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A Q-operator for the twisted XXX model

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Abstract
Taking the isotropic limit $\Delta \to 1$ in a recent representation theoretic construction of Baxter's Q-operators for the XXZ model with quasi-periodic boundary conditions we obtain new results for the XXX model. We show that quasi-periodic boundary conditions are needed to ensure convergence of the Q-operator construction and derive a quantum Wronskian relation which implies two different sets of Bethe ansatz equations, one above, the other below the 'equator' of total spin $S^z = 0$. We discuss the limit to periodic boundary conditions at the end and explain how this construction relates to the trace functional introduced by Boos *et al* in the context of correlation functions on the infinite lattice. We also identify a special subclass of solutions to the quantum Wronskian and numerically verify them up to spin chains of ten sites. This special type of solutions might persist for longer chains.

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1. Introduction

Historically Baxter's Q-operator was introduced as substitute means for the coordinate Bethe ansatz in solving the eight-vertex model [1–3], but has more recently seen wider applications in the field of integrable systems e.g. [4–9] making it an important and almost universal tool. To motivate his technique Baxter first discussed the concept of the Q-operator in the context of the six-vertex or XXZ model, where a direct comparison with the coordinate Bethe ansatz can be made. While our primary interest in this paper will be the XXX model, it is helpful to consider first the anisotropic or XXZ case. Denote by t the transfer matrix; then the Q-operator is implicitly defined through the functional equation

$$t(u)Q(u) = \chi\left(u - \tfrac{1}{2}\right)Q(u+1) + \chi\left(u + \tfrac{1}{2}\right)Q(u-1), \tag{1.1}$$

where $\chi(u) = \sin^M \gamma u$ is the XXZ quantum determinant with M being the number of lattice columns, respectively, the number of sites in the spin chain. In addition to this relation, known as TQ equation, one usually requires a number of properties such as 'analyticity' of the Q-operator in the spectral variable u and that $[t(u), Q(u')] = [Q(u), Q(u')] = 0$ for an arbitrary pair $u, u' \in \mathbb{C}$. The latter commutation relations allow one to discuss the TQ equation on the level of eigenvalues and this is where one makes contact with the coordinate Bethe ansatz [10] which determines the spectrum of the transfer matrix in terms of the solutions $\{v_k\}_{k=1}^n$ to the Bethe ansatz equations [11, 12],

$$\left(\frac{\sinh\gamma(v_j - \mathrm{i}/2)}{\sinh\gamma(v_j + \mathrm{i}/2)}\right)^M = \prod_{k\neq j}\frac{\sinh\gamma(v_j - v_k - \mathrm{i})}{\sinh\gamma(v_j - v_k + \mathrm{i})}, \qquad j = 1, 2, \ldots, \quad n = M/2 - S^z. \tag{1.2}$$

Here, γ is the crossing or coupling parameter of the six-vertex model and $S^z \geqslant 0$ the total spin operator. Postulating that the eigenvalues of the Q-operator are of the form [3]:

$$Q(u) = \prod_{j=1}^n \frac{\sinh\gamma(u - v_j)}{\sinh\gamma}, \tag{1.3}$$

the outcome of the coordinate Bethe ansatz then implies the TQ relation (1.1), which is the starting point for the construction of the operator Q. Note that this line of argument is based on the essential assumption that the coordinate Bethe ansatz yields a complete set of eigenstates of the transfer matrix with a finite set of Bethe roots v_j. It is this assumption which has to be treated with care in the isotropic limit $\gamma \to 0$ yielding the XXX model[1].

The transfer matrix of the XXX model as well as the associated Heisenberg spin chain is sl_2 symmetric, whence their eigenspaces decompose into sl_2 modules. As is well known, the finite solutions to the XXX Bethe ansatz equations (first derived by Bethe in [10] albeit in a different form),

$$\left(\frac{v_j - \mathrm{i}/2}{v_j + \mathrm{i}/2}\right)^M = \prod_{k\neq j}\frac{v_j - v_k - \mathrm{i}}{v_j - v_k + \mathrm{i}}, \tag{1.4}$$

now only yield the highest weight vectors in each sl_2 module [16] . The remaining states within each module are obtained through the action of the symmetry algebra and have been referred to as 'non-regular' Bethe states as they involve 'infinite rapidities' in the particular parametrization used in (1.4); see e.g. [17] for a discussion on how to recover the non-regular Bethe states through a limiting procedure. Thus, the obvious ansatz

$$Q(u) = \prod_{j=1}^n (u - v_j) \tag{1.5}$$

for the eigenvalues of an XXX Q-operator becomes problematic due to the presence of 'infinite rapidities', or more precisely not all states correspond to finite solutions of the Bethe ansatz equations (1.4). Clearly, there are ways out of this dilemma, either by choosing a different parametrization such that all rapidities stay finite (this is for instance the case in the coordinate Bethe ansatz, where the non-regular Bethe states correspond to the case that multiple quasi-momenta vanish), or by (continuously) breaking the sl_2 symmetry in such a manner that the assumption on the completeness of the Bethe ansatz becomes applicable again.

In this work we shall do the latter by introducing quasi-periodic boundary conditions, see e.g. [18–21]. This has the advantage that all relevant algebraic properties needed for the quantum inverse scattering method [22] stay intact and that we can take at the very end the limit to periodic boundary conditions making contact with previous investigations of Q-operators

[1] Similar problems occur for the XXZ model at roots of unity [13, 14] due to a partial loop algebra symmetry [15].

for the XXX model. Of particular interest will be aspects which are not accessible through the coordinate Bethe ansatz, namely the existence of two linearly independent solutions, say $Q^{\pm}$, to the TQ equation and, closely related to this question, the derivation of the following quantum Wronskian identity:

$$\frac{\omega Q_{\omega}^{+}\left(u-\frac{\mathrm{i}}{2}\right) Q_{\omega}^{-}\left(u+\frac{\mathrm{i}}{2}\right)-\omega^{-1} Q_{\omega}^{+}\left(u+\frac{\mathrm{i}}{2}\right) Q_{\omega}^{-}\left(u-\frac{\mathrm{i}}{2}\right)}{\omega-\omega^{-1}}=\chi(u), \tag{1.6}$$

which is a new result. Here, $\omega = \exp(\mathrm{i}\phi)$ is the twist parameter associated with the quasi-periodic boundary conditions and χ is the aforementioned quantum determinant, but now of the XXX model. Since the latter is explicitly known, e.g. $\chi(u) = u^M$ for the homogeneous case, one can employ the quantum Wronskian (1.6) rather than the generalization of the Bethe ansatz equations (1.4) to twisted boundary conditions when solving the model. Namely, making the ansatz (which will be justified through our construction of $Q_{\omega}^{\pm}$ in the text)

$$Q_{\omega}^{+}(u)=\prod_{j=1}^{n}\left(u-v_{j}^{+}\right) \qquad \text{and} \qquad Q_{\omega}^{-}(u)=\prod_{j=1}^{M-n}\left(u-v_{j}^{-}\right), \qquad n=\frac{M}{2}-S^{z} \tag{1.7}$$

for the eigenvalues of the two solutions to the TQ equation, the roots $v_j^{\pm} = v_j^{\pm}(\omega)$ are determined through (1.6). Here, S^z denotes the total spin component in the direction singled out by the quasi-periodic boundary conditions. Note that upon setting $u = v_j^{\pm} + \mathrm{i}/2, v_j^{\pm} - \mathrm{i}/2$ identity (1.6) implies two different sets of Bethe ansatz equations, one above, the other one below the equator $S^z = 0$. Due to the quasi-periodic boundary conditions, $\omega \neq 1$, the Bethe roots $v_j^{\pm}$ are all finite and the number of solutions matches the dimension of each fixed spin-sector signalling completeness; compare for example with the discussion in [23].

As discussed above this ceases to be true in the limit $\omega \to 1$ corresponding to periodic boundary conditions. From (1.6) we infer that this limit might indeed be singular unless the numerator and denominator vanish simultaneously. We will compare the outcome of this paper with the findings for periodic boundary conditions by Pronko and Stroganov [24], who have presented a similar quantum Wronskian without the denominator at $\omega = 1$ and a different degree for the second solution Q^-, namely deg $Q^- = M - n + 1$. Their Wronskian relation can be numerically solved but the resulting number of solutions is in general much smaller than the dimension of the state space $\binom{M}{n}$. In light of the previous remarks on the sl_2 symmetry, this is not surprising as their solutions only yield the highest weight vectors in each module. Taking the limit $\omega \to 1$ in the explicit solutions to (1.6) for small chains we indeed find that of those solutions $Q_{\omega}^{\pm}$ which stay finite, *both* approach the Q^+ solution of Pronko and Stroganov. We shall comment on this in more detail in the text, see section 5.2.

