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XXZ chain with a boundary

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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 $h \geqslant 0$, 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.

To the memory of Mr. Toyosaburo Taniguchi

1. Introduction

Modern mathematical physics has seen many remarkable interactions between quantum field theory and statistical mechanics. In particular, in the field of solvable models, there has been much progress recently. Among others the notion of intertwiners in the representation theory provides a key mathematical tool for conformal field theory (CFT) in the characterization of primary fields. The quantized version of these plays a similar role in massive integrable field theories and solvable lattice models (SLM).

Sometimes we must be careful in observing analogies between the lattice and continuum theories, because the same mathematical mechanism may work differently. For example, the physical spaces of states both in CFT and SLM are sums of tensor products of representation spaces. However, the physical interpretations of the tensor components are quite different. In CFT, the left and right tensor components represent the left- and right-moving particles, while in SLM they represent the left and right semi-infinite spin

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chains [21]. In other words, in the continuum theory, the tensor component appear in the momentum-space language, while in the lattice theory it appears in the coordinate-space language.

In this paper, we study the one-dimensional quantum spin chain called XXZ model, on a semi-infinite lattice. The recent paper by Ghoshal–Zamolodchikov [16] has stimulated us in this work. Before introducing our results, let us give our motivation in comparison to their work.

In Ref. [16], after general consideration of the boundary problems in massive integrable field theories, two examples are worked out — the Ising field theory and the sine–Gordon model. As for the Ising model, it was already solved on the lattice by McCoy–Wu (see Ref. [25]). Although the Ising model is one of the first and best examples in integrable models, the origin of its solvability is somewhat special in the sense that free fermions can be used. Because of this, not only the partition function and magnetization but also the correlation functions are explicitly obtained in this model. In the developments during the 70–80's, the mechanisms of the solvability of other lattice models have been revealed. These use the idea of commuting transfer matrices and the quantum inverse scattering method. By these methods, the ground states and the excitations are obtained. However, our knowledge of the correlation functions are very limited except for the Ising model. More recently, influenced by the developments in the conformal field theory and the massive integrable field theory, the structure of the space of states in some lattice models (other than the Ising model) was fully understood. For example, for the six-vertex model in the anti-ferromagnetic regime, the space of the eigenvectors of the corner transfer matrix was identified with an irreducible highest-weight module $\mathrm{V}(\Lambda_i)$ $(i = 0,1)$ of the quantum affine algebra $\mathrm{U}_q(\widehat{\mathrm{sl}}_2)$. As a byproduct, integral formulas for the correlation functions are obtained.

In the treatment of the boundary theory in Ref. [16], Ghoshal and Zamolodchikov propose two different approaches, different in the direction of the time development. In comparison with the space of states in the lattice theory mentioned above, the time development in the direction parallel to the boundary is more interesting. They propose a certain equation for the boundary states $|i\rangle_{\mathrm{B}}$ $(i = 0,1)$ under the actions of creation operators without explicit construction of these states. In the lattice theory, we can actually test this assumption by looking for such a vector in an appropriate completion of the space $\mathrm{V}(\Lambda_i)$. In fact, we prove that the ground-state vectors of the commuting transfer matrices, to which we can give exact expressions in terms of bosonization, satisfy the equation of Ghoshal–Zamolodchikov. Furthermore, starting from this result, we can diagonalize the boundary hamiltonian, compute the S-matrix and the correlation functions. In particular, we get the exact formula for the boundary excitation energy and the boundary polarization. These quantities are particularly interesting because they represent the boundary effect.

To avoid confusion, we should state that the lattice model considered in this paper is not a lattice regularization of the SG model. The continuum limit of the model is the su(2)-invariant Thirring model. We will not discuss this limit in this paper.

Now, we concentrate on lattice models. In the standard treatment of integrable quan-

tum spin chains, 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.

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 Ref. [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 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)

$$K_2(\zeta_2)R_{21}(\zeta_1\zeta_2)K_1(\zeta_1)R_{12}(\zeta_1/\zeta_2) = R_{21}(\zeta_1/\zeta_2)K_1(\zeta_1)R_{12}(\zeta_1\zeta_2)K_2(\zeta_2)\,. \quad (1.1)$$

Several groups have investigated the solutions of (1.1) along with the Bethe ansatz equations for the models associated with them [7–13]. For a recent review and further references, see Ref. [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 Refs. [18–20] for related works).

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

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

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

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

For a systematic account of this method, see Ref. [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",

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

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 $U_q(\widehat{sl}_2)$, and $\mathcal{H}^*$ its dual. Here,

$$\Delta = \frac{q+q^{-1}}{2}, \tag{1.5}$$

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:

$$|i\rangle_B = e^{F_i}\,|i\rangle\,, \tag{1.6}$$

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 (2.27)) corresponds to the binding energy of the boundary bound state of Ref. [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. Mathematically, 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

$$h_c^{(1)} = \frac{(1+q)^2}{-4q} = -\frac{\Delta+1}{2}, \qquad h_c^{(2)} = \frac{(1-q)^2}{-4q} = -\frac{\Delta-1}{2}. \tag{1.7}$$

Physically, the meaning of the critical fields is related to the existence of S-matrix poles in the physical sheet. The boundary S-matrix has a pole in the physical sheet if and only if the boundary field h satisfies $h < h_c^{(1)}$ or $h > h_c^{(2)}$. In this way, we can show that the state $|1\rangle_B$ is the boundary bound state corresponding to this pole.

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

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

The matrix $M^{(i)}(\xi)$ is therefore the boundary S-matrix, analogous to that formulated in Ref. [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,

$$-\frac{{}_{\mathrm{B}}\langle 0|\sigma_1^z|0\rangle_{\mathrm{B}}}{{}_{\mathrm{B}}\langle 0|0\rangle_{\mathrm{B}}} = 1 + 2\sum_{l=1}^{\infty} \frac{(-q^2)^l(1-r)^2}{(1-q^{2l}r)^2},$$

where

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

The values of h where both vacuum states $|i\rangle_{\mathrm{B}}$ 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 $|i\rangle_{\mathrm{B}}$. 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,

$$H_{\mathrm{B}}^{\mathrm{fin}} = -\tfrac{1}{2}\sum_{k=1}^{N-1}\left(\sigma_{k+1}^x\sigma_k^x + \sigma_{k+1}^y\sigma_k^y + \Delta\sigma_{k+1}^z\sigma_k^z\right) + h_-\sigma_1^z + h_+\sigma_N^z. \tag{2.1}$$

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 ζ is the multiplicative spectral parameter. We also specify a matrix $K(\zeta)$, corresponding to an interaction at the boundary, which satisfies the boundary YBE (1.1). Here, we consider only the diagonal solution [15]

$$K(\zeta) = K(\zeta;r) = \frac{1}{f(\zeta;r)}\begin{pmatrix} \dfrac{1-r\zeta^2}{\zeta^2-r} & 0 \\ 0 & 1 \end{pmatrix}. \tag{2.2}$$

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

The scalar $f(\zeta;r)$ in (2.2) is

$$f(\zeta;r)=\frac{\varphi(\zeta^{-2};r)}{\varphi(\zeta^{2};r)}\,,\qquad \varphi(z;r)=\frac{(q^4rz;q^4)_\infty}{(q^2rz;q^4)_\infty}\frac{(q^6z^2;q^8)_\infty}{(q^8z^2;q^8)_\infty}\,, \tag{2.3}$$

and is chosen in such a way that $\log f(\zeta;r)$ is holomorphic in the region $1\leqslant|\zeta|\leqslant|q^{-1/2}|$ and the K-matrix obeys the relations

$$K(\zeta)K(\zeta^{-1})=1\,,\qquad \text{(Boundary unitarity)}\,, \tag{2.4}$$

$$K_a^b(-q^{-1}\zeta^{-1})=\sum_{a',b'}R_{a'-b'}^{-a\ b}\left(-q\zeta^2\right)K_{b'}^{a'}(\zeta)\,,\qquad \text{(Boundary crossing)}\,. \tag{2.5}$$

These ensure that the transfer matrix (2.13) satisfies the unitarity and crossing relations (2.16), (2.17). See Subsection 2.4 for a further discussion on this normalization.

A commuting family of transfer matrices is constructed from R and K as follows [6]:

$$T_{\mathrm{B}}^{\mathrm{fin}}(\zeta)=\mathrm{tr}_{\mathrm{V}_0}\left(K_+(\zeta)\mathcal{T}(\zeta^{-1})^{-1}K_-(\zeta)\mathcal{T}(\zeta)\right). \tag{2.6}$$

Here

$$\mathcal{T}(\zeta)=R_{01}(\zeta)\ldots R_{0N}(\zeta)\in\mathrm{End}\ (\mathrm{V}_0\otimes\mathrm{V}_1\otimes\ldots\otimes\mathrm{V}_N)$$

denotes the monodromy matrix, V_j are copies of $\mathbb{C}^2$, and

$$K_-(\zeta)=K(\zeta;r_-),\qquad K_+(\zeta)=K(-q^{-1}\zeta^{-1};r_+)^t\in\mathrm{End}\ (\mathrm{V}_0)\ ,$$

where $r_\pm$ are arbitrary parameters. Graphically, the transfer matrix (2.6) is represented in Fig. 1.

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

(i) The transfer matrices (2.6) form a commutative family:

$$[T_{\mathrm{B}}^{\mathrm{fin}}(\zeta),T_{\mathrm{B}}^{\mathrm{fin}}(\zeta')]=0\qquad\forall\zeta,\zeta'.$$

(ii) The hamiltonian (2.1) is obtained as

$$\frac{\mathrm{d}}{\mathrm{d}\zeta}T_{\mathrm{B}}^{\mathrm{fin}}(\zeta)\bigg|_{\zeta=1}=\frac{4q}{1-q^2}H_{\mathrm{B}}^{\mathrm{fin}}+\mathrm{const}\,, \tag{2.7}$$

where Δ is defined by (1.5) and

$$h_\pm=\mp\frac{1-q^2}{-4q}\frac{1+r_\pm}{1-r_\pm}\,. \tag{2.8}$$

In Ref. [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 Refs. [4,5] using the coordinate Bethe ansatz.

