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Boundary *S*-matrix for the *XXZ* chain

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Abstract. We compute by means of the Bethe ansatz the boundary S-matrix for the open anisotropic spin-$\frac{1}{2}$ chain with diagonal boundary magnetic fields in the noncritical regime ($\Delta > 1$). Our result, which is formulated in terms of q-gamma functions, agrees with the vertex-operator result of Jimbo *et al*.

1. Introduction

The concept of the boundary S-matrix in (1+1)-dimensional integrable quantum field theory was precisely formulated by Ghoshal and Zamolodchikov in [1]. There they also developed a bootstrap approach for determining such S-matrices. Boundary S-matrices can also be computed for integrable quantum spin chains by a direct Bethe-ansatz approach which was proposed in [2]†. Until now this method has only been used for isotropic models [2, 6–8]. We recently simplified this method in [9]. In the present paper, we take advantage of this simplification to analyze an *anisotropic* model, namely the open XXZ spin chain:

$$\mathcal{H} = \frac{1}{4}\left\{ \sum_{n=1}^{N-1} \left(\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \cosh\eta\ \sigma_n^z \sigma_{n+1}^z\right) + \sinh\eta \coth(\eta\xi_-)\ \sigma_1^z \right.$$
$$\left. + \sinh\eta \coth(\eta\xi_+)\ \sigma_N^z \right\} \tag{1}$$

where the real parameters $\xi_\pm > \frac{1}{2}$ correspond to boundary magnetic fields. For simplicity, we restrict our attention to the case $\Delta \equiv \cosh\eta > 1$, which corresponds to the noncritical regime in which there is a nonzero gap (see, e.g., [10]). Our result for the boundary S-matrix, which is formulated in terms of q-gamma functions [11], agrees with the result found by Jimbo *et al* [12] by means of the vertex operator approach. In the limit $\eta \to 0$, we recover the results of [2] and [9].

2. The Bethe ansatz and the one-hole state

In this section we review the exact Bethe-ansatz (BA) solution of the open XXZ chain, and we compute the root and hole density for the BA state consisting of a single hole.

† This method is a generalization of the approach developed by Korepin–Andrei–Destri [3, 4] to calculate bulk two-particle S-matrices. See also [5].

The eigenvalues of $\mathcal{H}$ and $S^z = \frac{1}{2}\sum_{n=1}^{N}\sigma_n^z$ are given [13–15] by

$$E = -\frac{1}{2}\sinh^2\eta \sum_{\alpha=1}^{M} \frac{1}{\sin\eta\left(\lambda_\alpha - \frac{1}{2}\mathrm{i}\right)\sin\eta\left(\lambda_\alpha + \frac{1}{2}\mathrm{i}\right)} \tag{2}$$

$$S^z = \tfrac{1}{2}N - M \tag{3}$$

where $\lambda_1, \cdots, \lambda_M$ satisfy the BA equations

$$\frac{\sin\eta\left(\lambda_\alpha + \mathrm{i}(\xi_+ - \frac{1}{2})\right)}{\sin\eta\left(\lambda_\alpha - \mathrm{i}(\xi_+ - \frac{1}{2})\right)} \frac{\sin\eta\left(\lambda_\alpha + \mathrm{i}(\xi_- - \frac{1}{2})\right)}{\sin\eta\left(\lambda_\alpha - \mathrm{i}(\xi_- - \frac{1}{2})\right)} \left(\frac{\sin\eta\left(\lambda_\alpha + \frac{1}{2}\mathrm{i}\right)}{\sin\eta\left(\lambda_\alpha - \frac{1}{2}\mathrm{i}\right)}\right)^{2N}$$

$$= \prod_{\substack{\beta=1\\ \beta\neq\alpha}}^{M} \frac{\sin\eta\left(\lambda_\alpha - \lambda_\beta + \mathrm{i}\right)}{\sin\eta\left(\lambda_\alpha - \lambda_\beta - \mathrm{i}\right)} \frac{\sin\eta\left(\lambda_\alpha + \lambda_\beta + \mathrm{i}\right)}{\sin\eta\left(\lambda_\alpha + \lambda_\beta - \mathrm{i}\right)} \qquad \alpha = 1, \ldots, M. \tag{4}$$

(We neglect in (2) additional terms which are independent of $\{\lambda_\alpha\}$.)