The appearance of singularities in the limit of periodic boundary conditions can also be understood from the explicit construction of the Q-operator for twisted boundary conditions. The latter is given as the trace of a monodromy matrix with infinite-dimensional auxiliary space. In order to obtain a well-defined object one must ensure convergence of the trace. As we will see in the text this actually *requires* the introduction of quasi-periodic boundary conditions. Previous constructions of Q-operators for the XXX spin chain [25–27] have been for periodic boundary conditions only, where Q has been represented as an integral kernel (see also [28] for a related XXZ construction).

In contrast, the limit of the transfer matrix from quasi-periodic to periodic boundary conditions is well defined. In fact, this applies to all higher spin transfer matrices which can be expressed in terms of $Q_{\omega}^{\pm}$ as follows:

$$t(u;x)=\lim_{\omega\to 1}\frac{\omega^{x} Q_{\omega}^{+}\left(u-\frac{\mathrm{i}x}{2}\right) Q_{\omega}^{-}\left(u+\frac{\mathrm{i}x}{2}\right)-\omega^{-x} Q_{\omega}^{+}\left(u+\frac{\mathrm{i}x}{2}\right) Q_{\omega}^{-}\left(u-\frac{\mathrm{i}x}{2}\right)}{\omega-\omega^{-1}}. \tag{1.8}$$

When $x = n \in \mathbb{N}_{>0}$, the function $t(u; x = n)$ gives the spectrum of the transfer matrix with spin $s = (n-1)/2$ in the auxiliary space. However, if we take x to be an arbitrary complex parameter, the resulting spectrum belongs to a generalized transfer matrix used in the discussion of correlation functions for the infinite chain [29–32]. This result is the analogue of a previous discussion for the XXZ model [33, 34] and the discussion presented here is in accordance with these earlier results for the more general case when $\gamma \neq 0$. At the moment there appears to be no construction of a Q-operator for $\omega = 1$ which allows us to define (1.8). This is one of the main reasons for the construction presented in this paper.

In section 2, the basic definitions of the XXX model and its fusion hierarchy are stated. Section 3 contains the construction of the Q-operator which is simply the isotropic limit ($\gamma \to 0$) of earlier constructions for the XXZ model [34]. We briefly address the aforementioned conditions for convergence due to an infinite-dimensional auxiliary space and state the relevant functional equations with the transfer matrix. We omit most proofs for those results which readily follow from taking the isotropic limit in the XXZ construction. For instance, the eigenvalues of the Q-operator are discussed by making contact with the algebraic Bethe ansatz discussion in [33]. By comparison with the analogous results for the XXZ model, it is shown that the Q-operator factorizes into two linearly independent solutions to Baxter's TQ equation. We discuss how they are related via spin reversal. The relation with the fusion hierarchy and its analytic continuation (1.8) to 'complex spin' is presented in section 4. Section 5 gives the quantum Wronskian relation between the two independent solutions to Baxter's TQ equation, which is then compared against the one of Pronko and Stroganov [24]. A special subset of solutions to the twisted quantum Wronskian (1.6) is also discussed based on numerical results for chains of even length $\leqslant 10$. Their associated Bethe roots obey identities which imply (and are therefore more fundamental than) the Bethe ansatz equations. The conclusions are stated in section 6.

2. Definitions

Let us start by introducing our conventions for the definition of the XXX model. Denote by $\{\sigma^x = \sigma^1, \sigma^y = \sigma^2, \sigma^z = \sigma^3\}$ the Pauli matrices acting on $\mathbb{C}^2$ and let $\mathbb{P}$ be the permutation operator, $\mathbb{P}(v \otimes w) = w \otimes v$. Then the basic ingredient for constructing the XXX model is the following simple solution to the Yang–Baxter equation

$$r(\lambda) = \lambda + \frac{1}{2} + \sum_{\alpha=1}^{3} \sigma^\alpha \otimes \sigma^\alpha = \lambda + \mathbb{P} \in \mathrm{End}(\mathbb{C}^2 \otimes \mathbb{C}^2). \tag{2.1}$$

Note that we have changed our conventions from that in the introduction as it simplifies some of the following computations. The alternative definition of the XXX r-matrix also commonly used in the literature reads

$$\tilde{r}(u) := \mathrm{i}r(-\mathrm{i}u - 1/2) = u + \mathrm{i}\sum_{\alpha=1}^{3} \sigma^\alpha \otimes \sigma^\alpha = u - \mathrm{i}/2 + \mathrm{i}\mathbb{P}. \tag{2.2}$$

Both definitions only differ by a re-parametrization of the spectral parameter, $\lambda \to -\mathrm{i}u - 1/2$, and an overall factor $\mathrm{i} = \sqrt{-1}$. The XXX functional relations and equations stated in the introduction refer to this last convention (2.2).

In terms of (2.1) the transfer matrix of the inhomogeneous XXX model with quasi-periodic boundary conditions is defined as follows:

$$t_\omega(\lambda) = \mathrm{Tr}_{\mathbb{C}^2} \omega^{\sigma^z \otimes 1} r_M(\lambda - \lambda_M) \cdots r_1(\lambda - \lambda_1), \qquad \omega = \mathrm{e}^{\mathrm{i}\phi}. \tag{2.3}$$

Here, the trace is taken in the first factor of the r-matrix, i.e. $t_\omega \in \mathrm{End}(\mathbb{C}^2)^{\otimes M}$. The set $\{\lambda_m\}_{m=1}^M$ is some arbitrary generic inhomogeneity parameters, while the parameter $\omega = \exp(\mathrm{i}\phi)$ incorporates the twist angle ϕ which for the moment is allowed to be a generic complex number, but can be specialized later on to real values in order to ensure hermiticity. In the homogeneous limit $\lambda_1 = \cdots = \lambda_M = 0$ its meaning becomes apparent when writing down the associated spin-chain Hamiltonian

$$H_\omega = \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln \frac{t_\omega(\lambda)}{(\lambda+1)^M}\bigg|_{\lambda=0} = \frac{1}{2}\sum_{m=1}^{M}(\vec{\sigma}_m \cdot \vec{\sigma}_{m+1} - 1) \tag{2.4}$$

with the boundary conditions

$$\sigma_{M+1}^x \pm \mathrm{i}\sigma_{M+1}^y = \omega^{\pm 2}\left(\sigma_1^x \pm \mathrm{i}\sigma_1^y\right) \qquad \text{and} \qquad \sigma_{M+1}^z = \sigma_1^z. \tag{2.5}$$

These boundary conditions break for $\omega \neq 1$, the spherical symmetry of the Hamiltonian which unlike in the case of periodic boundary conditions is not sl_2 invariant. However, there is an axial symmetry, i.e. the total spin operator

$$S^z = \frac{1}{2}\sum_{m=1}^{M}\sigma_m^z \tag{2.6}$$

is preserved. This breaking of the spherical symmetry is significant for the Bethe ansatz analysis of the spectrum as for quasi-periodic boundary conditions all eigenvectors become regular Bethe states. In the case of periodic boundary conditions this is only true for the highest weight state in each sl_2-module spanning one of the degenerate subspaces of the transfer matrix respectively the Hamiltonian. This fact also plays an important role in the construction of the Q-operator.

