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A Q-operator identity for the correlation functions of the infinite XXZ spin-chain

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Abstract
An explicit construction for Q-operators of the finite XXZ spin chain with twisted boundary conditions is presented. The massless and the massive regimes are considered as well as the root of unity case. It is explained how these results yield an alternative expression for the trace function employed in the description of the correlation functions of the inhomogeneous XXZ model on the infinite lattice by Boos, Jimbo, Miwa, Smirnov and Takeyama.

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1. Introduction

The computation of correlation functions is one of the major challenges in integrable systems. Multidimensional integral formulae have been derived for the infinite [1–3] as well as the finite XXZ spin chain at zero [4, 5] and at finite temperature [6]. More recently it has been observed that some of these multidimensional integrals can be reduced to one-dimensional ones allowing for their explicit computation [7–9]. In a series of papers [10–12] this reducibility was connected to a duality between the solutions of the quantum Knizhnik–Zamolodchikov (qKZ) equations of level 0 and level -4 which the correlation functions of the model ought to obey [13].

In this paper we will refer to the subsequent work by Boos, Jimbo, Miwa, Smirnov and Takeyama on the correlation functions of the infinite XXZ spin chain [14],

$$H_{\mathrm{XXZ}} = \frac{1}{2}\sum_{j=-\infty}^{\infty}\left\{\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \frac{q+q^{-1}}{2}\sigma_j^z\sigma_{j+1}^z\right\}, \qquad q = \mathrm{e}^{\mathrm{i}\pi\nu}. \tag{1}$$

There it is explained that the correlation functions are particular solutions of a reduced set of qKZ equations which can be formulated in terms of a special trace of a certain monodromy matrix. The latter formally resembles in its algebraic structure the monodromy matrix of the inhomogeneous six-vertex model on a *finite* lattice whose number of columns is determined by the number of operators in the correlation function. It is the special trace of this finite monodromy matrix which we will identify as an analytic continuation of the six-vertex fusion hierarchy in terms of Q-operators. Before giving the technical details of the computation we state this result more explicitly. To this end we first briefly summarize the main outcome of the work [14].

1.1. Correlation functions and a generalized trace

Consider the correlation functions of the elementary matrices $\left(E_{\varepsilon_j,\bar{\varepsilon}_j}\right)_j$ acting on the jth site in the XXZ spin chain and interpret

$$h_p(\lambda_1,\ldots,\lambda_p)^{\varepsilon_1,\ldots,\varepsilon_p,\bar{\varepsilon}_p,\ldots,\bar{\varepsilon}_1} = \langle \mathrm{vac}|\left(E_{-\varepsilon_1,\bar{\varepsilon}_1}\right)_1\cdots\left(E_{-\varepsilon_p,\bar{\varepsilon}_p}\right)_p|\mathrm{vac}\rangle\prod_{j=1}^{p}(-\bar{\varepsilon}_j) \tag{2}$$

with $\varepsilon_j, \bar{\varepsilon}_j = \pm 1$ as the vector components of a function $h_p = h_p(\lambda_1,\ldots,\lambda_p)$ whose values lie in the tensor space $V^{\otimes 2p}$, $V = \mathbb{C}v_+ \oplus \mathbb{C}v_-$. Here $|\mathrm{vac}\rangle$ denotes the groundstate of the six-vertex model on an infinite lattice with inhomogeneity parameters $\{\lambda_j\}$. In the homogeneous limit $\lambda_j \to 0$ this becomes the groundstate of the Hamiltonian (1)[1]. The vector valued functions h_p are solutions of a set of reduced qKZ equations and according to [14] can be expressed as

$$h_p(\lambda_1,\ldots,\lambda_p) = \frac{\mathrm{e}^{\hat{\Omega}_p(\lambda_1,\ldots,\lambda_p)}}{2^p}\prod_{\ell=1}^{p}\mathfrak{s}_{\ell,\bar{\ell}}, \qquad \mathfrak{s} = v_+\otimes v_- - v_-\otimes v_+, \qquad \bar{\ell} = 2p+1-\ell \tag{3}$$

where $\hat{\Omega} = \sum_{i<j}\hat{\Omega}^{(i,j)}$ is a sum of operators of the form

$$\hat{\Omega}^{(i,j)}(\lambda_1,\ldots,\lambda_p) = \tilde{\omega}(\lambda_{ij})\tilde{W}^{(i,j)}(q^{\lambda_1},\ldots,q^{\lambda_p}) + \omega(\lambda_{ij})W^{(i,j)}(q^{\lambda_1},\ldots,q^{\lambda_p}) \tag{4}$$

with $\lambda_{ij} = \lambda_i - \lambda_j$ and $\omega, \tilde{\omega}$ being certain scalar functions. The operators $\tilde{W}, W$ depending rationally on $\{q^{\lambda_i}\}$ are defined through the aforementioned special trace of a monodromy matrix. For instance, setting $(i,j) = (1,2)$ and $\lambda_0 = (\lambda_1+\lambda_2)/2$ one considers the map $V^{\otimes 2(p-2)} \to V^{\otimes 2p}$

$${}_pX_{p-2}(\lambda_1,\ldots,\lambda_p) = \frac{\mathrm{Tr}_{\lambda_{12}}L_{\bar{2}}(\lambda_{02}-1)\cdots L_{\bar{p}}(\lambda_{0\bar{p}}-1)L_p(\lambda_{0p})\cdots L_2(\lambda_{02})}{[\lambda_{12}]_q\prod_{j=3}^{p}[\lambda_{1j}]_q[\lambda_{2j}]_q}\mathfrak{s}_{1,\bar{2}}\mathfrak{s}_{\bar{1},2} \tag{5}$$

which decomposes as

$${}_pX_{p-2}(\lambda_1,\ldots,\lambda_p) = -\lambda_{12}\cdot{}_p\tilde{G}_{p-2}(q^{\lambda_1},\ldots,q^{\lambda_p}) + {}_pG_{p-2}(q^{\lambda_1},\ldots,q^{\lambda_p}). \tag{6}$$

The two terms appearing in the above sum determine the two operators on the right-hand side in (4). For further details and the precise relation between $G, \tilde{G}$ and $W, \tilde{W}$ we refer the reader to [14]. For our purposes it will be sufficient to focus only on the following object in End $V^{\otimes 2p-2}$:

$$\boldsymbol{t} := \mathrm{Tr}_{\lambda_{12}}L_{\bar{2}}(\lambda-\lambda_2-1)\cdots L_{\bar{p}}(\lambda-\lambda_{\bar{p}}-1)L_p(\lambda-\lambda_p)\cdots L_2(\lambda-\lambda_2). \tag{7}$$

The operator $L_j \in U_q(sl_2)\otimes \mathrm{End}\,V_j$ is a quantum group intertwiner and

$$\mathrm{Tr}_\lambda \equiv \mathrm{Tr}_{\lambda,\zeta=q^\lambda} \tag{8}$$

denotes a linear function

$$\mathrm{Tr}_{\lambda,\zeta} : U_q(sl_2)\otimes\mathbb{C}[\zeta,\zeta^{-1}] \to \lambda\mathbb{C}[\zeta,\zeta^{-1}]\otimes\mathbb{C}[\zeta,\zeta^{-1}] \tag{9}$$

[1] We follow here the conventions in [14] and consider in the massive regime, where the groundstate is twofold degenerate, only matrix elements between the same vectors. Note further that unlike in the case of the XXX chain it is not known at the moment how to take the homogeneous directly in the ansatz of [14].

which for $\lambda = n+1$ yields the conventional trace over the quantum group representation $\pi^{(n)}$ of spin $n/2$,

$$\mathrm{Tr}_{\lambda=n+1}(x) = \mathop{\mathrm{Tr}}_{\pi^{(n)}} x, \qquad \forall x \in U_q(sl_2). \tag{10}$$

For our definition of $\pi^{(n)}$ see (20) in the text below. In particular, one has for the special elements $x = 1, q^h$ and the Casimir operator

$$\mathfrak{C} = \frac{q^{h-1} + q^{1-h}}{(q-q^{-1})^2} + ef \tag{11}$$

the following identities:

$$\mathrm{Tr}_{\lambda,\zeta} 1 = \lambda, \qquad \mathrm{Tr}_{\lambda,\zeta} q^{mh} = \frac{\zeta^m - \zeta^{-m}}{q^m - q^{-m}}, \qquad \mathrm{Tr}_{\lambda,\zeta} \mathfrak{C} = \frac{\zeta + \zeta^{-1}}{(q-q^{-1})^2}. \tag{12}$$

We will now explain the main point of this paper, namely, that there is an alternative expression for (7) which does not use the introduction of the abstract trace function (9) but relies on the two linearly independent solutions to Baxter's *TQ* equation for the inhomogeneous six-vertex model with twisted boundary conditions.

