Generalized $T$–$Q$ relations and the open XXZ chain

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Abstract. We propose a generalization of the Baxter $T$–$Q$ relation which involves more than one independent $Q(u)$. We argue that the eigenvalues of the transfer matrix of the open XXZ quantum spin chain are given by such generalized $T$–$Q$ relations, for the case that at most two of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are nonzero, and the bulk anisotropy parameter has values $\eta = i\pi/2, i\pi/4, \ldots$

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1. Introduction

The famous Baxter $T$–$Q$ relation [1], which schematically has the form

$$ t(u)Q(u) = Q(u') + Q(u''), $$

holds for many integrable models associated with the $sl_2$ Lie algebra and its deformations, such as the closed XXZ quantum spin chain. This relation provides one of the most direct routes to the Bethe ansatz expression for the eigenvalues of the transfer matrix $t(u)$.

We propose here a generalization of this relation which involves more than one $Q(u)$,

$$ t(u)Q_1(u) = Q_2(u') + Q_2(u''), $$
$$ t(u)Q_2(u) = Q_1(u''') + Q_1(u'''). $$

This structure arises naturally in the open XXZ quantum spin chain for special values of the bulk and boundary parameters. We expect that such generalized $T$–$Q$ relations, involving two or more independent $Q(u)$'s, may also appear in other integrable models.

The open XXZ chain with general integrable boundary terms [2] has a Hamiltonian which can be written as

$$ \mathcal{H} = \sum_{n=1}^{N-1} H_{n,n+1} + \frac{1}{2} \sinh \eta [\coth \alpha_- \tanh \beta_- \sigma_1^x + \cosech \alpha_- \sech \beta_- (\cosh \theta_- \sigma_1^x + i \sinh \theta_- \sigma_1^y)] $$
$$ - \coth \alpha_+ \tanh \beta_+ \sigma_N^x + \cosech \alpha_+ \sech \beta_+ (\cosh \theta_+ \sigma_N^x + i \sinh \theta_+ \sigma_N^y)], $$

where $H_{n,n+1}$ is given by

$$ H_{n,n+1} = \frac{1}{2} (\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \cosh \eta \sigma_n^z \sigma_{n+1}^z), $$

$\sigma^x, \sigma^y, \sigma^z$ are the usual Pauli matrices, $\eta$ is the bulk anisotropy parameter, $\alpha_+, \beta_+, \theta_+$ are boundary parameters, and $N$ is the number of spins.

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Although this model remains unsolved, the case of diagonal boundary terms ($\alpha_\pm$ or $\beta_\pm \to \pm \infty$) was solved long ago [3]–[5]. Moreover, the case of nondiagonal boundary terms when the boundary parameters obey the constraint

$$\alpha_- + \beta_- + \alpha_+ + \beta_+ = \pm (\theta_- - \theta_+) + \eta k,$$

(where $k \in [-(N+1), N+1]$ is an even/odd integer if $N$ is odd/even, respectively) has recently been solved by two approaches: generalized algebraic Bethe ansatz [6], and functional relations at roots of unity [7]–[9].

It would clearly be desirable to overcome this constraint, and find the solution for further values of the boundary parameters. Some progress was achieved recently using the functional relations approach [10]. Namely, Bethe ansätze were proposed for the special cases that at most one of the boundary parameters is nonzero, and the bulk anisotropy has values $\eta = i\pi/3, i\pi/5, \ldots$.

We find here (again by means of the functional relations approach) that by allowing the possibility of generalized $T$–$Q$ relations, we can obtain Bethe-ansatz-type expressions for the transfer matrix eigenvalues for the cases that at most two of the boundary parameters $\\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are nonzero, and the bulk anisotropy has values $\eta = i\pi/2, i\pi/4, \ldots$.

In order to make the paper self-contained, we summarize in section 2 the construction of the transfer matrix and the functional relations which it satisfies at roots of unity. In order to derive the generalized $T$–$Q$ relation, it is instructive to first understand why we are unable to obtain a conventional relation with a single $Q(u)$. We present this analysis in section 3. Finally, in section 4 we derive the generalized $T$–$Q$ relations. We conclude in section 5 with a brief discussion of our results and of some remaining open problems.