Besides the transfer matrix and the Hamiltonian it will be convenient to discuss the entire fusion hierarchy of the XXX model. To this end consider the Chevalley–Serre generators of sl_2,

$$[h, e] = 2e, \qquad [h, f] = -2f \qquad \text{and} \qquad [e, f] = h; \tag{2.7}$$

then the following defines a well-known Verma module π_x depending on a complex parameter $x \in \mathbb{C}$:

$$\begin{aligned} &\pi_x(e)|k\rangle = (x-k)k|k-1\rangle, \qquad \pi_x(e)|0\rangle = 0 \\ &\pi_x(f)|k\rangle = |k+1\rangle, \\ &\pi_x(h)|k\rangle = (x-2k-1)|k\rangle, \qquad k = 0, 1, \ldots, \infty. \end{aligned} \tag{2.8}$$

It is this Verma module which will form the auxiliary space for the Q-operator. Note that if $x = n \in \mathbb{N}_{>0}$ and one invokes the truncation condition $\pi_x(f)|n\rangle = 0$, the n-dimensional subspace spanned by the vectors $\{|k\rangle\}_{k=0}^{n-1}$ gives rise to the finite-dimensional modules $\pi^{(n-1)}$ known as spin $s = (n-1)/2$ representations in the physics literature. Set

$$L(\lambda) = \begin{pmatrix} \lambda + \frac{h+1}{2} & f \\ \mathrm{e} & \lambda - \frac{h-1}{2} \end{pmatrix} \in U(sl_2) \otimes \mathrm{End}\,\mathbb{C}^2; \tag{2.9}$$

then

$$L_{12}(\lambda)L_{13}(\lambda+\lambda')r_{23}(\lambda') = r_{23}(\lambda')L_{13}(\lambda+\lambda')L_{12}(\lambda) \tag{2.10}$$

and the higher spin transfer matrix $t_\omega^{(n)}$ is defined through

$$t_\omega^{(n)}(\lambda) = \mathrm{Tr}_{\pi^{(n)}}\omega^{h\otimes 1}L_M(\lambda-\lambda_M)\cdots L_1(\lambda-\lambda_1). \tag{2.11}$$

The two distinguished elements in this hierarchy are the previously introduced transfer matrix $t_\omega = t_\omega^{(1)}$ of spin 1/2 and the quantum determinant χ corresponding to the trivial representation of spin 0,

$$\chi(\lambda) = t^{(0)}(\lambda) = \prod_{m=1}^{M} \left(\lambda - \lambda_m + \frac{1}{2}\right). \tag{2.12}$$

From these two elements all the other members of the fusion hierarchy can be generated via the functional equation

$$t_\omega^{(n)}\left(\lambda + \frac{n+1}{2}\right) t_\omega^{(1)}(\lambda) = t^{(0)}\left(\lambda + \frac{1}{2}\right) t_\omega^{(n+1)}\left(\lambda + \frac{n}{2}\right) + t^{(0)}\left(\lambda - \frac{1}{2}\right) t_\omega^{(n-1)}\left(\lambda + \frac{n+2}{2}\right). \tag{2.13}$$

Instead of solving this functional relation in terms of $t_\omega^{(1)}, t^{(0)}$, which leads to quite involved formulae, it is simpler to consider an auxiliary linear problem, Baxter's TQ equation, which we discuss next.

3. The Q-operator and its spectrum

We extend the definition of the higher spin transfer matrix to the infinite-dimensional Verma module (2.8) introduced above and set

$$Q_\omega(\lambda; x) = \mathrm{Tr}_{\pi_x} \omega^{h\otimes 1} L_M\left(\lambda - \lambda_M + \frac{x}{2}\right) \cdots L_1\left(\lambda - \lambda_1 + \frac{x}{2}\right). \tag{3.1}$$

This definition of the Q-operator coincides with the isotropic limit of the definition for the XXZ model [34]. Note that the trace runs now over a (half) infinite-dimensional space, whence it is crucial to have quasi-periodic boundary conditions which upon the right choice of the twist parameter ω ensure convergence [33].

Since the matrix $Q_\omega(\lambda; x)$ preserves the total spin, $[Q_\omega(\lambda; x), S^z] = 0$, its matrix elements do always contain the same number of the Chevalley–Serre generators e and f. Using the Casimir relation,

$$\pi_x(C) = \frac{x^2 - 1}{2}, \qquad C = h^2/2 + h + 2fe, \tag{3.2}$$

we deduce that it suffices to ensure that the following expressions are finite:

$$\mathrm{Tr}_{\pi_x}\{\omega^h h^m\} = \omega^x \sum_{k=0}^{\infty} \omega^{-2k-1}(x - 2k - 1)^m < \infty, \qquad m = 0, 1, 2, \ldots, M. \tag{3.3}$$

This is obviously guaranteed as long as $|\omega| > 1$. Employing the geometric series to compute the trace, we then analytically continue this operator from the region of convergence to the whole complex ω plane. Note that there remains a pole at $\omega = 1$.

For instance, by construction $Q_\omega(\lambda; x)$ is a polynomial of degree M in λ and we have for the coefficient of the highest power λ^M,

$$Q_\omega(\lambda; x) = \mathrm{Tr}_{\pi_x}\{\omega^h\}\lambda^M + \cdots = \sum_{k=0}^{\infty} \omega^{x-2k-1}\lambda^M + \cdots = \frac{\omega^x}{\omega - \omega^{-1}}\lambda^M + \cdots, \tag{3.4}$$

where the last expression can be continued with respect to ω from the region of convergence into the complex plane. Henceforth, this analytic continuation from the region of convergence shall always be implicitly understood.

The crucial property of the Q-operator is the following functional equation, which strictly speaking is not yet Baxter's TQ equation:

$$t_\omega(\lambda)Q_\omega(\lambda;x) = Q_\omega(\lambda+1;x-1)\prod_{m=1}^{M}(\lambda-\lambda_m) + Q_\omega(\lambda-1;x+1)\prod_{m=1}^{M}(\lambda-\lambda_m+1). \quad (3.5)$$

We omit the proof as it follows from taking the isotropic limit in the analogous XXZ relations; see e.g. [33–35]. The difference with Baxter's TQ equation is the fact that the additional complex parameter x originating from the definition of the Verma module also shifts, instead of only a shift in the spectral variable λ. Thus, the above equation should rather be seen as an extension of the fusion hierarchy to 'infinite' spin. Nevertheless, the solutions to Baxter's TQ equation are obtained from $Q_\omega(\lambda;x)$ through special limits. Namely, as we will discuss below we have the following factorization:

$$Q_\omega(\lambda;x) = \frac{\omega^x}{\omega-\omega^{-1}}Q^+_\omega(\lambda)Q^-_\omega(\lambda+x), \quad (3.6)$$

where $Q^\pm_\omega$ are two linearly independent solutions to Baxter's TQ equation

$$t_\omega(\lambda)Q^\pm_\omega(\lambda) = \omega^{\mp 1}Q^\pm_\omega(\lambda+1)\prod_{m=1}^{M}(\lambda-\lambda_m) + \omega^{\pm 1}Q^\pm_\omega(\lambda-1)\prod_{m=1}^{M}(\lambda-\lambda_m+1). \quad (3.7)$$

We now turn to the discussion of the spectrum of the Q-operator where we will explain in more detail the above factorization into the solutions $Q^\pm_\omega$.

3.1. The algebraic Bethe ansatz analysis of Q

In the context of the XXZ model, the spectrum of the Q-operator has been analysed [33] using the formalism of the algebraic Bethe ansatz [22]. We recall that for twisted boundary conditions there is no problem with the Bethe ansatz as the sl_2 symmetry of the XXX model is broken and all eigenstates of the XXX transfer matrix are regular Bethe states; see for instance the discussion in [23] where the completeness of the Bethe ansatz in a neighbourhood of $\omega = 0$ has been shown. Using the analogous algebraic relations as in the XXZ case [33], one can show that the Bethe states are eigenvectors of the Q-operator[2]. Namely, decomposing the monodromy matrix of the XXX model in the usual manner

$$\boldsymbol{t}(\lambda) = \omega^{\sigma^z\otimes 1}r_M(\lambda-\lambda_M)\cdots r_1(\lambda-\lambda_1) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda)\end{pmatrix}, \quad (3.8)$$

one considers for $n = M/2 - S^z > 0$ an 'admissible' solution [23] to the Bethe ansatz equations above the equator (note that according to the conventions (2.1) and (2.2) the corresponding Bethe roots are related by $\xi^+_j \to -\mathrm{i}v^+_j - 1/2$)

$$\omega^{-1}\prod_{j=1}^{n}\left(\xi^+_i - \xi^+_j + 1\right)\prod_{m=1}^{M}\left(\xi^+_i - \lambda_m\right) + \omega\prod_{j=1}^{n}\left(\xi^+_i - \xi^+_j - 1\right)\prod_{m=1}^{M}\left(\xi^+_i - \lambda_m + 1\right) = 0. \quad (3.9)$$

Then it follows from the Yang–Baxter equation that the matrix elements $\{Q_{kl}\}_{k,l\in\mathbb{N}}$ of the monodromy matrix

$$\boldsymbol{Q}(\lambda) = \omega^{h\otimes 1}L_M\left(\lambda-\lambda_M+\frac{x}{2}\right)\cdots L_1\left(\lambda-\lambda_1+\frac{x}{2}\right)$$