1.2. Baxter's TQ equation and the six-vertex fusion hierarchy

Consider the inhomogeneous six-vertex model on a finite lattice with length $M = 2p-2 \in 2\mathbb{N}$, compare with (7). This model can be solved by finding solutions to Baxter's *TQ* equation [15–18],

$$t(\lambda)Q(\lambda) = Q(\lambda+1)\prod_{m=1}^{M}[\lambda-\lambda_m]_q + Q(\lambda-1)\prod_{m=1}^{M}[\lambda-\lambda_m+1]_q. \tag{13}$$

Here t denotes the six-vertex transfer matrix and Q is an auxiliary matrix. In terms of eigenvalues (13) is a difference equation of second order and hence will in general allow for two linearly independent solutions, say $Q^{\pm}$ [19–21]. However, they do not always possess the same analyticity properties. For instance, for generic q and when M is even, as it is the case here, there is only one solution which can be expressed as a product of the form

$$Q^{+}(\lambda) = \prod_{m=1}^{n_+}\left[\lambda - \xi_m^{+}\right]_q = \prod_{m=1}^{n_+}\frac{\sin\pi\nu\left[\lambda-\xi_m^{+}\right]}{\sin\pi\nu}, \qquad \xi_m^{+} \equiv \text{Bethe roots}, \tag{14}$$

the other, Q^-, contains terms linear in λ [21]. The situation is different for M odd where both solutions take the form of a product of sine functions. See also the discussion in [22] and [23–25] for the case when q is a root of unity and the second solution Q^- factorizes into Q^+ and a 'complete string' polynomial due to a loop algebra symmetry of the model [26]. Here we will remove the associated degeneracies in the spectrum.

In this paper we give an explicit construction of the Q-operators behind the two solutions $Q^{\pm}$ for even M and relate via a limiting procedure the linear terms in the second solution to the decomposition in (6). For the construction of Q-operators one in general assumes analyticity with respect to the variable $z = q^{2\lambda}$ by requiring that the Q-operators commute for arbitrary values of the spectral parameter, $[Q(z_1), Q(z_2)] = 0$ [18]. This usually prevents the appearance of linear terms in λ.

The key to obtain these terms is the introduction of quasi-periodic boundary conditions on the finite lattice taking the limit to periodic boundary conditions at the very end of the construction. The twisted boundary conditions depend on a generic twist parameter α where the value $\alpha = 0$ corresponds to ordinary periodic boundary conditions. For $\alpha \neq 0$ two linearly independent solutions to (13) without linear terms can be constructed and one finds a simplified expression for the six-vertex fusion hierarchy: denote by $t_\alpha^{(n)}$ the transfer matrix with spin $n/2$ in the auxiliary space; then one has

$$t_\alpha^{(n-1)}(\lambda) = \frac{q^{-n\alpha} Q_\alpha^+\big(\lambda + \frac{n}{2}\big) Q_\alpha^-\big(\lambda - \frac{n}{2}\big) - q^{n\alpha} Q_\alpha^+\big(\lambda - \frac{n}{2}\big) Q_\alpha^-\big(\lambda + \frac{n}{2}\big)}{q^{-S^z-\alpha} - q^{\alpha+S^z}}. \tag{15}$$

Here S^z denotes the total spin operator acting on the chain. By analytic continuation of this formula with respect to the spin variable $n/2$ of the transfer matrix one obtains in the limit $\alpha \to 0$ an alternative expression for (7),

$$\boldsymbol{t}(\lambda, \zeta) = \lim_{\alpha\to 0} \frac{\zeta^{-\alpha} Q_\alpha^+\big(q^\lambda \zeta^{\frac{1}{2}}\big) Q_\alpha^-\big(q^\lambda \zeta^{-\frac{1}{2}}\big) - \zeta^{\alpha} Q_\alpha^+\big(q^\lambda \zeta^{-\frac{1}{2}}\big) Q_\alpha^-\big(q^\lambda \zeta^{\frac{1}{2}}\big)}{q^{-S^z-\alpha} - q^{\alpha+S^z}}, \tag{16}$$

which reproduces all the desired properties (12) of the trace function, in particular the appearance of linear terms in λ,

$$q^{M\lambda} \boldsymbol{t}(\lambda, \zeta = q^\lambda) = \lambda \cdot \tilde{\boldsymbol{g}}(q^{2\lambda}) + \boldsymbol{g}(q^{2\lambda}). \tag{17}$$

In (16) we have identified on the right-hand side of the equation $Q_\alpha^\pm(\lambda) \equiv Q_\alpha^\pm(q^\lambda)$ and $\tilde{\boldsymbol{g}}(x), \boldsymbol{g}(x)$ in (17) are operator valued polynomials whose degrees in each fixed spin sector S^z are given by

$$\deg \tilde{\boldsymbol{g}}|_{S^z} = M - |S^z| \qquad \text{and} \qquad \deg \boldsymbol{g}|_{S^z} \leqslant M, \tag{18}$$

where the upper bound for $\deg \boldsymbol{g}|_{S^z}$ is assumed when $S^z \neq 0$ but it is strictly smaller than M when $S^z = 0$. This will be derived in section 4. Before that we present in section 3 our concrete construction of the Q-operators, which will relate the appearance of the extra variable ζ to a special restriction of a Verma module of the upper Borel subalgebra $U_q(b_+) \subset U_q(\widehat{sl}_2)$.

It should be emphasized that our construction of Q-operators for the quasi-periodic chain has applications beyond the focus of this paper and it would be interesting to see whether similar formulae also occur in the treatment of the correlation functions for the finite XXZ chain [4, 5, 6]. These approaches rely on the Bethe ansatz and we stress that the Bethe ansatz equations are also contained in (15) when setting $n = 1$ and shifting $\lambda \to \lambda + 1/2$,

$$\prod_{m=1}^{M} [\lambda - \lambda_m + 1]_q = \frac{q^{-\alpha} Q_\alpha^+(\lambda + 1) Q_\alpha^-(\lambda) - q^{\alpha} Q_\alpha^+(\lambda) Q_\alpha^-(\lambda + 1)}{q^{-S^z-\alpha} - q^{\alpha+S^z}}. \tag{19}$$

In the context of the Liouville model the analogue of this identity has been referred to as quantum Wronskian [20]. Evaluating it at $\lambda = \xi_m^\pm, \xi_m^\pm - 1$ gives the Bethe ansatz equations above and below the equator [19, 21]. However, the above equation (19) is of a simpler form than the Bethe ansatz equations and it is desirable to understand its consequences in the thermodynamic limit.

An analogous construction of Q-operators for the eight-vertex or XYZ model is currently under investigation [33].

2. The six-vertex fusion hierarchy

The inhomogeneous six-vertex model on a finite lattice is associated with the quantum loop algebra $U_q(\widetilde{sl}_2)$ in terms of which the transfer matrix and fusion hierarchy can be defined. Consider the spin $n/2$ representation $\pi^{(n)}$ of the finite quantum subgroup $U_q(sl_2) \subset U_q(\widetilde{sl}_2)$, i.e.

$$\begin{aligned} \pi^{(n)}(e)\,|k\rangle &= [n-k+1]_q [k]_q\,|k-1\rangle, \\ \pi^{(n)}(f)\,|k\rangle &= |k+1\rangle, \\ \pi^{(n)}(q^{\frac{h}{2}})\,|k\rangle &= q^{\frac{n}{2}-k}\,|k\rangle \end{aligned} \tag{20}$$

with $k = 0, 1, \ldots, n$. The transfer matrices of the model are built up from the intertwiners of the respective evaluation modules. Define

$$L = \begin{pmatrix} zq^{\frac{h}{2}+1} - q^{-\frac{h}{2}} & z(q-q^{-1})q^{\frac{h}{2}+1}f \\ (q-q^{-1})eq^{-\frac{h}{2}} & zq^{-\frac{h}{2}+1} - q^{\frac{h}{2}} \end{pmatrix} \in U_q(sl_2) \otimes \mathrm{End}\, V \tag{21}$$

where V is identified as the two-dimensional representation space of $\pi^{(1)}$ and $z = q^{2\lambda}$ as the spectral parameter. Then the inhomogeneous transfer matrix of spin $n/2$ is introduced by setting[2]

$$T_\alpha^{(n)}(z) = \operatorname*{Tr}_{\pi^{(n)}} q^{\alpha h \otimes 1} L_M\big(z\zeta_M^2\big) \cdots L_1\big(z\zeta_1^2\big) \in \mathrm{End}\, V^{\otimes M}. \tag{22}$$

For the moment the length of the spin chain M can be any positive integer and α is the twist angle. The set $\{\zeta_m = q^{-\lambda_m}\}_{m=1}^{M}$ are some unspecified 'generic' inhomogeneity parameters. The above transfer matrices constitute the six-vertex fusion hierarchy satisfying the functional equation [32]

$$T_\alpha^{(n)}(zq^{n+1})T_\alpha^{(1)}(z) = T_\alpha^{(n+1)}(zq^n)\prod_{m=1}^{M}\big(zq^2\zeta_m^2 - 1\big) + T_\alpha^{(n-1)}(zq^{n+2})\prod_{m=1}^{M}\big(z\zeta_m^2 - 1\big). \tag{23}$$

