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 boundary $S$ matrix in $1+1$ dimensional integrable quantum field theory was precisely formulated by Ghoshal and Zamolodchikov in Ref. [1]. They also developed there 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 Ref. [2]. This method has been used until now only for isotropic models [2], [6] - [8]. We recently simplified this method in Ref. [9]. In the present Letter, we take advantage of this simplification to analyze an anisotropic model, namely the open XXZ spin chain

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

(1)

where the real parameters $\xi^+ > 1/2$ 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. Ref. [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 Refs. [2] and [9].

2 Bethe Ansatz and 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.

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

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

(2)

$$S^z = \frac{N}{2} - M ,$$

(3)

\(1\)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].
where \( \lambda_1, \cdots, \lambda_M \) satisfy the BA equations

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

\[
= \prod_{\beta=1, \beta \neq \alpha}^{M} \frac{\sin \eta (\lambda_\alpha - \lambda_\beta + i) \sin \eta (\lambda_\alpha + \lambda_\beta + i)}{\sin \eta (\lambda_\alpha - \lambda_\beta - i) \sin \eta (\lambda_\alpha + \lambda_\beta - i)} , \quad \alpha = 1, \cdots, M . \tag{4}
\]

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

Introducing the notation

\[
e_n(\lambda) = \frac{\sin \eta \left( \lambda + \frac{in}{2} \right)}{\sin \eta \left( \lambda - \frac{in}{2} \right)} , \quad g_n(\lambda) = \frac{\cos \eta \left( \lambda + \frac{in}{2} \right)}{\cos \eta \left( \lambda - \frac{in}{2} \right)} , \tag{5}
\]

the BA equations take the more compact form

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

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)

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

Following [3], we focus now on the BA state consisting of a single hole. This state lies in the sector \( N = \text{odd} \) with \( M = \frac{N}{2} - \frac{1}{2} \) and \( \{\lambda_\alpha\} \) real. This state has \( S^z = +\frac{1}{2} \).

Since Eq. (8) 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

\[
h(\lambda) = \frac{1}{2\pi} \left\{ (2N+1)q_1(\lambda) + r_1(\lambda) + q_{2\xi_+^{-1}}(\lambda) + q_{2\xi_-^{-1}}(\lambda) \right. \\
- \left. \sum_{\beta=1}^{M} [q_2(\lambda - \lambda_\beta) + q_2(\lambda + \lambda_\beta)] \right\} , \tag{9}
\]
$q_n(\lambda)$ and $r_n(\lambda)$ are odd monotonic-increasing functions defined by
\begin{align}
q_n(\lambda) &= \pi + i \log e_n(\lambda), \quad -\pi < q_n(\lambda) \leq \pi, \quad (10) \\
r_n(\lambda) &= i \log g_n(\lambda), \quad -\pi < r_n(\lambda) \leq \pi, \quad (11)
\end{align}
and \{J_\alpha\} are certain integers which serve as “quantum numbers” that parametrize the BA state. (See e.g. [10].)

We shall need in the next section the root and hole density $\sigma(\lambda)$ for the one-hole BA state, which is defined by
\begin{equation}
\sigma(\lambda) = \frac{1}{N} \frac{dh(\lambda)}{d\lambda}. \quad (12)
\end{equation}
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 $\lambda = 0, \frac{\pi}{2\eta}$ of the BA equations are excluded, one can derive\footnote{The argument is a slight modification of the one presented in the appendix of Ref. [3].} for a state with $\nu$ holes the following general result:
\begin{equation}
\frac{1}{N} \sum_{\alpha=1}^{\nu} g(\lambda_\alpha) = \int_{0}^{\pi/2} d\lambda \sigma(\lambda) g(\lambda) - \frac{1}{N} \sum_{\alpha=1}^{\nu} g(\lambda_\alpha) - \frac{1}{2N} \left[ g(0) + g(\frac{\pi}{2\eta}) \right] \quad (13)
\end{equation}
(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{equation}
\sigma(\lambda) = 2a_1(\lambda) + \frac{1}{N} \left\{ 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}) \right\} - \int_{0}^{\pi/2} d\lambda' [a_2(\lambda' - \tilde{\lambda}) + a_2(\lambda' + \tilde{\lambda})] \sigma(\lambda'), \quad \lambda > 0 \quad (14)
\end{equation}
where $\tilde{\lambda}$ is the hole rapidity, and
\begin{align}
a_n(\lambda) &= \frac{1}{2\pi} \frac{d}{d\lambda} q_n(\lambda) = \frac{\eta}{\pi} \frac{\sinh(\eta\lambda)}{\cosh(\eta\lambda) - \cos(2\eta\lambda)}, \quad (15) \\
b_n(\lambda) &= \frac{1}{2\pi} \frac{d}{d\lambda} r_n(\lambda) = \frac{\eta}{\pi} \frac{\sinh(\eta\lambda)}{\cosh(\eta\lambda) + \cos(2\eta\lambda)} = a_n(\lambda \pm \frac{\pi}{2\eta}). \quad (16)
\end{align}
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 Eqs. (3), and the $b_2$ term originates from the last term in Eq. (13).

