} + \frac{q}{4[2]} a_{-2} a_{-1} + \frac{q(2q^2 + 1)}{6[2]^3} a_{-1}^3 \right) \otimes e^{A_0}, \\
G(3, 2, 1) &= q^6 \otimes e^{A_0 + 2\alpha}.
\end{align*}

From these data, we can write \(|0\rangle_B\) (see (3.4)) as a linear combination of the global basis vectors up to degree 6:

\begin{align*}
|0\rangle_B &= G(\phi) + qrG(2) + q^2r^2G(4) + q^3G(3, 1) + q^3r^3G(6) \\
&\quad + q^4[2]rG(4, 2) + q^4rG(5, 1) + \ldots. \quad (B.6)
\end{align*}

The global base vectors are regular and finite at \(q = 0\). We say \(|0\rangle_B\) is regular to mean that each coefficient in the expansion \((B.6)\), regarded as a function of \(q\) by setting \(r = \pm (q^2)\alpha\), is regular at \(q = 0\). Hence we find, up to this order, that this is the case if and only if \(|rq| \leq 1\).

Now, we expand \(|0\rangle_B\) in \(q\). Let

\[ G(Y) = |p_0(Y)\rangle + q|p_1(Y)\rangle + q^2|p_2(Y)\rangle + \cdots, \]

be the expansion of a global base vector \(G(Y)\), where \(|p_j(Y)\rangle\) is a finite or possibly infinite linear combination of paths

\[ |p_j(Y)\rangle = \sum_{Y'} c_j(Y', Y)|Y'\rangle. \]

We have, in particular,

\[ c_0(Y', Y) = \delta_{Y', Y}. \quad (B.7) \]

We have the following expansions.

\[ G(\phi) = |\phi\rangle + \varepsilon \sum_{k \geq 0} |k + 2, k\rangle + \varepsilon^2 \left( 2 \sum_{k \geq 0} |k + 4, k\rangle + \sum_{k \geq 1} |k + 2, k, l + 2, l\rangle \right) \]
\[ + \varepsilon^3 \left( \sum_{m \geq 0 \atop l \geq m+3 \atop k \geq k+4}^\infty |k+2, k, l+2, l, m+2, m\rangle + 2 \sum_{k \geq 0 \atop l \geq k+5} |l+2, l, k+4, k\rangle \right. \\
\left. + 2 \sum_{k \geq 0 \atop l \geq k+3} |l+4, l, k+2, k\rangle + \sum_{k \geq 0} |k+4, k+3, k+1, k\rangle + 5 \sum_{k \geq 0} |k+6, k\rangle \right) \\
- \sum_{k \geq 1} |k+2, k\rangle \right) + O(\varepsilon^4), \tag{B.8} \]

\[ G(2) = (1 - 4\varepsilon^2 + O(\varepsilon^4)) \left\{ |2\rangle + \varepsilon \left( -|0\rangle + 3|4\rangle + \sum_{k \geq 3} |k+2, k, 2\rangle \right) \right. \\
\left. + \varepsilon^2 \left( 9|6\rangle - 2|3, 1\rangle - \sum_{k \geq 3} |k+2, k\rangle + 2|4, 3, 1\rangle + 3 \sum_{k \geq 5} |k+2, k, 4\rangle \right) \\
+ 2 \sum_{k \geq 3} |k+4, k, 2\rangle + \sum_{k \geq 3 \atop l \geq k+3} |l+2, l, k+2, k, 2\rangle \right) + O(\varepsilon^3) \right\}, \tag{B.9} \]

\[ G(4) = |4\rangle + \varepsilon \left( -3|2\rangle + 5|6\rangle + |4, 2\rangle + |4, 3, 1\rangle + \sum_{k \geq 5} |k+2, k, 4\rangle \right) + O(\varepsilon^2). \tag{B.10} \]

Combining (B.6)–(B.10), we obtain the \(q\)-expansion of \(|0\rangle_B\). We have checked the equality between (B.6) for \(r = -1\) and (B.1), (B.3)–(B.5) up to the third order.

## C  Coherent states

We here summarize formulas concerning coherent states of bosons which are used in Section 4.