In the homogeneous limit, $\zeta_m \to 1$, we obtain from the transfer matrix T as logarithmic derivative the Hamiltonian for the finite XXZ chain,

$$\begin{aligned} H_{\mathrm{XXZ}} &= -(q-q^{-1})\, z\frac{\mathrm{d}}{\mathrm{d}z} \ln \frac{T_\alpha(z)}{(zq^2-1)^M}\bigg|_{z=1} \\ &= -\frac{1}{2}\sum_{m=1}^{M}\left\{\sigma_m^x\sigma_{m+1}^x + \sigma_m^y\sigma_{m+1}^y + \frac{q+q^{-1}}{2}\big(\sigma_m^z\sigma_{m+1}^z - 1\big)\right\}. \end{aligned} \tag{24}$$

Here the twisted boundary conditions manifest themselves in the identification

$$\sigma_{M+1}^{\pm} = q^{\pm 2\alpha}\sigma_1^{\pm}.$$

The well-known symmetries of the model are expressed in terms of the following commutators:

$$\big[T_\alpha^{(m)}(z), T_\alpha^{(n)}(w)\big] = \big[T_\alpha^{(n)}(z), S^z\big] = \big[T_\alpha^{(n)}(z), \mathfrak{S}\big] = 0, \tag{25}$$

and

$$\mathfrak{R}T_\alpha^{(n)}(z) = T_{-\alpha}^{(n)}(z)\mathfrak{R} \tag{26}$$

where the respective operators are defined as

$$S^z = \frac{1}{2}\sum_{m=1}^{M}\sigma_m^z, \quad \mathfrak{R} = \sigma^x \otimes \cdots \otimes \sigma^x = \prod_{m=1}^{M}\sigma_m^x, \quad \mathfrak{S} = \sigma^z \otimes \cdots \otimes \sigma^z = \prod_{m=1}^{M}\sigma_m^z. \tag{27}$$

These symmetries hold for spin chains of even as well as odd length. For later purposes we also compute the value of the transfer matrices at the origin,

$$T_\alpha^{(n-1)}(0) = (-)^M \operatorname*{Tr}_{\pi^{(n-1)}} q^{(\alpha - S^z)h} = (-)^M \frac{q^{n(S^z-\alpha)} - q^{-n(S^z-\alpha)}}{q^{S^z-\alpha} - q^{-S^z+\alpha}}. \tag{28}$$

[2] Note that we have changed our conventions in comparison with [22, 30, 31] and have made the following change in notation, $T^{(n)}(z) \to T^{(n-1)}(zq^n)$.

3. The auxiliary matrices

Our construction follows the main steps of the previous works [27] and [22, 28–31] with some minor modifications. We therefore only state the main results and briefly comment on the steps involved to accommodate twisted boundary conditions. The reader is referred to the aforementioned literature for the technical details.

3.1. Definition

For the definition of the auxiliary matrix we employ the following representations $\pi^\pm = \pi^\pm(z;r,s)$ of the upper Borel subalgebra $U_q(b_+)\subset U_q(\widetilde{sl}_2)$. Let $k\in\mathbb{N}_{\geqslant 0}$ then

$$\begin{aligned}&\pi^+(e_0)\,|k\rangle = z|k+1\rangle, \qquad \pi^+\big(q^{\frac{h_1}{2}}\big)\,|k\rangle = \pi^+\big(q^{-\frac{h_0}{2}}\big)\,|k\rangle = rq^{-2k-1}|k\rangle,\\ &\pi^+(e_1)\,|k\rangle = \frac{s+1-q^{2k}-sq^{-2k}}{(q-q^{-1})^2}|k-1\rangle, \qquad \pi^+(e_1)\,|0\rangle = 0, \qquad r,s,z\in\mathbb{C}\end{aligned} \tag{29}$$

and set

$$\pi^- := \pi^+\circ\omega \quad \text{with} \quad \big\{e_1,e_0,q^{\frac{h_1}{2}},q^{\frac{h_0}{2}}\big\} \stackrel{\omega}{\to} \big\{e_0,e_1,q^{\frac{h_0}{2}},q^{\frac{h_1}{2}}\big\}. \tag{30}$$

The representation π^- is a particular restriction of the representation introduced in [27]. When q is a primitive root of unity of order N we set $N'=N$ if the order is odd and $N'=N/2$ if it is even. Then the above infinite-dimensional representation becomes reducible and can be truncated [31],

$$\pi^+(e_0)|N'-1\rangle = 0. \tag{31}$$

For roots of unity this truncation will always be implicitly understood. In order to unburden the formulae we will often drop the explicit dependence on the parameters $\{z,r,s\}$ and the representation π^+. Set

$$\mathfrak{L} = \begin{pmatrix} z\frac{s}{r}q^{\frac{h_1}{2}+1}-q^{-\frac{h_1}{2}} & (q-q^{-1})e_0q^{-\frac{h_0}{2}} \\ (q-q^{-1})e_1q^{-\frac{h_1}{2}} & zrq^{-\frac{h_1}{2}+1}-q^{\frac{h_1}{2}} \end{pmatrix} \in U_q(b_+)\otimes \operatorname{End} V, \tag{32}$$

then $\mathfrak{L}_{\pi^+} = (\pi^+\otimes 1)\mathfrak{L}$ is the intertwiner of the tensor product $\pi^+\otimes\pi^{(1)}$. Note that the intertwiner for the representation π^- is obtained via spin reversal, i.e.

$$\mathfrak{L}_{\pi^-} = (1\otimes\sigma^x)\mathfrak{L}_{\pi^+}(1\otimes\sigma^x). \tag{33}$$

Define the auxiliary matrix in terms of the intertwiner $\mathfrak{L}$ as the trace of the following operator product:

$$Q_\alpha(z;r,s) = \operatorname*{Tr}_{\pi^+} q^{\alpha h_1\otimes 1}\mathfrak{L}_M\big(z\zeta_M^2;r,s\big)\cdots\mathfrak{L}_1\big(z\zeta_1^2;r,s\big). \tag{34}$$

For later purposes we also define the special limits

$$Q_\alpha^+(z) = \lim_{s\to 0} Q_\alpha(0;1,s)^{-1}Q_\alpha(z;1,s) \qquad \text{and} \qquad Q_\alpha^- = \mathfrak{R}Q_{-\alpha}^+\mathfrak{R}. \tag{35}$$

By definition of the auxiliary matrix the operators $Q_\alpha^\pm$ are well defined and we have for roots of unity

$$q^N=1: \quad Q_\alpha(0;r,s) = (-)^M r^{\alpha-S^z}\frac{1-q^{2N'(S^z-\alpha)}}{q^{\alpha-S^z}-q^{S^z-\alpha}}, \tag{36}$$

while for

$$\text{generic } q: \quad Q_\alpha(0;r,s) = \frac{(-)^M r^{\alpha-S^z}}{q^{\alpha-S^z}-q^{S^z-\alpha}} \quad \text{with} \quad \big|q^{-\alpha\pm\frac{M}{2}}\big| < 1 \text{ for } |q|^{\pm 1} > 1. \tag{37}$$

After a suitable renormalization (see section 4.1) the eigenvalues of the operators (35) yield the two linearly independent solutions to Baxter's TQ equation mentioned in the introduction.