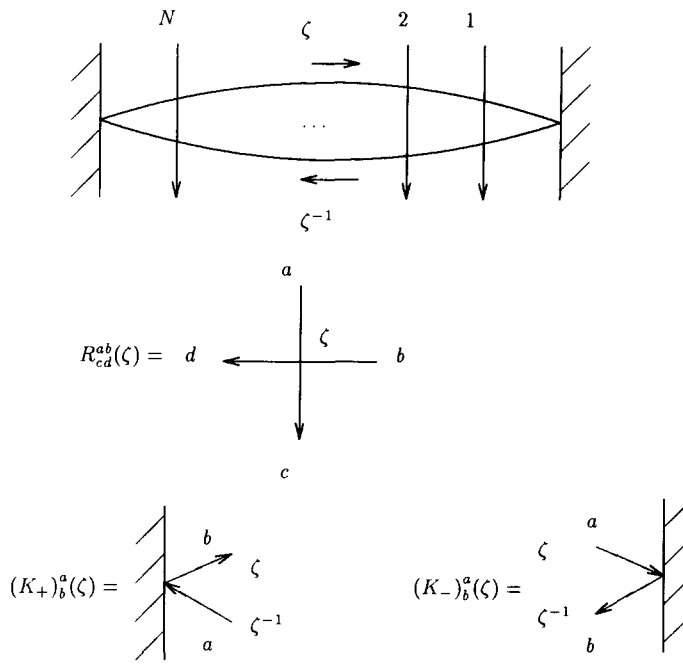

Fig. 1. Transfer matrix on a finite chain. The spectral parameters attached to the lines $1, \ldots, N$ are chosen to be 1.

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 $h \geqslant 0$, or

$$-1 \leqslant r \leqslant 1.$$

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 $\mathrm{U}_q(\mathrm{sl}_2)$ invariance [26].

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

In the naïve tensor product space $\ldots \otimes \mathrm{V} \otimes \mathrm{V} \otimes \mathrm{V}$, 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 $-2qH_{\mathrm{B}}$ scales to

$$H_{\mathrm{B},0} = \tfrac{1}{2} \sum_{k=1}^{\infty} (\sigma_{k+1}^z \sigma_k^z + 1) + \frac{1+r}{2(1-r)} \sigma_1^z \,, \tag{2.9}$$

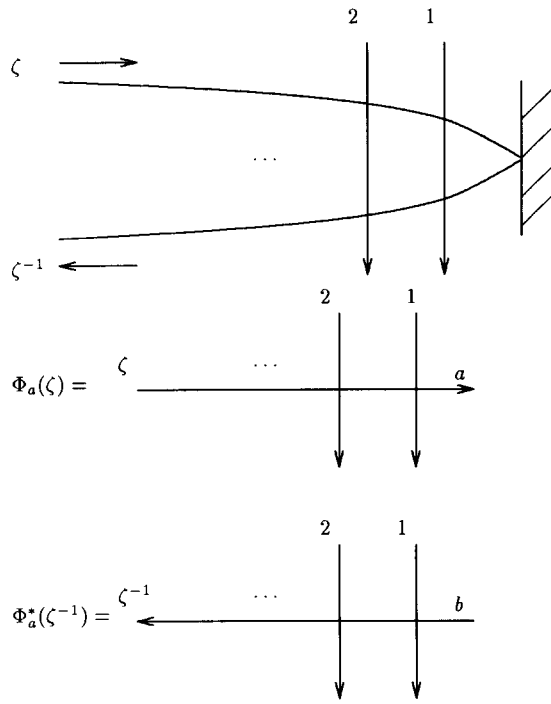

Fig. 2. Transfer matrix on the semi-infinite chain. By convention, the lattice sites are numbered $k = 1, 2, 3, \ldots$ from right to left.

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

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

$$|p^{(0)}\rangle = \ldots \otimes v_+ \otimes v_- \otimes v_+ \otimes v_- , \qquad |p^{(1)}\rangle = \ldots \otimes v_- \otimes v_+ \otimes v_- \otimes v_+ . \tag{2.10}$$

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 $p : \mathbb{Z}_{\geqslant 1} \to \{\pm\}$ satisfying the asymptotic boundary condition

$$p(k) = (-1)^{k+i} \quad \text{for } k \gg 1 . \tag{2.11}$$

When $r \neq -1$, the eigenvalues of $H_{\mathrm{B},0}$ corresponding to $|p^{(0)}\rangle$ and $|p^{(1)}\rangle$ differ:

$$H_{\mathrm{B},0}|p^{(0)}\rangle = -\frac{1+r}{2(1-r)}|p^{(0)}\rangle , \qquad H_{\mathrm{B},0}|p^{(1)}\rangle = \frac{1+r}{2(1-r)}|p^{(1)}\rangle .$$

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 $|i\rangle_{\mathrm{B}}$, unique up to a scalar multiple, which has the lowest energy in that sector. We call $|i\rangle_{\mathrm{B}}$ 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 Ref. [21]. Fig. 2 suggests (see chapter 4 of Ref. [23]) that we identify $\mathcal{H}^{(i)}$ with the integrable highest-weight module $\mathrm{V}(\Lambda_i)$ of $\mathrm{U}_q(\widehat{\mathrm{sl}}_2)$, $i = 0, 1$, and the horizontal lines with the components $\Phi_\varepsilon^{(1-i,i)}(\zeta)$ of the vertex operator of type I:

$$\Phi^{(1-i,i)}(\zeta) : \mathcal{H}^{(i)} \to \mathcal{H}^{(1-i)} \otimes \mathrm{V}, \qquad \Phi^{(1-i,i)}(\zeta) = \sum_\varepsilon \Phi_\varepsilon^{(1-i,i)}(\zeta) \otimes v_\varepsilon . \tag{2.12}$$

In the present case, the algebra $\mathrm{U}_q(\widehat{\mathrm{sl}}_2)$ 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 $\Phi_\varepsilon^{(1-i,i)}(\zeta)$ 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

$$T_{\mathrm{B}}^{(i)}(\zeta) = g \sum_{\varepsilon,\varepsilon'} \Phi_\varepsilon^{*(i,1-i)}(\zeta^{-1}) K_\varepsilon^{\varepsilon'}(\zeta) \Phi_{\varepsilon'}^{(1-i,i)}(\zeta) , \tag{2.13}$$

(cf. (2.6)). Here,

$$\Phi_\varepsilon^{*(i,1-i)}(\zeta) = \Phi_{-\varepsilon}^{(i,1-i)}\left(-q^{-1}\zeta\right) , \qquad g = \frac{\left(q^2;q^4\right)_\infty}{\left(q^4;q^4\right)_\infty} .$$

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))

$$\frac{\mathrm{d}}{\mathrm{d}\zeta} T_{\mathrm{B}}(\zeta) \bigg|_{\zeta=1} = \frac{4q}{1-q^2} H_{\mathrm{B}} . \tag{2.14}$$

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):

$$[T_{\mathrm{B}}(\zeta), T_{\mathrm{B}}(\zeta')] = 0 \qquad (\forall \zeta, \zeta') , \tag{2.15}$$

$$T_{\mathrm{B}}(1) = \mathrm{id}, \qquad T_{\mathrm{B}}(\zeta) T_{\mathrm{B}}(\zeta^{-1}) = \mathrm{id} , \tag{2.16}$$

$$T_{\mathrm{B}}\left(-q^{-1}\zeta^{-1}\right) = T_{\mathrm{B}}(\zeta) . \tag{2.17}$$

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,

$$T_{\mathrm{B}}(\zeta)|v\rangle = t(\zeta)|v\rangle\,, \tag{2.18}$$

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

$$t(1) = 1\,, \qquad t(\zeta)t(\zeta^{-1}) = 1\,, \qquad t\left(-q^{-1}\zeta^{-1}\right) = t(\zeta)\,. \tag{2.19}$$

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

$$\sum_{\varepsilon'} K_\varepsilon^{\varepsilon'}(\zeta)\Phi_{\varepsilon'}(\zeta)|v\rangle = t(\zeta)\Phi_\varepsilon(\zeta^{-1})|v\rangle \qquad (\varepsilon = \pm)\,. \tag{2.20}$$

Consider the region of the parameters where

$$1 < \zeta < 1+\varepsilon\,, \qquad -\varepsilon < q < 0\,, \qquad -1 < r < -1+\varepsilon\,, \tag{2.21}$$

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 $T_{\mathrm{B}}(\zeta)$ (see (2.14), and note that $q < 0$). In view of the study of $H_{\mathrm{B},0}$ in Subsection 2.2, we assume that (i) the largest eigenvalue of $T_{\mathrm{B}}^{(i)}(\zeta)$ has multiplicity one, and (ii) 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 $|i\rangle_{\mathrm{B}}$ of Subsection 2.2. We assume that

$$\Lambda^{(0)}(\zeta) = 1. \tag{2.22}$$

This assumption is related to our choice of the K-matrix in (2.13). Let us explain how to choose the factor $f(\zeta, r)$ so that one can expect (2.22) to be the largest eigenvalue. The process is analogous to the so-called inversion trick in the calculation of the partition function per site in the bulk theory, which we recall briefly. Consider the $M \times N$ lattice with cyclic boundary condition. The partition function Z_{MN} behaves as $Z_{MN} \sim \mu^{MN}$, where μ is called the partition function per site. The choice of $R(\zeta)$ in (A.1) is such that $\mu = 1$. (Or equivalently, $\mu = \kappa(\zeta)$ of (A.2) if the normalization is such that $R_{++}^{++}(\zeta) = R_{--}^{--}(\zeta) = 1$.)