2. Transfer matrix and functional relations at roots of unity

The transfer matrix $t(u)$ of the open XXZ chain with general integrable boundary terms, which satisfies the fundamental commutativity property

$$[t(u), t(v)] = 0,$$

(2.1)

is given by [5]

$$t(u) = \text{tr}_0 K_0^+(u) T_0(u) K_0^-(u) \hat{T}_0(u),$$

(2.2)

where $T_0(u)$ and $\hat{T}_0(u)$ are the monodromy matrices

$$T_0(u) = R_{0N}(u) \cdots R_{01}(u), \quad \hat{T}_0(u) = R_{01}(u) \cdots R_{0N}(u),$$

(2.3)

and $\text{tr}_0$ denotes trace over the ‘auxiliary space’ 0. The $R$ matrix is given by

$$R(u) = \begin{pmatrix}
\sinh(u + \eta) & 0 & 0 & 0 \\
0 & \sinh u & \sinh \eta & 0 \\
0 & \sinh \eta & \sinh u & 0 \\
0 & 0 & 0 & \sinh(u + \eta)
\end{pmatrix},$$

(2.4)
where $\eta$ is the bulk anisotropy parameter; and $K^{\pm}(u)$ are $2 \times 2$ matrices whose components are given by [2, 11]

\[
\begin{align*}
K_{11}^-(u) & = 2(\sinh \alpha_- \cosh \beta_- \cosh u + \cosh \alpha_- \sinh \beta_- \sinh u) \\
K_{22}^-(u) & = 2(\sinh \alpha_- \cosh \beta_- \cosh u - \cosh \alpha_- \sinh \beta_- \sinh u) \\
K_{12}^-(u) & = e^{\theta_-} \sinh 2u, \\
K_{21}^-(u) & = e^{-\theta_-} \sinh 2u,
\end{align*}
\]

(2.5)

and

\[
\begin{align*}
K_{11}^+(u) & = -2(\sinh \alpha_+ \cosh \beta_+ \cosh (u+\eta) - \cosh \alpha_+ \sinh \beta_+ \sinh (u+\eta)) \\
K_{22}^+(u) & = -2(\sinh \alpha_+ \cosh \beta_+ \cosh (u+\eta) + \cosh \alpha_+ \sinh \beta_+ \sinh (u+\eta)) \\
K_{12}^+(u) & = -e^{\theta_+} \sinh 2(u+\eta), \\
K_{21}^+(u) & = -e^{-\theta_+} \sinh 2(u+\eta),
\end{align*}
\]

(2.6)

where $\alpha_{\pm}, \beta_{\pm}, \theta_{\pm}$ are the boundary parameters. The transfer matrix ‘contains’ the Hamiltonian (1.3),

\[
\mathcal{H} = c_1 \frac{\partial}{\partial u} t(u) \bigg|_{u=0} + c_2 \mathbb{I},
\]

(2.7)

where

\[
\begin{align*}
c_1 & = -\frac{1}{16 \sinh \alpha_- \cosh \beta_- \sinh \alpha_+ \cosh \beta_+ \sinh^{2N-1} \eta \cosh \eta}, \\
c_2 & = -\frac{\sinh^2 \eta + N \cosh^2 \eta}{2 \cosh \eta},
\end{align*}
\]

(2.8)

and $\mathbb{I}$ is the identity matrix.

The transfer matrix eigenvalues $\Lambda(u)$ have $i\pi$ periodicity

\[
\Lambda(u+i\pi) = \Lambda(u),
\]

(2.9)

crossing symmetry

\[
\Lambda(-u-\eta) = \Lambda(u),
\]

(2.10)

and the asymptotic behaviour

\[
\Lambda(u) \sim -\cosh(\theta_- - \theta_+) \frac{e^{u(2N+4)+\eta(N+2)}}{2^{2N+1}} + \cdots \text{ for } u \to \infty.
\]

(2.11)

For bulk anisotropy values

\[
\eta = \frac{i\pi}{p+1}, \quad p = 1, 2, \ldots,
\]

(2.12)

so that $q \equiv e^\eta$ is a root of unity, the eigenvalues obey functional relations of order $p+1$ [7, 8]

\[
\begin{align*}
\Lambda(u)\Lambda(u+\eta) \cdots \Lambda(u+p\eta) - \delta(u)\Lambda(u+2\eta)\Lambda(u+3\eta) \cdots \Lambda(u+p\eta) \\
& - \delta(u+\eta)\Lambda(u)\Lambda(u+3\eta) \cdots \Lambda(u+p\eta) \\
& - \delta(u+2\eta)\Lambda(u)\Lambda(u+\eta) \cdots \Lambda(u+p\eta) - \cdots \\
& - \delta(u+p\eta)\Lambda(u+\eta)\Lambda(u+2\eta) \cdots \Lambda(u+(p-1)\eta) + \cdots = f(u).
\end{align*}
\]