[2] At the moment this has only been carried out for Bethe states with $n < 4$ due to the complicated and numerous unwanted terms, see the appendix in [33]. However, in the case of the XXZ model alternative proofs (based on functional relations) exist [36, 37] which match the algebraic Bethe ansatz result for arbitrary n. The spectrum for the XXX model presented here is the isotropic limit of the XXZ result [33, 34].

with respect to the infinite-dimensional auxiliary space corresponding to π_x satisfy certain commutation relations with the Yang–Baxter algebra $\{A, B, C, D\}$, for example [33]:

$$Q_{k,l}(\lambda)B(\xi) = \frac{\alpha_{l+1}\delta_l - \beta_{l+1}\gamma_l}{\alpha_k\alpha_{l+1}} B(\xi)Q_{k,l}(\lambda) + \frac{\beta_{l+1}}{\alpha_{l+1}} Q_{k,l+1}(\lambda)A(\xi) - \frac{\beta_k}{\alpha_k} Q_{k+1,l}(\lambda)D(\xi) + \frac{\beta_k\beta_{l+1}}{\alpha_k\alpha_{l+1}} Q_{k+1,l+1}(\lambda)C(\xi),$$

where the coefficients are determined through the matrix elements of the L-operator (2.9),

$$\alpha_k = \lambda - \xi + x - k, \qquad \beta_k = 1, \qquad \gamma_{k-1} = (x - k)k, \qquad \delta_k = \lambda - \xi + k + 1. \tag{3.10}$$

For a complete list of the algebraic identities we refer the reader to [33]. Employing these commutation relations one can identify the eigenvalue of the Q-operator on a Bethe state. Denoting by $|0\rangle$ the pseudo-vacuum, i.e. the state with all spins up, the Bethe vector associated with an admissible solution to (3.9) is an eigenstate of the Q-operator with eigenvalue

$$Q_\omega(\lambda; x)B\left(\xi_1^+\right)\cdots B\left(\xi_n^+\right)|0\rangle = \frac{\omega^x}{\omega - \omega^{-1}} Q_\omega^+(\lambda)Q_\omega^-(\lambda + x)B\left(\xi_1^+\right)\cdots B\left(\xi_n^+\right)|0\rangle, \tag{3.11}$$

where

$$Q_\omega^+(\lambda) = \prod_{j=1}^{n}\left(\lambda - \xi_j^+\right) \tag{3.12}$$

and

$$Q_\omega^-(\lambda) = (\omega - \omega^{-1})Q_\omega^+(\lambda)\sum_{k=0}^{\infty} \frac{\omega^{-2k-1}\prod_m(\lambda - \lambda_m - k)}{Q_\omega^+(\lambda - k)Q_\omega^+(\lambda - k - 1)}. \tag{3.13}$$

Note that Q_ω^- is polynomial in λ due to the Bethe ansatz equations. In fact, by the very construction of the Q-operator it must be a polynomial of degree $M - n$,

$$Q_\omega^-(\lambda) = \prod_{j=1}^{M-n}(\lambda - \xi_j^-). \tag{3.14}$$

Exploiting the completeness of the Bethe ansatz for generic quasi-periodic boundary conditions and inhomogeneity parameters [23], we obtain the factorization of the Q-operator into the previously introduced, linearly independent solutions $Q_\omega^\pm$ of Baxter's TQ equation (3.7). We might define them implicitly as operators through the following limits:

$$\lim_{x\to-\lambda} Q_\omega(\lambda; x) = \frac{\omega^{-\lambda}}{\omega - \omega^{-1}} Q_\omega^+(\lambda)Q_\omega^-(0) \tag{3.15}$$

and

$$\lim_{\lambda\to 0} Q_\omega(\lambda; x) = \frac{\omega^x}{\omega - \omega^{-1}} Q_\omega^+(0)Q_\omega^-(x). \tag{3.16}$$

We shall denote the operators and eigenvalues by the same symbol. In contrast to the XXZ case [34], the operators $Q_\omega^\pm(0)$ are not easily determined and we are missing at the moment concrete operator expressions for them. However, explicit computation of the Q-operators in the various spin sectors for small lattice sizes ($M \leqslant 6$) shows that the following expressions drastically simplify:

$$\omega^\lambda Q_\omega(\lambda; -\lambda)Q_\omega(0; 0)^{-1} = Q_\omega^+(\lambda)Q_\omega^+(0)^{-1} \tag{3.17}$$

and

$$\omega^{-\lambda} Q_\omega(0; 0)^{-1}Q_\omega(0; \lambda) = Q_\omega^-(0)^{-1}Q_\omega^-(\lambda). \tag{3.18}$$

Both (3.12) and (3.14) are obviously solutions to Baxter's TQ equation (3.7) and are normalized to the identity matrix at the origin $\lambda = 0$. The inverse matrices exist as long as none of the Bethe roots $\xi_j^{\pm}$ vanishes, which is the case as long as $\omega \neq 1$. Despite this lack of information on the normalization constants, our Q-operator analysis yields computational advantages. Before we address the latter, let us first discuss the relationship between $Q_\omega^{\pm}(\lambda)$ under spin reversal.

3.2. Spin reversal

Define the spin-reversal operator by setting $\mathfrak{R} = \prod_{m=1}^{M} \sigma_m^x$. Due to the twisted boundary conditions spin-reversal symmetry is broken and we have for the transfer matrix the identity

$$\mathfrak{R} t_\omega(\lambda) \mathfrak{R} = t_{\omega^{-1}}(\lambda). \tag{3.19}$$

Let us now investigate the transformation of the Q-operator under spin reversal. From the equality

$$(1 \otimes \sigma^x) L(\lambda)(1 \otimes \sigma^x) = -\begin{pmatrix} -\lambda - 1 + \frac{h+1}{2} & -e \\ -f & -\lambda - 1 - \frac{h-1}{2} \end{pmatrix} \tag{3.20}$$

it follows for the homogeneous model $\lambda_1 = \cdots = \lambda_M = 0$ that

$$\mathfrak{R} Q_\omega(\lambda; x) \mathfrak{R} = (-)^M Q_\omega(-\lambda - 1 - x; x)^t. \tag{3.21}$$

Alternatively, we can compute the spectrum of $\check{Q}_\omega := \mathfrak{R} Q_\omega \mathfrak{R}$ from the algebraic Bethe ansatz similar as before. In terms of the matrix elements of the associated monodromy matrices the basic relation we need is

$$\check{Q}_{k,l} B = \left(\frac{\alpha_l}{\delta_k} - \frac{\gamma_{l-1}\beta_l}{\delta_k \delta_{l-1}} \right) B \check{Q}_{k,l} + \frac{\gamma_{l-1}}{\delta_{l-1}} \check{Q}_{k,l-1} A - \frac{\gamma_k}{\delta_k} \check{Q}_{k+1,l} D + \frac{\gamma_k \gamma_{l-1}}{\delta_k \delta_{l-1}} \check{Q}_{k+1,l-1} C. \tag{3.22}$$

Here, the coefficients are the same as in (3.10). This then leads to the following eigenvalues corresponding to Bethe states:

$$\begin{aligned} &\mathfrak{R} Q_\omega(\lambda; x) \mathfrak{R} B\left(\xi_1^+\right) \cdots B\left(\xi_n^+\right)|0\rangle \\ &\quad = Q_{\omega^{-1}}^+(\lambda + x) Q_{\omega^{-1}}^+(\lambda) \sum_{k=0}^{\infty} \frac{\omega^{x-2k-1} \prod_m (\lambda - \lambda_m + k + 1)}{Q_{\omega^{-1}}^+(\lambda + k) Q_{\omega^{-1}}^+(\lambda + k + 1)} B\left(\xi_1^+\right) \cdots B\left(\xi_n^+\right)|0\rangle. \end{aligned}$$

As already previously mentioned, for generic inhomogeneity parameters λ_m and a suitable neighbourhood of $\omega = 0$ (or $\omega = \infty$), the Bethe ansatz yields a complete set of eigenstates [23]. This fact now implies the operator equation

$$\mathfrak{R} Q_\omega(\lambda; x) \mathfrak{R} = Q_{\omega^{-1}}(\lambda + x; -x) = -\frac{\omega^x}{\omega - \omega^{-1}} Q_{\omega^{-1}}^+(\lambda + x) Q_{\omega^{-1}}^-(\lambda). \tag{3.23}$$

Therefore, under spin reversal the roles of Q_ω^+, Q_ω^- are interchanged. These relations match the analogous ones derived for the six-vertex model [33, 34, 37].