The inversion trick works as follows. We start from the normalization of R such that the largest Boltzmann weights $R_{-+}^{+-}(\zeta) = R_{+-}^{-+}(\zeta)$ are 1. Because of the unitarity and crossing relations, the partition function per site $\mu(\zeta)$ obeys the functional relations:

$$\mu(\zeta)\mu(\zeta^{-1}) = \frac{(1-q^2)^2}{(1-q^2\zeta^2)(1-q^2\zeta^{-2})}\,, \qquad \mu(-q^{-1}\zeta^{-1}) = \mu(\zeta)\,.$$

Assuming the analyticity of $\log\mu(\zeta)$ in the region $1 \leqslant |\zeta| \leqslant |q^{-1/2}|$, the solution $\mu(\zeta)$ is uniquely determined.

The partition function Z_{MN} and the transfer matrix T_N are related as $Z_{MN} = \mathrm{tr}\,(T_N)^M \sim (\Lambda_N)^M$, where Λ_N is the largest eigenvalue of T_N. Therefore, once we normalize the Boltzmann weights in such a way that $\mu = 1$, Λ_N is finite for $N \to \infty$. In the vertex operator approach, we identify the semi-infinite transfer matrix with the type I vertex operator. In this identification, the eigenvalues of the transfer matrix are finite, and therefore, the corresponding Boltzmann weights are such that $\mu = 1$.

Now, let us consider the boundary problem. If $\mu = 1$, the partition function behaves as

$$Z_{\mathrm{B},MN} \sim \nu^M .$$

The surface term ν is related to the largest eigenvalue $\Lambda_{\mathrm{B},N}$ of the boundary transfer matrix as $\nu = \lim_{N\to\infty} \Lambda_{\mathrm{B},N}$. In the vertex operator approach, ν is equal to the largest eigenvalue $\Lambda^{(0)}(\zeta)$ of $T_{\mathrm{B}}(\zeta)$. The problem is to determine $\Lambda^{(0)}(\zeta)$, which is dependent on the choice of the $K(\zeta)$. In the analogy of the inversion trick we proceed as follows. Starting from the normalization of $K(\zeta)$ such that the largest matrix element $K_-^-(\zeta)$ to be 1, we derive relations for $\nu = \nu(\zeta)$ similar to (2.19). Again assuming the analyticity of $\log \nu(\zeta)$ in the region $1 \leqslant |\zeta| \leqslant |q^{-1/2}|$ we obtain the unique solution for $\nu(\zeta)$. After renormalization by $\nu(\zeta)$, we get the K-matrix in (2.2), and in this normalization we have (2.22).

As supporting evidence for (2.22), we use it to construct $|0\rangle_{\mathrm{B}}$ in Section 3. We then use the result to calculate, in Appendix B, the q-expansion of $|0\rangle_{\mathrm{B}}$ (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 $|p^{(0)}\rangle + \mathrm{O}(q)$, as required in Subsection 2.3. Therefore, we conclude that (2.22) is the correct lowest eigenvalue.

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

$$\Lambda(\zeta;r) = \frac{K_+^+(\zeta;r)}{K_-^-(\zeta;r^{-1})} = \frac{1}{\zeta^2}\frac{\Theta_{q^4}(r\zeta^2)}{\Theta_{q^4}(r\zeta^{-2})}\frac{\Theta_{q^4}(q^2r\zeta^{-2})}{\Theta_{q^4}(q^2r\zeta^2)} , \tag{2.23}$$

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

$$\Lambda^{(1)}(\zeta;r) = \Lambda(\zeta;r) . \tag{2.24}$$

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

$$\nu\Phi_{\varepsilon}^{(0,1)}(\zeta)\nu = \Phi_{-\varepsilon}^{(1,0)}(\zeta) . \tag{2.25}$$

Noting the relation

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

we find that

$$\nu^{-1}T_{\mathrm{B}}^{(1)}(\zeta;r)\nu = \Lambda(\zeta;r)T_{\mathrm{B}}^{(0)}(\zeta;r^{-1}) . \tag{2.26}$$

If r is close to -1, the eigenvalue 1 of $T_{\mathrm{B}}^{(0)}(\zeta;r^{-1})$ is the largest. Hence the largest eigenvalue of $T_{\mathrm{B}}^{(1)}(\zeta;r)$ is given by (2.24).

Now, let us compare the two energy levels $e^{(0)}(r)$ and $e^{(1)}(r)$ of H_{B}, corresponding to $|0\rangle_{\mathrm{B}}$ and $|1\rangle_{\mathrm{B}}$, 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 α is real and positive. From (2.22) 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 (2.23) and (2.14), we find

$$\Delta e(r) = \begin{cases} \epsilon(1)\ \mathrm{sn}(2K'\alpha, k') & \text{if } -1 \leqslant r < 0\,; \\ \dfrac{\epsilon(1)}{k'\ \mathrm{sn}(2K'\alpha, k')} & \text{if } 0 < r < 1\,, \end{cases} \tag{2.27}$$

where the Jacobi elliptic functions refer to the nome $-q = \exp(-\pi K'/K)$ (see 7.5 in Ref. [23]), and

$$\epsilon(\xi) = \frac{2K}{\pi} \sinh \frac{\pi K'}{K}\ \mathrm{dn}\left(\frac{2K}{\pi}\theta, k\right), \qquad \xi = -i\,\mathrm{e}^{i\theta}, \tag{2.28}$$

$$\epsilon(1) = \frac{2Kk'}{\pi} \sinh \frac{\pi K'}{K}\,. \tag{2.29}$$

In Fig. 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 $0 \leqslant h < h_{\mathrm{c}}^{(1)}$, and from $\epsilon(1)/k'$ (which is the maximum of the one-particle energy $\varepsilon(\xi)$, as pointed out by A. Klümper) to ∞ when $h_{\mathrm{c}}^{(2)} < h \leqslant \infty$. In the latter region, the energy of $|1\rangle_{\mathrm{B}}$ 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 Ref. [16], although it does not occur in the Ising model. When $h_{\mathrm{c}}^{(1)} < h < h_{\mathrm{c}}^{(2)}$, the state $|1\rangle_{\mathrm{B}}$ is well defined, as we shall argue in Subsection 3.1.

In the next section we shall find the vacuum vectors $|0\rangle_{\mathrm{B}}$ and $|1\rangle_{\mathrm{B}}$ 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 II, $\Psi_{\mu}^{*}(\xi)$ ($\mu = \pm$), in much the same way as in the bulk theory (see Ref. [23]). The commutation relations (A.8) imply that

$$\Psi_{\mu_1}^{*}(\xi_1) \cdots \Psi_{\mu_m}^{*}(\xi_m)|i\rangle_{\mathrm{B}}$$

is an eigenstate of $T_{\mathrm{B}}(\zeta)$ with eigenvalue $\Lambda^{(i)}(\zeta) \prod_{j=1}^{m} \tau_{\mathrm{B}}(\zeta, \xi_j)$, where

$$\tau_{\mathrm{B}}(\zeta, \xi) = \tau(\zeta/\xi)\tau(\zeta\xi) \tag{2.30}$$

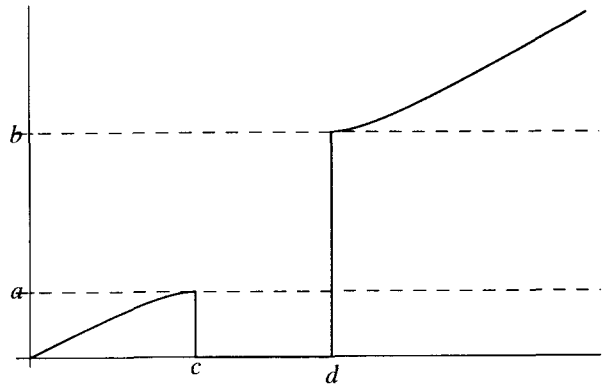

Fig. 3. The energy difference $\Delta e(r)$ between the vacuum states as a function of h, when $q = -0.15$. The energy $a = \epsilon(1)$, and $b = \epsilon(1)/k'$. The critical field $c = h_c^{(1)}$ and $d = h_c^{(2)}$.

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

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

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 (1.6), with

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

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

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

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

$$\alpha_n = -q^{6n}, \qquad \beta_n^{(0)} = -\frac{q^{7n/2}r^n}{[2n]} - \theta_n \frac{q^{5n/2}(1-q^n)}{[2n]},$$

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 $|0\rangle_{\mathrm{B}}$ found in this manner satisfies also the relation (2.20) with $\varepsilon = +$. Using

$$\mathrm{e}^{Q(z)}|0\rangle_{\mathrm{B}} = \varphi(z^{-1};r)\,\mathrm{e}^{P(z^{-1})}|0\rangle_{\mathrm{B}},$$
$$\mathrm{e}^{S^-(w)}|0\rangle_{\mathrm{B}} = (1-q^6w^{-2})(1-q^4rw^{-1})\,\mathrm{e}^{R^-(q^6w^{-1})}|0\rangle_{\mathrm{B}},$$

the verification is reduced to showing that

$$\oint \frac{\mathrm{d}w}{2\pi i w}\frac{(1-rz)(w^2-q^6)(w-rq^4)}{(w-q^2z)(w-q^4z)(w-q^4z^{-1})} \times \exp\left(R^-(w)+R^-(q^6w^{-1})\right)|0\rangle = (z \leftrightarrow z^{-1}).$$

Here the contour encircles $w = 0,\ q^4z^{\pm1}$ but not $q^2z^{\pm1}$. The desired equality can be shown by the change of variable $w \to q^6w^{-1}$.

