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A Q-operator for the quantum transfer matrix

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Abstract

Baxter's concept of a Q-operator is generalized to the quantum transfer matrix of the XXZ spin-chain by employing the representation theory of quantum groups. The spectrum of this Q-operator is discussed and novel functional relations which describe the finite temperature regime of the XXZ spin-chain are derived. For a non-vanishing magnetic field the previously known Bethe ansatz equations can be replaced by a system of quadratic equations which is an important advantage for numerical studies. For vanishing magnetic field and rational coupling values it is argued that the quantum transfer matrix exhibits a loop algebra symmetry closely related to the one of the classical six-vertex transfer matrix at roots of unity. The quantum-classical crossover is also discussed in terms of the eigenvalues of the Q-operator for a few special examples.

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1. Introduction

In this work we present new identities for the description of the spectrum of the quantum transfer matrix for the XXZ spin-chain with a non-vanishing external magnetic field h [1],

$$H_{\mathrm{XXZ}} = \frac{1}{2}\sum_{\ell=1}^{L}\left\{\sigma_\ell^x\sigma_{\ell+1}^x + \sigma_\ell^y\sigma_{\ell+1}^y + \Delta\left(\sigma_\ell^z\sigma_{\ell+1}^z - 1\right)\right\} - \frac{h}{2}\sum_{\ell=1}^{L}\sigma^z. \tag{1.1}$$

Here $\Delta = (q + q^{-1})/2$ is an anisotropy parameter and we will consider the two cases q real and q on the unit circle. This spin-chain serves as a prototype model for other more complicated integrable systems. It is an important toy model for the exact computation of physical quantities such as magnetic, electric or thermal conductivities. In this context the study of the finite temperature behaviour of the spin-chain is of crucial importance. One method to achieve this is the so-called quantum transfer matrix (see, e.g., [2]),

$$\tau(z;w) = \operatorname*{Tr}_0 q^{\alpha\sigma_0^z\otimes 1} R_{0N}(zw)R^{t_{N-1}}_{(N-1)0}(w/z)\cdots R_{02}(zw)R^{t_1}_{10}(w/z), \qquad q^\alpha := \mathrm{e}^{\beta h/2} \tag{1.2}$$

in terms of which the partition function of the XXZ spin-chain can be expressed:

$$Z_L = \operatorname*{Tr}_{(\mathbb{C}^2)^{\otimes L}} \mathrm{e}^{-\beta H_{\mathrm{XXZ}}} = \lim_{N\to\infty} \operatorname*{Tr}_{(\mathbb{C}^2)^{\otimes N}} \tau(z=1; w=\mathrm{e}^{-\beta'/N})^L, \qquad \beta' = \beta(q-q^{-1}). \tag{1.3}$$

Let us explain the various objects appearing in the definition. The variable $\beta > 0$ denotes the inverse temperature of the system and for convenience we have introduced a 'twist angle' $\alpha = \beta h/2\ln q$, with h being the magnetic field in (1.1). The quantum transfer matrix is built out of the well-known six-vertex R-matrix which acts on the tensor product $\mathbb{C}^2 \otimes \mathbb{C}^2$:

$$R = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & c & 0 \\ 0 & c' & b & 0 \\ 0 & 0 & 0 & a \end{pmatrix}. \tag{1.4}$$

Here the parametrization of the Boltzmann weights a, b, c, c' is chosen as follows[1]:

$$a = 1, \qquad b = \frac{(1-z)q}{1-zq^2}, \qquad c = \frac{1-q^2}{1-zq^2}, \qquad c' = cz. \tag{1.5}$$

The upper index t_i in (1.2) stands for transposition in the ith factor. We recall that the six-vertex R-matrix gives rise to a classical statistical mechanics system which is described by the *classical* six-vertex transfer matrix (as opposed to *quantum*) [8]:

$$t_{6\mathrm{v}}(z) = \operatorname*{Tr}_0 R_{0L}(z)\cdots R_{01}(z). \tag{1.6}$$

This classical physical system is connected with the above quantum spin-chain through the relation (we set temporarily $h = 0$)

$$H_{\mathrm{XXZ}} = (q-q^{-1})\, z\frac{\mathrm{d}}{\mathrm{d}z}\ln t_{6\mathrm{v}}(z)\Big|_{z=1}. \tag{1.7}$$

The prefactor in the last equation explains the introduction of the renormalized temperature variable β' in (1.3). As an immediate consequence of (1.7) one has the following identity for the density matrix:

$$\lim_{N\to\infty} (t_{6\mathrm{v}}(1)^{-1} t_{6\mathrm{v}}(\mathrm{e}^{-\beta'/N}))^N = \mathrm{e}^{-\beta H_{\mathrm{XXZ}}}. \tag{1.8}$$

