Separation of Variables in the open XXX chain

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Abstract

We apply the Sklyanin method of separation of variables to the reflection algebra underlying the open spin-$\frac{1}{2}$ XXX chain with non-diagonal boundary fields. The spectral problem can be formulated in terms of a $TQ$-equation which leads to the known Bethe equations for boundary parameters satisfying a constraint. For generic boundary parameters we study the asymptotic behaviour of the solutions of the $TQ$-equation.

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1 Introduction

Exact solutions of spin chain models have provided many insights into the properties of interacting many-body systems subject to strong quantum fluctuations. Various methods have been established to study the spectrum and nature of their low-lying excitations of such models as well as their thermodynamical properties and even correlation functions without the need to revert to perturbational approaches. At the same time various problems concerning systems with open boundaries are still not solved completely. Even for the prototype spin-$\frac{1}{2}$ XXZ chain with general open boundary conditions techniques for the solution of the spectral problem have been developed only recently [1, 4, 11–14]. This model, apart from being the simplest starting point for studies of boundary effects in a correlated system, allows to investigate the approach to a stationary state in one-dimensional diffusion problems for hard-core particles [7, 8] and transport through one-dimensional quantum systems [5]. Its Hamiltonian is given by

$$H = \sum_{j=1}^{L-1} \left[ \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + (\sigma_j^z \sigma_{j+1}^z - 1) \cosh \eta \right] - \cosh \eta$$

$$+ \left[ \sigma_L^x \coth \xi^- + \frac{2\kappa^-}{\sinh \xi^-}(\sigma_L^x \cosh \theta^- + i\sigma_L^y \sinh \theta^-) \right] \sinh \eta$$

$$+ \left[ \sigma_1^x \coth \xi^+ + \frac{2\kappa^+}{\sinh \xi^+}(\sigma_1^x \cosh \theta^+ + i\sigma_1^y \sinh \theta^+) \right] \sinh \eta \tag{1.1}$$

where $\sigma_j^\alpha$, $\alpha = x, y, z$ denote the usual Pauli matrices at site $j$ and the parameters $\xi^\pm, \kappa^\pm, \theta^\pm$ refer to the left and right boundary respectively. The Hamiltonian (1.1) is a member of a commuting family of operators generated by a transfer matrix based on a representation of Sklyanin’s reflection algebra [16]. While this establishes the integrability the actual solution of the spectral problem through application of Bethe ansatz methods has been impeded by the absence of a reference state, such as the ferromagnetically polarized state with all spins up for the case of diagonal boundary fields. Interestingly, by imposing certain constraints obeyed by the left and right boundary fields, the eigenvalues of the spin-$\frac{1}{2}$ XXZ chain and of the isotropic spin-$S$ model can be obtained by means of the algebraic Bethe ansatz [4, 12]. In an alternative approach, Nepomechie et al. have been able to derive Bethe type equations whose roots parametrize the eigenvalues of the Hamiltonian for special values of the anisotropy $\eta = i\pi/(p + 1)$ with $p$ a positive integer and where the transfer matrix obeys functional equations of finite order [13]. Their approach relies on the periodicity of the underlying trigonometric $R$-matrix of the model which is missing in the rational limit $\eta \to 0$ of the isotropic chain. For generic values of the anisotropy the spectral problem has been formulated as a $TQ$-equation assuming that the large $j$-limit of the transfer matrices with spin $j$ in auxiliary space exists [19]. No such constraints are needed in the derivation of a different set of recursion relations for the diagonalization of (1.1) based on the representation theory of the $q$-Onsager algebra [1]. Very recently, Galleas has formulated another functional approach to determine the eigenvalues of (1.1) in the generic case without a reference state [11]. Taking certain matrix elements of the transfer matrix involving the ferromagnetic pseudo vacuum and the unknown eigenstates he derives the Bethe equations of Nepomechie et al. without the need to restrict the anisotropy to roots of unity. Unfortunately, this approach yields no
information on the eigenstates, therefore further studies of correlation functions are out of reach for now.

In this paper we approach the problem by means of a different method which circumvents the difficulties of the algebraic Bethe ansatz in the absence of a reference state. Within Sklyanin’s functional Bethe ansatz (or separation of variables method) [17] the eigenvalue problem is formulated using a suitably chosen representation of the underlying Yang-Baxter algebra on a space of certain functions. This approach was independently confirmed by use of Manin matrices [6] and has proven its strength in particular in models with non-compact target space lacking a reference state, e.g. the Toda chain [15] or the sinh-Gordon model [3,18] where the spectral problem can be formulated in terms of separable functional equations on this space which then have to be solved by exploiting the analytical properties of the problem.

The article is organized as follows. In sections 2 and 3 we will review the basic properties of the reflection algebra and its representation for the open XXZ spin chain. Then in section 4 we will implement the functional Bethe ansatz for the restriction to the open XXX spin chain following Sklyanin’s original article [17]. Finally in section 5 we address the problem of extracting the solution of the spectral problem from the resulting second order difference equations and study the analytical properties of their eigenfunctions. The last section is devoted to a concluding summary.

2 Integrable Boundary Conditions

Sklyanin’s construction [16] of integrable systems involving boundaries is valid for a general class of integrable systems characterized by an $R$-matrix of difference form $R(\lambda, \mu) = R(\lambda - \mu) \in \text{End}(V \otimes V) \ (V \text{ is a vector space with dim} \ V \in \mathbb{N}$ ) which not only satisfies the Yang-Baxter equation

$$R_{12}(\lambda - \mu) R_{13}(\lambda - \nu) R_{23}(\mu - \nu) = R_{23}(\mu - \nu) R_{13}(\lambda - \nu) R_{12}(\lambda - \mu)$$

(2.1)

but also several conditions such as symmetry with respect to the permutation operator $P$ on $V \otimes V \ (P \ x \otimes y = y \otimes x)$,

$$R(\lambda) = PR(\lambda)P ,$$

(2.2)

unitarity involving some complex function $\rho(\lambda)$,

$$R(\lambda)R(-\lambda) = \rho(\lambda)$$

(2.3)

and crossing unitarity for another complex function $\tilde{\rho}(\lambda)$,

$$R^{t_1}(\lambda)R^{t_1}(-\lambda - 2\eta) = \tilde{\rho}(\lambda) .$$

(2.4)

The parameter $\eta$ characterizes the $R$-matrix and the superscript $t_j$ denotes the transposition with respect to the $j$th space in the tensor product $V \otimes V$. Here we will need the well-known 6-vertex model solution

$$R(\lambda, \mu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(\lambda, \mu) & c(\lambda, \mu) & 0 \\ 0 & c(\lambda, \mu) & b(\lambda, \mu) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$b(\lambda, \mu) = \frac{\sinh(\lambda - \mu)}{\sinh(\lambda - \mu + \eta)}$$

(2.5)

$$c(\lambda, \mu) = \frac{\sinh(\lambda - \mu + \eta)}{\sinh(\lambda - \mu + \eta)}$$
of the Yang-Baxter equation \((2.1)\). It generates the Hamiltonian of the spin-\(\frac{1}{2}\) XXZ chain with
\[
\rho(\lambda) = 1, \quad \tilde{\rho}(\lambda) = \frac{\sinh \lambda \sinh (\lambda + 2\eta)}{\sinh^2(\lambda + \eta)}.
\] (2.6)
Each solution \(R(\lambda)\) of the Yang-Baxter equation fixes the structure constants of a Yang-Baxter algebra
\[
R_{12}(\lambda - \mu)T_1(\lambda)T_2(\mu) = T_2(\mu)T_1(\lambda)R_{12}(\lambda - \mu)
\] (2.7)
with generators \(T_{\alpha \beta}(\lambda)\), \(\alpha, \beta = 1, 2\); where \(T_1(\lambda) = T(\lambda) \otimes I\), \(T_2(\lambda) = I \otimes T(\lambda)\) are the embeddings of the monodromy matrix \(T(\lambda)\).