3.2. Spin conservation and reversal

The matrix (34) commutes by construction with the fusion hierarchy and preserves two of the symmetries (25) [28, 29],

$$[Q_\alpha(z; r, s), S^z] = [Q_\alpha(z; r, s), \mathfrak{S}] = 0. \tag{38}$$

Because of spin conservation the dependence of the auxiliary matrix Q on the parameter r can be easily extracted,

$$Q_\alpha(z; r, s) = r^{\alpha - S^z} Q_\alpha(z; 1, s) \equiv r^{\alpha - S^z} Q_\alpha(z; s). \tag{39}$$

Without loss of generality we can therefore set $r = 1$ in order to discuss the behaviour of the auxiliary matrix under spin reversal. Employing once more spin conservation we easily find from

$$\langle v_+ | \mathfrak{L} | v_+ \rangle = zsq^{1+\frac{h_1}{2}} - q^{-\frac{h_1}{2}} = (-zsq)\left(z^{-1}q^{-2}s^{-1}q^{1-\frac{h_1}{2}} - q^{\frac{h_1}{2}}\right)$$
$$\langle v_- | \mathfrak{L} | v_- \rangle = zq^{1-\frac{h_1}{2}} - q^{\frac{h_1}{2}} = (-zq)\left(z^{-1}q^{-2}s^{-1}sq^{1+\frac{h_1}{2}} - q^{-\frac{h_1}{2}}\right)$$

the identities

$$\mathfrak{R} Q_\alpha(z; s, \{\zeta_m\}) \mathfrak{R} = (-z)^M q^M s^{\frac{M}{2} - S^z} Q_\alpha\left(z^{-1}q^{-2}s^{-1}; s, \left\{\zeta_m^{-1}\right\}\right)^t \prod_m \zeta_m^2 \tag{40}$$

and

$$\mathfrak{R} Q_\alpha(z, q; s) \mathfrak{R} = Q_{-\alpha}(zq^2 s, q^{-1}; s^{-1})^t. \tag{41}$$

3.3. Commutation of the auxiliary matrices

For generic q we can employ the concept of the universal R-matrix and the fact that $\pi^+(z; r, s)$ is the restriction of a well-known evaluation Verma module of $U_q(\widehat{sl}_2)$ to conclude that the intertwiner, say S, of the tensor product

$$\pi^+(z; r, s) \otimes \pi^+(w; r', s')$$

exists. Consequently, the Yang–Baxter relation $S_{12}\mathfrak{L}_{13}\mathfrak{L}'_{23} = \mathfrak{L}'_{23}\mathfrak{L}_{13}S_{12}$ holds and the auxiliary matrices commute among each other,

$$[Q_\alpha(z; r, s), Q_\alpha(w; r', s')] = 0. \tag{42}$$

Here we have implicitly used that

$$[\mathfrak{L}, \pi^+(h_1) \otimes \sigma^z] = [S, \pi^+(h_1) \otimes \pi^+(h_1)'] = 0 \tag{43}$$

in order to ensure compatibility with the quasi-periodic boundary conditions. The above commutation relations are a direct consequence of the intertwining property of $\mathfrak{L}$ and S.

When q is a root of unity we cannot use the existence of the universal R -matrix and have to construct the intertwiners S explicitly. This has been done for $N = 3, 4, 6$ in [29, 31]. Numerical checks have been carried out for $N = 5, 7, 8$ and the commutation relation was found to hold. *We therefore assume as a working hypothesis that the intertwiner S also exists in the root of unity case for general N.*

From (42) it follows that the eigenvalues of the auxiliary matrix are polynomial in the parameters z, s and that the eigenvectors of the Q-operator do not depend on them.

3.4. The TQ equation

One of the essential properties of the auxiliary matrix Q_α is that it satisfies the functional equation

$$T_\alpha(z)Q_\alpha(z;r,s) = Q_\alpha(zq^2;rq^{-1},sq^{-2})\prod_m\left(z\zeta_m^2-1\right)+Q_\alpha(zq^{-2};rq,sq^2)\prod_m\left(z\zeta_m^2q^2-1\right) \tag{44}$$

which one derives from the following non-split exact sequence of representations [27, 28]:

$$0\to\pi^+(zq^2;rq^{-1},sq^{-2})\hookrightarrow\pi^+(z;r,s)\otimes\pi_z^{(1)}\to\pi^+(zq^{-2},rq,sq^2)\to 0. \tag{45}$$

The proof can be found in [27, 28], here we have only to incorporate twisted boundary conditions. To this end note for instance that the inclusion $\imath\,:\,\pi^+(zq^2;rq^{-1},sq^{-2})\hookrightarrow\pi^+(z;r,s)\otimes\pi_z^{(1)}$ in (45) is given in the following form:

$$|k\rangle\hookrightarrow|k+1\rangle\otimes v_+ + c_k\,|k\rangle\otimes v_-$$

where c_k is some coefficient whose explicit form is not relevant here. Then one easily verifies that

$$\imath\circ\pi^+(q^{\alpha h_1};z,rq^{-1},sq^{-2}) = \pi^+(q^{\alpha h_1};z,r,s)\circ\imath.$$

Similarly one shows that the projection $p:\pi^+(z;r,s)\otimes\pi_z^{(1)}\to\pi^+(zq^{-2},rq,sq^2)$,

$$p:\quad |k\rangle\mapsto c_k'\,|k\rangle\otimes v_+$$

in (45) commutes with the twist operator as well,

$$p\circ\pi^+(q^{\alpha h_1};z,r,s) = \pi^+(q^{\alpha h_1};z,rq,sq^2)\circ p.$$

Setting $r=1$ and taking the limit $s\to 0$ we find

$$T_\alpha(z)Q_\alpha^\pm(z) = q^{\pm(S^z-\alpha)}Q_\alpha^\pm(zq^2)\prod_m\left(z\zeta_m^2-1\right)+q^{\pm(\alpha-S^z)}Q_\alpha^\pm(zq^{-2})\prod_m\left(z\zeta_m^2q^2-1\right).$$

As we will see below, this relation is identical to Baxter's famous *TQ* equation mentioned in the introduction after an appropriate rescaling of the auxiliary matrix; see section 4.1. The eigenvalues of the operators $Q_\alpha^\pm$ defined in (35) then coincide with the two linearly independent solutions of (13) discussed in the introduction.

As an immediate consequence of the *TQ* equation and the fusion relation we have in terms of eigenvalues the identity

$$T_\alpha^{(n-1)}(z) = q^{-(n+1)(\alpha-S^z)}Q_\alpha^+(zq^{-n})Q_\alpha^+(zq^n)\sum_{\ell=1}^{n}\frac{q^{2\ell(\alpha-S^z)}\prod_m\left(z\zeta_m^2q^{2\ell-n}-1\right)}{Q_\alpha^+(zq^{2\ell-n})Q_\alpha^+(zq^{2\ell-n-2})}. \tag{46}$$

This formula is easily proved by induction.

3.5. Functional equation at roots of unity

When q is a root of unity the vital information on the spectrum of the auxiliary matrix is encoded in the following functional equation which is a straightforward generalization of a previous result [22] to twisted boundary conditions[3];

$$Q_\alpha(zq^2/s;s)Q_\alpha(z;t) = q^{S^z-\alpha}Q_\alpha(zq^2/s;stq^{-2})$$
$$\times\left[\prod_m\left(z\zeta_m^2q^2-1\right)+q^{N'(S^z-\alpha)}T_\alpha^{(N'-2)}(zq^{N'+1})\right]. \tag{47}$$

[3] In order to facilitate the comparison with [22, 31] note that we have made the following changes. In order to match the result in [22] set $s=\mu^{-2}$ and $r=\mu^{-1}$. We have also redefined the fusion hierarchy, $T^{(n)}(z)\to T^{(n-1)}(zq^n)$, and shifted the parameter r in [31] by $r\to rq^{-1}$.

It implies the following decomposition of the eigenvalues:

$$Q_\alpha(z;s) = Q_\alpha(0)Q_\alpha^+(z)Q_\alpha^-(zs), \qquad Q_\alpha^\pm(z) = \prod_{i=1}^{n_\pm}\left(1 - zx_i^\pm\right) \tag{48}$$

where the last factors $Q_\alpha^\pm$ are polynomials with a total of $M = n_+ + n_-$ roots and are related by the following formula:

$$Q_\alpha(0)Q_\alpha^-(z) = q^{(2N'+1)(S^z-\alpha)}Q_\alpha^+(z)\sum_{\ell=1}^{N'}\frac{q^{2\ell(\alpha-S^z)}\prod_m\left(z\zeta_m^2q^{2\ell}-1\right)}{Q_\alpha^+(zq^{2\ell})Q_\alpha^+(zq^{2\ell-2})}. \tag{49}$$

Employing the transformation laws (40), (41) of the auxiliary matrix under spin reversal we deduce that

$$n_\pm = \frac{M}{2} \mp S^z. \tag{50}$$

From the above identity (49) between the eigenvalues of $Q_\alpha^\pm$ we now derive the following expression for the fusion hierarchy:

$$\begin{aligned}
&q^{-n(\alpha-S^z)}Q_\alpha(0)Q_\alpha^+(zq^{2n})Q_\alpha^-(z) - q^{n(\alpha-S^z)}Q_\alpha(0)Q_\alpha^+(z)Q_\alpha^-(zq^{2n}) \\
&\quad = q^{(2N'+1+n)(S^z-\alpha)}Q_\alpha^+(zq^{2n})Q_\alpha^+(z)\sum_{\ell=1}^{N'}\frac{q^{2\ell(\alpha-S^z)}\prod\left(z\zeta_m^2q^{2\ell}-1\right)}{Q_\alpha^+(zq^{2\ell})Q_\alpha^+(zq^{2\ell-2})} \\
&-q^{(2N'+1+n)(S^z-\alpha)}Q_\alpha^+(z)Q_\alpha^+(zq^{2n})\left\{\sum_{\ell=n+1}^{N'}\cdots + q^{2N'(\alpha-S^z)}\sum_{\ell=1}^{n}\cdots\right\} \\
&\quad = (q^{2N'(S^z-\alpha)}-1)T_\alpha^{(n-1)}(zq^n).
\end{aligned}$$

After inserting the value for $Q_\alpha(0)$ we obtain

$$T_\alpha^{(n-1)}(z) = (-)^M\frac{q^{n(S^z-\alpha)}Q_\alpha^+(zq^n)Q_\alpha^-(zq^{-n}) - q^{n(\alpha-S^z)}Q_\alpha^+(zq^{-n})Q_\alpha^-(zq^n)}{q^{S^z-\alpha}-q^{\alpha-S^z}}. \tag{51}$$

As long as $\alpha \neq 0 \bmod N', S^z$ this expression holds true for M, N even and odd. In particular we have for $n = 1$ the identity

$$\prod_{m=1}^{M}\left(1 - z\zeta_m^2q\right) = \frac{q^{S^z-\alpha}Q_\alpha^+(zq)Q_\alpha^-(zq^{-1}) - q^{\alpha-S^z}Q_\alpha^+(zq^{-1})Q_\alpha^-(zq)}{q^{S^z-\alpha}-q^{\alpha-S^z}} \tag{52}$$

which has been called 'quantum Wronskian' in the literature [20].