(2.13)
For example, for the case \( p = 3 \), the functional relation is

\[
\Lambda(u)\Lambda(u + \eta)\Lambda(u + 2\eta)\Lambda(u + 3\eta) - \delta(u)\Lambda(u + 2\eta)\Lambda(u + 3\eta) - \delta(u + \eta)\Lambda(u)\Lambda(u + 3\eta) - \delta(u + 2\eta)\Lambda(u + \eta) - \delta(u + 3\eta)\Lambda(u + \eta)\Lambda(u + 2\eta) + \delta(u)\delta(u + 2\eta) + \delta(u + \eta)\delta(u + 3\eta) = f(u). \tag{2.14}
\]

The functions \( \delta(u) \) and \( f(u) \) are given in terms of the boundary parameters \( \alpha_{\mp}, \beta_{\mp}, \theta_{\mp} \) by

\[
\delta(u) = \delta_0(u)\delta_1(u), \quad f(u) = f_0(u)f_1(u), \tag{2.15}
\]

where

\[
\delta_0(u) = (\sinh u \sinh(u + 2\eta))^2 \frac{\sinh 2u \sinh(2u + 4\eta)}{\sinh(2u + \eta) \sinh(2u + 3\eta)}, \tag{2.16}
\]

\[
\delta_1(u) = 2^4 \sinh(u + \eta + \alpha_-) \sinh(u + \eta - \alpha_-) \cosh(u + \eta + \beta_-) \cosh(u + \eta - \beta_-) \\
\times \sinh(u + \eta + \alpha_+) \sinh(u + \eta - \alpha_+) \cosh(u + \eta + \beta_+) \cosh(u + \eta - \beta_+), \tag{2.17}
\]

and therefore,

\[
\delta(u + i\pi) = \delta(u), \quad \delta(-u - 2\eta) = \delta(u). \tag{2.18}
\]

For \( p \) odd,

\[
f_0(u) = (-1)^{N+1}2^{-2pN} \sinh^{2N}((p + 1)u) \tanh^2((p + 1)u), \tag{2.19}
\]

\[
f_1(u) = -2^{3-2p} \cosh((p + 1)\alpha_-) \cosh((p + 1)\beta_-) \cosh((p + 1)\alpha_+) \cosh((p + 1)\beta_+) \\
\times \sinh^2((p + 1)u) - \sinh((p + 1)\alpha_-) \sinh((p + 1)\beta_-) \sinh((p + 1)\alpha_+) \\
\times \sinh((p + 1)\beta_+) \cosh^2((p + 1)u) + (-1)^N \cosh((p + 1)(\theta_- - \theta_+)) \\
\times \sinh^2((p + 1)u) \cosh^2((p + 1)u)). \tag{2.20}
\]

For \( p \) even,

\[
f_0(u) = (-1)^{N+1}2^{-2pN} \sinh^{2N}((p + 1)u), \tag{2.21}
\]

\[
f_1(u) = (-1)^{N+1}2^{3-2p} \sinh((p + 1)\alpha_-) \cosh((p + 1)\beta_-) \sinh((p + 1)\alpha_+) \cosh((p + 1)\beta_+) \\
\times \cosh^2((p + 1)u) - \cosh((p + 1)\alpha_-) \sinh((p + 1)\beta_-) \cosh((p + 1)\alpha_+) \\
\times \sinh((p + 1)\beta_+) \sinh^2((p + 1)u) + (-1)^N \cosh((p + 1)(\theta_- - \theta_+)) \\
\times \sinh^2((p + 1)u) \cosh^2((p + 1)u)). \tag{2.22}
\]

Hence, \( f(u) \) satisfies

\[
f(u + \eta) = f(u), \quad f(-u) = f(u). \tag{2.23}
\]

We also note the identity

\[
f_0(u)^2 = \prod_{j=0}^{p} \delta_0(u + j\eta). \tag{2.24}
\]
3. An attempt to obtain a conventional $T$–$Q$ relation

In order to obtain Bethe ansatz expressions for the transfer matrix eigenvalues, we try (following [12]) to recast the functional relations as the condition that the determinant of a certain matrix vanishes. To this end, let us consider again the $(p + 1) \times (p + 1)$ matrix given by [8]

$$
\mathcal{M}(u) = \begin{pmatrix}
\Lambda(u) - \frac{\delta(u)}{h(u + \eta)} & 0 & \ldots & 0 & -h(u) \\
-h(u + \eta) & \Lambda(u + \eta) - \frac{\delta(u + \eta)}{h(u + 2\eta)} & \ldots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
-\frac{\delta(u - \eta)}{h(u)} & 0 & \ldots & -h(u + p\eta) & \Lambda(u + p\eta)
\end{pmatrix},
$$