Sklyanin’s construction of open spin chains is based on the representations of two algebras \(T^{(+)}\) and \(T^{(-)}\) defined by the relations
\[
R_{12}(\lambda - \mu)T_1^{(-)}(\lambda)R_{12}(\lambda + \mu)T_2^{(-)}(\mu) = T_2^{(-)}(\mu)R_{12}(\lambda + \mu)T_1^{(-)}(\lambda)R_{12}(\lambda - \mu)
\] (2.8)
\[
R_{12}(-\lambda + \mu)T_1^{(+)t_1}(\lambda)R_{12}(-\lambda - \mu - 2\eta)T_2^{(+)t_2}(\mu) =
= T_2^{(+)t_2}(\mu)R_{12}(-\lambda - \mu - 2\eta)T_1^{(+)t_1}(\lambda)R_{12}(-\lambda + \mu).
\] (2.9)
We shall call \(T^{(+)}\) and \(T^{(-)}\) right and left reflection algebras respectively. The transfer matrix
\[
t(\lambda) = \text{tr} T^{(+)}(\lambda)T^{(-)}(\lambda)
\] (2.10)
as a trace in auxiliary space is the central object under consideration because it generates with \([t(\lambda), t(\mu)] = 0\) a commuting family of operators.

The explicit construction of integrable open boundary conditions for models arising from the Yang-Baxter algebra starts with the \(2 \times 2\) matrix
\[
K(\lambda, \xi) = \frac{1}{\sinh \xi \cosh \lambda}
\begin{pmatrix}
\sinh(\lambda + \xi) & \kappa e^\theta \sinh(2\lambda) \\
\kappa e^{-\theta} \sinh(2\lambda) & -\sinh(\lambda - \xi)
\end{pmatrix}
\] (2.11)
originally found by de Vega et al. [9]. It constitutes the known \(c\)-number representations \(K^{(+)}(\lambda) = \frac{1}{2}K(\lambda + \eta, \xi^+)\) and \(K^{(-)}(\lambda) = K(\lambda, \xi^-)\) of the reflection algebras with the obvious properties
\[
\text{tr} K(\lambda, \xi) = 2, \quad K^{(-)}(0) = I, \quad \text{tr} K^{(+)}(0) = 1.
\] (2.12)

The Hamiltonian \((1.1)\) involving two neighbour sites for the interaction is connected, up to a factor, to the first derivative of \(t(\lambda)\) by looking at the expansion \(t(\lambda) = 1 + 2\lambda \mathcal{H} + \ldots\) around the point \(\lambda = 0\). Considering local \(L\)-matrices building up the two representations \(T^{(+)}(\lambda) = L_L(\lambda) \cdots L_{M+1}(\lambda)\) and \(T^{(-)}(\lambda) = L_M(\lambda) \cdots L_1(\lambda)\) of \((2.7)\) then by construction
\[
T^{(-)}(\lambda) = T^{(-)}(\lambda)K^{(-)}(\lambda)T^{(-)}(\lambda)^{-1}(-\lambda)
\]
\[
T^{(+)}(\lambda) = T^{(+)}(\lambda)K^{(+)}(\lambda)(T^{(+)}(\lambda)^{-1})^t(-\lambda)
\] (2.13)
are representations of the reflection algebras such that the normalized transfer matrix

\[ t(\lambda) = K(\lambda)T(\lambda)K(-\lambda)T^{-1}(-\lambda) \quad , \quad t(0) = 1 \quad (2.14) \]

is independent of the factorization of \( T(\lambda) = T^{(+)}(\lambda)T^{(-)}(\lambda) \). Thus we are free to choose

\[ T^{(+)}(\lambda) = K^{(+)}(\lambda) \quad , \quad T^{(-)}(\lambda) = T(\lambda)K^{(-)}(\lambda)T^{-1}(-\lambda) \quad . \quad (2.15) \]

In order to gain more symmetric arguments and to avoid inconvenient scalar functions after applying the inversion formula

\[ T^{-1}(\lambda) = \frac{1}{(d_qT)(\lambda - \eta/2)}\sigma^y T^t(\lambda - \eta)\sigma^y \quad (2.16) \]

it is instructive to define the new object \( U(\lambda + \eta/2) \equiv T^{(-)}(\lambda)(d_qT)(-\lambda - \eta/2) \) consisting of

\[ U(\lambda) = T(\lambda - \eta/2)K^{(-)}(\lambda - \eta/2)\sigma^y T^t(-\lambda - \eta/2)\sigma^y \quad . \quad (2.17) \]

It is still a representation of the left reflection algebra with a \( 2 \times 2 \) matrix in auxiliary space,

\[ U(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix} \quad . \quad (2.18) \]

The quantum determinant \((d_qT)(\lambda)\) is the central element (Casimir) of the Yang-Baxter algebra \((2.7)\). With the one-dimensional projector \( P_{12} \) onto the antisymmetric (singlet) state in the tensor product \( V \otimes V \) of auxiliary spaces the definition reads

\[ (d_qT)(\lambda) = \text{tr}_{12} P_{12} T_1(\lambda - \eta/2)T_2(\lambda + \eta/2) \]

\[ = A(\lambda + \eta/2)D(\lambda - \eta/2) - B(\lambda + \eta/2)C(\lambda - \eta/2) \quad . \quad (2.19) \]

Here, the trace \( \text{tr}_{12} \) is to be taken in both auxiliary spaces 1 and 2 of the tensor product \( V \otimes V \) and the monodromy matrix \( T \) enters with the usual representation

\[ T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix} \quad . \quad (2.20) \]

### 3 Quantum Determinants

Like the Casimir for the Yang-Baxter algebra there exists a similar object for the left reflection algebra. It is defined as

\[ (\Delta_q U)(\lambda) = \text{tr}_{12} P_{12} U_1(\lambda - \eta/2)R_{12}(2\lambda - \eta)U_2(\lambda + \eta/2) \quad . \quad (3.1) \]

To express \((\Delta_q U)(\lambda)\) in terms of the generators \( A(\lambda) \), \( B(\lambda) \), \( C(\lambda) \) and \( D(\lambda) \) it is instructive to use the combinations

\[ \tilde{D}(\lambda) \equiv \sinh(2\lambda)D(\lambda) - \sinh \eta A(\lambda) \quad , \quad \tilde{C}(\lambda) \equiv \sinh(2\lambda + \eta)C(\lambda) \quad (3.2) \]
borrowed from the algebraic Bethe ansatz. Then the suggestive form of the quantum determinant reads
\[
(\Delta_q U)(\lambda) = A(\lambda + \eta/2) \tilde{D}(\lambda - \eta/2) - B(\lambda + \eta/2) \tilde{C}(\lambda - \eta/2) .
\] (3.3)

In case of the \(c\)-number representation \(K(\lambda - \eta/2, \xi)\) for \(U(\lambda)\) connected to the left reflection algebra the relation
\[
(\Delta_q K)(\lambda - \eta/2, \xi) = \frac{\sinh(2\lambda - 2\eta) \cosh \lambda}{\cosh(\lambda - \eta)} \det K(\lambda, \xi) \tag{3.4}
\]
holds. Note that this relation is only valid for the shifted argument \(\lambda - \eta/2\) because the arising expressions are no longer of difference form.