3.6. The algebraic Bethe ansatz for generic q

In [30] the spectrum of auxiliary matrices constructed in [27] have been investigated on the basis of the algebraic Bethe ansatz. The results in [30] apply to the inhomogeneous XXZ chain with twisted boundary conditions. Denote the monodromy matrices associated with the transfer and auxiliary matrix by

$$\mathcal{T} = (\pi^{(1)}\otimes 1)q^{\alpha h\otimes 1}L_M\cdots L_1 = \begin{pmatrix}\mathcal{A} & \mathcal{B}\\ \mathcal{C} & \mathcal{D}\end{pmatrix}$$

and

$$\mathcal{Q} = (\pi^+\otimes 1)q^{\alpha h_1\otimes 1}\mathfrak{L}_M\cdots\mathfrak{L}_1 = (\mathcal{Q}_{k\ell})_{k,\ell\geqslant 0}, \qquad \mathcal{Q}_{k\ell} = \langle k|\mathcal{Q}|\ell\rangle,$$

respectively. If the quantum space $\mathcal{H}$ carries a highest (or lowest) weight representation of the quantum group with highest weight vector $|0\rangle_{\mathcal{H}}$ then the eigenvectors and eigenvalues of the Q-operator can be computed via the algebraic Bethe ansatz. Setting $r = 1$ in (29) and denoting by $\mathfrak{L}^{\ell,\varepsilon'}_{k,\varepsilon} = \langle \ell, \varepsilon' | \mathfrak{L} | k, \varepsilon \rangle$ the matrix elements of the $\mathfrak{L}$-operator one finds

$$Q_\alpha(z) \prod_{j=1}^{n_+} \mathcal{B}\big(x_j^+\big)\, |0\rangle_{\mathcal{H}}$$
$$= \left\{ \sum_{k\geqslant 0} \langle 0 | \mathcal{Q}_{kk}(z) | 0 \rangle_{\mathcal{H}} \prod_{j=1}^{n_+} \left(\frac{\mathfrak{L}^{k,-}_{k,-}\big(zx_j^+\big)}{\mathfrak{L}^{k,+}_{k,+}\big(zx_j^+\big)} - \frac{\mathfrak{L}^{k+1,+}_{k,-}\big(zx_j^+\big)\mathfrak{L}^{k,-}_{k+1,+}\big(zx_j^+\big)}{\mathfrak{L}^{k+1,+}_{k+1,+}\big(zx_j^+\big)\mathfrak{L}^{k,+}_{k,+}\big(zx_j^+\big)} \right) \right\} \prod_{j=1}^{n_+} \mathcal{B}\big(x_j^+\big)\, |0\rangle_{\mathcal{H}}$$
$$= \left\{ \sum_{k\geqslant 0} \langle 0 | \mathcal{Q}_{kk}(z) | 0 \rangle_{\mathcal{H}} \prod_{j=1}^{n_+} \frac{q^{-2k-1}\big(1 - zx_j^+\big)\big(1 - zx_j^+ s\big)}{\big(1 - zx_j^+ s q^{-2k}\big)\big(1 - zx_j^+ s q^{-2k-2}\big)} \right\} \prod_{j=1}^{n_+} \mathcal{B}\big(x_j^+\big)\, |0\rangle_{\mathcal{H}}\,,$$

where x_j^+ are the Bethe roots above the equator. This formula has been proved directly for $n_+ = 1, 2, 3$ in [30] and further checked for consistency for arbitrary n_+. In the present case of the XXZ chain we have

$$|0\rangle_{\mathcal{H}} = v_+ \otimes \cdots \otimes v_+, \qquad \mathcal{H} = (\mathbb{C}^2)^{\otimes M} \tag{53}$$

and

$$\langle 0 | \mathcal{Q}_{kk}(z) | 0 \rangle_{\mathcal{H}} = q^{-\alpha(2k+1)} \prod_m q^{k+\frac{1}{2}} \big(zs\zeta_m^2 q^{-2k} - 1\big). \tag{54}$$

The above expression from the algebraic Bethe ansatz then yields for the case of generic q the same information on the spectrum which we had previously derived from the functional equation (47) at a root of unity,

$$Q_\alpha(z) \prod_{j=1}^{n_+} \mathcal{B}\big(x_j^+\big) |0\rangle_{\mathcal{H}}$$
$$= \left\{ q^{S^z-\alpha} Q^+_\alpha(z) Q^+_\alpha(zs) \sum_{k\geqslant 0} \frac{q^{2k(S^z-\alpha)} \prod \big(zs\zeta_m^2 q^{-2k} - 1\big)}{Q^+_\alpha(zsq^{-2k}) Q^+_\alpha(zsq^{-2k-2})} \right\} \prod_{j=1}^{n_+} \mathcal{B}\big(x_j^+\big) |0\rangle_{\mathcal{H}},$$

where we have set as before

$$Q^+_\alpha(z) = \prod_{j=1}^{n_+} \big(1 - zx_j^+\big), \qquad n_+ = \frac{M}{2} - S^z. \tag{55}$$

Thus, the analogous result concerning the decomposition of the eigenvalues into $Q^\pm_\alpha$ applies also here. Note that for generic q one has to put further restrictions on the twist parameter α [30],

$$|q^{-\alpha\pm M/2}| < 1 \qquad \text{for} \quad |q|^{\pm 1} \geqslant 1,$$

in order to ensure absolute convergence. Analytically continuing from this region the relation (51) holds also true for generic q.

An alternative to the Bethe ansatz is to follow the analogous line of argument as presented in [20]. Note that when we set $s = q^{2n}$ in (29) it follows that

$$s = q^{2n}: \quad e_1 |n\rangle = 0. \tag{56}$$

Hence, the infinite-dimensional module π^+ splits into a finite n-dimensional part $W_{<n}$ given by the linear span of the basis vectors $\{|k\rangle\}_{k=0}^{n-1}$ and an infinite-dimensional space $W_{\geqslant n}$ which is the linear span of the vectors $\{|k\rangle\}_{k=n}^{\infty}$. Note that $W_{\geqslant n}$ is left invariant under the action of $U_q(b_+)$. Restricting the $\mathfrak{L}$-operator onto these two spaces, one finds

$$\{\pi^+(z; 1, s = q^{2n}) \otimes 1\}\mathfrak{L}|_{W_{<n}} = \big(1 \otimes q^{-\frac{n}{2}\sigma^z}\big)\{\pi^{(n-1)} \otimes 1\} L(zq^n)(1 \otimes q^{n\sigma^z}) \tag{57}$$

and

$$\{\pi^+(z;1,s=q^{2n})\otimes 1\}\mathfrak{L}|_{W_{\geqslant n}}=\big(1\otimes q^{-n\sigma^z}\big)\{\pi^+(zq^{2n};1,s=q^{-2n})\otimes 1\}\mathfrak{L}\big(1\otimes q^{2n\sigma^z}\big). \quad (58)$$

Employing these identities together with the invariance of $W_{\geqslant n}$ one can split the trace in the definition of the auxiliary matrix into two parts leading to

$$Q_\alpha(z;s=q^{2n})=q^{n(S^z-\alpha)}T_\alpha^{(n-1)}(zq^n)+q^{2n(S^z-\alpha)}Q_\alpha(zq^{2n};s=q^{-2n}). \quad (59)$$

Apart from the factorization of Q_α into $Q_\alpha^\pm$ this corresponds to the identity (51). As it turns out this result is already sufficient for our present purposes, i.e. the analytic continuation of the fusion hierarchy in the spin variable. See equation (71) below.

4. The trace function

In order to make contact with the trace function used in [14] we now reparametrize the fusion hierarchy and the Q-operator and take M to be even.