(3.1)

where $h(u)$ is a function which is $\pi$-periodic, but otherwise not yet specified. Evidently, successive rows of this matrix are obtained by simultaneously shifting $u \mapsto u + \eta$ and cyclically permuting the columns to the right. Hence, this matrix has the symmetry property

$$
SM(u)S^{-1} = M(u + \eta),
$$

(3.2)

where $S$ is the $(p + 1) \times (p + 1)$ matrix given by

$$
S = \begin{pmatrix}
0 & 1 & 0 & \ldots & 0 & 0 \\
0 & 0 & 1 & \ldots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & 0 & 1 \\
1 & 0 & 0 & \ldots & 0 & 0
\end{pmatrix}, \quad S^{p+1} = 1.
$$

(3.3)

This symmetry implies that the corresponding $T$–$Q$ relation would involve only one $Q(u)$. Indeed, if we assume $\det \mathcal{M}(u) = 0$ (which, as we discuss below, turns out to be false for the cases which we consider here), then $\mathcal{M}(u)$ has a null eigenvector,

$$
\mathcal{M}(u)v(u) = 0.
$$

(3.4)

The symmetry (3.2) is consistent with

$$
Sv(u) = v(u + \eta),
$$

(3.5)

which in turn implies that $v(u)$ has the form

$$
v(u) = (Q(u), Q(u + \eta), \ldots, Q(u + p\eta)), \quad Q(u + i\pi) = Q(u).
$$

(3.6)

That is, all the components of $v(u)$ are determined by a single function $Q(u)$. The null eigenvector condition (3.4) together with the explicit forms (3.1), (3.6) of $\mathcal{M}(u)$ and $v(u)$ would then lead to a conventional $T$–$Q$ relation.

One can verify that the condition $\det \mathcal{M}(u) = 0$ indeed implies the functional relations (2.13), if $h(u)$ satisfies

$$
f(u) = \prod_{j=0}^{p} h(u + j\eta) + \prod_{j=0}^{p} \frac{\delta(u + j\eta)}{h(u + j\eta)}.
$$

(3.7)
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Setting

$$z(u) \equiv \prod_{j=0}^{p} h(u + j\eta), \quad (3.8)$$

it immediately follows from (3.7) that $z(u)$ is given by

$$z(u) = \frac{1}{2} \left( f(u) \pm \sqrt{\Delta(u)} \right), \quad (3.9)$$

where $\Delta(u)$ is defined by

$$\Delta(u) \equiv f(u)^2 - 4 \prod_{j=0}^{p} \delta(u + j\eta). \quad (3.10)$$

We wish to focus here on new special cases that $\Delta(u)$ is a perfect square\(^1\). For odd values of $p$, $\Delta(u)$ is also a perfect square if at most two of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are nonzero. We henceforth restrict to such parameter values. In particular, we assume that $\eta$ is given by (2.12), with $p$ odd (i.e., bulk anisotropy values $\eta = i\pi/2, i\pi/4, \ldots$). For definiteness, here we present results for the case that $\alpha_-, \beta_+ \neq 0$ and $\alpha_+ = \beta_+ = \theta_+ = 0$. (In the appendix, we present results for the case that $\alpha_\pm \neq 0$ and $\beta_\pm = \theta_\pm = 0$; and similar results hold for the other cases.) Moreover, we also restrict to even values of $N$. (We expect similar results to hold for odd $N$.)

For such parameter values, it is easy to arrive at a contradiction. Indeed, on the one hand, the definition (3.8) together with the assumed $i\pi$-periodicity of $h(u)$ (which is required for the symmetry (3.2)) imply the result $z(u) = z(u + \eta)$. On the other hand, (3.10) together with (2.15)–(2.20) and (2.24) imply

$$\sqrt{\Delta(u)} = 2^{3-2p} f_0(u) (\cosh((p + 1)\alpha_-) + \cosh((p + 1)\beta_-)) \sinh^2((p + 1)u) \cosh((p + 1)u). \quad (3.11)$$

Hence, it follows from (3.9) that $z(u) \neq z(u + \eta)$, which contradicts the earlier result. We conclude that, for such parameter values, it is not possible to find a function $h(u)$ which is $i\pi$-periodic and satisfies the condition (3.7). Hence, for such parameter values, the matrix $\mathcal{M}(u)$ given by (3.1) does not lead to the solution of the model, and we fail to obtain a conventional $T$–$Q$ relation.