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

$${}_{\mathrm{B}}\langle i|T_{\mathrm{B}}(\zeta) = \Lambda^{(i)}(\zeta)\,{}_{\mathrm{B}}\langle i|.$$

The analog of (2.20) is

$$\sum_{\varepsilon} {}_{\mathrm{B}}\langle i|\Phi_\varepsilon^*(\zeta^{-1})K_\varepsilon^{\varepsilon'}(\zeta) = \Lambda^{(i)}(\zeta)\,{}_{\mathrm{B}}\langle i|\Phi_{\varepsilon'}^*(\zeta) \qquad (\varepsilon' = \pm). \tag{3.3}$$

The results are summarized as follows:

$$|i\rangle_{\mathrm{B}} = \mathrm{e}^{F_i}|i\rangle, \qquad F_i = \tfrac{1}{2}\sum_{n=1}^{\infty}\frac{n\alpha_n}{[2n][n]}a_{-n}^2 + \sum_{n=1}^{\infty}\beta_n^{(i)}a_{-n}, \tag{3.4}$$

$${}_{\mathrm{B}}\langle i| = \langle i|\,\mathrm{e}^{G_i}, \qquad G_i = \tfrac{1}{2}\sum_{n=1}^{\infty}\frac{n\gamma_n}{[2n][n]}a_n^2 + \sum_{n=1}^{\infty}\delta_n^{(i)}a_n, \tag{3.5}$$

where

$$\alpha_n = -q^{6n}, \qquad \gamma_n = -q^{-2n}, \tag{3.6}$$

$$\beta_n^{(i)} = -\theta_n \frac{q^{5n/2}(1-q^n)}{[2n]} + \begin{cases} -\dfrac{q^{7n/2}r^n}{[2n]} & (i=0)\ ; \\ +\dfrac{q^{3n/2}r^{-n}}{[2n]} & (i=1)\ , \end{cases} \tag{3.7}$$

$$\delta_n^{(i)} = \theta_n \frac{q^{-3n/2}(1-q^n)}{[2n]} + \begin{cases} -\dfrac{q^{-5n/2}r^n}{[2n]} & (i=0)\ ; \\ +\dfrac{q^{-n/2}r^{-n}}{[2n]} & (i=1)\ . \end{cases} \tag{3.8}$$

The relation (2.26) suggests that the two vacuum vectors should be related by

$$\nu\left(|0\rangle_{\mathrm{B}}\right)\Big|_{r\to r^{-1}} = |1\rangle_{\mathrm{B}}\,. \tag{3.9}$$

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

$$T_{\mathrm{B}}^{(i)}(\zeta;t) = g\sum_{\varepsilon,\varepsilon'} \Phi_\varepsilon^{*(i,1-i)}(t\zeta^{-1})K_\varepsilon^{\varepsilon'}(\zeta)\Phi_{\varepsilon'}^{(1-i,i)}(t\zeta)\,, \tag{3.10}$$

which corresponds to changing the spectral parameters for the vertical lines from 1 to t^{-1}. The properties (2.15)–(2.17) are unaffected by this change. The vacuum vectors for (3.10) are obtained by replacing

$$a_n \to t^{-2n}a_n\,, \qquad a_{-n} \to t^{2n}a_{-n} \qquad (n>0)$$

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

$$_{\mathrm{B}}\langle 0|\Phi_-^*(t\zeta^{-1})\Phi_-(t\zeta) = \lambda(\zeta^2)\,_{\mathrm{B}}\langle 0|\,, \quad \Phi_-^*(t\zeta^{-1})\Phi_-(t\zeta)|0\rangle_{\mathrm{B}} = \lambda(\zeta^2)|0\rangle_{\mathrm{B}}\,,$$
$$_{\mathrm{B}}\langle 1|\Phi_+^*(t\zeta^{-1})\Phi_+(t\zeta) = \lambda(\zeta^2)\,_{\mathrm{B}}\langle 1|\,, \quad \Phi_+^*(t\zeta^{-1})\Phi_+(t\zeta)|1\rangle_{\mathrm{B}} = \lambda(\zeta^2)|1\rangle_{\mathrm{B}}\,,$$

with

$$\lambda(z) = \frac{(q^8z^2;q^8)_\infty}{(q^6z^2;q^8)_\infty}\frac{(q^4z^{-2};q^8)_\infty}{(q^2z^{-2};q^8)_\infty}.$$

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

Next, consider the small-q expansion of the vectors $|i\rangle_{\mathrm{B}}$ $(i=0,1)$. 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 $|i\rangle_{\mathrm{B}}$ 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 $|0\rangle_{\mathrm{B}}$ in terms of the global base vectors. Although we have no proof to all orders, the expansion suggests that $|0\rangle_{\mathrm{B}}$ is well defined

when $h \geqslant 0$, but not when $|r| \geqslant 1/|q|$, i.e., $-h_c^{(2)} \leqslant h \leqslant -h_c^{(1)}$. 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 $h \geqslant 0$:

(i) $0 \leqslant h < h_c^{(1)}$: Both $|0\rangle_B$ and $|1\rangle_B$ are well defined;
(ii) $h_c^{(1)} \leqslant h \leqslant h_c^{(2)}$: $|0\rangle_B$ is well defined, but $|1\rangle_B$ is not well defined;
(iii) $h_c^{(2)} < h \leqslant \infty$: 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 (2.30) 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 ${}_B\langle i|$ and $|i\rangle_B$, we find

$$\Psi^*_\mu(\xi)|i\rangle_B = M^{(i)\mu}_\mu(\xi)\Psi^*_\mu(\xi^{-1})|i\rangle_B\,, \tag{3.11}$$
$${}_B\langle i|\Psi_\mu(\xi^{-1}) = {}_B\langle i|\Psi_\mu(\xi)M^{(i)\mu}_\mu(\xi)\,. \tag{3.12}$$

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

$$M^{(0)\mu}_\mu(\xi) = M^\mu_\mu(\xi;r)\,, \qquad M^{(1)\mu}_\mu(\xi) = M^{-\mu}_{-\mu}(\xi;r^{-1})\,, \tag{3.13}$$

where

$$M(\xi;r) = \frac{1}{\overline{f}(\xi;r)}\begin{pmatrix} \dfrac{1-rq^{-1}\xi^2}{\xi^2-rq^{-1}} & 0 \\ 0 & 1 \end{pmatrix} \tag{3.14}$$

and

$$\overline{f}(\xi;r) = -\xi^2\frac{\overline{\varphi}(\xi^{-2};r)}{\overline{\varphi}(\xi^2;r)}\,, \qquad \overline{\varphi}(z;r) = \frac{(q^3rz;q^4)_\infty}{(qrz;q^4)_\infty}\frac{(q^2z^2;q^8)_\infty}{(q^8z^2;q^8)_\infty}\,.$$

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 $r \to rq^{-1}$. The M-matrix has properties similar to those of the K-matrix:

$$M_2(\xi_2)S_{12}(\xi_2\xi_1)M_1(\xi_1)S_{21}(\xi_1/\xi_2) = S_{12}(\xi_1/\xi_2)M_1(\xi_1)S_{21}(\xi_1\xi_2)M_2(\xi_2)\,,$$
$$M(\xi)M(\xi^{-1}) = 1\,,$$
$$M^b_a(-q^{-1}\xi^{-1}) = \sum_{a',b'} S^{b'\,-a'}_{-b\,a}(-q\xi^2)M^{a'}_{b'}(\xi)\,. \tag{3.15}$$

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 Ref. [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 Ref. [16]. The boundary S-matrix is given by

$$R_h(\theta) = i \tanh\left(\frac{\pi i}{4} - \frac{\theta}{2}\right) \frac{\kappa - i\sinh\theta}{\kappa + i\sinh\theta}, \tag{3.16}$$

where θ 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 $0 \leqslant h < \sqrt{2m}$, the pole of $R_h(\theta)$ at $\theta = \frac{1}{2}\pi i - iv$, where $\kappa = \cos v$, stays in the physical strip, $0 < \operatorname{Im}\theta \leqslant \pi$. When $h \geqslant \sqrt{2m}$, the pole moves away from the physical strip.

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

We recognize that $|1\rangle_{\mathrm{B}}$ 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 $\Psi_+^*(\xi)|0\rangle_{\mathrm{B}}$ has a series of simple poles at

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

By explicit computation, we find that the state $|1\rangle_{\mathrm{B}}$ can be obtained as the residue at the first pole:

$$\operatorname{Res}_{\xi^2=q^{-1}r}\left({}_{\mathrm{B}}\langle 0|\Psi_+(\xi^{-1})\frac{\mathrm{d}\xi^2}{\xi^2}\right) = gc(r^{-1})\ {}_{\mathrm{B}}\langle 1|, \tag{3.17}$$

$$\operatorname{Res}_{\xi^2=q^{-1}r}\left(\Psi_+^*(\xi)|0\rangle_{\mathrm{B}}\frac{\mathrm{d}\xi^2}{\xi^2}\right) = gc(r^{-1})\ |1\rangle_{\mathrm{B}}, \tag{3.18}$$

where $c(z) = (q^2z^2;q^8)_\infty/(q^4z^2;q^8)_\infty$. Eqs. (3.17), (3.18) are also valid if we replace ${}_{\mathrm{B}}\langle 0|\Psi_+(\xi^{-1}) \to {}_{\mathrm{B}}\langle 1|\Psi_-(\xi^{-1})$, $\Psi_+^*(\xi)|0\rangle_{\mathrm{B}} \to \Psi_-^*(\xi)|1\rangle_{\mathrm{B}}$ and $r \to r^{-1}$. The formulas above allow us to interpret $|i\rangle_{\mathrm{B}}$ 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:

$$P^{(i)}_{\varepsilon_1\dots\varepsilon_N}(\zeta_1,\dots,\zeta_N) = \frac{{}_{\mathrm{B}}\langle i|\Phi^{(i,1-i)}_{\varepsilon_1}(\zeta_1)\Phi^{(1-i,i)}_{\varepsilon_2}(\zeta_2)\dots\Phi^{(1-i,i)}_{\varepsilon_N}(\zeta_N)|i\rangle_{\mathrm{B}}}{{}_{\mathrm{B}}\langle i|i\rangle_{\mathrm{B}}}. \tag{4.1}$$