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

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

(17)

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

$$f(\lambda) = \frac{\eta}{\pi} \sum_{k=-\infty}^{\infty} e^{-2i\eta k\lambda} \hat{f}(k), \quad \hat{f}(k) = \int_{-\pi/2}^{\pi/2} d\lambda e^{2i\eta k\lambda} f(\lambda).$$

(18)

Indeed, we find

$$\sigma_s(\lambda) = 2s(\lambda) + \frac{1}{N} r_{(+)}(\lambda),$$

(19)

where

$$r_{(+)}(\lambda) = s(\lambda) + K(\lambda) + J(\lambda) + L(\lambda) + J_{(+)}^{(+)}(\lambda) + J_{(-)}^{(+)}(\lambda) + J(\lambda - \tilde{\lambda}) + J(\lambda + \tilde{\lambda}),$$

(20)

and

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

(21)

with

$$\hat{a}_n(k) = e^{-\eta|k|}, \quad \hat{b}_n(k) = (-)^k \hat{a}_n(k).$$

(22)

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

### 3 Boundary $S$ Matrix

The boundary $S$ matrix has the diagonal form

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

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

we obtain by a calculation completely analogous to the one in Ref. [9] the result

$$\Phi^{(+)}(\tilde{\lambda}) \equiv \phi(\tilde{\lambda}, \xi_{+}) + \phi(\tilde{\lambda}, \xi_{-}) = 2\pi \int_{0}^{\tilde{\lambda}} r^{(+)}(\lambda) \, d\lambda + \text{const.} \tag{25}$$

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

$$\int_{0}^{\tilde{\lambda}} \left[ J(\lambda - \tilde{\lambda}) + J(\lambda + \tilde{\lambda}) \right] \, d\lambda = \int_{0}^{\tilde{\lambda}} 2J(2\lambda) \, d\lambda \tag{26}$$

we obtain

$$\phi(\tilde{\lambda}, \xi_{\pm}) = \pi \int_{0}^{\tilde{\lambda}} \left[ s(\lambda) + K(\lambda) + J(\lambda) + L(\lambda) + 2J(2\lambda) + 2J^{(+)}_{\pm}(\lambda) \right] \, d\lambda. \tag{27}$$

We now use Eqs. (18), (21), (22) to explicitly write the integrand as a Fourier series. Performing the $\lambda$ integration, using the identity

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

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

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

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

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

We turn now 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

$$S_z = M - \frac{N}{2},$$

and there is a change $\xi_\pm \to -\xi_\pm$ in the BA Eqs. (I).

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

$$J^{(-)}_\pm(\lambda) = -\frac{\tilde{a}_{2\xi_\pm+1}}{1 + \tilde{a}_2}. \tag{32}$$

We observe that

$$\frac{\beta(\tilde{\lambda},\xi_-) \beta(\tilde{\lambda},\xi_+)}{\alpha(\lambda,\xi_-) \alpha(\lambda,\xi_+)} = e^{i2\pi \int_0^\lambda [r^{(-)}(\lambda) - r^{(+)}(\lambda)] d\lambda}. \tag{33}$$

Using the identity

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

we conclude that

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

We have fixed the sign in Eq. (35) by demanding that $K(\tilde{\lambda},\xi_\pm)$ 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

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

6
where $\alpha(\lambda, \xi_{\pm})$ is given by Eq. (30). It can be shown that this result agrees with the one 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 of 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 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.

5 Acknowledgments

This work was supported in part by the National Science Foundation under Grant PHY-9507829.

6 Appendix

Here we prove the identity

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

(37)

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

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

(38)

It is convenient to first consider the sum

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

(39)
Expanding the denominator in an infinite series and then interchanging the order of summations, we obtain

\[
S(x) = \sum_{k=1}^{\infty} e^{-2\eta k x} \sum_{n=0}^{\infty} (-)^n e^{-2\eta k n}
\]

\[
= \sum_{n=0}^{\infty} (-)^n \sum_{k=1}^{\infty} e^{-2\eta k (x+n)}
\]

\[
= \sum_{m=0}^{\infty} \left\{ \frac{e^{-2\eta (x+2m)}}{1 - e^{-2\eta (x+2m)}} - \frac{e^{-2\eta (x+2m+1)}}{1 - e^{-2\eta (x+2m+1)}} \right\}
\]

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

where

\[
\psi_q(x) = \frac{d}{dx} \log \Gamma_q(x)
\]

\[
= -\log(1-q) + \log q \sum_{j=0}^{\infty} \frac{q^{x+j}}{1-q^{x+j}}.
\]

Integrating the result \((43)\) with respect to \(x\), and evaluating the integration constant by considering the limit \(x \to \infty\), we obtain the desired identity Eq. (37).

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