We remark that if either $\alpha_+$ or $\alpha_-$ is zero, then the Hamiltonian is no longer given by (1.3), since the coefficient $c_1$ (2.8) is singular. Indeed, as noted in [10], $t''(0)$ is then proportional to $\sigma_N^\tau$. Hence, in order to obtain a nontrivial integrable Hamiltonian, one must consider the second derivative of the transfer matrix. For the case $\alpha_-, \beta_+ \neq 0$,

$$t''(0) = -16 \sinh^{2N-1} \eta \cosh \eta \left( \sinh \alpha_- \cosh \beta_- \left\{ \sum_{n=1}^{N-1} H_{n,n+1} \right\} \right)$$

$$\quad \quad \quad \quad + \sinh \alpha_- \cosh \beta_-(N \cosh \eta + \sinh \eta \tanh \eta) \sigma_N^\tau \right) \sigma_N^\tau + \sinh \eta (\sigma_1^\tau + \sinh \beta_- \cosh \alpha_- \sigma_1^\tau) \sigma_N^\tau \right), \quad (3.12)$$

where $H_{n,n+1}$ is given by (1.4). The case $\alpha_\pm \neq 0$, for which the Hamiltonian instead has a conventional local form, is discussed in the appendix.

\(^1\) When the constraint (1.5) is satisfied, $\Delta(u)$ is a perfect square; these are the cases studied in [8]. For even values of $p$, $\Delta(u)$ is also a perfect square if at most one of the boundary parameters is nonzero; these are the cases studied in [10].

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4. The generalized $T$–$Q$ relations

Instead of demanding the symmetry (3.2), let us now demand only the weaker symmetry

$$TM(u)T^{-1} = M(u + 2\eta), \quad T \equiv S^2,$$

(4.1)

where $S$ is given by (3.3). Indeed, (3.2) implies (4.1), but the converse is not true. A matrix $M(u)$ with such symmetry is given by

$$M(u) = \begin{pmatrix}
\Lambda(u) - \frac{\delta(u)}{h^{(1)}(u)} & 0 & \ldots & 0 & -\frac{\delta(u - \eta)}{h^{(2)}(u - \eta)} \\
-h^{(1)}(u) & \Lambda(u + \eta) - h^{(2)}(u + \eta) & \ldots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
-h^{(2)}(u - \eta) & 0 & 0 & \ldots & -h^{(1)}(u + (p - 1)\eta) & \Lambda(u + p\eta)
\end{pmatrix},$$

(4.2)

where $h^{(1)}(u)$ and $h^{(2)}(u)$ are functions which are $i\pi$-periodic, but otherwise not yet specified.

This symmetry implies that the corresponding $T$–$Q$ relations will involve two $Q(u)$’s. Indeed, assuming again that

$$\det M(u) = 0,$$

(4.3)

then $M(u)$ has a null eigenvector $v(u),$

$$M(u)v(u) = 0.$$  

(4.4)

The symmetry (4.1) is consistent with

$$Tv(u) = v(u + 2\eta),$$

(4.5)

which implies that $v(u)$ has the form

$$v(u) = (Q_1(u), Q_2(u), \ldots, Q_1(u - 2\eta), Q_2(u - 2\eta)),$$

(4.6)

with

$$Q_1(u) = Q_1(u + i\pi), \quad Q_2(u) = Q_2(u + i\pi).$$

(4.7)

That is, the components of $v(u)$ are determined by two independent functions, $Q_1(u)$ and $Q_2(u)$. The null eigenvector condition (4.4) together with the explicit forms (4.2), (4.6) of $M(u)$ and $v(u)$ now lead to generalized $T$–$Q$ relations,

$$\Lambda(u) = \frac{\delta(u)}{h^{(1)}(u)} \frac{Q_2(u)}{Q_1(u)} + \frac{\delta(u - \eta)}{h^{(2)}(u - \eta)} \frac{Q_2(u - 2\eta)}{Q_1(u - \eta)},$$

(4.8)

$$= h^{(1)}(u - \eta) \frac{Q_1(u - \eta)}{Q_2(u - \eta)} + h^{(2)}(u) \frac{Q_1(u + \eta)}{Q_2(u - \eta)}.$$  

(4.9)

Since $\Lambda(u)$ has the crossing symmetry (2.10) and $\delta(u)$ has the crossing property (2.18), it is natural to have the two terms in (4.8) transform into each other under crossing. Hence, we set

$$h^{(2)}(u) = h^{(1)}(-u - 2\eta),$$

(4.10)

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and we make the ansatz

\[ Q_1(u) = \prod_{j=1}^{M_1} \sinh(u - u_j^{(1)}) \sinh(u + u_j^{(1)} + \eta), \]

\[ Q_2(u) = \prod_{j=1}^{M_2} \sinh(u - u_j^{(2)}) \sinh(u + u_j^{(2)} + 3\eta), \]

which is consistent with the required periodicity (4.7) and crossing properties

\[ Q_1(u) = Q_1(-u - \eta), \quad Q_2(u) = Q_2(-u - 3\eta). \]  