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

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

Since the total spin is conserved, (4.1) is nontrivial 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 (2.25), one obtains

$$P^{(1)}_{\varepsilon_1\dots\varepsilon_N}(\zeta_1,\dots,\zeta_N) = P^{(0)}_{-\varepsilon_1\dots-\varepsilon_N}(\zeta_1,\dots,\zeta_N)\Big|_{r\to r^{-1}}. \tag{4.2}$$

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

$$\begin{aligned} P^{(i)}_{\varepsilon_1\dots\varepsilon_N}(\zeta_1,\dots,\zeta_N) &= (-q^3)^{N^2/4+iN/2-\sum_{a\in\mathrm{A}} a}(1-q^2)^{N/2} \\ &\quad\times\prod_{j=1}^N \zeta_j^{(1+\epsilon_j)/2-j+N+i}\prod_{j<k}\frac{(q^2z_k/z_j;q^4)_\infty}{(q^4z_k/z_j;q^4)_\infty} \\ &\quad\times\prod_{a\in\mathrm{A}}\oint_{C_a}\frac{\mathrm{d}w_a w_a^{1-i}}{2\pi\sqrt{-1}}\frac{\prod_{a<b}(w_a-w_b)(w_a-q^2w_b)}{\prod_{j\leqslant a}(z_j-q^{-2}w_a)\prod_{a\leqslant j}(w_a-q^4z_j)} \\ &\quad\times I^{(i)}(\{z_j\},\{w_a\}), \end{aligned} \tag{4.3}$$

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

$$I^{(i)}(\{z_j\},\{w_a\}) = \frac{{}_{\mathrm{B}}\langle i|\exp\left(\sum_{n=1}^\infty a_{-n}X_n\right)\exp\left(-\sum_{n=1}^\infty a_nY_n\right)|i\rangle_{\mathrm{B}}}{{}_{\mathrm{B}}\langle i|i\rangle_{\mathrm{B}}},$$

$$X_n = \frac{q^{7n/2}}{[2n]}\sum_{j=1}^N z_j^n - \frac{q^{n/2}}{[n]}\sum_a w_a^n,$$

$$Y_n = \frac{q^{-5n/2}}{[2n]} \sum_{j=1}^{N} z_j^{-n} - \frac{q^{n/2}}{[n]} \sum_a w_a^{-n} .$$

Next let us calculate the expectation value $I^{(i)}(\{z_j\},\{w_a\})$. By using the Bogoliubov transformation (3.2), we obtain

$$I^{(i)}(\{z_j\},\{w_a\}) = \frac{\langle i|\, \mathrm{e}^{G_i}\, \mathrm{e}^{F_i} \exp\left(\sum_{n=1}^{\infty} a_{-n}(X_n - \alpha_n Y_n)\right) |i\rangle}{{}_{\mathrm{B}}\langle i|i\rangle_{\mathrm{B}}}$$
$$\times \exp\left(-\sum_{n=1}^{\infty} \frac{[2n][n]}{n} \beta_n^{(i)} Y_n\right) \exp\left(\tfrac{1}{2}\sum_{n=1}^{\infty} \frac{[2n][n]}{n} \alpha_n Y_n^2\right) .$$

We then insert between e^{G_i} and e^{F_i} the completeness relation of the coherent states (C.4) and use the integration formula (C.5). As a result we find

$$I^{(i)}(\{z_j\},\{w_a\}) \times \prod_{n=1}^{\infty} (1-\alpha_n\gamma_n)^{1/2}$$
$$= \exp\Bigg(\sum_{n=1}^{\infty} \frac{[2n][n]}{n} \frac{1}{1-\alpha_n\gamma_n} \{\tfrac{1}{2}\gamma_n X_n^2 - \alpha_n\gamma_n X_n Y_n$$
$$+\tfrac{1}{2}\alpha_n Y_n^2 + (\delta_n^{(i)} + \gamma_n\beta_n^{(i)}) X_n - (\beta_n^{(i)} + \alpha_n\delta_n^{(i)}) Y_n\}\Bigg) , \tag{4.4}$$

$${}_{\mathrm{B}}\langle i|i\rangle_{\mathrm{B}} \times \prod_{n=1}^{\infty} (1-\alpha_n\gamma_n)^{1/2}$$
$$= \exp\left(\tfrac{1}{2}\sum_{n=1}^{\infty} \frac{[2n][n]}{n} \frac{1}{1-\alpha_n\gamma_n} \left\{\gamma_n\beta_n^{(i)2} + \alpha_n\delta_n^{(i)2} + 2\beta_n^{(i)}\delta_n^{(i)}\right\}\right) . \tag{4.5}$$

The sums in the right-hand sides are evaluated by making use of the following formulas:

$$\exp\left(\sum_{n=1}^{\infty} \frac{[n]}{n} q^{-5n/2} z^n \beta_n^{(i)}\right) = \left(\frac{(q^4z^2;q^4)_\infty}{(q^2z^2;q^4)_\infty}\right)^{-1/2} \begin{cases} \varphi(z;r)^{-1} , \\ \left[(1-r^{-1}z)\varphi(z;r^{-1})\right]^{-1} , \end{cases}$$

$$\exp\left(\sum_{n=1}^{\infty} \frac{[2n]}{n} q^{an} w^n \beta_n^{(i)}\right) = \left(\frac{1-q^{2a+5}w^2}{1-q^{2a+7}w^2}\right)^{1/2} \begin{cases} 1-q^{a+7/2}rw , \\ (1-q^{a+3/2}r^{-1}w)^{-1} , \end{cases}$$

$$\exp\left(\sum_{n=1}^{\infty} \frac{[n]}{n} q^{3n/2} z^n \delta_n^{(i)}\right) = \left(\frac{(q^4z^2;q^4)_\infty}{(q^2z^2;q^4)_\infty}\right)^{1/2} \begin{cases} (1-rz)\varphi(z;r) , \\ \varphi(z;r^{-1}) , \end{cases}$$

$$\exp\left(\sum_{n=1}^{\infty} \frac{[2n]}{n} q^{an} w^n \delta_n^{(i)}\right) = \left(\frac{1-q^{2a-1}w^2}{1-q^{2a-3}w^2}\right)^{1/2} \begin{cases} 1-q^{a-5/2}rw , \\ (1-q^{a-1/2}r^{-1}w)^{-1} . \end{cases}$$

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:

$$ {}_{\mathrm{B}}\langle 0|0\rangle_{\mathrm{B}} = \frac{(q^4r^2;q^8)_\infty}{(q^6;q^8)_\infty(q^2r^2;q^8)_\infty}, \tag{4.6} $$

$$ {}_{\mathrm{B}}\langle 1|1\rangle_{\mathrm{B}} = \frac{(q^4/r^2;q^8)_\infty}{(q^6;q^8)_\infty(q^2/r^2;q^8)_\infty}. \tag{4.7} $$

The N-point function:

$$ \begin{aligned} &P^{(i)}_{\varepsilon_1\ldots\varepsilon_N}(\zeta_1,\ldots,\zeta_N) \\ &= (-q^3)^{N^2/4-\sum_{a\in\mathrm{A}}a}\left(\frac{\{q^6\}_\infty}{\{q^8\}_\infty}\right)^N (q^2;q^2)_\infty^{N/2}\prod_{j=1}^N \zeta_j^{(1+\varepsilon_j)/2-j+N} \\ &\quad\times\prod_{j<k}\frac{\{q^6z_jz_k\}_\infty\{q^6z_j/z_k\}_\infty\{q^6z_k/z_j\}_\infty\{q^2/z_jz_k\}_\infty}{\{q^8z_jz_k\}_\infty\{q^8z_j/z_k\}_\infty\{q^8z_k/z_j\}_\infty\{q^4/z_jz_k\}_\infty} \\ &\quad\times\prod_{j=1}^N\frac{[q^{10}z_j^2]_\infty[q^{14}z_j^2]_\infty[q^{10}/z_j^2]_\infty[q^6/z_j^2]_\infty}{[q^{12}z_j^2]_\infty[q^{16}z_j^2]_\infty[q^{12}/z_j^2]_\infty[q^8/z_j^2]_\infty} \\ &\quad\times\prod_{a\in\mathrm{A}}\oint_{C_a^{(i)}}\frac{\mathrm{d}w_a}{2\pi\sqrt{-1}}\frac{w_a^{N-2a}(q^{-2}w_a^2;q^4)_\infty(q^6/w_a^2;q^4)_\infty}{\prod_{j\leqslant a}(z_j-q^{-2}w_a)\prod_{a\leqslant j}(w_a-q^4z_j)} \\ &\quad\times\frac{\prod_{a<b}(q^{-2}w_aw_b;q^2)_\infty(q^4w_a/w_b;q^2)_\infty(w_b/w_a;q^2)_\infty(q^6/w_aw_b;q^2)_\infty}{\prod_a\prod_j(q^2z_jw_a;q^4)_\infty(q^8z_j/w_a;q^4)_\infty(q^2w_a/z_j;q^4)_\infty(q^4/z_jw_a;q^4)_\infty} \\ &\quad\times\begin{cases}\displaystyle\prod_{j=1}^N\frac{(q^2rz_j;q^4)_\infty}{(q^4rz_j;q^4)_\infty}\prod_a\frac{w_a}{1-q^{-2}rw_a} & (\text{for } i=0)\,, \\ \displaystyle(-q^3)^{N/2}\prod_{j=1}^N\zeta_j\frac{(r^{-1}z_j^{-1};q^4)_\infty}{(q^2r^{-1}z_j^{-1};q^4)_\infty}\prod_a\frac{1}{1-q^2r^{-1}w_a^{-1}} & (\text{for } i=1)\,. \end{cases} \end{aligned} \tag{4.8} $$

Here, the contour $C_a^{(0)}$ encircles the points $q^{4l}z_j^{-1}$ (for all j), $q^{4l}z_j$ $(a \leqslant j)$ and $q^{4+4l}z_j$ $(a > j)$, $l = 1,2,3,\ldots$ but not the point q^2r^{-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

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

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

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 $\langle\sigma_1^z\rangle$.