4.1. Reparametrization

Henceforth we set $z=q^{2\lambda}$, $\zeta_m=q^{-\lambda_m}$ and define the rescaled fusion hierarchy as

$$T_\alpha^{(n)}(z)\to t_\alpha^{(n)}(\lambda):=\frac{(zq)^{-\frac{M}{2}}T_\alpha^{(n)}(z)}{(q-q^{-1})^M}\prod_m\zeta_m^{-1}. \quad (60)$$

This renormalization corresponds to the following choice of the six-vertex R-matrix which is in accordance with the conventions used in [14],

$$r(\lambda)=\begin{pmatrix}[\lambda+1]_q & 0 & 0 & 0\\ 0 & [\lambda]_q & 1 & 0\\ 0 & 1 & [\lambda]_q & 0\\ 0 & 0 & 0 & [\lambda+1]_q\end{pmatrix}. \quad (61)$$

Thus, the fusion hierarchy is now expressed as

$$t_\alpha^{(n)}\left(\lambda+\frac{n+1}{2}\right)t_\alpha(\lambda)=t_\alpha^{(n+1)}\left(\lambda+\frac{n}{2}\right)\prod_m[\lambda-\lambda_m+1]_q+t_\alpha^{(n-1)}\left(\lambda+\frac{n+2}{2}\right)\prod_m[\lambda-\lambda_m]_q \quad (62)$$

with the quantum determinant being

$$t_\alpha^{(0)}(\lambda)=t^{(0)}(\lambda)=\prod_m\left[\lambda-\lambda_m+\frac{1}{2}\right]_q. \quad (63)$$

Let us now turn to the re-definition of the auxiliary matrix. With respect to the decomposition

$$\mathfrak{L}(\lambda)=\begin{pmatrix}\mathfrak{L}_+^+ & \mathfrak{L}_-^+\\ \mathfrak{L}_+^- & \mathfrak{L}_-^-\end{pmatrix}$$

the matrix entries are now chosen as

$$\begin{aligned}
\mathfrak{L}_+^+&=\zeta^{-\frac12}\frac{\zeta^2/rq^{\lambda+\frac{h_1+1}{2}}-q^{-\lambda-\frac{h_1+1}{2}}}{q-q^{-1}}, \qquad s=\zeta^2, z=q^{2\lambda}\\
\mathfrak{L}_-^+&=\zeta^{-\frac12}q^{-\lambda}e_0q^{-\frac{h_0+1}{2}},\\
\mathfrak{L}_+^-&=\zeta^{-\frac12}q^{-\lambda}q^{-\frac{h_1-1}{2}}e_1,\\
\mathfrak{L}_-^-&=\zeta^{-\frac12}\frac{rq^{\lambda-\frac{h_1-1}{2}}-q^{-\lambda+\frac{h_1-1}{2}}}{q-q^{-1}}.
\end{aligned} \quad (64)$$

Note that this re-definition corresponds to the overall scaling factor

$$Q_\alpha(z;r,s=\zeta^2)\to Q_\alpha(\lambda;r,\zeta):=\frac{(zq\zeta)^{-\frac{M}{2}}}{(q-q^{-1})^M}Q_\alpha(z;r,s=\zeta^2)\prod_m\zeta_m^{-1} \tag{65}$$

and the eigenvalues of the auxiliary matrix in each spin sector have now the following decomposition:

$$Q_\alpha(\lambda;r,\zeta=q^{\lambda'})=\mathfrak{N}_\alpha r^{\alpha-S^z}q^{\lambda'S^z}Q_\alpha^+(\lambda)Q_\alpha^-(\lambda+\lambda') \tag{66}$$

with

$$\mathfrak{N}_\alpha=\begin{cases} q^{-N'(S^z+\alpha)}\frac{[N'(\alpha+S^z)]_q}{[\alpha+S^z]_q}, & \text{if}\quad q^N=1\\ \frac{1}{q^{\alpha+S^z}-q^{-S^z-\alpha}}, & \text{if}\quad q\ \text{generic}\end{cases}$$

and

$$Q_\alpha^\pm(\lambda)=\prod_{i=1}^{n_\pm}\left[\lambda-\xi_i^\pm\right]_q,\qquad x_i^\pm=q^{-2\xi_i^\pm}. \tag{67}$$

Here we have used the sum rule

$$q^{-M}\prod_{i=1}^{n_+}x_i^+\prod_{i=1}^{n_-}x_i^-\prod_m\zeta_m^{-2}=\frac{Q_{-\alpha}(0,q^{-1})}{Q_\alpha(0,q)}=\frac{q^{S^z-\alpha}-q^{\alpha-S^z}}{q^{-S^z-\alpha}-q^{\alpha+S^z}}$$

which follows from combining (40) with (41) and setting $z=0$. Employing this decomposition the *TQ* equation is equivalent to

$$t_\alpha(\lambda)Q_\alpha^\pm(\lambda)=q^{-\alpha}Q_\alpha^\pm(\lambda+1)\prod_{m=1}^M[\lambda-\lambda_m]_q+q^\alpha Q_\alpha^\pm(\lambda-1)\prod_{m=1}^M[\lambda-\lambda_m+1]_q. \tag{68}$$

The expression for the transfer matrices of the fusion hierarchy is now

$$t_\alpha^{(n-1)}(\lambda)=\frac{q^{-n\alpha}Q_\alpha^+\left(\lambda+\frac{n}{2}\right)Q_\alpha^-\left(\lambda-\frac{n}{2}\right)-q^{n\alpha}Q_\alpha^+\left(\lambda-\frac{n}{2}\right)Q_\alpha^-\left(\lambda+\frac{n}{2}\right)}{q^{-S^z-\alpha}-q^{\alpha+S^z}},\qquad n\in\mathbb{N}. \tag{69}$$

It is the last expression respectively (51) which we want to analytically continue in n in order to obtain the trace function used in the description of the correlation functions of the infinite XXZ chain.

4.2. *Analytic continuation and the limit* $\alpha\to 0$

As mentioned in the introduction we now analytically continue the expression for the fusion hierarchy (51), (59) in the spin variable $n/2$ by defining the following operator:

$$\boldsymbol{T}_\alpha(z,\zeta)=(-)^M\frac{\zeta^{S^z-\alpha}Q_\alpha^+(z\zeta)Q_\alpha^-(z\zeta^{-1})-\zeta^{\alpha-S^z}Q_\alpha^+(z\zeta^{-1})Q_\alpha^-(z\zeta)}{q^{S^z-\alpha}-q^{\alpha-S^z}} \tag{70}$$

$$=\frac{\zeta^{\alpha-S^z}Q_\alpha(z\zeta^{-1};s=\zeta^2)-\zeta^{S^z-\alpha}Q_\alpha(z\zeta;s=\zeta^{-2})}{q^{S^z-\alpha}-q^{\alpha-S^z}}Q_\alpha(0)^{-1}. \tag{71}$$

Note that this analytic continuation is unambiguous as the operators on the right-hand side of (71) have only a polynomial dependence on the spectral parameter z by construction. The rescaled counterpart of (71) gives the result (16) stated in the introduction,

$$\boldsymbol{t}_\alpha(\lambda,\zeta)\equiv\frac{\boldsymbol{T}_\alpha(z=q^{2\lambda},\zeta)}{q^{M(\lambda+1/2)}(q-q^{-1})^M}\prod_m\zeta_m^{-1}. \tag{72}$$

First note that we recover the fusion hierarchy (51) respectively (59) when setting $\zeta = q^n$,

$$\boldsymbol{T}_\alpha(z, \zeta = q^n) = T_\alpha^{(n-1)}(z). \tag{73}$$

Now, as an easy example for the occurrence of terms linear in λ in the matrix elements we evaluate (70) at the origin $z = 0$. Then we have for nonzero spin $S^z \neq 0$

$$(-)^M \lim_{\alpha\to 0} \boldsymbol{T}_\alpha(0, \zeta) = \lim_{\alpha\to 0} \frac{\zeta^{-\alpha+S^z} - \zeta^{\alpha-S^z}}{q^{-\alpha+S^z} - q^{\alpha-S^z}} = \frac{\zeta^{S^z} - \zeta^{-S^z}}{q^{S^z} - q^{-S^z}}. \tag{74}$$

For vanishing spin $S^z = 0$ we set $\zeta = q^\lambda$ and obtain

$$(-)^M \lim_{\alpha\to 0} T_\alpha(0, \zeta = q^\lambda) = \lambda. \tag{75}$$

These last two relations correspond to the defining equations (5.3) in [14], see also (12) in the introduction of this paper. The occurrence of linear terms λ in the matrix elements is not restricted to the zero spin sector but occurs more generally. To see this we now derive the analogue of lemma 5.1 in [14].