The coherent states \(|\xi\rangle_i\) and \(i\langle\bar{\xi}|\) in the Fock spaces \(\mathcal{H}^{(i)}, \mathcal{H}^{*(i)}, \ i = 0, 1\), are defined by

\[ |\xi\rangle_i = \exp \left( \sum_{n=1}^\infty \frac{n}{|n|2n} \xi_n a_{-n} \right) |i\rangle, \tag{C.1} \]

\[ i\langle\bar{\xi}| = \langle i| \exp \left( \sum_{n=1}^\infty \frac{n}{|n|2n} \bar{\xi}_n a_n \right), \tag{C.2} \]

where \(\xi_n\) and \(\bar{\xi}_n\) are complex conjugate parameters.

Noting that the highest weight states \(|i\rangle\) and \(\langle i|\) are annihilated by the boson oscillators \(a_n\) and \(a_{-n}\) with \(n \geq 1\), respectively, one can easily verify

\[ a_n |\xi\rangle_i = \xi_n |\xi\rangle_i, \quad i \langle\bar{\xi}| a_{-n} = \bar{\xi}_n i \langle\bar{\xi}|. \tag{C.3} \]
One can also show that the coherent states \(\{|ξ_i⟩\}\) (resp. \(\langle i|(ξ)\})\) form a complete basis in the Fock space \(H^{(i)}\) (resp. \(H^{∗(i)}\)). Namely one can verify the completeness relation

\[
\text{id}_{H^{(i)}} = \int \prod_{n=1}^{∞} \frac{ndξ_n d\bar{ξ}_n}{[n][2n]} e^{-\sum_{n=1}^{∞} \frac{n}{[2n]}|ξ_n|^2|ξ_n⟩i⟨\bar{ξ}_n|}.
\]

(C.4)

Here the integration is taken over the entire complex plane with the measure \(dξ d\bar{ξ} = dx dy\) for \(ξ = x + iy\). In the proof, the following integration formula is used:

\[
\int \prod_{n=1}^{∞} \frac{ndξ_n d\bar{ξ}_n}{[n][2n]} \exp \left(-\frac{1}{2} \sum_{n=1}^{∞} \frac{n}{[n][2n]}(ξ_n, \bar{ξ}_n)A_n \left(\bar{ξ}_n, ξ_n\right) + \sum_{n=1}^{∞} (ξ_n, ξ_n) B_n\right) = \prod_{n=1}^{∞} \left(-\det A_n\right)^{-1/2} \exp \left(\frac{1}{2} \sum_{n=1}^{∞} \frac{[n][2n]}{n}B_n^t A_n^{-1}B_n\right),
\]

(C.5)

where \(A_n\) are invertible constant \(2×2\) matrices and \(B_n\) are constant \(2\) component vectors.

References

[1] McCoy, B. M. and Wu, T. T., Theory of Toeplitz determinants and the spin correlation functions of the two-dimensional Ising model. IV, Phys. Rev. 162 436–475 (1967).

[2] McCoy, B. M. and Wu, T. T., Theory of Toeplitz determinants and the spin correlation functions of the two-dimensional Ising model. V, Phys. Rev. 174 546–559 (1968).

[3] Bariev, R. Z., Correlation functions of the semi-infinite two-dimensional Ising model, Theoret. Math. Phys. 40 623–626 (1979).

[4] Gaudin, M., Boundary energy of a bose gas in one dimension, Phys. Rev. A 4 386–394 (1971).

[5] Alcaraz, F. C., Barber, M. N., Batchelor, M. T., Baxter, R. and Quispel, G. R. W., Surface exponents of the quantum XXZ, Ashkin-Teller and Potts models, J. Phys. A 20 6397–6409 (1987).

[6] Sklyanin, E. K., Boundary conditions for integrable quantum systems, J. Phys. A 21 2375–2389 (1988).

[7] Kulish, P. P. and Sklyanin, E. K., The general \(U_q[sl(2)]\) invariant XXZ integrable quantum spin chain, J. Phys. A 24 L435–L439 (1991).
[8] Mezincescu, L. and Nepomechie, R. I., Integrability of open spin chains with quantum algebra symmetry, *Int. J. Mod. Phys. A* 6 5231–5248 (1991); *Int. J. Mod. Phys. A* 7 5657–55659 (1992).

[9] Mezincescu, L. and Nepomechie, R. I., Analytical Bethe ansatz for quantum-algebra-invariant spin chains, *Nucl. Phys. B* 372 597–621 (1992).

[10] Grisaru, M. T., Mezincescu, L. and Nepomechie, R. I., Direct calculation of the boundary $S$ matrix for the Heisenberg chain, *preprint* UMTG-177, hep-th/9407089, to appear in *J. Phys. A*.