Appropriately transforming the boundary parameters \(\xi\) and \(\kappa\) according to the mapping
\[
\sinh \alpha \cosh \beta = \frac{\sinh \xi}{2\kappa} , \quad \cosh \alpha \sinh \beta = \frac{\cosh \xi}{2\kappa} \tag{3.5}
\]
the determinant \(\det K(\lambda, \xi)\) factorizes and its quantum version decomposes to product form
\[
(\Delta_q K)(\lambda - \eta/2, \xi) = -\sinh(2\lambda - 2\eta) \frac{\sinh(\lambda - \alpha) \cosh(\lambda - \beta)}{\sinh \alpha \cosh \beta \cosh(\lambda - \eta)} \frac{\sinh(\lambda + \alpha) \cosh(\lambda + \beta)}{\sinh \alpha \cosh \beta \cosh \lambda} .
\] (3.6)

It is obvious that in the parametrization (3.5) the model is invariant under the simultaneous transformations \(\alpha \rightarrow -\alpha\) and \(\beta \rightarrow i\pi - \beta\).

As the quantum determinant respects co-multiplication, applying it to the full representation (2.17) of the left reflection algebra with monodromy matrices \(T\) yields
\[
(\Delta_q U)(\lambda) = (d_q T)(\lambda - \eta/2) (\Delta_q K)(\lambda - \eta/2, \xi) (d_q T)(-\lambda - \eta/2) .
\] (3.7)

Example. Consider the inhomogeneous periodic chain with inhomogeneities \(s_j \in \mathbb{C}\) at each lattice site \(j = 1 \ldots L\). Then the quantum determinant of a fundamental \(L\)-matrix \(L_j(\lambda) = R(\lambda - s_j)\) takes the scalar value
\[
(d_q L_j)(\lambda) = \sinh(\lambda - s_j + 3\eta/2) \sinh(\lambda - s_j - \eta/2) \tag{3.8}
\]
yielding \((d_q T)(\lambda - \eta/2) = \left[ \prod_{j=1}^L \sinh(\lambda - s_j + \eta) \sinh(\lambda - s_j - \eta) \right]\) for a chain of \(L\) local spins \(1/2\).
4 Functional Bethe Ansatz

The entries of the monodromy matrix $U(\lambda)$ can be expressed in terms of the operators $A(\lambda)$, $B(\lambda)$, $C(\lambda)$ and $D(\lambda)$ of the periodic monodromy matrix $T(\lambda)$, i.e.

$$
\mathcal{B}(\lambda) = -\frac{\sinh(\lambda - \eta/2 + \xi^-) \cosh(\lambda - \eta/2) \sinh(2\lambda - \eta)}{\sinh(2\lambda) \cosh(\lambda - \eta/2) \sinh(2\lambda)} B(-\lambda - \eta/2) A(\lambda - \eta/2)
-\frac{\sinh(\lambda + \eta/2 - \xi^-) \cosh(\lambda - \eta/2) \sinh(2\lambda - \eta)}{\sinh(2\lambda) \cosh(\lambda - \eta/2) \sinh(2\lambda)} B(\lambda - \eta/2) A(-\lambda - \eta/2)
+ \frac{\kappa^- e^{\theta^-}}{\sinh(\lambda - \eta/2) \cosh(\lambda - \eta/2)} A(\lambda - \eta/2) A(-\lambda - \eta/2)
- \frac{\kappa^- e^{\theta^-}}{\sinh(\lambda - \eta/2) \cosh(\lambda - \eta/2)} B(\lambda - \eta/2) B(-\lambda - \eta/2) \ .
$$

(4.1)

Obviously there is no easy pseudo vacuum $|0\rangle$ for an algebraic Bethe ansatz to work ($\mathcal{B}(\lambda)|0\rangle = 0$) for non-diagonal boundaries ($\kappa^- \neq 0$) in $K^-$. Instead we can apply Sklyanin’s functional Bethe ansatz [17].

Henceforth let us restrict to the rational case. Then we can choose the boundary matrices diagonal in favour of a twisted monodromy matrix $T(\lambda)$ as demonstrated in the following

**Example.** Applying the rational limit\(^1\) to the parametrization of the boundary matrix $K(\lambda, \xi)$ yields the similarity transformation independent of the spectral parameter

$$
K(\lambda, \xi) = MS \begin{pmatrix} \frac{\alpha + \lambda}{\alpha} & 0 \\ 0 & \frac{\alpha - \lambda}{\alpha} \end{pmatrix} (MS)^{-1}
$$

(4.2)

with the diagonal matrix to be a solution to the reflection algebra and the $2 \times 2$ number matrices

$$
M = \begin{pmatrix} e^{\theta/2} & 0 \\ 0 & e^{-\theta/2} \end{pmatrix} \quad , \quad S = \frac{1}{\sqrt{2 \cosh \beta}} \begin{pmatrix} e^{\beta/2} & -e^{-\beta/2} \\ e^{-\beta/2} & e^{\beta/2} \end{pmatrix} \ .
$$

(4.3)

Thus in the transfer matrix $t(\lambda) = \text{tr} K^-(\lambda) T(\lambda) K^+(\lambda) T^{-1}(-\lambda)$ we are free to consider a diagonal outer boundary matrix $K^+$ together with the c-number twist $(M^+(S^+))^{-1} T(\lambda)$ of $T(\lambda)$\(^2\).

**Operator-Valued Zeroes**

The main goal of the functional Bethe ansatz is to treat the spectral problem of the transfer matrix in a representation space of symmetric functions manipulated by some shift operators, which descent from operator-valued zeroes of the $\mathcal{B}$-operator. Starting from $\mathcal{B}(\lambda)$ in the

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\(^1\)‘Rational limit’ means to scale the arguments by a small parameter $\varepsilon \to 0$ and calling $\eta \to \varepsilon \eta \iota c$. Here only $\alpha$ is rescaled whereas $\beta$ remains unchanged. This immediately follows from (3.5).

\(^2\)The $gl(2)$ symmetry of the rational model allows to remove the twist of the monodromy matrix in favour of a twisted boundary matrix $\tilde{K}^-(\lambda) = (M^+(S^+))^{-1} K^-(\lambda) M^+(S^+)$, see Ref. [12].
rational limit reading
\[ B(\lambda) = -\frac{2\lambda - ic}{\xi^-} \left[ \frac{\lambda + \xi^- - ic/2}{2\lambda} B(-\lambda - ic/2)A(\lambda - ic/2) \right. \]
\[ \quad + \frac{-\lambda + \xi^- - ic/2}{-2\lambda} B(\lambda - ic/2)A(-\lambda - ic/2) \]
\[ \left. - \kappa^- e^{\theta^-} A(\lambda - ic/2)A(-\lambda - ic/2) \right) \]
\[ + \kappa^- e^{-\theta^-} B(\lambda - ic/2)B(-\lambda - ic/2) \] (4.4)
we observe the expression in the square brackets to be symmetric with respect to \( \lambda \to -\lambda \) and having no pole at \( \lambda = 0 \). As the operators \( A, B, C \) and \( D \) are polynomials of degree \( L \) with the known asymptotics
\[ A \sim \frac{\exp(\beta^+ + \theta^+)}{\sqrt{2 \cosh \beta^+}} \lambda^L, \quad B \sim \frac{\exp(\theta^- - \beta^+)}{\sqrt{2 \cosh \beta^+}} \lambda^L \]
\[ C \sim -\frac{\exp(-\beta^+ + \theta^+)}{\sqrt{2 \cosh \beta^+}} \lambda^L, \quad D \sim \frac{\exp(\beta^+ + \theta^+)}{\sqrt{2 \cosh \beta^+}} \lambda^L \] (4.5)
we can factorize the square brackets in terms of \( \lambda^2 \). The asymptotic pre-factors arise from the twist \( S^{-1}M^{-1} \) of the periodic monodromy matrix \( T(\lambda) \).

Thus \( B(\lambda) \) is polynomial with a simple zero at \( \lambda = ic/2 \) and operator-valued coefficients assembling
\[ B(\lambda) = -\frac{2\lambda - ic}{(-1)^L \xi^-} \frac{1 - 2\kappa^- \sinh(\theta^- - \theta^+ - \beta^+)}{2 \cosh \beta^+} \left[ \prod_{l=1}^L (\lambda^2 - \hat{x}_l^2) \right] . \] (4.6)
As \( [B(\lambda), B(\mu)] = 0 \), according to the reflection algebra, we can deduce \( [\hat{x}_j^2, \hat{x}_k^2] = 0 \) for all \( j, k = 1 \ldots L \) with the spectrum shown in the next Example.