Analyticity of \( \Lambda(u) \) (4.8), (4.9) implies Bethe-ansatz-type equations for the zeros \( \{u_j^{(1)}, u_j^{(2)}\} \) of \( Q_1(u), Q_2(u) \), respectively,

\[ \frac{\delta(u_j^{(1)}) h_j^{(2)}(u_j^{(1)} - \eta)}{\delta(u_j^{(1)} - \eta) h_j^{(1)}(u_j^{(1)})} = \frac{-Q_2(u_j^{(1)} - 2\eta)}{Q_2(u_j^{(1)})}, \quad j = 1, 2, \ldots, M_1, \]

\[ \frac{h_j^{(1)}(u_j^{(2)})}{h_j^{(2)}(u_j^{(2)} + \eta)} = \frac{Q_1(u_j^{(2)} + 2\eta)}{Q_1(u_j^{(2)})}, \quad j = 1, 2, \ldots, M_2. \]

Note that the function \( h_j^{(1)}(u) \) has not yet been specified, nor has the important assumption that \( \mathcal{M}(u) \) has a vanishing determinant (4.3) yet been verified. These problems are closely related, and we now address them both.

One can verify that the condition \( \det \mathcal{M}(u) = 0 \) indeed implies the functional relations (2.13), if \( h_j^{(1)}(u) \) satisfies

\[ f(u) = w(u) \prod_{j=0,2,\ldots}^{p-1} \delta(u + j\eta) + \frac{1}{w(u)} \prod_{j=1,3,\ldots}^p \delta(u + j\eta), \]

where

\[ w(u) = \frac{\prod_{j=1,3,\ldots}^p h_j^{(2)}(u + j\eta)}{\prod_{j=0,2,\ldots}^{p-1} h_j^{(1)}(u + j\eta)}. \]

It immediately follows from (4.14) that \( w(u) \) is given by

\[ w(u) = \frac{f(u) \pm \sqrt{\Delta(u)}}{2 \prod_{j=0,2,\ldots}^{p-1} \delta(u + j\eta)}, \]

where \( \Delta(u) \) is the same quantity defined in (3.10).

Let us recall that we are considering the case that \( p \) is odd, and that at most \( \alpha_- \) and \( \beta_- \) are nonzero. For this case, \( \sqrt{\Delta(u)} \) is given by (3.11). It follows from (4.16) that for \( p = 3, 7, 11, \ldots \) the two solutions for \( w(u) \) are given by

\[ w(u) = \coth^{2N}(\frac{1}{2}(p + 1)u), \]

\[ w(u) = \left( \frac{\cosh((p + 1)u) - \cosh((p + 1)\alpha_-)}{\cosh((p + 1)u) + \cosh((p + 1)\alpha_-)} \right) \left( \frac{\cosh((p + 1)u) - \cosh((p + 1)\beta_-)}{\cosh((p + 1)u) + \cosh((p + 1)\beta_-)} \right) \times \coth^{2N}(\frac{1}{2}(p + 1)u), \quad p = 3, 7, 11, \ldots; \]
and for \( p = 1, 5, 9, \ldots \) the two solutions for \( w(u) \) are given by

\[
w(u) = \begin{cases} \frac{\cosh((p+1)u) - \cosh((p+1)\alpha_-)}{\cosh((p+1)u) + \cosh((p+1)\alpha_-)} \coth(2N) \left( \frac{1}{2} (p+1)u \right), \\
\frac{\cosh((p+1)u) + \cosh((p+1)\beta_-)}{\cosh((p+1)u) - \cosh((p+1)\beta_-)} \coth(2N) \left( \frac{1}{2} (p+1)u \right),
\end{cases}
\]

for \( p = 1, 5, 9, \ldots \) \( (4.18) \).