4. Fusion hierarchy and complex dimension

One of the aforementioned advantages of our Q-operator analysis is that the relation between $Q_\omega(\lambda; x)$ and the higher spin transfer matrices $t_\omega^{(n-1)}$ is particularly simple allowing one through analytic continuation to compactly present the information on the entire fusion hierarchy. Specializing $x \to n \in \mathbb{N}$, it was already pointed out earlier that the infinite-dimensional Verma module (2.8) contains a finite-dimensional subrepresentation spanned by the vectors $\{|k\rangle\}_{k=0}^{n-1}$ and which is isomorphic to the sl_2 representation $\pi^{(n-1)}$ of spin $s = (n-1)/2$. The remaining space spanned by $\{|k\rangle\}_{k=n}^{\infty}$ can be identified again as the Verma module π_x with $x = -n$. This simple representation theoretic fact translates into the following functional relation when splitting the trace over the aforementioned subspaces:

$$t_\omega^{(n-1)}(\lambda) = Q_\omega\left(\lambda - \frac{n}{2}; n\right) - Q_\omega\left(\lambda + \frac{n}{2}; -n\right). \qquad (4.1)$$

Thus the spectrum of the higher spin transfer matrices takes a particularly simple form in terms of the spectrum of $Q_\omega(\lambda; x)$. In contrast, the expression from the algebraic Bethe ansatz and the fusion relation (2.13) is more involved. Furthermore, we might analytically continue expression (4.1) in the spin variable n setting

$$t_\omega(\lambda; x) = Q_\omega\left(\lambda - \frac{x}{2}; x\right) - Q_\omega\left(\lambda + \frac{x}{2}; -x\right). \qquad (4.2)$$

The last object combines the information of the entire fusion hierarchy. Note that in (4.1) respectively (4.2) one can safely take the limit to periodic boundary conditions, i.e. the following object is well defined:

$$t(\lambda; x) = \lim_{\omega\to 1} t_\omega(\lambda; x) = \lim_{\omega\to 1}\left[Q_\omega\left(\lambda - \frac{x}{2}; x\right) - Q_\omega\left(\lambda + \frac{x}{2}; -x\right)\right]. \qquad (4.3)$$

In this manner one recovers the XXX model with periodic boundary conditions. The transfer matrix $t(\lambda; x)$ with 'complex dimension' x coincides with the generalized trace construction [29] in the context of correlation functions on the infinite lattice. This complex dimension occurs as the coefficient of the highest power in the polynomial $t(\lambda; x)$,

$$t(\lambda; x) = x\lambda^M + \sum_{m=0}^{M-1} t_m(x)\lambda^m. \qquad (4.4)$$

In comparison, the analogous result in the context of the six-vertex or XXZ model showed the appearance of logarithmic terms; see [34].

4.1. The trace functional: a simple example $M = 4$, $S^z = 0$

It is instructive to verify for a simple example whether the construction (4.3) coincides with the definition through the trace functional given in [29]. Setting $M = 4$ and $S^z = 0$, we consider a diagonal matrix element of the Q-operator,

$$Q_\omega(\lambda; x)^{\alpha_1,\ldots,\alpha_4}_{\alpha_1,\ldots,\alpha_4} = \sum_{k=0}^{\infty} \omega^{x-2k-1}(\lambda + x - k)^2(\lambda + k + 1)^2. \qquad (4.5)$$

Here, $\alpha_i = \pm 1$ are the eigenvalues of σ_i^z acting on the ith lattice site with $i = 1, 2, 3, 4$ and $\sum_i \alpha_i = 0$. Using the formula for the geometric series and analytically continuing the result in ω afterwards to take the limit $\omega \to 1$ in (4.3) we arrive at

$$t(\lambda; x)^{\alpha_1\ldots\alpha_4}_{\alpha_1\ldots\alpha_4} = \frac{32x - 20x^3 + 3x^5}{240} + \frac{4x - x^3}{6}\lambda + \frac{10x - x^3}{6}\lambda^2 + 2x\lambda^3 + x\lambda^4. \qquad (4.6)$$

The action of the trace functional $\mathrm{Tr}_x : U(sl_2) \otimes \mathbb{C}[x] \to \mathbb{C}[x]$ introduced in [29] (not to be mistaken for $\mathrm{Tr}_{\pi_x} \neq \mathrm{Tr}_x$) on the powers of the Cartan generators is defined through

$$\mathrm{Tr}_x\{\mathrm{e}^{zh}\} = \frac{\sinh(zx)}{\sinh z} = x + \frac{x^3 - x}{6}z^2 + \frac{7x - 10x^3 + 3x^5}{360}z^4 + \cdots. \qquad (4.7)$$

By the action of the trace functional on the monodromy matrix of L-operators we compute

$$\begin{aligned}\mathrm{Tr}_x L(\lambda)^{\alpha_4}_{\alpha_4} L(\lambda)^{\alpha_3}_{\alpha_3} L(\lambda)^{\alpha_2}_{\alpha_2} L(\lambda)^{\alpha_1}_{\alpha_1} &= \mathrm{Tr}_x\left\{\left(\lambda + \frac{h+1}{2}\right)^2\left(\lambda - \frac{h-1}{2}\right)^2\right\}\\ &= \frac{\mathrm{Tr}_x\{1 - 2h^2 + h^4\}}{16} + \frac{\mathrm{Tr}_x\{1 - h^2\}}{2}\lambda + \frac{\mathrm{Tr}_x\{3 - h^2\}}{2}\lambda^2 + 2\,\mathrm{Tr}_x\{1\}\lambda^3 + \mathrm{Tr}_x\{1\}\lambda^4\\ &= t(\lambda; x)^{\alpha_1,\ldots,\alpha_4}_{\alpha_1,\ldots,\alpha_4},\end{aligned}$$

Table 1. Spectrum of the transfer matrix with complex dimension x.

P	$t(\lambda; x)$
π	$\frac{x}{2} - \frac{x^3}{2} + \frac{x^5}{16} + \frac{2x-x^3}{2}\lambda + \frac{4x-x^3}{2}\lambda^2 + 2x\lambda^3 + x\lambda^4$
π	$\frac{x}{6} - \frac{x^3}{12} - \frac{x^5}{48} + \frac{4x-x^3}{6}\lambda + \frac{10x-x^3}{6}\lambda^2 + 2x\lambda^3 + x\lambda^4$
0	$\frac{x}{6} - \frac{x^3}{6} + \frac{x^5}{16} + \frac{2x-x^3}{2}\lambda + \frac{4x-x^3}{2}\lambda^2 + 2x\lambda^3 + x\lambda^4$
0	$-\frac{x}{30} + \frac{x^3}{12} + \frac{x^5}{80} + \frac{x^3\lambda}{2} + \frac{2x+x^3}{2}\lambda^2 + 2x\lambda^3 + x\lambda^4$
$\pi/2$	$\frac{8\mathrm{i}x+(4-8\mathrm{i})x^3-x^5}{48} + \frac{(4+2\mathrm{i})x-(1+2\mathrm{i})x^3}{6}\lambda + \frac{10x-x^3}{6}\lambda^2 + 2x\lambda^3 + x\lambda^4$
$\pi/2$	$-\frac{8\mathrm{i}x-(4+8\mathrm{i})x^3+x^5}{48} + \frac{(4-2\mathrm{i})x-(1-2\mathrm{i})x^3}{6}\lambda + \frac{10x-x^3}{6}\lambda^2 + 2x\lambda^3 + x\lambda^4$

where the last line is obtained after inserting the values from expansion (4.7). Thus, we find agreement with (4.3). To illustrate the generalized transfer matrix of complex dimension further we present its eigenvalues for each total momentum $P = -\mathrm{i}\ln t(0)$ sector in table 1. Specializing x to be an integer >0 one obtains the eigenvalues of each element in the fusion hierarchy.