**Example.** Setting \( L = 1 \) in the explicit expression (4.6) for a spin 1/2 representation with inhomogeneity \( s_1 \) yields for the argument \( \lambda = 0 \) the form
\[ \hat{x}_1^2 = \left( \frac{(s_1 + ic/2)^2}{(s_1 - ic/2)^2} \right) \] (4.7)
of the operator-valued zero \( \hat{x}_1^2 \) reading in a diagonalized form. This fixes discrete sets \( \Lambda_j \equiv \{ s_j - ic/2, s_j + ic/2 \} \) representing the spectra of the coordinates \( \hat{x}_j \) except for a global sign and resembling \( \mathbb{X}^L \equiv \Lambda_1 \times \ldots \times \Lambda_L \).

For the forthcoming relations, to work with the simple zeroes \( \hat{x}_j \) instead of \( \hat{x}_j^2 \), we refer to the supplemental

**Remark.** Let \( \hat{x}_j \) be the operator-valued zeroes satisfying \( \lambda = \pm \hat{x}_j \mid B(\lambda) = 0 \). Then all \( \hat{x}_j^2 \) can be simultaneously diagonalized such that for all \( j, k = 1 \ldots L \)
\[ [\hat{x}_j, \hat{x}_k] = 0, \quad \hat{x}_j = \left( \begin{array}{c} s_j + ic/2 \\ s_j - ic/2 \end{array} \right) . \] (4.8)
Conjugated Momenta

With the operators $\hat{x}_j$ the next problem is to calculate the expression for the transfer matrix in the $\hat{x}$-representation. For this let us introduce first the ‘conjugated momenta’ to the ‘coordinates’ $\hat{x}_j$.

Considering $A(\lambda)$ and $\tilde{D}(\lambda)$ as polynomials and inserting the operator valued zeroes of $B(\lambda)$ by ‘substitution from the left’ yields the new operators

$\lambda=\tilde{x}_j \mid A(\lambda) = \sum p \hat{x}^p_j A_p \equiv X^-_j$ \hspace{1cm} \hspace{1cm} (4.9)

$\lambda=\tilde{x}_j \mid \tilde{D}(\lambda) = \sum p \hat{x}^p_j \tilde{D}_p \equiv X^+_j$ .

Here $A_p$ and $\tilde{D}_p$ denote operator-valued expansion coefficients. The commutation relations with the coordinates $\hat{x}_j$ are summarized in

**Theorem 1.** Let $\tilde{x}_j$ be the operator-valued zeroes of $B(\lambda)$ and $X^\pm_j$ their conjugated momenta related by the reflection algebra. Then

$X^\pm_j \hat{x}_k = (\tilde{x}_k \pm ic\delta_{jk})X^\pm_j$. \hspace{1cm} (4.10)

**Proof.** Consider the commutation relation

$A(\lambda)B(\mu) = \frac{\sinh(\lambda + \mu - \eta) \sinh(\lambda - \mu - \eta)}{\sinh(\lambda + \mu) \sinh(\lambda - \mu)} B(\mu)A(\lambda)$

$\hspace{1cm} + \frac{\sinh \eta \sinh(2\mu - \eta)}{\sinh(2\mu) \sinh(\lambda + \mu)} B(\lambda)A(\mu)$

$\hspace{1cm} - \frac{\sinh \eta}{\sinh(2\mu) \sinh(\lambda + \mu)} B(\lambda)\tilde{D}(\mu)$ \hspace{1cm} (4.11)

of $A(\lambda)$ and $B(\mu)$ and multiply it by $\sinh(\lambda + \mu) \sinh(\lambda - \mu)$. Then take its rational limit and insert the coordinates $\tilde{x}_j$ by ‘substitution from the left’. The expression reduces to

$(\tilde{x}_j - \lambda)(\tilde{x}_j + \lambda)X^-_j B(\lambda) = (\tilde{x} + \lambda - ic)(\tilde{x} - \lambda - ic)B(\lambda)X^-_j$. \hspace{1cm} (4.12)

Replacing $B(\lambda)$ by its factorized form, cancelling the constant asymptotics and multiplying by the inverse $(\tilde{x}^2_j - \lambda^2)^{-1}$ from the left the commutation relation

$X^-_j \left[ \prod_{l=1}^L (\lambda^2 - \tilde{x}_l^2) \right] = \left[ \lambda^2 - (\tilde{x}_j - ic)^2 \right] \left[ \prod_{l=1, l \neq j}^L (\lambda^2 - \tilde{x}_l^2) \right] X^-_j$ \hspace{1cm} (4.13)

remains. Implying all expressions to be symmetric in $\tilde{x}_j$ to act on we arrive at the desired relation. Analogously the elementary commutation of $X^+_j$ with the coordinates arises from the commutation of $B$ and $\tilde{D}$. \hspace{1cm} $\Box$

The next natural step would be establishing the commutation relation between two $X^\pm$’s. However, it cannot be done directly because $X^\pm_j$ exceed per definition the representation space.
Representation space

Following Sklyanin’s approach the square brackets in operator (4.6) can be expanded into $\lambda^2L - \hat{b}_1\lambda^{2(L-1)} \pm \ldots + \hat{b}_L$ with commuting operators $\hat{b}_j$ thus sharing a common system of eigenfunctions $f_\alpha$,

$$\hat{b}_j f_\alpha = b^\alpha_\alpha f_\alpha \quad , \quad \alpha = 1 \ldots 2^L \quad (4.14)$$

where $2^L$ represents spin-$1/2$. To every point $b^\alpha = (b^\alpha_1, \ldots, b^\alpha_L) \in \mathbb{B}^L \subset \mathbb{C}^L$ there corresponds only one eigenfunction $f_\alpha$ and the representation space $W$ (e.g. for the XXX chain we have $W = (\mathbb{C}^2)^{\otimes L}$) is isomorphic to the space $\text{Fun} \mathbb{B}^L$.

Example. A possible realization of the eigenfunctions $f_\alpha$ is

$$\left(\hat{b}_j f_\alpha\right)(b^\beta) = b^\alpha_\beta f_\alpha(b^\beta) \quad (4.15)$$

where $\hat{b}_j$ act as multiplication operators. Let $\{t_\alpha \in (\mathbb{C}^2)^{\otimes L} | (t_\alpha)^\beta = f_\alpha(b^\beta)\}$ be a basis of $W$ then, with the constraint $f_\alpha(b^\beta) = \delta_\alpha^\beta$, it is indeed orthonormal and complete.