Introducing the notation

$$e_n(\lambda) = \frac{\sin\eta\left(\lambda + \frac{1}{2}\mathrm{i}n\right)}{\sin\eta\left(\lambda - \frac{1}{2}\mathrm{i}n\right)} \qquad g_n(\lambda) = \frac{\cos\eta\left(\lambda + \frac{1}{2}\mathrm{i}n\right)}{\cos\eta\left(\lambda - \frac{1}{2}\mathrm{i}n\right)} \tag{5}$$

the BA equations take the more compact form

$$e_{2\xi_+-1}(\lambda_\alpha)\; e_{2\xi_--1}(\lambda_\alpha)\; g_1(\lambda_\alpha)\; e_1(\lambda_\alpha)^{2N+1} = -\prod_{\beta=1}^{M} e_2(\lambda_\alpha - \lambda_\beta)\; e_2(\lambda_\alpha + \lambda_\beta). \tag{6}$$

Note that the factor $g_1(\lambda_\alpha)$ is absent in the isotropic limit $\eta \to 0$.

Without loss of generality, we restrict $\eta > 0$. Moreover, the requirement that BA solutions correspond to independent BA states leads to the restriction (see [2] and references therein)

$$\mathrm{Re}\,(\lambda_\alpha) \in \left[0, \frac{\pi}{2\eta}\right] \qquad \lambda_\alpha \neq 0, \frac{\pi}{2\eta}. \tag{7}$$

Following [9], we now focus on the BA state consisting of a single hole. This state lies in the sector $N =$ odd with $M = \frac{1}{2}N - \frac{1}{2}$ and $\{\lambda_\alpha\}$ real. This state has $S^z = +\frac{1}{2}$.

Since equation (6) involves only products of phases, it is useful to take the logarithm. In this way we arrive at the desired form of the BA equations:

$$h(\lambda_\alpha) = J_\alpha \tag{8}$$

where the so-called counting function $h(\lambda)$ is given by

$$h(\lambda) = \frac{1}{2\pi}\Bigg\{(2N+1)q_1(\lambda) + r_1(\lambda) + q_{2\xi_+-1}(\lambda) + q_{2\xi_--1}(\lambda)$$

$$- \sum_{\beta=1}^{M}\left[q_2(\lambda - \lambda_\beta) + q_2(\lambda + \lambda_\beta)\right]\Bigg\}. \tag{9}$$

Here $q_n(\lambda)$ and $r_n(\lambda)$ are odd monotonically increasing functions defined by

$$q_n(\lambda) = \pi + \mathrm{i}\log e_n(\lambda) \qquad -\pi < q_n(\lambda) \leqslant \pi \tag{10}$$

$$r_n(\lambda) = \mathrm{i}\log g_n(\lambda) \qquad -\pi < r_n(\lambda) \leqslant \pi \tag{11}$$

and $\{J_\alpha\}$ are certain integers which serve as 'quantum numbers' that parametrize the BA state (see, e.g., [16]).

In section 3 we shall need the root and hole density $\sigma(\lambda)$ for the one-hole BA state, which is defined by

$$\sigma(\lambda) = \frac{1}{N}\frac{\mathrm{d}h(\lambda)}{\mathrm{d}\lambda}. \tag{12}$$

To calculate this quantity, we must pass with care from the sum in $h(\lambda)$ to an integral. Indeed, with the help of the Euler–Maclaurin formula for approximating sums by integrals, and using the fact that the solutions $\lambda = 0, \pi/2\eta$ of the BA equations are excluded, one can derive the following general result for a state with ν holes†:

$$\frac{1}{N}\sum_{\alpha=1}^{M} g(\lambda_\alpha) = \int_0^{\pi/2\eta} \mathrm{d}\lambda\, \sigma(\lambda)\; g(\lambda) - \frac{1}{N}\sum_{\alpha=1}^{\nu} g(\tilde{\lambda}_\alpha) - \frac{1}{2N}\left[g(0) + g\left(\frac{\pi}{2\eta}\right)\right] \tag{13}$$

(plus terms that are of higher order in $1/N$), where $g(\lambda)$ is an arbitrary function, and $\{\tilde{\lambda}_\alpha\}$ are the hole rapidities.

Using the above result, we obtain the integral equation

$$\begin{aligned}\sigma(\lambda) = 2a_1(\lambda) + \frac{1}{N}\big\{&a_1(\lambda) + b_1(\lambda) + a_2(\lambda) + b_2(\lambda) + a_{2\xi_+-1}(\lambda) + a_{2\xi_--1}(\lambda) + a_2(\lambda - \tilde{\lambda})\\ &+a_2(\lambda + \tilde{\lambda})\big\} - \int_0^{\pi/2\eta} \mathrm{d}\lambda'\; \big[a_2(\lambda - \lambda') + a_2(\lambda + \lambda')\big]\,\sigma(\lambda') \qquad \lambda > 0\end{aligned} \tag{14}$$