Let L be a linear operator on the n-fold tensor product of the two-dimensional space $\mathrm{V}\otimes\cdots\otimes\mathrm{V}$. 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 [22,23]. Explicitly, if L is the spin operator at the nth site

$$\sigma_n^\alpha = \sigma^\alpha \otimes \underbrace{\mathrm{id}\otimes\cdots\otimes\mathrm{id}}_{n-1} \qquad (\alpha = \pm, z)\,,$$

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

$$\mathcal{L}^{(i)\pm} = E^{(i)}_{\pm\mp}(1,\dots,1)\,, \tag{4.9}$$

$$\mathcal{L}^{(i)z} = E^{(i)}_{++}(1,\dots,1) - E^{(i)}_{--}(1,\dots,1)\,, \tag{4.10}$$

where

$$\begin{aligned} E^{(i)}_{\varepsilon\varepsilon'}(\zeta_1,\dots,\zeta_n) = g^n \sum_{\varepsilon_1,\dots,\varepsilon_{n-1}} & \Phi^{*(i,1-i)}_{\varepsilon_1}(\zeta_1)\dots\Phi^{*(\iota,1-\iota)}_{\varepsilon_{n-1}}(\zeta_{n-1})\Phi^{*(1-\iota,\iota)}_{\varepsilon}(\zeta_n) \\ & \times\Phi^{(\iota,1-\iota)}_{\varepsilon'}(\zeta_n)\Phi^{(1-\iota,\iota)}_{\varepsilon_{n-1}}(\zeta_{n-1})\dots\Phi^{(1-i,i)}_{\varepsilon_1}(\zeta_1) \end{aligned} \tag{4.11}$$

with $\iota = i$ for even n and $\iota = 1-i$ 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:

$$\begin{aligned} & {}_{\mathrm{B}}\langle i|E^{(i)}_{\varepsilon_n\varepsilon'_n}(\zeta_1,\dots,\zeta_n)E^{(i)}_{\varepsilon_{n-1}\varepsilon'_{n-1}}(\zeta_1,\dots,\zeta_{n-1})\dots E^{(i)}_{\varepsilon_1\varepsilon'_1}(\zeta_1)|i\rangle_{\mathrm{B}} \\ & = g^n\,{}_{\mathrm{B}}\langle i|\Phi^{*(i,1-i)}_{\varepsilon_1}(\zeta_1)\dots\Phi^{*(1-\iota,\iota)}_{\varepsilon_n}(\zeta_n)\Phi^{(\iota,1-\iota)}_{\varepsilon'_n}(\zeta_n)\dots\Phi^{(1-i,i)}_{\varepsilon'_1}(\zeta_1)|i\rangle_{\mathrm{B}}\,. \end{aligned}$$

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

$$\begin{aligned} & \varepsilon_1,\varepsilon_2,\dots,\varepsilon_N \to -\varepsilon_1,\dots,-\varepsilon_n,\varepsilon'_n,\dots,\varepsilon'_1\,, \\ & \zeta_1,\zeta_2,\dots,\zeta_N \to -q^{-1}\zeta_1,\dots,-q^{-1}\zeta_n,\zeta_n,\dots,\zeta_1\,. \end{aligned}$$

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

$$\begin{aligned} \mathcal{M}^{(i)}(\zeta;r) &= \frac{{}_{\mathrm{B}}\langle i|\left(E^{(i)}_{++}(\zeta) - E^{(i)}_{--}(\zeta)\right)|i\rangle_{\mathrm{B}}}{{}_{\mathrm{B}}\langle i|i\rangle_{\mathrm{B}}} \\ &= g\left(P^{(i)}_{-+}(-q^{-1}\zeta,\zeta) - P^{(i)}_{+-}(-q^{-1}\zeta,\zeta)\right). \end{aligned}$$

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

$$\mathcal{M}^{(i)}(\zeta^{-1};r) = \mathcal{M}^{(i)}(\zeta;r)\,. \tag{4.12}$$

From (4.2) we have in addition

$$\mathcal{M}^{(1)}(\zeta;r) = -\mathcal{M}^{(0)}(\zeta;r^{-1})\,, \tag{4.13}$$

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

Specializing the integral formula (4.8) to $N=2$, $\zeta_1=-q^{-1}\zeta$ and $\zeta_2=\zeta$, we obtain

$$gP^{(i)}_{\mp\pm}(-q^{-1}\zeta,\zeta)=\mp g(z)p^{(i)}_{\pm}(z,r)\,, \tag{4.14}$$

where

$$g(z)=\frac{(q^2;q^2)^4_\infty}{(q^4;q^4)^2_\infty}\frac{\Theta_{q^4}(z^2)}{1-z^2}=g(z^{-1})\,,$$

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

$$F(w,z,r)=\frac{(1-rz)(1-q^{-2}wz)}{z(1-q^{-2}wr)}\frac{\Theta_{q^4}(q^2w^2)}{\Theta_{q^2}(wz)\Theta_{q^2}(w/z)}\,.$$

The contour $C^{(0)}_{--}$ encircles the points $q^{2l}z$, $q^{2l}z^{-1}$ with $l=1,2,\ldots$, but not the point q^2r^{-1}. The contour $C^{(0)}_{++}$ 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 $w\to q^4/w$ we find

$$P^{(1)}_{\varepsilon_1,\varepsilon_2}(-q^{-1}\zeta,\zeta)=P^{(0)}_{-\varepsilon_1,-\varepsilon_2}(-q^{-1}\zeta,\zeta)\Big|_{r\to r^{-1}}\,, \tag{4.15}$$

$$p^{(0)}_{\pm}(z,r)=-p^{(0)}_{\mp}(z^{-1},r^{-1})+G(z,r)\,, \tag{4.16}$$

where

$$\begin{aligned}G(z,r)&=-\mathrm{Res}_{w=q^2r}F(w,z^{-1},r^{-1})\\&=(1-rz)(1-r/z)\frac{\Theta_{q^4}(q^2r^2)}{\Theta_{q^2}(rz)\Theta_{q^2}(r/z)}\,.\end{aligned}$$

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

$$\begin{aligned}&-\left(\mathcal{M}^{(0)}(\zeta;r)+\mathcal{M}^{(0)}(\zeta;r^{-1})\right)\\&=g(z)\left(p^{(0)}_{+}(z^{-1},r)+p^{(0)}_{-}(z^{-1},r)+p^{(0)}_{+}(z,r^{-1})+p^{(0)}_{-}(z,r^{-1})\right)\\&=2g(z)G(z,r)\,.\end{aligned} \tag{4.17}$$

The integral for $p^{(0)}_{\pm}(z,r)$ 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

$$\begin{aligned}-\mathcal{M}^{(0)}(\zeta;r)&=g(z)\left(p^{(0)}_{+}(z,r)+p^{(0)}_{-}(z,r)\right)\\&=1+2\sum_{l=1}^{\infty}\frac{(-q^2)^l(1-rz)(1-r/z)}{(1-q^{2l}rz)(1-q^{2l}r/z)}\,.\end{aligned} \tag{4.18}$$

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

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

$$\mathcal{M}^{(i)}(r) = \frac{{}_{\mathrm{B}}\langle i|\sigma_1^z|i\rangle_{\mathrm{B}}}{{}_{\mathrm{B}}\langle i|i\rangle_{\mathrm{B}}} = \mathcal{M}^{(i)}(1;r)\,.$$

Noting (4.13), we have

$$-\mathcal{M}^{(0)}(r) = \mathcal{M}^{(1)}(r^{-1}) = 1 + 2\sum_{l=1}^{\infty} \frac{(-q^2)^l(1-r)^2}{(1-q^{2l}r)^2}\,, \tag{4.19}$$

$$\mathcal{M}^{(1)}(r) - \mathcal{M}^{(0)}(r) = 2\frac{(q^2;q^2)_\infty^4}{(q^2;q^4)_\infty^2}\frac{(q^2r^2;q^4)_\infty(q^2/r^2;q^4)_\infty}{(q^2r;q^2)_\infty^2(q^2/r;q^2)_\infty^2}\,. \tag{4.20}$$

When r takes the values $r_{\mathrm{c}}^{(1)} = q$ and $r_{\mathrm{c}}^{(2)} = -q$, corresponding to the critical fields $h_{\mathrm{c}}^{(1)}$ and $h_{\mathrm{c}}^{(2)}$, 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 $|0\rangle_{\mathrm{B}}$ for $h \geqslant 0$ and $|1\rangle_{\mathrm{B}}$ for $h \leqslant 0$, 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

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

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 (2.27), that the following relation holds:

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

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 nontrivial boundary term, it is necessary to scale r near the point $r = 1$. Setting

$$r = (q^2)^\alpha$$

the hamiltonian (1.2) scales to

$$H_{\mathrm{B}}^{\mathrm{bare}} = \tfrac{1}{2}\sum_{k=1}^{\infty}\left(-\sigma_{k+1}^x\sigma_k^x - \sigma_{k+1}^y\sigma_k^y + \sigma_{k+1}^z\sigma_k^z\right) + h\sigma_1^z\,,$$

where $h = 1/2\alpha$. It turns out that we should also scale the parameter ξ 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,

$$\begin{aligned} M_-^-(\xi;r) &= (q^2)^{-\sqrt{-1}\lambda} \\ &\times \frac{\Gamma_{q^4}\left(\frac{1}{4}+\frac{1}{2}(\alpha+\sqrt{-1}\lambda)\right)}{\Gamma_{q^4}\left(\frac{1}{4}+\frac{1}{2}(\alpha-\sqrt{-1}\lambda)\right)}\frac{\Gamma_{q^4}\left(\frac{3}{4}+\frac{1}{2}(\alpha-\sqrt{-1}\lambda)\right)}{\Gamma_{q^4}\left(\frac{3}{4}+\frac{1}{2}(\alpha+\sqrt{-1}\lambda)\right)} \\ &\times \frac{\Gamma_{q^8}\left(\frac{1}{4}-\frac{1}{2}\sqrt{-1}\lambda\right)}{\Gamma_{q^8}\left(\frac{1}{4}+\frac{1}{2}\sqrt{-1}\lambda\right)}\frac{\Gamma_{q^8}\left(1+\frac{1}{2}\sqrt{-1}\lambda\right)}{\Gamma_{q^8}\left(1-\frac{1}{2}\sqrt{-1}\lambda\right)}. \end{aligned}$$