5. The quantum Wronskian

The second computational advantage from the Q-operator analysis is of great practical importance in the actual computation of the spectra of the Hamiltonian and the transfer matrices. Instead of solving the quite intricate Bethe ansatz equations, one can now turn the ideology around and rather interpret relation (4.2) for $x = 1$, named the quantum Wronskian, as the fundamental identity,

$$\prod_{m=1}^{M}(\lambda - \lambda_m) = \frac{\omega Q_\omega^+(\lambda - 1)Q_\omega^-(\lambda) - \omega^{-1}Q_\omega^+(\lambda)Q_\omega^-(\lambda - 1)}{\omega - \omega^{-1}}. \tag{5.1}$$

Here we have exploited the factorization (3.6). In terms of eigenvalues (3.12), (3.14), the above relation incorporates the Bethe ansatz equations above and below the equator with respect to the parametrization (2.1),

$$\prod_{m=1}^{M}\frac{\xi_i^\pm - \lambda_m}{\xi_i^\pm - \lambda_m + 1} = \omega^{\pm 2}\prod_{j=1}^{n_\pm}\frac{\xi_i^\pm - \xi_j^\pm - 1}{\xi_i^\pm - \xi_j^\pm + 1}, \qquad n_\pm = M/2 \mp S^z, \tag{5.2}$$

and is therefore sufficient to analyse the spectrum. Introducing the elementary symmetric polynomials $e_k^\pm = e_k\left(\xi_1^\pm, \ldots, \xi_{n_\pm}^\pm\right)$ in the Bethe roots

$$Q_\omega^\pm(\lambda) = \sum_{k=0}^{n_\pm}(-)^k e_k^\pm \lambda^{n_\pm - k}, \tag{5.3}$$

the quantum Wronskian (5.1) becomes the following identity:

$$e_{M-m}(\lambda_1, \ldots, \lambda_M) = \sum_{k=0}^{m}\sum_{\ell \geqslant m-k}\binom{\ell}{m-k}\frac{\omega e_{n-\ell}^+ e_{M-n-k}^- - \omega^{-1}e_{n-k}^+ e_{M-n-\ell}^-}{\omega - \omega^{-1}}, \tag{5.4}$$

which is quadratic in the M unknowns $e_k^\pm$. Here, $e_m(\lambda_1, \ldots, \lambda_M)$ is the mth elementary symmetric polynomial in the inhomogeneity parameters. Furthermore, we use the convention $e_k^\pm \equiv 0$ for $k < 0$ and $k > n_\pm = M/2 \mp S^z$. In contrast, the Bethe ansatz equations (5.2) are of order M. The approach based on the quantum Wronskian (5.1), therefore, leads to a significant advantage in numerical computations for long spin chains.

Note that in the limits $\omega \to 0, \infty$ we can easily establish the completeness of the Bethe ansatz for generic inhomogeneity parameters by a similar line of argument as it has been used in [23]. Namely, assuming all inhomogeneity parameters $\{\lambda_j\}$ to be mutually distinct we infer from the quantum Wronskian (5.1) the solutions

$$\omega = \infty: \quad Q^+_\infty(\lambda) = \prod_{j=1}^{n} (\lambda - \lambda_{m_j} + 1) \qquad \text{and} \qquad Q^-_\infty(\lambda) = \prod_{j=1}^{M-n} (\lambda - \lambda_{m_{j+n}})$$

for any permutation $(m_1, \dots, m_M)$ of the index set $\{1, 2, \dots, M\}$. Obviously, the number of distinct solutions is then $\binom{M}{n}$ which coincides with the dimension of the associated spin sector. For $\omega = 0$ the roles of $Q^\pm$ are interchanged. Using the implicit function theorem one can then argue that the number of solutions stays the same in the vicinity of the point $\omega = \infty$ respectively $\omega = 0$.

5.1. Special solutions for homogeneous chains of even length and $S^z = 0$

Let $M \in 2\mathbb{N}$ and consider the spin sector $S^z = 0$. Then, according to our previous discussion Q^+_ω and Q^-_ω have the same polynomial degree $n = M/2$ and in light of (3.21), (3.23) one might expect a simple relationship between them. In fact, based on numerical studies of homogeneous spin chains up to length $M = 10$ and $\omega = e^{i\phi}$, $\phi \in \mathbb{R}$, one confirms that there exist $2^{M/2}$ solutions to the quantum Wronskian which satisfy

$$M \in 2\mathbb{N}, \qquad S^z = 0: \qquad Q^-_\omega(\lambda) = (-1)^{\frac{M}{2}} Q^+_\omega(-\lambda - 1). \tag{5.5}$$

Notably, for the mentioned examples $M = 2, 4, 6, 8, 10$ the eigenvalue of the transfer matrix which belongs to the ground state in the limit $\omega \to 1$ always appears to be among this set of special solutions.

For the numerical investigation, it is more convenient to use the second parametrization (2.2) of the XXX model, since then the coefficients (not the roots) of the polynomials

$$\tilde{Q}^\pm_\omega(u) = i^{n_\pm} Q^\pm_\omega(-iu - 1/2) = \prod_{j=1}^{n_\pm} (u - v^\pm_j)$$

are always real numbers. In this parametrization the special relationship (5.5) simply becomes

$$M \in 2\mathbb{N}, \qquad S^z = 0: \qquad \tilde{Q}^-_\omega(u) = (-1)^{\frac{M}{2}} \tilde{Q}^+_\omega(-u). \tag{5.6}$$

At the moment there is no derivation from first principles for this simplification; however, it can be motivated by (3.21) which states that left and right eigenvectors of the Q-operator are related by spin reversal. As the spin zero sector is invariant under the action of the spin-reversal operator it can happen that some left and right eigenvectors of Q coincide leading via (3.21) to the simplification (5.5) respectively (5.6). Assuming the latter to hold true, one can verify it for chains of length $M > 10$ by inserting this special subset of solutions into the Wronskian relation which then simplifies to

$$u^M = (-1)^{\frac{M}{2}} \frac{\omega \tilde{Q}^+_\omega\left(u - \frac{i}{2}\right) \tilde{Q}^+_\omega\left(-u - \frac{i}{2}\right) - \omega^{-1} \tilde{Q}^+_\omega\left(u + \frac{i}{2}\right) \tilde{Q}^+_\omega\left(-u + \frac{i}{2}\right)}{\omega - \omega^{-1}}. \tag{5.7}$$

Specializing the spectral parameter to $u = v^+_j + \frac{i}{2}$ and $u = v^+_j - \frac{i}{2}$ we now obtain the following sets of equations for the Bethe roots v^+_j of this subclass of solutions:

$$\left(v^+_j + i/2\right)^M = \frac{\omega^{-1}}{\omega^{-1} - \omega} \prod_{k=1}^{M/2} \left(v^+_j - v^+_k + i\right)\left(v^+_j + v^+_k\right) \tag{5.8}$$

Table 2. Ground-state eigenvalues of the transfer matrix and Q-operator in the spin zero sector for various twist parameters. For $\phi = \pi/2$ the ground state is two-fold degenerate.

ϕ	$M = 10$
$\frac{\pi}{2}$	$Q^+ = u^5 \mp 0.776\,9661\, u^4 - 0.323\,1618\, u^3 \pm 0.111\,7312\, u^2 + 0.011\,891\, u \mp 0.011\,8901$ $t = \pm 1.553\,932\, u^8 \pm 6.047\,51\, u^6 \pm 9.740\,55\, u^4 \pm 7.584\,83\, u^2 \pm 2.375\,84$
$\frac{\pi}{20}$	$Q^+ = u^5 - 0.069\,3516\, u^4 - 0.403\,661\, u^3 + 0.010\,5767\, u^2 - 0.016\,6721\, u - 0.000\,1079$ $t = 1.975\,38\, u^{10} + 7.429\,36\, u^8 + 13.5893\, u^6 + 14.8551\, u^4 + 9.333\,35\, u^2 + 2.590\,13$
$\frac{\pi}{200}$	$Q^+ = u^5 - 0.006\,9288\, u^4 - 0.404\,443\, u^3 + 0.001\,0573\, u^2 - 0.016\,7203\, u - 0.000\,1079$ $t = 1.999\,75\, u^{10} + 7.499\,29\, u^8 + 13.6758\, u^6 + 14.9119\, u^4 + 9.352\,24\, u^2 + 2.592\,41$
0	$Q^+ = u^5 - 0.404\,451\, u^3 - 0.016\,7203\, u$ $t = 2u^{10} + \frac{15}{2}\, u^8 + 13.6767\, u^6 + 14.9125\, u^4 + 9.352\,43\, u^2 + 2.592\,43$

and

$$\left(v_j^+ - \mathrm{i}/2\right)^M = \frac{\omega}{\omega - \omega^{-1}} \prod_{k=1}^{M/2} \left(v_j^+ - v_k^+ - \mathrm{i}\right)\left(v_j^+ + v_k^+\right), \tag{5.9}$$

respectively. Since ω lies on the unit circle, both equations are equivalent under complex conjugation as the Bethe roots v_j^+ are either real or occur in complex conjugate pairs. Dividing these two equations yields the familiar Bethe ansatz equations for twisted boundary conditions,

$$\left(\frac{v_j^+ + \mathrm{i}/2}{v_j^+ - \mathrm{i}/2}\right)^M = \omega^{-2} \prod_{k \neq j}^{M/2} \frac{v_j^+ - v_k^+ + \mathrm{i}}{v_j^+ - v_k^+ - \mathrm{i}}. \tag{5.10}$$