where $\tilde{\lambda}$ is the hole rapidity, and

$$a_n(\lambda) = \frac{1}{2\pi}\frac{\mathrm{d}}{\mathrm{d}\lambda}q_n(\lambda) = \frac{\eta}{\pi}\frac{\sinh(\eta n)}{\cosh(\eta n) - \cos(2\eta\lambda)} \tag{15}$$

$$b_n(\lambda) = \frac{1}{2\pi}\frac{\mathrm{d}}{\mathrm{d}\lambda}r_n(\lambda) = \frac{\eta}{\pi}\frac{\sinh(\eta n)}{\cosh(\eta n) + \cos(2\eta\lambda)} = a_n\left(\lambda \pm \frac{\pi}{2\eta}\right). \tag{16}$$

Note that the $b_n(\lambda)$ terms are absent from the integral equation in the isotropic limit. The b_1 term originates from the factor g_1 in the BA equations (6), and the b_2 term originates from the last term in (13).

The symmetric density $\sigma_s(\lambda)$ defined by

$$\sigma_s(\lambda) = \begin{cases}\sigma(\lambda) & \lambda > 0\\ \sigma(-\lambda) & \lambda < 0\end{cases} \tag{17}$$

can now readily be found with the help of Fourier transforms, for which we use the following conventions:

$$f(\lambda) = \frac{\eta}{\pi}\sum_{k=-\infty}^{\infty} \mathrm{e}^{-2\mathrm{i}\eta k\lambda}\hat{f}(k) \qquad \hat{f}(k) = \int_{-\pi/2\eta}^{\pi/2\eta} \mathrm{d}\lambda\; \mathrm{e}^{2i\eta k\lambda} f(\lambda). \tag{18}$$

Indeed, we find that

$$\sigma_s(\lambda) = 2s(\lambda) + \frac{1}{N}r^{(+)}(\lambda) \tag{19}$$

† The argument is a slight modification of that presented in the appendix of [2].

where

$$r^{(+)}(\lambda) = s(\lambda) + K(\lambda) + J(\lambda) + L(\lambda) + J_+^{(+)}(\lambda) + J_-^{(+)}(\lambda) + J(\lambda - \tilde{\lambda}) + J(\lambda + \tilde{\lambda}) \tag{20}$$

and

$$\hat{s} = \frac{\hat{a}_1}{1+\hat{a}_2} \qquad \hat{J} = \frac{\hat{a}_2}{1+\hat{a}_2} \qquad \hat{J}_\pm^{(+)} = \frac{\hat{a}_{2\xi_\pm - 1}}{1+\hat{a}_2} \qquad \hat{K} = \frac{\hat{b}_1}{1+\hat{a}_2} \qquad \hat{L} = \frac{\hat{b}_2}{1+\hat{a}_2} \tag{21}$$

with

$$\hat{a}_n(k) = \mathrm{e}^{-\eta n|k|} \qquad \hat{b}_n(k) = (-)^k\ \hat{a}_n(k). \tag{22}$$

Note that the Fourier series for $J_\pm^{(+)}(\lambda)$ converges for $\xi_\pm > \frac{1}{2}$.

3. The boundary *S*-matrix

The boundary S-matrix has the diagonal form

$$\mathcal{K}(\tilde{\lambda}, \xi_\pm) = \begin{pmatrix} \alpha(\tilde{\lambda}, \xi_\pm) & 0 \\ 0 & \beta(\tilde{\lambda}, \xi_\pm) \end{pmatrix}. \tag{23}$$

The matrix elements $\alpha(\tilde{\lambda}, \xi_\pm)$ and $\beta(\tilde{\lambda}, \xi_\pm)$ are the boundary scattering amplitudes for one-hole states with $S^z = +\frac{1}{2}$ and $S^z = -\frac{1}{2}$, respectively.

We first compute $\alpha(\tilde{\lambda}, \xi_\pm)$. Setting

$$\alpha(\tilde{\lambda}, \xi_\pm) = \mathrm{e}^{i\phi(\tilde{\lambda}, \xi_\pm)} \tag{24}$$

by a calculation completely analogous to that in [9] we obtain the result

$$\Phi^{(+)}(\tilde{\lambda}) \equiv \phi(\tilde{\lambda}, \xi_+) + \phi(\tilde{\lambda}, \xi_-) = 2\pi \int_0^{\tilde{\lambda}} r^{(+)}(\lambda)\ \mathrm{d}\lambda + \text{constant}. \tag{25}$$