In the limit $q \to -1$, the q-gamma function is the ordinary gamma function, and

$$\frac{M_+^+(\lambda;\alpha)}{M_-^-(\lambda;\alpha)} = \frac{\sqrt{-1}\lambda+\alpha-\frac{1}{2}}{\sqrt{-1}\lambda-\alpha+\frac{1}{2}}.$$

Denoting by $\mathcal{R}(\lambda)$ and $\mathcal{K}(\lambda;\alpha)$ the R- and K-matrices in Ref. [10] (see Eqs. (5.17), (5.19), (5.30) and (5.36) in Ref. [10]),

$$\begin{aligned} \lim S_{12}(\xi_1/\xi_2) &= -\sigma_1^z\mathcal{R}(\lambda_1-\lambda_2)\sigma_2^z, \\ \lim M(\xi;r) &= -\sigma^z\mathcal{K}(\lambda;\alpha). \end{aligned}$$

Following Ref. [29], p. 99, let us modify the signs and define the limiting states by

$$|\lambda_n,\dots,\lambda_1\rangle_{\mu_n,\dots,\mu_1;(i)B} = \prod_{j:\mathrm{odd}}(-\mu_j)\lim \Psi^*_{\mu_n}(\xi_n)\dots\Psi^*_{\mu_1}(\xi_1)|i\rangle_{\mathrm{B}}, \tag{5.1}$$

where $\xi_j = \sqrt{-1}(q^2)^{\sqrt{-1}\lambda_j/2}$. Notice that

$$|-\lambda_1\rangle_{\mu_1;(i)B} = \lim \Psi^*_{\mu_1}(-\xi_1^{-1})|i\rangle_{\mathrm{B}} = (-1)^{i+(1-\mu)/2}\lim \Psi^*_{\mu_1}(\xi_1^{-1})|i\rangle_{\mathrm{B}}.$$

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 $\alpha = \frac{1}{2}$, and it is the limit of our $h_c^{(2)}$. The pole in the boundary S-matrix at $\lambda = \sqrt{-1}(\frac{1}{2}-\alpha)$ is in the physical strip, $0 < \mathrm{Im}\,\lambda \leqslant 1$, when $h > h_c^{(2)} = 1$. The energy difference and the boundary magnetization in this limit are:

$$\begin{aligned} \lim \Delta e(r) &= \frac{\pi}{\sin \pi\alpha}, \\ \lim \mathcal{M}^{(0)}(r) &= -1 - 2\sum_{l=1}^{\infty}(-1)^l\frac{\alpha^2}{(l+\alpha)^2} \\ &= 1 + \frac{\alpha^2}{2}\left(\psi'\left(\frac{\alpha+1}{2}\right) - \psi'\left(\frac{\alpha}{2}\right)\right), \end{aligned}$$

where $\psi'(x) = (\mathrm{d}^2/\mathrm{d}x^2)\log\Gamma(x)$.

6. Discussion

In conclusion, we have obtained the following results for the XXZ hamiltonian on the semi-infinite chain (1.2): (i) the space of states and the renormalized transfer matrix (2.13), (ii) the vacuum vectors (3.4) and the energy difference between them (2.27), (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 $U_q(\widehat{sl}_2)$, 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 Fig. 2). Therefore, the corner transfer matrix is not diagonalized by our vertex operators, since in Refs. [21–23] 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 Ref. [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 $|i\rangle_{\mathrm{B}}$ bears some resemblance to the expression for $|B\rangle$, e.g. (3.38) of Ref. [16]. However, the two states exist in different spaces. The states $|i\rangle_{\mathrm{B}}$ correspond (see (3.18)) to the "boundary bound states" of Ref. [16].

Although there exists a Bethe ansatz for the model [4–6], the excitation structure has 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 nondiagonal K-matrix, corresponding to a boundary 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 hamiltonian, as for the bulk case.

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Appendix A

Vertex operators

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

A.1. R-matrix

The R-matrix for the six-vertex model is

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

where

$$\kappa(\zeta) = \zeta \frac{(q^4\zeta^2;q^4)_\infty (q^2\zeta^{-2};q^4)_\infty}{(q^4\zeta^{-2};q^4)_\infty (q^2\zeta^2;q^4)_\infty}, \qquad (z;p)_\infty = \prod_{n=0}^{\infty}(1-zp^n). \tag{A.2}$$

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

$$R(\zeta)\left(v_{\varepsilon_1'} \otimes v_{\varepsilon_2'}\right) = \sum_{\varepsilon_1,\varepsilon_2} v_{\varepsilon_1} \otimes v_{\varepsilon_2} R_{\varepsilon_1\varepsilon_2}^{\varepsilon_1'\varepsilon_2'}(\zeta)\,.$$

As usual, when copies V_j of V are involved, $R_{ij}(\zeta)$ acts as $R(\zeta)$ on the ith and jth components and as the identity elsewhere. The Yang–Baxter equation satisfied by (A.1) is

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

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

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

$$R^{\varepsilon_2'\varepsilon_1}_{\varepsilon_2\varepsilon_1'}(\zeta_2/\zeta_1) = R^{-\varepsilon_1'\,\varepsilon_2'}_{-\varepsilon_1\,\varepsilon_2}\left(-q^{-1}\zeta_1/\zeta_2\right)\,. \tag{A.5}$$

A.2. Vertex operators

We list here the commutation relations for the vertex operators:

$$\Phi_{\varepsilon_2}(\zeta_2)\Phi_{\varepsilon_1}(\zeta_1) = \sum_{\varepsilon_1',\varepsilon_2'} R^{\varepsilon_1'\,\varepsilon_2'}_{\varepsilon_1\,\varepsilon_2}(\zeta_1/\zeta_2)\Phi_{\varepsilon_1'}(\zeta_1)\Phi_{\varepsilon_2'}(\zeta_2)\,, \tag{A.6}$$

$$\Psi^*_{\mu_1'}(\xi_1)\Psi^*_{\mu_2'}(\xi_2) = -\sum_{\mu_1,\mu_2} R^{\mu_1'\,\mu_2'}_{\mu_1\,\mu_2}(\xi_1/\xi_2)\Psi^*_{\mu_2}(\xi_2)\Psi^*_{\mu_1}(\xi_1)\,, \tag{A.7}$$

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

Here

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

The type I vertex operators satisfy the invertibility

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

where g is given by

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

For the type II operators the corresponding property is

$$\Psi^{(i,1-i)}_{\mu_1}(\xi_1)\Psi^{*(1-i,i)}_{\mu_2}(\xi_2) = \frac{g\delta_{\mu_1\mu_2}}{1-\xi_2^2/\xi_1^2}\left(\frac{\xi_2}{\xi_1}\right)^{i+(1-\mu_1)/2} + \dots \qquad (\xi_1 \to \pm\xi_2)\,, \tag{A.12}$$

where

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

and ... means regular terms.

A.3. Bosonization

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

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

The commutation relations of a_n are

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

On the symbols e^γ, the operators e^β, z^∂ act as

$$\mathrm{e}^\beta \cdot \mathrm{e}^\gamma = \mathrm{e}^{\beta+\gamma} , \qquad z^\partial \cdot \mathrm{e}^\gamma = z^{[\partial,\gamma]}\, \mathrm{e}^\gamma ,$$

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 $|i\rangle = 1 \otimes \mathrm{e}^{\Lambda_i}$.

We have the following bosonic realization for the vertex operators:

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

$$\Phi_+^{(1-i,i)}(\zeta) = \oint_{C_1} \frac{\mathrm{d}w}{2\pi i} \frac{(1-q^2) w\zeta}{q(w - q^2\zeta^2)(w - q^4\zeta^2)} : \Phi_-^{(1-i,i)}(\zeta) X^-(w) : , \tag{A.14}$$

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

$$\Psi_+^{*(1-i,i)}(\zeta) = \oint_{C_2} \frac{\mathrm{d}w}{2\pi i} \frac{q^2(1-q^2)\zeta}{(w - q^2\zeta^2)(w - q^4\zeta^2)} : \Psi_-^{*(1-i,i)}(\zeta) X^+(w) : , \tag{A.16}$$

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

where

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

$$\begin{aligned} R^\pm(z) &= \pm \sum_{n=1}^{\infty} \frac{a_{-n}}{[n]} q^{\mp n/2} z^n , \\ S^\pm(z) &= \mp \sum_{n=1}^{\infty} \frac{a_n}{[n]} q^{\mp n/2} z^{-n} . \end{aligned} \tag{A.19}$$

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

$C_1 : q^4\zeta^2$ is inside and $q^2\zeta^2$ is outside,

$C_2 : q^4\zeta^2$ is outside and $q^2\zeta^2$ is inside.