There are many solutions of \((4.15)\) for \( h^{(1)}(u) \) (with \( h^{(2)}(u) \) given by \((4.10)\)) corresponding to the above expressions for \( w(u) \), which also have the required \( \pi \) periodicity. We consider here the solutions

\[
h^{(1)}(u) = -4 \sinh(2N(u + 2\eta)), \quad M_2 = \frac{1}{2} N + p - 1, \quad M_1 = M_2 + 2, \quad p = 3, 7, 11, \ldots
\]

\[(4.19)\]

and

\[
h^{(1)}(u) = \begin{cases} -2 \cosh(u + \alpha_-) \cosh(u - \alpha_-) \cosh(2u) \sinh(2N(u + 2\eta)), \\
M_1 = M_2 = \frac{1}{2} N + 2p - 1, \quad p = 9, 17, 25, \ldots \end{cases}
\]

\[
2 \cosh(u + \alpha_-) \cosh(u - \alpha_-) \cosh(2u) \sinh(2N(u + 2\eta)),
\]

\[
M_1 = M_2 = \frac{1}{2} N + \frac{3}{2} (p - 1), \quad p = 5, 13, 21, \ldots
\]

\[
2 \cosh(u + \alpha_-) \cosh(u - \alpha_-) \cosh(2u) \sinh(2N(u + 2\eta)),
\]

\[
M_1 = M_2 = \frac{1}{2} N + 2, \quad p = 1,
\]

\[(4.20)\]

corresponding to the first solutions for \( w(u) \) given in \((4.17), (4.18)\), respectively. We have searched for solutions largely by trial and error, verifying numerically (along the lines explained in [9]) for small values of \( N \) that the eigenvalues can indeed be expressed as \((4.8), (4.9)\) with \( Q(u) \)'s of the form \((4.11)\).

Note that the values of \( M_1 \) and \( M_2 \) (i.e., the number of zeros of \( Q_1(u) \) and \( Q_2(u) \), respectively) depend on the particular choice for the function \( h^{(1)}(u) \). Our reason for choosing \((4.19), (4.20)\) over the other solutions which we found is that the former solutions gave the lowest values of \( M_1 \) and \( M_2 \), for given values of \( N \) and \( p \). (It would be interesting to know whether there exist other solutions for \( h^{(1)}(u) \) which give even lower values of \( M_1 \) and \( M_2 \).) Our conjectured values of \( M_1 \) and \( M_2 \) given in \((4.19), (4.20)\) are consistent with the asymptotic behaviour \((2.11)\). Moreover, these values have been checked numerically for small values of \( N \) (up to \( N = 6 \)) and \( p \) (up to \( p = 21 \)). That is, we have verified numerically that, with the above choice of \( h^{(1)}(u) \), the generalized \( T-Q \) relations \((4.8), (4.9)\) correctly give all \( 2^N \) eigenvalues, with \( Q_1(u) \) and \( Q_2(u) \) of the form \((4.11)\) and with \( M_1 \) and \( M_2 \) given in \((4.19), (4.20)\). We expect that similar results can be obtained corresponding to the second solutions for \( w(u) \).

To summarize, we propose that for the case that \( p \) is odd and that at most \( \alpha_- \), \( \beta_- \) are nonzero, the eigenvalues \( \Lambda(u) \) of the transfer matrix \( t(u) \) \((2.2)\) are given by the generalized \( T-Q \) relations \((4.8), (4.9)\), with \( Q_1(u) \) and \( Q_2(u) \) given by \((4.11), h^{(2)}(u) \) given by \((4.10)\), and \( h^{(1)}(u) \) given by \((4.19), (4.20)\). The zeros \( \{u^{(1)}_i, u^{(2)}_i\} \) of \( Q_1(u) \) and \( Q_2(u) \) are solutions of the Bethe ansatz equations \((4.13)\). We expect that there are sufficiently many such equations to determine all the zeros. As already mentioned, similar results hold for the case that at most two of the boundary parameters \( \{\alpha_-, \alpha_+, \beta_-, \beta_+\} \) are nonzero.

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5. Discussion

We have argued that the eigenvalues of the transfer matrix of the open XXZ chain, for the special case that $p$ is odd and that at most two of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are nonzero, can be given by generalized $T$–$Q$ relations (4.8), (4.9) involving more than one $Q(u)$. Although we have not ruled out the possibility of expressing these eigenvalues in terms of a conventional $T$–$Q$ relation, the analysis in section 3 suggests to us that this is unlikely.

Many interesting problems remain to be explored. It should be possible to explicitly construct operators $Q_1(u), Q_2(u)$ which commute with each other and with the transfer matrix $t(u)$, and whose eigenvalues are given by (4.11). There may be further special cases for which the quantity $\Delta(u)$ is a perfect square, in which case it should not be difficult to find the corresponding Bethe ansatz solution. The general case that $\Delta(u)$ is not a perfect square and/or that $\eta \neq i\pi/(p + 1)$ remains to be understood.

Generalized $T$–$Q$ relations are novel structures, which merit further investigation. The corresponding Bethe ansatz equations (e.g., (4.13)) have some resemblance to the ‘nested’ equations which are characteristic of higher-rank models. Such generalized $T$–$Q$ relations, involving two or even more $Q(u)$’s, may also lead to further solutions of integrable open chains of higher rank and/or higher-dimensional representations. (For recent progress on such models, see e.g. [13].)