Recalling the result (20) for $r^{(+)}(\lambda)$, and using the fact that

$$\int_0^{\tilde{\lambda}} \left[J(\lambda - \tilde{\lambda}) + J(\lambda + \tilde{\lambda})\right] \mathrm{d}\lambda = \int_0^{\tilde{\lambda}} 2J(2\lambda)\ \mathrm{d}\lambda \tag{26}$$

we obtain

$$\phi(\tilde{\lambda}, \xi_\pm) = \pi \int_0^{\tilde{\lambda}} \left[s(\lambda) + K(\lambda) + J(\lambda) + L(\lambda) + 2J(2\lambda) + 2J_\pm^{(+)}(\lambda)\right] \mathrm{d}\lambda. \tag{27}$$

We now use equations (18), (21), (22) to write the integrand explicitly as a Fourier series. Performing the λ integration, using the identity

$$\sum_{k=1}^{\infty} \frac{\mathrm{e}^{-2\eta k x}}{1+\mathrm{e}^{-2\eta k}} \frac{1}{k} = \log\left[\frac{\Gamma_{q^4}(\frac{1}{2}x)}{\Gamma_{q^4}\left(\frac{1}{2}(x+1)\right)}\right] - \frac{1}{2}\log(1-q^4) \tag{28}$$

where $q = \mathrm{e}^{-\eta}$ and $\Gamma_q(x)$ is the q-analogue of the Euler gamma function (see the appendix), and also using the q-analogue of the duplication formula [11]

$$\Gamma_q(2x)\ \Gamma_{q^2}(\tfrac{1}{2}) = (1+q)^{2x-1}\ \Gamma_{q^2}(x)\ \Gamma_{q^2}(x+\tfrac{1}{2}) \tag{29}$$

we obtain the following result for $\alpha(\tilde\lambda, \xi_\pm)$ (up to a rapidity-independent phase factor):

$$\alpha(\tilde\lambda, \xi_\pm) = q^{-4\mathrm{i}\tilde\lambda} \frac{\Gamma_{q^8}\big(-\frac{1}{2}\mathrm{i}\tilde\lambda+\frac{1}{4}\big)}{\Gamma_{q^8}\big(\frac{1}{2}\mathrm{i}\tilde\lambda+\frac{1}{4}\big)} \frac{\Gamma_{q^8}\big(\frac{1}{2}\mathrm{i}\tilde\lambda+1\big)}{\Gamma_{q^8}\big(-\frac{1}{2}\mathrm{i}\tilde\lambda+1\big)} \frac{\Gamma_{q^4}\big(-\frac{1}{2}\mathrm{i}\tilde\lambda+\frac{1}{4}(2\xi_\pm-1)\big)}{\Gamma_{q^4}\big(\frac{1}{2}\mathrm{i}\tilde\lambda+\frac{1}{4}(2\xi_\pm-1)\big)}$$
$$\times \frac{\Gamma_{q^4}\big(\frac{1}{2}\mathrm{i}\tilde\lambda+\frac{1}{4}(2\xi_\pm+1)\big)}{\Gamma_{q^4}\big(-\frac{1}{2}\mathrm{i}\tilde\lambda+\frac{1}{4}(2\xi_\pm+1)\big)}. \tag{30}$$

We now turn to the computation of $\beta(\tilde\lambda, \xi_\pm)$, for which we must consider a one-hole state with $S^z = -\frac{1}{2}$. Instead of taking the pseudovacuum to be the ferromagnetic state with all spins up as we have done so far, we now take the pseudovacuum to be the ferromagnetic state with all spins down. The expression (2) for the energy eigenvalues remains the same, the expression (3) for the S^z eigenvalues becomes

$$S^z = M - \tfrac{1}{2}N \tag{31}$$

and there is a change $\xi_\pm \to -\xi_\pm$ in the BA equations (4) [15].

We focus on the BA state consisting of one hole ($M = \frac{1}{2}N - \frac{1}{2}$ with $\{\lambda_\alpha\}$ real), which evidently has $S^z = -\frac{1}{2}$. The corresponding function $r^{(-)}(\lambda)$ is the same as $r^{(+)}(\lambda)$ (see equation (20)), except that $J_\pm^{(+)}(\lambda)$ is now replaced by $J_\pm^{(-)}(\lambda)$, with the Fourier transform

$$\hat J_\pm^{(-)} = -\frac{\hat a_{2\xi_\pm+1}}{1+\hat a_2}. \tag{32}$$

We observe that

$$\frac{\beta(\tilde\lambda, \xi_-)\ \beta(\tilde\lambda, \xi_+)}{\alpha(\tilde\lambda, \xi_-)\ \alpha(\tilde\lambda, \xi_+)} = \exp\left(2\pi\mathrm{i}\int_0^{\tilde\lambda}\left[r^{(-)}(\lambda) - r^{(+)}(\lambda)\right]\,\mathrm{d}\lambda\right). \tag{33}$$