Since $\hat{b}_n$ are the symmetric polynomials of the roots $\widetilde{x}_j^n$ we are led to consider the mapping

$$\theta : \mathbb{C}^L \rightarrow \mathbb{C}^L , \quad x \mapsto b \quad (4.16)$$

given by the formula $b_n(x) = s_n(x)$. The $s_n(x)$ are the elementary symmetric polynomials of degree $n = 1 \ldots L$ of $c$-number variables

$$s_1(x) = x_1^2 + x_2^2 + \ldots + x_L^2$$

$$\vdots$$

$$s_L(x) = x_1^2 x_2^2 \ldots x_L^2 . \quad (4.17)$$

The diagram

$$\begin{array}{c}
\mathbb{X}^L \xrightarrow{\theta} \mathbb{B}^L \xrightarrow{f} \{0, 1\} \subset \mathbb{C} \\
\rotatebox{90}{$g$} \quad \rotatebox{90}{$g$} \\
\mathbb{X}^L \xrightarrow{f \circ \theta} \{0, 1\} \subset \mathbb{C}
\end{array}$$

of the combined mapping $f \circ \theta$ reveals the isomorphism between $\text{Fun} \mathbb{B}^L \cong W$ and the space of symmetric functions $\text{SymFun} \mathbb{X}^L$. The set $\{0, 1\}$ is the range of $f$ in the example above. Thus the operator roots $\widetilde{x}_j^2$ can be thought of multiplication operators

$$\widetilde{x}_j^2 g(y_1, \ldots, y_L) = y_j^2 g(y_1, \ldots, y_L) \quad (4.18)$$

in an extended representation space $\text{Fun} \mathbb{X}^L \cong \widetilde{W}$ which is a non physical one. Recall all the results should only use the original space $\text{SymFun} \mathbb{X}^L \cong W$, as the operators $\mathcal{A}, \mathcal{B}, \mathcal{C}$ and $\mathcal{D}$ map $\text{SymFun} \mathbb{X}^L \rightarrow \text{SymFun} \mathbb{X}^L$ or more sloppy $W \rightarrow W$. So for plainness we will use in the following the terms $W$ and $\widetilde{W}$ for the representation spaces instead.

For the action of $X_j^\pm$ on a function $s \in \text{SymFun} \mathbb{X}^L$ we need first to extend the operators from $W$ to $\widetilde{W}$ by the constant function

$$\omega(x) = 1 \text{ for all } x \in \mathbb{X}^L . \quad (4.19)$$
Obviously \( \omega \) is symmetric and thus belongs to the representation space \( W \). Now define the action of \( X_j^\pm \) on \( \omega \) by

\[
(X_j^\pm \omega)(x) \equiv \Delta_j^\pm(x)
\]

Then the functions \( \Delta_j^\pm(x) \) uniquely determine the action of \( X_j^\pm \) on any vector \( s \) which is identified due to the isomorphism with some symmetric function \( s(x_1, \ldots, x_L) = (\tilde{s} \omega)(x) \) created from the cyclic vector \( \omega \) by the operator \( \tilde{s} = s(\tilde{x}_1, \ldots, \tilde{x}_L) \). Thus

\[
(X_j^\pm s)(x) = (X_j^\pm \tilde{s} \omega)(x) = s(E_j^\pm x)(X_j^\pm \omega)(x) = s(E_j^\pm x)\Delta_j^\pm(x) .
\]

Here we introduced the shift operators

\[
E_j^\pm : \mathbb{C}^L \to \mathbb{C}^L : (x_1, \ldots, x_j, \ldots, x_L) \mapsto (x_1, \ldots, x_j \pm \text{i}c, \ldots, x_L)
\]

acting on some \( L \)-tuple of \( c \)-numbers. In the extended representation space \( \tilde{W} \) of not necessarily symmetric functions the action of \( X_j^\pm \) then reads

\[
X_j^\pm = \Delta_j^\pm E_j^\pm
\]

with \( \Delta_j^\pm = \Delta_j^\pm(x) \). By the operator relation (4.23) we can now calculate the commutations of the momenta in

\[\text{Theorem 2.}\]

Let \( X_j^\pm \) be the conjugated momenta related to the coordinates \( \tilde{x}_j \) by the reflection algebra. Then

\[
\begin{align*}
[X_j^\pm, X_k^\pm] &= 0 \text{ for all } j, k = 1 \ldots L \\
[X_j^\pm, X_k^\mp] &= 0 \text{ for all } j, k = 1 \ldots L \text{ but } j \neq k .
\end{align*}
\]

\[\text{Proof.}\]

Let us start with \( X^- \) where the first assertion is obvious for \( j = k \). Then it is enough to consider the cases \( j = 1, k = 2 \). Taking the rational limit of

\[
[A(\lambda), A(\mu)] = \frac{\sinh \eta}{\sinh(\lambda + \mu)} [B(\mu)C(\lambda) - B(\lambda)C(\mu)]
\]

and inserting \( \lambda = \tilde{x}_1 \) and \( \mu = \tilde{x}_2 \) by ‘substitution from the left’ the RHS turns into zero and for the LHS we get

\[
\begin{align*}
\lambda = \tilde{x}_1, \mu = \tilde{x}_2 | A(\lambda)A(\mu) &= \sum_{m,n} \tilde{x}_1^m \tilde{x}_2^n A_mA_n = \sum_{m,n} \tilde{x}_2^n \tilde{x}_1^m A_mA_n \\
&= \sum_n \tilde{x}_2^n X_1^- A_n = X_1^- \sum_n \tilde{x}_2^n A_n = X_1^- X_2^- .
\end{align*}
\]

In the same way starting from \( A(\mu)A(\lambda) \) one obtains \( X_2^- X_1^- \) and the assertion is proven. The commutation of \( X^+ \)'s and mixed commutators excluding the cases \( j = k \) can be treated analogously by considering

\[
\begin{align*}
[\tilde{D}(\lambda), \tilde{D}(\mu)] &= -\sinh(2\lambda + \eta) \sinh(2\mu + \eta) [A(\lambda), A(\mu)] \\
[\tilde{D}(\lambda), A(\mu)] &= \frac{\sinh(\lambda + \mu) \sinh(2\lambda + \eta)}{\sinh(\lambda - \mu)} [A(\lambda), A(\mu)]
\end{align*}
\]

in the rational limit. \(\square\)
The remaining commutation involving the quantum determinant $\Delta_q$ is summarized in

**Theorem 3.** Let $\hat{x}_j$ and $X_j^\pm$ be the coordinates and conjugated momenta related by the reflection algebra and $\Delta_q(\lambda)$ is the quantum determinant. Then

$$X_j^\pm X_k^\mp = \Delta_q(\tilde{x}_j \pm ic/2) \text{ for all } j, k = 1 \ldots L \ .$$  \hspace{1cm} (4.28)

**Proof.** Substituting the operator-valued zeroes $\hat{x}_j$ into the quantum determinant $[3.7]$ one obtains

$$\Delta_q(\tilde{x}_j - ic/2) = \sum_{m,n} \hat{x}_j^m(\tilde{x}_j - ic)^n A_m D_n = \sum_{m,n} (\tilde{x}_j - ic)^n \hat{x}_j^m A_m D_n$$

$$= \sum_n (\tilde{x}_j - ic)^n X_j^- D_n = X_j^- \sum_n \hat{x}_j^n D_n$$ \hspace{1cm} (4.29)

and analogously $\Delta_q(\tilde{x}_j + ic/2) = X_j^+ X_j^-$ exerting the reflection algebra. \hfill \Box

**Remark.** The remaining zero $ic/2$ of $\mathcal{B}(\lambda)$ is an exception and renders the operators $A(ic/2) = d_q(-ic/2)$ and $D(ic/2) = 0$ to be constant yielding $\Delta_q(ic) = 0$.