[11] de Vega, H. J. and González Ruiz, A., Boundary $K$-matrices for the six vertex and the $n(2n−1)$ $A_{n−1}$ vertex models, *J. Phys. A* 26 L519–524 (1993).

[12] Inami, T. and Konno, H., Integrable XYZ spin chain with boundaries, *preprint* YITP/K-1084, hep-th/9409138, to appear in *J. Phys. A. Letts.*.

[13] Hou, B.-Y., Shi, K.-J. Fan, H. and Yang, Z.-X., Solution of reflection equation, *preprint* NWU-IMP-931201 (1993).

[14] Yung, C. M. and Batchelor, M. T., Integrable vertex and loop models on the square lattice with open boundaries via reflection matrices, *preprint* MRR042-94, hep-th/9410042 (1994).

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

[16] Ghoshal, S. and Zamolodchikov, A., Boundary $S$-matrix and boundary state in two-dimensional integrable quantum field theory, *Int. J. Mod. Phys. A* 21 3841–3885 (1994).

[17] Cardy, J. L., Effect of boundary conditions on the operator content of two-dimensional conformally invariant theories, *Nucl. Phys. B* 275[FS] 200–218 (1986).

[18] Fendley, P. and Saleur, H., Deriving boundary $S$ matrices, *preprint* USC-94-001, hep-th/9402045 (1994), *to appear in Nucl. Phys.*

[19] Fring, A. and Köberle, R., Factorized scattering in the presence of reflecting boundaries, *Nucl. Phys. B* 421 159–172 (1994).

[20] Corrigan, E., Dorey, P. E. and Sasaki, R., Affine Toda field theory on a half-line, *Phys. Lett. B* 333 83–91 (1994).
[21] Davies, B., Foda, O., Jimbo, M., Miwa, T. and Nakayashiki, A., Diagonalization of the XXZ Hamiltonian by vertex operators, Commun. Math. Phys. 151, 89–153 (1993).

[22] 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).

[23] Jimbo, M. and Miwa, T., Algebraic Analysis of Solvable Lattice Models, RIMS preprint 981 (1994), to appear in CBMS Regional Conference Series in Mathematics, vol.85, AMS.

[24] Frenkel, I. B. and Jing, N., Vertex representations of quantum affine algebras, Proc. Natl. Acad. Sci. USA, 85 9373–9377 (1988).

[25] McCoy, B. M. and Wu, T. T., The two dimensional Ising model, Harvard University Press, Cambridge, Massachusetts, 1973.

[26] Pasquier, V. and Saleur, H., Common structures between finite systems and conformal field theories through quantum groups, Nucl.Phys. B330 523 (1990).

[27] Etingof, P. I., On spectral theory of quantum vertex operators, preprint, hep-th/9410208 (1994).

[28] Baxter, R. J., Spontaneous staggered polarization of the $F$ model, J. Stat. Phys., 9 145–182 (1973).

[29] Smirnov, F. A., Form Factors in Completely Integrable Models of Quantum Field Theory, Advanced Series in Mathematical Physics 14, World Scientific, Singapore 1992.

[30] Reshetikhin, N. Yu. and Semenov-Tian-Shansky, M. A., Central extensions of quantum current groups, Lett. Math. Phys. 19 133–142 (1990).

[31] Ishibashi, N., The boundary and crosscap states in conformal field theories, Mod. Phys. Lett. A 4 251–264 (1989).

[32] Callan, C. G., Klebanov, I. R., Ludwig, A. W. W. and Maldacena, J. M., Exact solution of a boundary conformal field theory, Nucl. Phys. B422 [FS] 417–448 (1994).

[33] Foda, O. and Miwa, T., Corner transfer matrices and quantum affine algebras, Int. J. Mod. Phys. A 7 Suppl. 1A, 279–302 (1992).
\[
\zeta^{b} (K - a) b (\zeta) = (K + a) b (\zeta) = R_{cd}^{ab} (\zeta) = N_{2}
\]

Figure 1: Transfer matrix on a finite chain. The spectral parameters attached to the lines 1, \cdots, N are chosen to be 1.
Figure 2: Transfer matrix on the semi-infinite chain. By convention, the lattice sites are numbered $k = 1, 2, 3, \cdots$ from right to left.
Figure 3: The energy difference $\Delta e(r)$ between the vacuum states as a function of $h$, when $q = -0.15$. The energy $a = \epsilon(1)$, and $b = \epsilon(1)/k'$. The critical field $c = h_c^{(1)}$ and $d = h_c^{(2)}$. 