Using the identity

$$J_\pm^{(-)}(\lambda) - J_\pm^{(+)}(\lambda) = -a_{2\xi_\pm-1}(\lambda) \tag{34}$$

we conclude that

$$\frac{\beta(\tilde\lambda, \xi_\pm)}{\alpha(\tilde\lambda, \xi_\pm)} = -e_{2\xi_\pm-1}(\tilde\lambda). \tag{35}$$

We have fixed the sign in (35) by demanding that $\mathcal{K}(\tilde\lambda, \xi_\pm)$ be proportional to the unit matrix for $\tilde\lambda = 0$.

4. Discussion

Our final result for the boundary S-matrix of the XXZ chain is

$$\mathcal{K}(\tilde\lambda, \xi_\pm) = \alpha(\tilde\lambda, \xi_\pm)\begin{pmatrix} 1 & 0 \\ 0 & -e_{2\xi_\pm-1}(\tilde\lambda)\end{pmatrix} \tag{36}$$

where $\alpha(\lambda, \xi_\pm)$ is given by equation (30). It can be shown that this result agrees with that found by Jimbo *et al* [12] by means of the vertex operator approach. In the isotropic limit $\eta \to 0$, we see that $q \to 1$ and $\Gamma_q(x) \to \Gamma(x)$; hence, we recover the boundary S-matrix of the XXX chain [2, 9].

It would be interesting to see if this Bethe-ansatz method can be extended to the critical regime $|q| = 1$, which is outside the domain of the vertex operator approach.

The R-matrix for the XXZ chain is associated with the fundamental representation of $A_1^{(1)}$. The present work opens the way to calculating boundary S-matrices for spin chains whose R-matrices are associated with the fundamental representation of any (simply-laced) affine Lie algebra. For higher representations, the ground state involves complex strings, and the analysis is more complicated. We hope to address these and related questions in the near future.

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Appendix

Here we prove the identity

$$\sum_{k=1}^{\infty} \frac{\mathrm{e}^{-2\eta kx}}{1+\mathrm{e}^{-2\eta k}} \frac{1}{k} = \log\left[\frac{\Gamma_{q^4}\left(\frac{1}{2}x\right)}{\Gamma_{q^4}\left(\frac{1}{2}(x+1)\right)}\right] - \frac{1}{2}\log(1-q^4) \tag{A1}$$

where $q = \mathrm{e}^{-\eta}$ and $\Gamma_q(x)$ is the q-analogue of the Euler gamma function, which is defined [11] as

$$\Gamma_q(x) = (1-q)^{1-x} \prod_{j=0}^{\infty} \left[\frac{\left(1-q^{1+j}\right)}{\left(1-q^{x+j}\right)}\right] \qquad 0 < q < 1. \tag{A2}$$

It is convenient first to consider the sum

$$S(x) = \sum_{k=1}^{\infty} \frac{\mathrm{e}^{-2\eta kx}}{1+\mathrm{e}^{-2\eta k}}. \tag{A3}$$

Expanding the denominator in an infinite series and then interchanging the order of summations, we obtain

$$S(x) = \sum_{k=1}^{\infty} \mathrm{e}^{-2\eta kx} \sum_{n=0}^{\infty} (-)^n \mathrm{e}^{-2\eta kn} \tag{A4}$$

$$= \sum_{n=0}^{\infty} (-)^n \sum_{k=1}^{\infty} \mathrm{e}^{-2\eta k(x+n)} \tag{A5}$$

$$= \sum_{m=0}^{\infty} \left\{ \frac{\mathrm{e}^{-2\eta(x+2m)}}{1-\mathrm{e}^{-2\eta(x+2m)}} - \frac{\mathrm{e}^{-2\eta(x+2m+1)}}{1-\mathrm{e}^{-2\eta(x+2m+1)}} \right\} \tag{A6}$$

$$= \frac{1}{\log q^4}\left[\psi_{q^4}\left(\frac{x}{2}\right) - \psi_{q^4}\left(\frac{x+1}{2}\right)\right] \tag{A7}$$

where

$$\psi_q(x) = \frac{\mathrm{d}}{\mathrm{d}x} \log \Gamma_q(x) \tag{A8}$$

$$= -\log(1-q) + \log q \sum_{j=0}^{\infty} \frac{q^{x+j}}{1-q^{x+j}}. \tag{A9}$$

Integrating the result (A7) with respect to x, and evaluating the integration constant by considering the limit $x \to \infty$, we obtain the desired identity (A1).

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