**Representation of $\Delta^\pm$**

Applying $X_j^\pm X_k^\mp = \Delta_j^\pm E_j^\pm \Delta_j^\mp E_j^\mp$ to an arbitrary function $g \in \hat{W}$ induces the sequence

$$(X_j^\pm X_k^\mp g)(x) = (\Delta_j^\pm E_j^\pm \Delta_j^\mp E_j^\mp g)(x) = \Delta_j^\pm(\Delta_j^\mp x)(E_j^\mp g(x))$$

$$= \Delta_j^\pm(\Delta_j^\mp(E_j^\pm x))(E_j^\mp g)(E_j^\mp x)$$

$$= \Delta_j^\pm(E_j^\pm x)g(x)$$ \hspace{1cm} (4.30)

relating the representations $\Delta_j^\pm$ to the quantum determinant $\Delta_q$. In the case of a finite dimensional representation of the generators \{\hat{x}_j, X_j^\pm\}_{j=1}^L such that the spectrum $X^L$ shows no multiple points the problem of constructing such a representation is equivalent to that of determining the functions \{\Delta_j^\pm\}_{j=1}^L on $X^L$ satisfying

$$\Delta_m^n(x)\Delta_m^\pm(E_m^\pm x) = \Delta_m^n(x)\Delta_m^\pm(E_m^\pm x) \text{ for all } n, m$$

$$\Delta_m^n(x)\Delta_n^\pm(E_m^\pm x) = \Delta_n^\pm(x)\Delta_m^\pm(E_m^\pm x) \text{ for all } n, m \text{ but } n \neq m$$ \hspace{1cm} (4.31)

$$\Delta_q(\tilde{x}_j \pm ic/2) = \Delta_j^\pm(E_j^\pm x) \text{ for all } j$$

arising from theorems[2] and [3]. The above relations are not defined when the shifts $E_j^\pm$ move the point $x$ out of $X^L = \Lambda_1 \times \ldots \times \Lambda_L$. This means \{\Delta_j^\pm\}_{j=1}^L have to vanish on the boundary

$$\partial X_j^\pm \equiv \{x \in X^L | E_j^\pm x \in \mathbb{C}^L \setminus X^L\}$$ \hspace{1cm} (4.32)

of the set $X^L$. For the open XXX chain with $\Lambda_j = \{s_j - ic/2, s_j + ic/2\}$ this is clear from the following
Example. The vanishing of $\Delta_\pm(x)$ on the boundary $\partial \Omega_\pm$ can be directly seen from the explicit factorization of $\Delta_q(\lambda) = \Delta^- (\lambda + \eta/2) \Delta^+ (\lambda - \eta/2)$ into

$$
\Delta^- (\lambda) = \frac{\lambda - ic/2 + \alpha^-}{(-1)^L \alpha^-} \left[ \prod_{l=1}^L (\lambda - s_l + ic/2)(\lambda + s_l + ic/2) \right] 
$$

$$
\Delta^+ (\lambda) = -(2\lambda - ic) \frac{\lambda + ic/2 - \alpha^-}{(-1)^L \alpha^-} \left[ \prod_{l=1}^L (\lambda - s_l - ic/2)(\lambda + s_l - ic/2) \right]
$$

considered in the rational limit indicated by $\varepsilon \to 0$.

Spectral Analysis

Now let us return to the original problem, the spectral analysis of the new transfer matrix $\tau(\lambda) \equiv \text{tr} K(\lambda + \eta/2, \xi^+) U(\lambda)/2$ in the rational limit

$$
\tau(\lambda) = \frac{(\lambda + ic/2)(\lambda + \xi^+ - ic/2)}{2\lambda \xi^+} A(\lambda) - \frac{1}{\varepsilon} \frac{\lambda - \xi^+ + ic/2}{4\lambda \xi^+} \tilde{D}(\lambda)
$$

$$
+ \frac{(\lambda + ic/2)\kappa^+}{\xi^+} \left[ e^{\theta^+} C(\lambda) + e^{-\theta^+} B(\lambda) \right]
$$

and mind the scaling factor $\varepsilon \to 0$. To plug in the zeroes $\tilde{x}_j$ by ‘substitution from the left’ we have to get rid of $C(\lambda)$ by diagonalizing $K^+$. Thus only the first line remains. The diagonalization does not change the quantum determinant $\Delta_q(\lambda)$ and the eigenvalue problem $\tau(\lambda) \varphi = \Lambda(\lambda) \varphi$ can be solved by ‘substitution from the left’ reading

$$
\lambda = \tilde{x}_j \ | \tau(\lambda) = \frac{(\tilde{x}_j + ic/2)(\tilde{x}_j + \alpha^+ - ic/2)}{2\tilde{x}_j \alpha^+} X^- - \frac{1}{\varepsilon} \frac{\tilde{x}_j - \alpha^+ + ic/2}{4\tilde{x}_j \alpha^+} X^+ .
$$

With this representation at hand one observes ‘separation of variables’ suggesting the product ansatz

$$
\varphi = \left[ \prod_{l=1}^L Q(x_l) \right]
$$

for the eigenfunction $\varphi \in \text{SymFun} \times \Omega^L \cong W$ symmetric in its arguments $x_l$. To explicitly apply the operator-valued expression (4.35) one should clarify its behaviour by the following

Lemma. The action of the combined expression $\tilde{x}_j X_j^\pm$ by ‘substitution from the left’ onto a symmetric function $s = s(x_1, \ldots, x_L)$ is given by

$$
\tilde{x}_j X_j^\pm s(x) = (\tilde{x}_j X_j^\pm s)(x) = x_j (X_j^\pm s)(x) = x_j \Delta_j^\pm(x) s(E_j^\pm x) .
$$

Then applying (4.35) to $\varphi$ only the $j$th argument is affected such that the problem separates and

$$
\Lambda(x_j)Q(x_j) = \frac{(x_j + ic/2)(x_j + \alpha^+ - ic/2)}{2x_j \alpha^+} \Delta^- (x_j)Q(x_j - ic)
$$

$$
- \frac{1}{\varepsilon} \frac{x_j - \alpha^+ + ic/2}{4x_j \alpha^+} \Delta^+ (x_j)Q(x_j + ic)
$$

(4.38)
holds. Here we used (4.37) with the allowed arguments \( x_j \in \Lambda_j = \{ s_j - ic/2, s_j + ic/2 \} \) on the grid entering \( \Delta_j^{\pm}(x) = \Delta^{\pm}(x_j) \).

Remark. Along with the normalization \( (d_q T)(-\lambda) \), c.f. (3.8), and a shift in the arguments the original transfer matrix \( t(\lambda) \) is related to \( \tau(\lambda) \) via \( \tau(\lambda) = (d_q T)(-\lambda) t(\lambda - \eta/2) \).

## 5 TQ-Equations

The eigenvalue problem as formulated in Eq. (4.38) reduces to a system of homogeneous linear equations due to the fact that \( \Delta^{\pm}(x_j^{\pm}) = 0 \) at the points \( x_j^{\pm} = s_j \pm ic/2 \):

\[
\Lambda(x_j^+)Q(x_j^+) = \frac{(x_j^+ + ic/2)(x_j^+ + \alpha^+ - ic/2)}{2x_j^+ \alpha^+} \Delta^-(x_j^+)Q(x_j^-) \\
\Lambda(x_j^-)Q(x_j^-) = -\frac{1}{\varepsilon} \frac{x_j^- - \alpha^+ + ic/2}{4x_j^+ \alpha^+} \Delta^+(x_j^-)Q(x_j^+) .
\]  

(5.1)

For pairwise different inhomogeneities, \( s_j \neq s_k \) for \( j \neq k \), these linear equations allow for a non-trivial solution provided that the following functional equation for the eigenvalues \( \Lambda \) are satisfied\(^4\)

\[
\Lambda(s_j + ic/2)\Lambda(s_j - ic/2) = -\frac{s_j + ic}{2\varepsilon} \frac{s_j - \alpha^+}{(2s_j - ic)\alpha^+} \frac{s_j + \alpha^+}{(2s_j + ic)\alpha^+} \Delta_q(s_j), \quad j = 1 \ldots L .
\]  

(5.2)

Using the known asymptotic form of the even polynomial \( \Lambda(\lambda) = \Lambda(-\lambda) \) we are led to the ansatz

\[
\Lambda(\lambda) = \frac{(-1)^L \sinh \beta^+ \sinh \beta^- + \cosh(\theta^+ - \theta^-)}{\cosh \beta^+ \cosh \beta^-} \lambda^{2L+2} + a_{2L} \lambda^{2L} + a_{2L-2} \lambda^{2L-2} + \ldots + a_0 .
\]  

(5.3)

The \( (L+1) \) unknown coefficients \( a_j \) are determined by Eqs. (5.2) and the constraint \( \Lambda(ic/2) = d_q(-ic/2) \) with the quantum determinant \( d_q(\lambda) \) of the periodic chain. Thus the solution of the spectral problem amounts to finding the common roots \( \{ a_j^{(\nu)} \}_{j=0}^L, \nu = 1 \ldots 2^L \) of these polynomial equations. This task is of the same complexity as finding the eigenvalues of the spin chain Hamiltonian directly and therefore this approach is limited to small system sizes where we have checked numerically that it does indeed yield the complete spectrum.