Thus, we infer that extending the assumption (5.6) beyond the numerically checked examples of spin chains of length $M \leqslant 10$ (compare with table 2) is compatible with the Bethe ansatz. The corresponding eigenvalues of the transfer matrix are of the form

$$\tilde{t}(u) = \mathrm{i}^M t(-\mathrm{i}u - 1/2) = (\omega + \omega^{-1})u^M + \sum_{m=1}^{M/2} \tilde{t}_m u^{M-2m}, \tag{5.11}$$

i.e. only even powers of the spectral parameter u occur. In addition, the parameters $\tilde{t}_m$ are real and the eigenvalue corresponding to the ground state in the limit of periodic boundary conditions $\omega \to 1$ is distinguished by the fact that all coefficients have the same sign, $\operatorname{sgn} \tilde{t}_m = \operatorname{sgn}(\omega + \omega^{-1})$. We leave a more detailed study of these solutions to future work as it involves more extensive numerical calculations.

5.2. Eigenvalues in the limit of periodic boundary conditions

Let us make contact with the discussion of Pronko and Stroganov for the XXX model with periodic boundary conditions $\phi = 0$ respectively $\omega = 1$ [24]. Starting from the TQ equation on the level of eigenvalues they reported the following quantum Wronskian relation with respect to the parametrization (2.2):

$$\mathcal{Q}^-\left(u + \frac{\mathrm{i}}{2}\right) \mathcal{Q}^+\left(u - \frac{\mathrm{i}}{2}\right) - \mathcal{Q}^-\left(u - \frac{\mathrm{i}}{2}\right) \mathcal{Q}^+\left(u + \frac{\mathrm{i}}{2}\right) = u^M, \tag{5.12}$$

with the crucial difference that the degree of the second linearly independent solution $\mathcal{Q}^-$ is now increased by 1,

$$\mathcal{Q}^-(u) = \frac{-\mathrm{i}}{2S^z + 1} \prod_{k=1}^{M-n+1} (u - v_k^-). \tag{5.13}$$

Table 3. Number of solutions to (5.12) in comparison with the dimension of the spin sector.

M	3	4	5	6	7	8	9	10
S^z	1/2	0	1/2	0	1/2	0	1/2	0
dim	3	6	10	20	35	70	126	252
No	2	2	5	5	14	14	42	42

Table 4. Solutions to the quantum Wronskian (5.12) for $M = 6$, $S^z = 0$ and the corresponding eigenvalues of the transfer matrix.

$\mathrm{i}\mathcal{Q}^-(u)$	$\mathcal{Q}^+(u)$	$\tilde{t}(u)$
$u^4 - \frac{3}{2}u^2 - \frac{1}{48}$	$u\left(u + \frac{1}{4}\right)$	$-\frac{25}{32} + \frac{15}{8}u^2 + \frac{9}{2}u^4 + 2u^6$
$u^4 + \frac{4\mp\sqrt{13}}{2}u^2 - \frac{7\mp 2\sqrt{13}}{16}$	$u^3 + \frac{5\mp 2\sqrt{13}}{12}u$	$\frac{31\pm 8\sqrt{13}}{32} + \frac{7\pm 8\sqrt{13}}{8}u^2 + \frac{9}{2}u^4 + 2u^6$
$u^4 + u^2 \pm \frac{u}{2\sqrt{3}} - \frac{1}{16}$	$u^3 + \frac{u}{12} \pm \frac{1}{4\sqrt{3}}$	$-\frac{1}{32} \mp \sqrt{3}u + \frac{23}{8}u^2 + \frac{9}{2}u^4 + 2u^6$

The degree of the other solution, $\mathcal{Q}^+$, describing the well-known Bethe roots above the equator remains unchanged,

$$\mathcal{Q}^+(u) = \prod_{k=1}^{n}\left(u - v_k^+\right). \tag{5.14}$$

We have deliberately denoted their solutions $\mathcal{Q}^\pm$ by a different symbol to distinguish them from the solutions $Q_\omega^\pm$ obtained from our operator construction at quasi-periodic boundary conditions. As already pointed out in the introduction, the quantum Wronskian (5.12) has a restricted number of solutions which is much smaller than the dimension of the respective spin sector fixed by the degree $n = M/2 - S^z$. These solutions must correspond to regular Bethe states which yield the highest weight vectors of the various sl_2 modules, while the 'missing' states are simply descendant states from highest weight vectors which lie in a different (higher) spin sector. For instance, in the case of even M the possible number of highest weight states in the sector $S^z = 0$ is given by $\binom{M}{M/2} - \binom{M}{M/2-1}$ and we find that this number is matched by the solutions to (5.12); see table 3.

The simplified expression for the transfer matrix in terms of the two linearly independent solutions $\mathcal{Q}^\pm$ remains formally the same [24]; however, we remind the reader that the degree of $\mathcal{Q}^-$ has changed in comparison with (4.1),

$$\tilde{t}(u) = \mathcal{Q}^-(u+\mathrm{i})\mathcal{Q}^+(u-\mathrm{i}) - \mathcal{Q}^-(u-\mathrm{i})\mathcal{Q}^+(u+\mathrm{i}). \tag{5.15}$$

See table 4 for a concrete example. Naturally, one wonders how the solutions $\mathcal{Q}^\pm$ are related to those at quasi-periodic boundary conditions, $\tilde{Q}_\omega^\pm(u)$, when the limit $\omega \to 1$ is taken. One finds that only a subset of the solutions $Q_\omega^\pm$ stays finite; the other solutions diverge. In the explicit construction of the Q-operator this is due to the fact that the trace over the infinite-dimensional auxiliary space does not converge any longer. The number of finite solutions, i.e. those for which the limit $\omega \to 1$ is well defined, approach the solution $\mathcal{Q}^+$ of Pronko and Stroganov:

$$\text{if} \quad \lim_{\omega\to 1}\left|\tilde{Q}_\omega^\pm(u)\right| < \infty, \qquad \text{then} \quad \lim_{\omega\to 1}\tilde{Q}_\omega^\pm(u) = \mathcal{Q}^+(u). \tag{5.16}$$

The above relation has been numerically verified for spin chains up to length $M = 10$. Note that both solutions Q_ω^+ and Q_ω^- approach in the limit $\omega \to 1$ the same solution $\mathcal{Q}^+$ above the equator. This is to be expected as the degree $M - n$ of Q_ω^- can become smaller in the limit of periodic boundary conditions but not greater. At the moment there appears to be no Q-operator construction which would yield the other solution $\mathcal{Q}^-$ and at the same time have the analogous factorization property (3.6). The constructions suggested in the literature for periodic boundary conditions [25–27] all have degree $\leqslant M$ for the spin 1/2 chain of M sites, while the maximal degree of Q^- is $M+1$.

6. Conclusions

In this work, we have presented the isotropic limit of a previous Q-operator construction for the XXZ model [33, 34, 36, 37] in order to discuss the XXX model with quasi-periodic boundary conditions. The motivation for this discussion has been twofold. On the one hand, this construction enables one to formulate an analytic continuation of the fusion hierarchy to complex dimension as it has been recently used in the description of correlation functions in the form of a trace functional [29]. In this context, it should be noted that previous constructions of Q-operators for the XXX model [25–27] have always been for periodic boundary conditions where an analogous formulation does not exist. This is due to the fact that the trace over an infinite-dimensional auxiliary space has to be taken whose convergence is not necessarily guaranteed. Moreover, due to the sl_2 symmetry the set of solutions to the Bethe ansatz equations is reduced (i.e. only the highest weight states in each sl_2 module are proper Bethe states), whence certain functional relations such as the quantum Wronskian for periodic boundary conditions [24] do not yield the complete set of eigenvalues; compare with table 3.