Lemma. *For M even the analytically continued fusion hierarchy (70) decomposes in the limit $\alpha \to 0$ into a sum*

$$\lim_{\alpha\to 0} \boldsymbol{T}_\alpha(z, \zeta = q^\lambda) = \lambda \cdot \tilde{\boldsymbol{G}}(z) + \boldsymbol{G}(z) \tag{76}$$

where the operators $\tilde{\boldsymbol{G}}, \boldsymbol{G}$ are polynomial in the spectral variable z and in each fixed spin sector $S^z \neq 0$ have degrees

$$\deg \tilde{\boldsymbol{G}}|_{S^z} = M - |S^z| \qquad \textit{and} \qquad \deg \boldsymbol{G}|_{S^z} = M. \tag{77}$$

If $S^z = 0$ then

$$\deg \tilde{\boldsymbol{G}}|_{S^z=0} = M \qquad \textit{and} \qquad \deg \boldsymbol{G}|_{S^z} < M. \tag{78}$$

According to the rescaling (70) this obviously implies (18).

Remark 1. For comparison with lemma 5.1 in [14] we have to identify $z \to \zeta_1^2$ and $M = 2p - 2$, compare with (7) in this paper. Moreover, we do consider here the degree of an operator in a whole spin sector, not a single matrix element as in [14].

Remark 2. Note that for M odd the linear terms in λ are absent, since the terms containing $\mathrm{Tr}_{\pi^+} q^{\alpha h_1}$ which contains a pole in the limit $\alpha \to 0$ can never occur in a matrix element of the Q-operator. See the proof below for an explanation.

Note further, at roots of unity and periodic boundary conditions $\alpha = 0$ the linear terms have not been observed in [22] and [23, 24]. This is explained by the fact that the root of unity limit does not commute with the limit $\alpha \to 0$. As long as $\alpha \neq 0$ (and generic) the root of unity symmetries discussed in [22, 23, 25, 26] are not present, whence we arrive here at a different result.

Proof. Since we are only interested in determining the maximal degree of the respective polynomials in z we can set $\zeta_m = 1$ without loss of generality. As an additional preparatory step we need to make contact with the Casimir operator which has also been used to define the trace function in [14]. Set $r = 1$ in (29), then we have

$$[e_1, e_0] = z \frac{s q^{h_1} - q^{-h_1}}{q - q^{-1}} \tag{79}$$

and

$$\mathfrak{C} = z \frac{s q^{h_1 - 1} + q^{-h_1+1}}{(q - q^{-1})^2} + e_1 e_0 = z \frac{1 + s}{(q - q^{-1})^2}. \tag{80}$$

This identity corresponds to equation (5.4) in [14], see (12) in this paper. Now consider a general matrix element of the auxiliary matrix

$$Q_\alpha(z;s)^{\underline{\varepsilon}'}_{\underline{\varepsilon}} = \operatorname*{Tr}_{\pi^+} q^{\alpha h_1 \otimes 1} \mathfrak{L}^{\varepsilon'_M}_{\varepsilon_M} \cdots \mathfrak{L}^{\varepsilon'_1}_{\varepsilon_1}, \qquad \sum_m \varepsilon_m = \sum_m \varepsilon'_m = 2S^z. \tag{81}$$

Since the Q-operator preserves the total spin the matrix elements $\mathfrak{L}^{\pm}_{\mp}$ always occur in pairs and we compute

$$\begin{aligned}\operatorname*{Tr}_{\pi^+}\left\{X\mathfrak{L}^{\pm}_{\mp}\mathfrak{L}^{\mp}_{\pm}\right\} &= zq \operatorname*{Tr}_{\pi^+}\{X(q-q^{-1})^2\mathfrak{C} - sq^{h_1\pm 1} - q^{-h_1\mp 1}\} \\ &= zq \operatorname*{Tr}_{\pi^+}\{X(1+s-q^{-h_1\mp 1} - sq^{h_1\pm 1})\}.\end{aligned} \tag{82}$$

The numbers of the various operators $\mathfrak{L}^{\varepsilon'}_{\varepsilon}$ occurring in a matrix element is given by

$$\#\mathfrak{L}^{\pm}_{\pm} + \#\mathfrak{L}^{\mp}_{\pm} = \frac{M}{2} \pm S^z = n_{\mp} \qquad \text{and} \qquad \#\mathfrak{L}^{+}_{-} = \#\mathfrak{L}^{-}_{+} = \sum_m \frac{1-\varepsilon_m\varepsilon'_m}{2} =: n_{\underline{\varepsilon},\underline{\varepsilon}'}. \tag{83}$$

Using the above relations any matrix element of the Q-operator in a fixed spin sector can be expressed as a linear combination of terms of the form

$$\begin{aligned}Q_\alpha(z\zeta; s=\zeta^{-2})^{\underline{\varepsilon}'}_{\underline{\varepsilon}} = (zq)^{n_{\underline{\varepsilon},\underline{\varepsilon}'}} \sum c_{\underline{\varepsilon},\underline{\varepsilon}'} \operatorname*{Tr}_{\pi^+}\Bigg\{ & q^{\alpha h_1}\big(\zeta^{-1} z q^{1+\frac{h_1}{2}} - q^{-\frac{h_1}{2}}\big)^{n_- - n_{\underline{\varepsilon},\underline{\varepsilon}'}} \\ & \times \big(\zeta z q^{1-\frac{h_1}{2}} - q^{\frac{h_1}{2}}\big)^{n_+ - n_{\underline{\varepsilon},\underline{\varepsilon}'}} \prod_{i=1}^{n_{\underline{\varepsilon},\underline{\varepsilon}'}} \zeta^{\sigma_i} q^{-\sigma_i h_1}\Bigg\}\end{aligned}$$

where the coefficients $c_{\underline{\varepsilon},\underline{\varepsilon}'}$ do not depend on z and $\sigma_i = 0, \pm 1$ can vary in each factor, but there can be terms present for which all the σ_i are equal. To see this note that $\left[\mathfrak{L}^+_+, \mathfrak{L}^-_-\right] = 0$, while the commutation of $\mathfrak{L}^{\pm}_{\mp}$ with $\mathfrak{L}^{\mp}_{\pm}$ only produces powers in q. The operators $\mathfrak{L}^+_-$ and $\mathfrak{L}^-_+$ commute according to (79). Let us distinguish the two cases $n_{\underline{\varepsilon},\underline{\varepsilon}'} = 0$ and $n_{\underline{\varepsilon},\underline{\varepsilon}'} \neq 0$.

Choose a matrix element with $n_{\underline{\varepsilon},\underline{\varepsilon}'} = 0$, i.e. $\varepsilon_m = \varepsilon'_m$. This is possible in all spin sectors. Then the term of maximal degree has the coefficient

$$\begin{aligned}Q_\alpha(z\zeta; s=\zeta^{-2})^{\underline{\varepsilon}}_{\underline{\varepsilon}} = \operatorname*{Tr}_{\pi^+}\Big\{ & q^{\alpha h_1}\big(\zeta^{-1} z q^{1+\frac{h_1}{2}} - q^{-\frac{h_1}{2}}\big)^{\frac{M}{2}-|S^z|}\big(\zeta z q^{1-\frac{h_1}{2}} - q^{\frac{h_1}{2}}\big)^{\frac{M}{2}-|S^z|} \\ & \times \big(\zeta^{-\sigma} z q^{1+\sigma\frac{h_1}{2}} - q^{-\sigma\frac{h_1}{2}}\big)^{2|S^z|}\Big\} = (zq)^M \zeta^{-2S^z} \operatorname*{Tr}_{\pi^+} q^{\alpha(1+S^z)h_1} + \cdots.\end{aligned}$$

Here we have set $\sigma = \operatorname{sgn} S^z$. From this we infer using (71) that

$$\begin{aligned}&\frac{\zeta^{S^z-\alpha} Q_\alpha(z\zeta; s=\zeta^{-2}) - \zeta^{\alpha-S^z} Q_\alpha(z\zeta^{-1}; s=\zeta^2)}{(q^{S^z-\alpha} - q^{\alpha-S^z})Q_\alpha(0)} \\ &\qquad = (zq)^M \frac{\zeta^{-S^z-\alpha} - \zeta^{\alpha+S^z}}{(q^{S^z-\alpha} - q^{\alpha-S^z})Q_\alpha(0)} \operatorname*{Tr}_{\pi^+} q^{\alpha(1+S^z)h_1} + \cdots.\end{aligned}$$

Setting $\zeta = q^\lambda$ we conclude similarly to our previous calculation at $z = 0$ that the linear terms in λ originate from coefficients containing $\operatorname{Tr}_{\pi^+} q^{\alpha h_1}$ which develops a pole in the limit $\alpha \to 0$. Thus, we deduce that $\deg \tilde{\boldsymbol{G}} = M$ and $\deg \boldsymbol{G} < M$ when $S^z = 0$. When $S^z \neq 0$, on the other hand, we have as degrees $\deg \boldsymbol{G} = M$ and $\deg \tilde{\boldsymbol{G}} = M - |S^z|$. Note that for this it is crucial that $2|S^z|$ is an even integer which is only the case when M is even.