To compute the eigenvalue of the transfer matrix or the spin chain Hamiltonian in the thermodynamic limit \( L \to \infty \) the functional equations introduced above need to be analyzed beyond the set \( X^L \) using explicitly the analytic properties of the functions therein.

Remark. Note that the functional equations (5.2) hold at the discrete points \( s_j \) only: treating the \( s_j \) as a continuous variable and applying standard Fourier techniques one can compute

\[^4\]If \( n \) of the inhomogeneities coincide the \( (n - 1) \) derivatives of this equation at this value of \( s_j \) have to be taken into account in addition.
\( \ln \Lambda(\lambda) \) and thereby the corresponding eigenvalue of the spin chain Hamiltonian \( \mathcal{H} = ic (\partial_\lambda \ln \tau)(ic/2) = ic t'(0) \) in the homogeneous limit. For \( |\alpha^\pm| > c/2 \) one obtains

\[
\frac{ic}{\partial \lambda} \ln \Lambda(i/2) = \psi(|\alpha^+|/2c) - \psi(|\alpha^+|/2c + 1/2) + c/|\alpha^+| \\
+ \psi(|\alpha^-|/2c) - \psi(|\alpha^-|/2c + 1/2) + c/|\alpha^-| \\
+ \pi - 2 \ln 2 - 1 + (2 - 4 \ln 2)L
\]

which is for imaginary \( \alpha^\pm \) the known energy eigenvalue of the XXX spin chain with diagonal boundary fields \cite{10} (\( \psi \) is the digamma function). However, the non-diagonal contributions and corrections of the order \( 1/L \) are not included. This is a consequence of neglecting the corrections to Eqs. (5.2) away from the points \( s_j \).

Instead we go back one step and consider the Eqs. (4.38) for general arguments \( x_j \to \lambda \). Formally, this is a second order difference equation reminiscent of Baxter’s \( TQ \)-equation \cite{2}. The analysis above leading to Eqs. (5.2) has been based on the singular points of the \( TQ \)-equation at the boundaries \( \partial X^L \), i.e. points where one of the coefficients \( \Delta^\pm \) vanishes. Away from these points there exist two independent solutions to (4.38) and one needs some information on the properties of the unknown functions \( Q(\lambda) \) in this formulation of the spectral problem which has to be solved for polynomial eigenvalues \( \Lambda(\lambda) \) of the transfer matrix.

In cases where a pseudo vacuum exists and the algebraic Bethe ansatz is applicable to the solution of the problem the \( Q \)-functions are known to be symmetric polynomials

\[ Q(\lambda) = \prod_{\ell=1}^{M} (\lambda - v_\ell)(\lambda + v_\ell) \]

with roots \( v_\ell \) satisfying Bethe ansatz equations. Note that only in these cases the constant function \( \omega = 1 \) introduced in the construction of the representation of the Yang-Baxter algebra on the space \( \hat{\mathcal{W}} \) can be identified with the pseudo vacuum \( |0\rangle \).

In general, the \( TQ \) equation can be rewritten as a recursion relation

\[ Q(\lambda + ic) = a(\lambda)Q(\lambda) + b(\lambda)Q(\lambda - ic) \]

for the function \( Q(\lambda) \) or equivalently, with the auxiliary function \( P(\lambda + ic) \equiv Q(\lambda) \),

\[ \begin{pmatrix} Q(\lambda + ic) \\ P(\lambda + ic) \end{pmatrix} = \begin{pmatrix} a(\lambda) & b(\lambda) \\ 1 & 0 \end{pmatrix} \begin{pmatrix} Q(\lambda) \\ P(\lambda) \end{pmatrix} \] (5.6)

The coefficients \( a(\lambda) \) and \( b(\lambda) \) are obtained from the \( TQ \)-equation (4.38) and show constant asymptotics for large values of their arguments

\[ a(\lambda) = -\frac{\Lambda(\lambda)}{\Delta^+(\lambda)} \frac{4\varepsilon\lambda\alpha^+}{\lambda - \alpha^+ + ic/2} \sim 2 \frac{\sinh \beta^+ \sinh \beta^- + \cosh(\theta^+ - \theta^-)}{\cosh \beta^+ \cosh \beta^-}, \]

\[ b(\lambda) = \frac{\Delta^-(\lambda)}{\Delta^+(\lambda)} \frac{2(\lambda + ic/2)(\lambda + \alpha^- - ic/2)\varepsilon}{\lambda - \alpha^+ + ic/2} \sim -1. \] (5.7)

This allows to solve the recursion relations in the asymptotic regime \( |\lambda| \gg 1 \) yielding

\[ Q(\lambda + inc) = \frac{\lambda_1^n - \lambda_2^n}{\lambda_1 - \lambda_2} Q(\lambda + ic) - \lambda_1 \lambda_2 \frac{\lambda_1^{n-1} - \lambda_2^{n-1}}{\lambda_1 - \lambda_2} Q(\lambda). \] (5.8)
Here $n$ is an integer and $\lambda_{1,2} = e^{\pm \phi}$ are the eigenvalues of the asymptotical matrix of coefficients in (5.6), $\cosh \phi = (\sinh \beta^+ \sinh \beta^- + \cosh (\theta^+ - \theta^-))/(\cosh \beta^+ \cosh \beta^-)$. Ordering the eigenvalues as $|\lambda_1| > |\lambda_2|$ we obtain for fixed $\lambda$ and large $n$ the leading term $Q(\lambda + inc) \sim \lambda_1^n$ suggesting the following ansatz for the asymptotic form

$$Q(\lambda) \sim \exp \left( \frac{\lambda \phi}{ic} \right) \times \text{polynomial in } \lambda \quad .$$

(5.9)

Here the polynomial form of the subleading part assures that the eigenvalue $\Lambda(\lambda)$ of the transfer matrix remains polynomial. Note, that since $\Lambda(\lambda)$ is an even function of its argument there exists always a second solution $Q(-\lambda)$ to the $TQ$ equation which decays exponentially for $\lambda \to \infty$.

Only in two cases, namely $\phi = 0$ and $i\pi$ or, equivalently,

$$\cosh(\theta^+ - \theta^-) = \pm \cosh(\beta^+ \mp \beta^-) \quad ,$$

(5.10)

the exponential factor disappears and the $TQ$ equation can be solved by an even polynomial: in the first case Eq. (5.9) implies that $Q(\lambda) = \prod_{i=1}^{M^{(+)}(\lambda)} (\lambda - v_i)(\lambda + v_i)$. For $\phi = i\pi$, the exponential factors can be removed by the transformation $Q(\lambda) = \exp(i\lambda\pi/ic)Q'(\lambda)$ resulting in a $TQ$ equation for $Q'$:

$$\Lambda(x_j)Q'(x_j) = - \frac{(x_j + ic/2)(x_j + \alpha^+ - ic/2)}{2x_j\alpha^+} \Delta^-(x_j)Q'(x_j - ic)$$

$$+ \frac{1}{\varepsilon} \prod_{j=1}^{M^{(-)}(\lambda - v_k)} (\lambda - v_k)(\lambda + v_k) \Delta^{+}(x_j)Q'(x_j + ic) .$$

(5.11)

Again, it follows from the asymptotic analysis that this equation allows for a polynomial solution $Q'(\lambda) = \prod_{i=1}^{M^{(-)}(\lambda - v_k)} (\lambda - v_k)(\lambda + v_k)$ whose existence has been verified by numerical analysis for small systems.