This provided additional motivation for investigating a Q-operator for the twisted XXX model. Via this construction one is lead to a quantum Wronskian for quasi-periodic boundary conditions (see (5.1)), which now yields the complete set of eigenstates, all of them being Bethe states, and eigenvalues of the transfer matrix. Our derivation relied on previous algebraic Bethe ansatz results for the Q-operator of the XXZ model [33]. As emphasized in the text, the quantum Wronskian has a simpler structure than the Bethe ansatz equations and based on numerical computations we found special solutions for spin chains of even length and vanishing total spin satisfying more fundamental identities. For instance, the Bethe roots of the aforementioned subset of solutions obey the set of equations,

$$\left(v_j^+ + \mathrm{i}/2\right)^M = \frac{\omega^{-1}}{\omega^{-1}-\omega}\prod_{k=1}^{M/2}\left(v_j^+ - v_k^+ + \mathrm{i}\right)\left(v_j^+ + v_k^+\right)$$

and are either real or occur in complex conjugate pairs; see the discussion in section 5.2. Among these special solutions is the eigenvalue which corresponds to the ground state in the limit of periodic boundary conditions and has real Bethe roots. The present numerical data only include chains up to length $M = 10$ and further investigation is needed to see whether they persist for longer chains. This is particularly important in order to make contact with the thermodynamic Bethe ansatz and the string hypothesis [10, 16, 38]. As has been discussed in the literature, there might be a critical length beyond which certain solutions cease to exist, see e.g. [10, 39]. We leave this problem of a more extensive numerical study to future work.

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References

[1] Baxter R J 1972 Partition function of the eight-vertex lattice model *Ann. Phys., NY* **70** 193–228

[2] Baxter R J 1973 Eight-vertex model in lattice statistics and one-dimenisional anisotropic Heisenberg chain I–III *Ann. Phys., NY* **76** 1–24, 25–47, 48–71

[3] Baxter R J 1982 *Exactly Solved Models in Statistical Mechanics* (London: Academic)

[4] Pasquier V and Gaudin M 1992 The periodic Toda chain and a matrix generalization of the Bessel function recursion relations *J. Phys. A: Math. Gen.* **25** 5243–52

[5] Krichever I, Lipan O, Wiegmann P and Zabrodin A 1997 Quantum integrable models and discrete classical Hirota equations *Commun. Math. Phys.* **188** 267–304

[6] Bazhanov V, Lukyanov S and Zamolodchikov A 1997 Integrable structure of conformal field theory II: Q-operator and DDV equation *Commun. Math. Phys.* **190** 247–78

[7] Kuznetsov V and Sklyanin E K 1998 On Bäcklund transformations for many-body systems *J. Phys. A: Math. Gen.* **31** 22241–51

[8] Sklyanin E K 2000 Bäcklund transformations and Baxter's Q-operator *Integrable Systems: from Classical to Quantum (Montreal, QC, 1999) (CRM Proc. Lecture Notes* vol 26*)* (Providence, RI: American Mathematical Society) pp 227–50

[9] Faddeev L D, Kashaev R and Volkov A Y 2001 Strongly coupled quantum discrete Liouville theory I: algebraic approach and duality *Commun. Math. Phys.* **219** 199–219

[10] Bethe H 1931 Zur theorie der metalle: I. Eigenwerte und eigenfunktionen der linearen atomkette *Z. Phys.* **71** 205–26

[11] Lieb E H 1967 Exact solution of the two-dimensional Slater KDP model of a ferroelectric *Phys. Rev. Lett.* **19** 108–10

[12] Sutherland B 1967 Exact solution of a two-dimensional model for hydrogen-bonded crystals *Phys. Rev. Lett.* **19** 103–4

[13] Fabricius K and McCoy B M 2001 Bethe's equation is incomplete for the XXZ model at roots of unity *J. Stat. Phys.* **103** 647–78

[14] Baxter R J 2002 Completeness of the Bethe ansatz for the six and eight-vertex models *J. Stat. Phys.* **108** 1–48

[15] Deguchi T, Fabricius K and McCoy B M 2001 The sl_2 loop algebra symmetry of the six-vertex model at roots of unity *J. Stat. Phys.* **102** 701–36

[16] Takhtajan L A and Faddeev L D 1981 Spectrum and scattering of stimuli of excitations in the one-dimensional isotropic Heisenberg model *Zap. Nauch. Semin. LOMI* **109** 134

[17] Deguchi T 2001 Non-regular eigenstate of the XXX model as some limit of the Bethe state *J. Phys. A: Math. Gen.* **34** 9755–75

[18] Byers N and Yang C 1961 Theoretical considerations concerning quantized magnetic flux in superconducting cylinders *Phys. Rev. Lett.* **7** 46–9

[19] de Vega H J 1984 Families of commuting transfer matrices and integrable models with disorder *Nucl. Phys.* B **240** 495–513

[20] Alcaraz F C, Barber M N and Batchelor M T 1988 Conformal invariance, the XXZ chain and the operator content of two-dimensional critical systems *Ann. Phys., NY* **182** 280–343

[21] Yu N and Fowler M 1992 Twisted boundary conditions and the adiabatic ground state for the attractive XXZ Luttinger liquid *Phys. Rev.* B **46** 14583–93

[22] Faddeev L D, Sklyanin E K and Takhtajan L A 1979 Quantum inverse problem I *Theor. Math. Phys.* **40** 194–220

[23] Tarasov V and Varchenko A 1995 Bases of Bethe vectors and difference equations with regular singular points *Int. Math. Res. Not.* **13** 637–69

[24] Pronko G P and Stroganov Y G 1999 Bethe equations on the wrong side of equator *J. Phys. A: Math. Gen.* **32** 2333–40

[25] Derkachov S E 1999 Baxter's Q-operator for the homogeneous XXX spin chain *J. Phys. A: Math. Gen.* **32** 5299–316

[26] Pronko G P 2000 On the Baxter's Q-operator for the XXX spin chain *Commun. Math. Phys.* **212** 687–701

[27] Derkachov S E 2005 Factorization of the R-matrix and Baxter's Q-operator *Preprint* math.QA/0507252

[28] Derkachov S E, Karakhanyan D and Kirschner R 2005 Baxter's Q-operators of the XXZ chain and R-matrix factorization *Preprint* hep-th/0511024

[29] Boos H, Jimbo M, Miwa T, Smirnov F and Takeyama Y 2006 A recursion formula for the correlation functions of an inhomogeneous XXX model *St. Petersburg Math. J.* **17** 85–117

[30] Boos H, Jimbo M, Miwa T, Smirnov F and Takeyama Y 2006 Reduced qKZ equation and correlation functions of the XXZ model *Commun. Math. Phys.* **261** 245–76

[31] Boos H, Jimbo M, Miwa T, Smirnov F and Takeyama Y 2005 Traces on the Sklyanin algebra and correlation functions of the eight-vertex model *J. Phys. A: Math. Gen.* **38** 7629–60

[32] Boos H, Jimbo M, Miwa T, Smirnov F and Takeyama Y 2005 Density matrix of a finite sub-chain of the Heisenberg anti-ferromagnet *Preprint* hep-th/0506171

[33] Korff C 2004 Auxiliary matrices for the six-vertex model and the algebraic Bethe ansatz *J. Phys. A: Math. Gen.* **37** 7227–53

[34] Korff C 2005 A Q-operator identity for the correlation functions of the infinite XXZ spin-chain *J. Phys. A: Math. Gen.* **38** 6641–57

[35] Rossi M and Weston R 2002 A generalized Q-operator for $U_q(\hat{sl}_2)$ vertex models *J. Phys. A: Math. Gen.* **35** 10015–32

[36] Korff C 2004 Auxiliary matrices for the six-vertex model at roots of unity: II. Bethe roots, complete strings, and the Drinfeld polynomial *J. Phys. A: Math. Gen.* **37** 385–406

[37] Korff C 2005 Auxiliary matrices on both sides of the equator *J. Phys. A: Math. Gen.* **38** 47–67

[38] Takahashi M 1971 One-dimensional Heisenberg model at finite temperature *Prog. Theor. Phys.* **46** 401–15

[39] Essler F H L, Korepin V E and Schoutens K 1992 Fine structure of the Bethe ansatz for the spin-1/2 Heisenberg XXX model *J. Phys. A: Math. Gen.* **25** 4115–26