These operators act also on the dual (right) modules $\mathcal{H}^{*(i)}$, which are defined analogously by replacing $e^{\Lambda_i+n\alpha}$ with $e^{-(\Lambda_i+n\alpha)}$. In particular the highest-weight vector is $\langle i| = 1 \otimes e^{-\Lambda_i}$. The right actions of e^β and z^∂ are given by

$$e^\gamma \cdot e^\beta = e^{\gamma+\beta}, \qquad e^\gamma \cdot z^\partial = e^\gamma z^{[\gamma,\partial]}.$$

Appendix 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 $\otimes_{k\geqslant 1} V_k$ (see (2.11)):

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

where

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

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 nonnegative integers

$$Y = (f_1, f_2, \ldots, f_n), \qquad f_1 > f_2 > \ldots > f_n,$$

given via the correspondence

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

We also use the convention that $|f_1, \ldots, f_n, 0\rangle = |f_1, \ldots, f_n\rangle$. The degree of Y is $f_1 + \ldots + f_n$. 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

$$|0\rangle_B = |\phi\rangle + \sum_{j\geqslant 1} \varepsilon^j v_j \tag{B.1}$$

be the expansion of the ground-state vector for (1.2), where $\varepsilon = -1/2\Delta = -q/(1+q^2)$. Each v_j is a linear combination of paths

$$v_j = \sum_{Y\neq\phi} c_j(Y)|Y\rangle. \tag{B.2}$$

Here we demanded that ϕ never appears in v_j $(j \geqslant 1)$, by multiplying a scalar to $|0\rangle_{\mathrm{B}}$ as necessary.

We are going to solve the following eigenvalue equation order by order in ε:

$$\left(\sum_{k\geqslant 1} \tfrac{1}{2}(\sigma^z_{k+1}\sigma^z_k + 1 + c_k(\varepsilon)) - 2\varepsilon Q\right)|0\rangle_{\mathrm{B}} = 0\,,$$

where

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

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

Up to the third order, we obtain

$$v_1 = 2|2\rangle + \sum_{k\geqslant 1}|k+2,k\rangle\,, \tag{B.3}$$

$$v_2 = 6|4\rangle + 2\sum_{k\geqslant 1}|k+4,k\rangle + 2\sum_{k\geqslant 3}|k+2,k,2\rangle + \sum_{\substack{k\geqslant 1\\ l\geqslant k+3}}|l+2,l,k+2,k\rangle\,, \tag{B.4}$$

$$\begin{aligned} v_3 = {} & -4|2\rangle + 20|6\rangle - 3|3,1\rangle + 2|4,2\rangle - \sum_{k\geqslant 3}|k+2,k\rangle \\ & +5\sum_{k\geqslant 1}|k+6,k\rangle + 4|4,3,1\rangle + 4\sum_{k\geqslant 3}|k+4,k,2\rangle \\ & +6\sum_{k\geqslant 5}|k+2,k,4\rangle + \sum_{k\geqslant 1}|k+4,k+3,k+1,k\rangle \\ & +2\sum_{\substack{k\geqslant 1\\ l\geqslant k+5}}|l+2,l,k+4,k\rangle + 2\sum_{\substack{k\geqslant 1\\ l\geqslant k+3}}|l+4,l,k+2,k\rangle \\ & +2\sum_{\substack{k\geqslant 3\\ l\geqslant k+3}}|l+2,l,k+2,k,2\rangle + \sum_{\substack{k\geqslant 1\\ l\geqslant k+3\\ m\geqslant l+3}}|m+2,m,l+2,l,k+2,k\rangle\,. \end{aligned} \tag{B.5}$$

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

Next, we expand the bosonic expression for the vector $|0\rangle_{\mathrm{B}}$ (3.4) in terms of paths. Since $|0\rangle_{\mathrm{B}}$ 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 $|0\rangle_{\mathrm{B}}$ belongs to the upper crystal lattice (see Ref. [21]), although we have no proof. On the other hand, the global basis vectors have a q-expansion in terms of paths. (For the meaning of this statement, see Refs. [33,21], in particular, the remark at the end of p. 99 of Ref. [21] and Ref. [27].) 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

Table B.1

Degree	Path	Monomials
0	ϕ	1
1	(1)	e^{α}
2	(2)	a_{-1}
3	(3), (2, 1)	$a_{-1}e^{\alpha}$, $e^{-\alpha}$
4	(4), (3, 1)	a_{-1}^2, a_{-2}
5	(5), (4, 1), (3, 2)	$a_{-1}e^{-\alpha}$, $a_{-1}^2e^{\alpha}$, $a_{-2}e^{\alpha}$
6	(6), (5, 1), (4, 2), (3, 2, 1)	a_{-3}, $a_{-1}a_{-2}$, a_{-1}^3, $e^{2\alpha}$

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 Ref. [21]). Up to degree 6, the possible paths and monomials in the bosons are denoted in Table B.1.

In the second column we abbreviated $X \otimes e^{\Lambda_0+\beta}$ to Xe^{β}.

The following is the explicit relation between the two bases:

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

$$G(4,2) = q^{5/2}\left(-\frac{q(q^2-1)}{[6]}a_{-3} + \frac{q}{[4][2]}a_{-2}a_{-1} + \frac{q(2q^2+1)}{6[2]^3}a_{-1}^3\right) \otimes e^{\Lambda_0},$$
$$G(3,2,1) = q^6 \otimes e^{\Lambda_0+2\alpha}.$$

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:

$$|0\rangle_B = G(\phi) + qrG(2) + q^2r^2G(4) + q^3G(3,1) + q^3r^3G(6)$$
$$+q^4[2]rG(4,2) + q^4rG(5,1) + \dots. \tag{B.6}$$

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 $|rq| \leqslant 1$.

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

$$G(Y) = |p_0(Y)\rangle + q|p_1(Y)\rangle + q^2|p_2(Y)\rangle + \dots$$

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,

$$c_0(Y',Y) = \delta_{Y',Y}. \tag{B.7}$$

We have the following expansions:

$$G(\phi) = |\phi\rangle + \varepsilon\sum_{k\geqslant 0}|k+2,k\rangle + \varepsilon^2\left(2\sum_{k\geqslant 0}|k+4,k\rangle + \sum_{\substack{l\geqslant 0\\ k\geqslant l+3}}|k+2,k,l+2,l\rangle\right)$$
$$+\varepsilon^3\Bigg(\sum_{\substack{m\geqslant 0\\ l\geqslant m+3\\ k\geqslant l+3}}|k+2,k,l+2,l,m+2,m\rangle + 2\sum_{\substack{k\geqslant 0\\ l\geqslant k+5}}|l+2,l,k+4,k\rangle$$
$$+2\sum_{\substack{k\geqslant 0\\ l\geqslant k+3}}|l+4,l,k+2,k\rangle + \sum_{k\geqslant 0}|k+4,k+3,k+1,k\rangle + 5\sum_{k\geqslant 0}|k+6,k\rangle$$
$$-\sum_{k\geqslant 1}|k+2,k\rangle\Bigg) + O(\varepsilon^4), \tag{B.8}$$

$$G(2) = (1-4\varepsilon^2+O(\varepsilon^4))\left\{|2\rangle + \varepsilon\left(-|0\rangle + 3|4\rangle + \sum_{k\geqslant 3}|k+2,k,2\rangle\right)\right.$$
$$+\varepsilon^2\Bigg(9|6\rangle - 2|3,1\rangle - \sum_{k\geqslant 3}|k+2,k\rangle + 2|4,3,1\rangle + 3\sum_{k\geqslant 5}|k+2,k,4\rangle$$

$$+2\sum_{k\geqslant 3}|k+4,k,2\rangle+\sum_{\substack{k\geqslant 3\\ l\geqslant k+3}}|l+2,l,k+2,k,2\rangle\Bigg)+\mathrm{O}(\varepsilon^3)\Bigg\}, \tag{B.9}$$

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

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

Appendix 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 ξ_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 $n\geqslant 1$, respectively, one can easily verify

$$a_n|\xi\rangle_i=\xi_n|\xi\rangle_i,\qquad {}_i\langle\bar{\xi}|a_{-n}=\bar{\xi}_n\,{}_i\langle\bar{\xi}|\,. \tag{C.3}$$

One can also show that the coherent states $\{|\xi\rangle_i\}$ (resp. $\{{}_i\langle\bar{\xi}|\}$) form a complete basis in the Fock space $\mathcal{H}^{(i)}$ (resp. $\mathcal{H}^{*(i)}$). Namely one can verify the completeness relation

$$\mathrm{id}_{\mathcal{H}^{(i)}}=\int\prod_{n=1}^{\infty}\frac{n\,\mathrm{d}\xi_n\,\mathrm{d}\bar{\xi}_n}{[n][2n]}\exp\left(-\sum_{n=1}^{\infty}\frac{n}{[n][2n]}|\xi_n|^2\right)|\xi_n\rangle_{ii}\langle\bar{\xi}_n|\,. \tag{C.4}$$

Here the integration is taken over the entire complex plane with the measure $\mathrm{d}\xi\,\mathrm{d}\bar{\xi}=\mathrm{d}x\,\mathrm{d}y$ for $\xi=x+iy$. In the proof, the following integration formula is used:

$$\int\prod_{n=1}^{\infty}\frac{n\,\mathrm{d}\xi_n\,\mathrm{d}\bar{\xi}_n}{[n][2n]}\exp\left(-\tfrac{1}{2}\sum_{n=1}^{\infty}\frac{n}{[n][2n]}(\bar{\xi}_n,\xi_n)\mathcal{A}_n\begin{pmatrix}\bar{\xi}_n\\ \xi_n\end{pmatrix}+\sum_{n=1}^{\infty}(\bar{\xi}_n,\xi_n)\mathcal{B}_n\right)$$

$$= \prod_{n=1}^{\infty} (-\det \mathcal{A}_n)^{-1/2} \exp\left(\frac{1}{2} \sum_{n=1}^{\infty} \frac{[n][2n]}{n} \mathcal{B}_n^t \mathcal{A}_n^{-1} \mathcal{B}_n \right), \tag{C.5}$$

where $\mathcal{A}_n$ are invertible constant 2×2 matrices and $\mathcal{B}_n$ are constant 2 component vectors.

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