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Appendix: the case $\alpha_\pm \neq 0$ and $\beta_\pm = \theta_\pm = 0$

Here we consider the case that $\alpha_\pm \neq 0$ and $\beta_\pm = \theta_\pm = 0$, for which the Hamiltonian is local,

$$H = \sum_{n=1}^{N-1} H_{n,n+1} + \frac{1}{2} \sinh \eta (\text{cosech } \alpha_- \sigma^x_1 + \text{cosech } \alpha_+ \sigma^x_N),$$

(A.1)
as follows from (1.3). For this case, the quantity $\sqrt{\Delta(u)}$ is given by (3.11) with $\beta_-$ replaced by $\alpha_+$, namely,

$$\sqrt{\Delta(u)} = 2^{3-2p} f_0(u) \left( \cosh((p+1)\alpha_-) + \cosh((p+1)\alpha_+) \right) \sinh^2((p+1)u) \cosh((p+1)u).$$

(A.2)

It follows that the two solutions for $w(u)$ (4.16) are given by

$$w(u) = \coth^{2N\left(\frac{1}{2} + 1\right)}((p+1)u),$$

$$w(u) = \left( \frac{\cosh((p+1)u) - \cosh((p+1)\alpha_-)}{\cosh((p+1)u) + \cosh((p+1)\alpha_-)} \right) \left( \frac{\cosh((p+1)u) - \cosh((p+1)\alpha_+)}{\cosh((p+1)u) + \cosh((p+1)\alpha_+)} \right) \times \coth^{2N\left(\frac{1}{2} + 1\right)}((p+1)u), \quad p = 3, 7, 11, \ldots,$$

(A.3)
and
\[ w(u) = \coth^{2N+2}(\frac{1}{2}(p+1)u), \]
\[ w(u) = \left( \frac{\cosh((p+1)u) - \cosh((p+1)\alpha_-)}{\cosh((p+1)u) + \cosh((p+1)\alpha_-)} \right) \left( \frac{\cosh((p+1)u) - \cosh((p+1)\alpha_+)}{\cosh((p+1)u) + \cosh((p+1)\alpha_+)} \right) \times \coth^{2N+2}(\frac{1}{2}(p+1)u), \quad p = 1, 5, 9, \ldots \]  
(A.4)

For simplicity, let us once again consider just the first solutions for \( w(u) \) given in (A.3) and (A.4), which are independent of \( \alpha_\pm \). Corresponding solutions of (4.15) for \( h^{(1)}(u) \) (with \( h^{(2)}(u) \) given by (4.10)) are
\[ h^{(1)}(u) = 4 \sinh^2(u + 2\eta), \quad M_2 = \frac{1}{2}N + \frac{1}{2}(3p - 1), \]  
\[ M_1 = M_2 + 2, \quad p = 3, 7, 11, \ldots \]  
(A.5)

and
\[ h^{(1)}(u) = \begin{cases} 
-2 \cosh(2u) \sinh^2 u \sinh^2(u + 2\eta), & M_1 = M_2 = \frac{1}{2}N + 2p - 1, \\
2 \cosh(2u) \sinh^2 u \sinh^2(u + 2\eta), & M_1 = M_2 = \frac{1}{2}N + \frac{3}{2}(p - 1), \\
2 \cosh(2u) \sinh^2 u \sinh^2(u + 2\eta), & M_1 = M_2 = \frac{1}{2}N + 2, \\
p = 9, 17, 25, \ldots & M_1 = M_2 = \frac{1}{2}N + 2p - 1, \\
p = 5, 13, 21, \ldots & M_1 = M_2 = \frac{1}{2}N + \frac{3}{2}(p - 1), \quad p = 3, 7, 11, \ldots \end{cases} \]  
(A.6)

That is, the eigenvalues \( \Lambda(u) \) of the transfer matrix \( t(u) \) (2.2), for \( \eta \) values (2.12) with \( p \) odd and for \( \alpha_\pm \neq 0 \) and \( \beta_\pm = \theta_\pm = 0 \), are given by the generalized \( T-Q \) relations (4.8), (4.9), with \( Q_1(u) \) and \( Q_2(u) \) given by (4.11), \( h^{(2)}(u) \) given by (4.10), and \( h^{(1)}(u) \) given by (A.5), (A.6). The zeros \( \{u_j^{(1)}, u_j^{(2)}\} \) of \( Q_1(u) \) and \( Q_2(u) \) are solutions of the Bethe ansatz equations (4.13).

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