In both cases the spectrum is determined by the roots of these polynomials. To guarantee analyticity of the transfer matrix eigenvalues $\Lambda(\lambda)$ the $v_j$, $j = 1 \ldots M^{(\pm)}$, have to satisfy the Bethe ansatz equations

$$\frac{v_j + \alpha^- - ic/2}{v_j - \alpha^- + ic/2} \frac{v_j + \alpha^+ - ic/2}{v_j - \alpha^+ + ic/2} \left[ \prod_{l=1}^{L} v_j - s_l + ic/2 \right] = \prod_{l=1}^{M^{(\pm)}} v_j - v_k + ic v_j + v_k + ic$$

(5.12)

$$= \prod_{k=1, k \neq j}^{M^{(\pm)}} v_j - v_k + ic \frac{v_j + v_k + ic}{v_j - v_k - ic} .$$

Note that Eq. (5.10) is equivalent to the constraint that the boundary matrices $K^{(\pm)}$ can be simultaneously diagonalized or brought to triangular form. In this case Eqs. (5.12) can be obtained by means of the algebraic Bethe ansatz [12] or in the rational limit from the $TQ$-equation approach for the open $XXZ$ chain [19]. In this trigonometric case the complete set of eigenvalues is obtained from two sets of Bethe equations which both reduce to (5.12). This is due to the invariance of the model under the change of parameters $\alpha \to -\alpha$ and $\beta \to i\pi - \beta$ which maps $\phi = 0 \leftrightarrow i\pi$, see Eq. (3.5). As another difference to the situation in the $XXZ$ model the number of Bethe roots is not restricted by the constraint on the boundary fields and we have to consider solutions of the $TQ$-equations 'beyond the equator', $M^{(\pm)} > L/2$.  


6 Summary

In this paper we have extended Sklyanin’s functional Bethe ansatz method to the open XXX chain with non-diagonal boundary fields. Within this framework we have derived a single $TQ$-equation (4.38) which determines the spectrum of this model for any values of the boundary parameters. This supports the approach of Yang et al. [19] who obtain a $TQ$-equation for the XXZ model assuming the existence of a certain limit in the auxiliary space.

The $TQ$-equation allows for a solution in terms of polynomials for the function $Q$ provided that a constraint between the left and right boundary field is satisfied. In this case the solution is parametrized by the roots of one set of Bethe ansatz equations. In our numerical study of small systems we obtain the complete spectrum from these equations, when solutions ‘beyond the equator’, i.e. polynomial $Q$ with degree $> L/2$, are taken into account. This is in contrast to the trigonometric case where two types of Bethe equations are required and the degrees of the corresponding $Q$-functions are fixed by the constraint. We suppose that this feature of the XXX case is a consequence of the rational limit.

If the constraint between the boundary fields is missing only the asymptotic (exponential) behaviour of the $Q$-functions is obtained from the $TQ$ equation, the subleading terms have to be chosen such that the eigenvalues of the transfer matrix remain polynomial. In Sklyanin’s approach the $Q$-functions contain all the information on the eigenstates of the model. Therefore, their determination for generic boundary parameters is necessary to tackle the problem of computing norms and scalar products within this approach. To make progress in this direction it should be useful to investigate how the recent construction of Galleas [11] connects to the $TQ$-equation (4.38). His solution of the spectral problem for XXZ chains with non-diagonal boundaries is given in terms of the zeroes of the transfer matrix eigenvalues and two complementary sets of numbers which parametrize matrix elements of certain elements of the Yang-Baxter algebra. They satisfy equations reminiscent of the nested Bethe ansatz used to solve models of higher-rank symmetries. Further studies are necessary to see whether this parametrization of the spectrum in terms of $O(L)$ complex numbers can be used to obtain a closed expression for generic (non-polynomial) $Q$-functions. This would be of great importance for the applicability of the $TQ$-equation to solve the spectral problem of integrable quantum chains.

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References

[1] P. Baseilhac and K. Koizumi, Exact spectrum of the XXZ open spin chain from the $q$-Onsager algebra representation theory, J. Stat. Mech. (2007), P09006, arXiv:hep-th/0703106

[2] R. J. Baxter, Exactly solved models in statistical mechanics, Academic Press, London, 1982.
[3] A. G. Bytsko and J. Teschner, *Quantization of models with non-compact quantum group symmetry: modular XXZ magnet and lattice sinh-Gordon model*, J. Phys. A **39** (2006), 12927–12981, arXiv:hep-th/0602093.

[4] J. Cao, H.-Q. Lin, K.-J. Shi, and Y. Wang, *Exact solution of XXZ spin chain with unparallel boundary fields*, Nucl. Phys. B **663** (2003), 487–519, arXiv:cond-mat/0212163.

[5] J. Cao and Y. Wang, *Spin current in quantum XXZ spin chain*, Nucl. Phys. B **792** (2008), 284–299.

[6] A. Chervov and G. Falqui, *Manin matrices and Talalaev’s formula*, (2007), arXiv:math.QA/0711.2236.

[7] J. de Gier and F. H. L. Essler, *Bethe ansatz solution of the asymmetric exclusion process with open boundaries*, Phys. Rev. Lett. **95** (2005), 240601, arXiv:cond-mat/0508707.

[8] ———, *Exact spectral gaps of the asymmetric exclusion process with open boundaries*, J. Stat. Mech. (2006), no. 12, P12011, arXiv:cond-mat/0609645.

[9] H. J. de Vega and A. González-Ruiz, *Boundary K-matrices for the six vertex and the n(2n − 1)A_{n−1} vertex models*, J. Phys. A **26** (1993), L519–L524, arXiv:hep-th/9211114.

[10] H. Frahm and A. A. Zvyagin, *The open spin chain with impurity: an exact solution*, J. Phys. Condens. Matter **9** (1997), 9939–9946.

[11] W. Galleas, *Functional relations from the Yang-Baxter algebra: Eigenvalues of the XXZ model with non-diagonal twisted and open boundary conditions*, Nucl. Phys. B **790** (2008), 524–542, arXiv:0708.0009.

[12] C. S. Melo, G. A. P. Ribeiro, and M. J. Martins, *Bethe ansatz for the XXX-S chain with non-diagonal open boundaries*, Nucl. Phys. B **711** (2005), 565–603, arXiv:nlin/0411038.

[13] R. Murgan, R. I. Nepomechie, and C. Shi, *Exact solution of the open XXZ chain with general integrable boundary terms at roots of unity*, J. Stat. Mech. (2006), P08006, arXiv:hep-th/0605223.

[14] R. I. Nepomechie, *Bethe ansatz solution of the open XXZ chain with nondiagonal boundary terms*, J. Phys. A **37** (2004), 433–440, arXiv:hep-th/0304092.

[15] E. K. Sklyanin, *The quantum Toda chain*, Non-linear Equations in Classical and Quantum Field Theory (N. Sanchez, ed.), Lecture Notes in Physics, vol. 226, Springer Verlag, Berlin, 1985, p. 196.

[16] ———, *Boundary conditions for integrable quantum systems*, J. Phys. A **21** (1988), 2375–2389.

[17] ———, *Quantum Inverse Scattering Method. Selected topics*, Quantum Group and Quantum Integrable Systems (M.-L. Ge, ed.), Nankai Lectures in Mathematical Physics, World Scientific, Singapore, 1992, pp. 63–97, arXiv:hep-th/9211111.
[18] J. Teschner, *On the spectrum of the sinh-Gordon model in finite volume*, (2007), arXiv:hep-th/0702214.

[19] W.-L. Yang, R. I. Nepomechie, and Y.-Z. Zhang, *Q-operator and T-Q relation from the fusion hierarchy*, Phys. Lett. B 633 (2006), 664-670, arXiv:hep-th/0511134.