Now choose a matrix element with $n_{\underline{\varepsilon},\underline{\varepsilon}'} \neq 0$. This is always possible as long as $|S^z| < M/2$. All we need to show is that the just derived degrees are not exceeded. The term of maximal degree has now coefficients of the form

$$Q_\alpha(z\zeta; s=\zeta^{-2})^{\underline{\varepsilon}'}_{\underline{\varepsilon}} = (zq)^{M-n_{\underline{\varepsilon},\underline{\varepsilon}'}} \sum c_{\underline{\varepsilon},\underline{\varepsilon}'} \zeta^{-2S^z} \operatorname*{Tr}_{\pi^+} q^{(\alpha+S^z)h_1} \prod_{i=1}^{n_{\underline{\varepsilon},\underline{\varepsilon}'}} \zeta^{\sigma_i} q^{-\sigma_i h_1} + \cdots.$$

As in the earlier examples we need to determine the maximal degree of the term which contains $\mathrm{Tr}_{\pi^+} q^{\alpha h_1}$ yielding the linear dependence on λ in the limit $\alpha \to 0$. The degree of $\tilde{\boldsymbol{G}}$ is maximized by choosing a matrix element with $n_{\underline{\varepsilon},\underline{\varepsilon}'} = |S^z|$, where the coefficient of the term with all $\sigma_i = \mathrm{sgn}\, S^z$ is non-vanishing. Then we have

$$\zeta^{S^z-\alpha} Q_\alpha(z\zeta;\zeta^{-2})^{\underline{\varepsilon}'}_{\underline{\varepsilon}} - \zeta^{\alpha-S^z} Q_\alpha(z\zeta^{-1};\zeta^2)^{\underline{\varepsilon}'}_{\underline{\varepsilon}} = \mathrm{const}(zq)^{M-|S^z|}(\zeta^{-\alpha}-\zeta^{\alpha}) \mathop{\mathrm{Tr}}_{\pi^+} q^{\alpha h_1} + \cdots$$

from which we infer in the limit $\alpha \to 0$ that the maximal degree of $\tilde{\boldsymbol{G}}$ in a fixed spin sector is again $M - |S^z|$. For the remainder polynomial $\boldsymbol{G}$ we find as before that its degree is strictly smaller than M if $S^z = 0$. □

4.2.1. Example: $M = 4$ and $S^z = 1$. Let us consider a simple example for the homogeneous chain to show how the linear term in λ emerges in a matrix element of the operator (70). Setting $M = 4$ and $S^z = 1$ we choose the matrix element

$$\begin{aligned} Q_\alpha(z;s)^{-+++}_{+-++} &= \mathop{\mathrm{Tr}}_{\pi^+} q^{\alpha h_1}\big(zsq^{1+\frac{h_1}{2}} - q^{-\frac{h_1}{2}}\big)^2 zq(1+s-q^{-h_1-1}-sq^{h_1+1}) \\ &= zq \mathop{\mathrm{Tr}}_{\pi^+} q^{\alpha h_1}(z^2s^2q^{2+h_1} - 2zsq + q^{-h_1})(1+s-q^{-h_1-1}-sq^{h_1+1}) \\ &= -zsq^2\{z^2s+1+2z(1+s)\}\mathop{\mathrm{Tr}}_{\pi^+} q^{\alpha h_1} + \cdots. \end{aligned} \tag{84}$$

In the last line we have only written out the terms which will give rise to the linear dependence in λ. Namely, inserting this expression into (70) we find

$$\begin{aligned} \boldsymbol{T}_\alpha(z;\zeta)^{-+++}_{+-++} &= \frac{\zeta^{1-\alpha}Q_\alpha(z\zeta;\zeta^{-2}) - \zeta^{\alpha-1}Q_\alpha(z\zeta^{-1};\zeta^2)}{Q_\alpha(0)(q^{1-\alpha}-q^{\alpha-1})} \\ &= -zq^2(z^2+1+2z(\zeta+\zeta^{-1}))\frac{\zeta^{-\alpha}-\zeta^{\alpha}}{Q_\alpha(0)(q^{1-\alpha}-q^{\alpha-1})}\mathop{\mathrm{Tr}}_{\pi^+} q^{\alpha h_1} + \cdots \\ &= -zq^2(z^2+1)\frac{\zeta^{-\alpha}-\zeta^{\alpha}}{Q_\alpha(0)(q^{1-\alpha}-q^{\alpha-1})}\mathop{\mathrm{Tr}}_{\pi^+} q^{\alpha h_1} + \cdots. \end{aligned} \tag{85}$$

Let us distinguish the case when q is generic and when it is a root of unity. If $q^N = 1$ then

$$Q_\alpha(0) = \frac{1-q^{-2N'\alpha}}{q^{\alpha-1}-q^{1-\alpha}} \qquad \text{and} \qquad \mathop{\mathrm{Tr}}_{\pi^+} q^{\alpha h_1} = \frac{1-q^{-2N'\alpha}}{q^{\alpha}-q^{-\alpha}}. \tag{86}$$

On the other hand we have for generic q

$$Q_\alpha(0) = \frac{1}{q^{\alpha-1}-q^{1-\alpha}} \qquad \text{and} \qquad \mathop{\mathrm{Tr}}_{\pi^+} q^{\alpha h_1} = \frac{1}{q^{\alpha}-q^{-\alpha}}, \tag{87}$$

where these expressions are understood as analytic continuation from the region where the trace converges. Thus, setting $\zeta = q^\lambda$ we arrive at

$$\begin{aligned} \lim_{\alpha\to 0} \boldsymbol{T}_\alpha(z;\zeta)^{-+++}_{+-++} &= -zq^2(z^2+1+2z(q^\lambda+q^{-\lambda}))\lim_{\alpha\to 0}\frac{q^{\alpha\lambda}-q^{-\alpha\lambda}}{q^\alpha-q^{-\alpha}} + \cdots \\ &= -\lambda zq^2(z^2+1+2z(q^\lambda+q^{-\lambda})) + \cdots \end{aligned} \tag{88}$$

where the coefficient of λ is of degree $M - |S^z| = 3$ in z in accordance with our lemma.

5. Conclusions

In this paper we continued a previous study [22, 28–31] on the explicit construction of operator solutions to Baxter's TQ equation (13). In terms of eigenvalues this equation is a second-order difference equation and its theory resembles closely that of second-order ordinary differential equations. In the case of the XXZ chain we discussed the existence of two linearly independent solutions when quasi-periodic boundary conditions are imposed by explicitly constructing the relevant Q-operators using representation theory. Because it is usually required that Q-operators should commute for arbitrary values of the spectral parameter, $[Q(z), Q(w)] = 0$, this precludes by choice of the construction method the possibility of obtaining 'non-analytic' solutions to the TQ equation: that is, solutions which obtain the linear terms discussed in the text and which have been postulated in [21] for even chains with periodic boundary conditions and when q is generic. The result of this paper is that such solutions can arise by taking the limit from quasi-periodic to periodic boundary conditions in the explicitly constructed Q-operators. Recall that for generic q this limit required a careful analysis. First one had to choose the twist parameter α such that convergence of the trace over the infinite-dimensional auxiliary space is guaranteed. In a second step we then analytically continued the matrix elements in α from the region of convergence to the complex plane which enabled us in the final step to discuss the limit $\alpha \to 0$. To complete the investigation by computing the spectra of the Q-operators in this limit one would need to know the explicit dependence of the Bethe roots on the twist parameter. This is a rather formidable challenge as the solutions to the Bethe ansatz equations are in general not known.

The main motivation for our construction of this 'non-analytic' Q-operator has been the relation with the recent developments in the computation of correlation functions as explained in detail in the introduction. The alternative expression (16) for the special trace of the monodromy matrix (7) entering the ansatz in [14] shows that there is a more fundamental quantity in which the correlation functions can be expressed and provides a different point of view on the role of the trace function (74). In future work it needs to be explored whether there are concrete practical implications of the identity (16) which facilitate the computation of correlation functions. For instance, one might ask whether one can insert each of the two terms in the difference (16) separately in the ansatz for the correlation functions and if they satisfy identities analogous to the quantum Knizhnik–Zamolodchikov equations. Of course one has to keep in mind that in order to perform the limit $\alpha \to 0$ both terms will be needed at the end. However, such an investigation might yield further insight into the analytic structure.

Note added in proof. After this paper was completed the work [34] appeared which extends the investigation of correlation functions to the inhomogeneous eight-vertex or XYZ model. An analogous Q-operator for this model would be helpful as it would simplify the computation of the analogue of the trace function over the Sklyanin algebra. The present discussion provides a first step towards this aim.

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