This rewriting is inspired by the Trotter formula in the path-integral formalism of quantum field theory and N is referred to as Trotter number [4]. The last expression (1.8) can be conveniently expressed in terms of the quantum transfer matrix (1.2); see the review [3] and references therein for details. Note, in particular, that for this construction to work the Trotter number N has to be even and we shall work throughout this paper with the convention

$$N = 2n. \tag{1.9}$$

In the thermodynamic limit when the physical system size L tends to infinity the partition function (1.3) can be approximated by the largest eigenvalue Λ_N of the quantum transfer matrix (1.2):

$$L \gg 1 : Z_L = \lim_{N\to\infty} \operatorname*{Tr}_{(\mathbb{C}^2)^{\otimes N}} \tau(1; \mathrm{e}^{-\beta'/N})^L \approx \lim_{N\to\infty} (\Lambda_N)^L. \tag{1.10}$$

Thus, the introduction of the quantum transfer matrix (1.2) allows one to efficiently investigate the finite temperature regime. Instead of having to compute multiple excited states and energies

[1] In what follows we will compare the results in this paper with the known properties about the quantum transfer matrix as they can be found in, e.g., [3]. To this end it is helpful to identify the definition of the Boltzmann weights in [3] on page 11, equation (2) with ours by setting $z = \mathrm{e}^{\mathrm{i}\gamma w}$ and $q = \mathrm{e}^{\mathrm{i}\gamma}$. Note that on page 16 in [3] a rotation in the complex plane is performed replacing $w \to \mathrm{i}v$; see equations (23) and (24) therein.

of the quantum spin-chain (1.1) at finite temperature, one only needs to compute a single eigenvalue and eigenstate of the quantum transfer matrix (1.2). Similar simplifications occur also in the computation of finite temperature correlation functions; see, for instance, [5].

There are some technical complications, however. We refer the reader for the following statements to [3] and references therein. The algebraic properties of the quantum transfer matrix resemble closely those of the classical six-vertex transfer matrix (1.6) and as a result one can compute the eigenstates and eigenvalues of the quantum transfer matrix by similar methods as in the classical case—i.e. the algebraic Bethe ansatz. Via this route one obtains expressions for the eigenvalues of (1.2). In particular, the largest eigenvalue Λ_N can be cast into the form

$$\Lambda_N(u) = \frac{\mathrm{e}^{-\frac{\beta h}{2}}\phi(u-\mathrm{i})\mathcal{Q}(u+2\mathrm{i}) + \mathrm{e}^{\frac{\beta h}{2}}\phi(u+\mathrm{i})\mathcal{Q}(u-2\mathrm{i})}{\mathcal{Q}(u)\big[\sinh\frac{\gamma}{2}(u-2\mathrm{i}+\mathrm{i}\tau)\sinh\frac{\gamma}{2}(u+2\mathrm{i}-\mathrm{i}\tau)\big]^{\frac{N}{2}}}, \tag{1.11}$$

where we have set $z = \mathrm{e}^{\gamma u}$, $w = \mathrm{e}^{-\beta'/N} = \mathrm{e}^{-\mathrm{i}\gamma\tau}$, $q = \mathrm{e}^{\mathrm{i}\gamma}$ and introduced the functions

$$\phi(u) = \Big[\sinh\frac{\gamma}{2}(u-\mathrm{i}+\mathrm{i}\tau)\sinh\frac{\gamma}{2}(u-2\mathrm{i}+\mathrm{i}\tau)\Big]^n, \qquad \mathcal{Q}(u) = \prod_{j=1}^{n}\sinh\frac{\gamma}{2}(u-u_j). \tag{1.12}$$

The quantities u_j are solutions of the following system of nonlinear equations:

$$\frac{\phi(u_j+\mathrm{i})}{\phi(u_j-\mathrm{i})} = -\mathrm{e}^{\beta h}\frac{\mathcal{Q}(u_j+2\mathrm{i})}{\mathcal{Q}(u_j-2\mathrm{i})}, \qquad j = 1,\dots,n. \tag{1.13}$$

Compare with equations (25)–(30) in [3]. The analytic solutions to the last set of equations, known as Bethe ansatz equations, are not known. Furthermore, in the Trotter limit $N \to \infty$ the distribution of the Bethe roots u_j remains discrete and cannot be approximated by continuous density functions as it is the case for the classical transfer matrix (1.6). Instead one has to rely on the numerical solution of a nonlinear integral equation. The derivation of this integral equation as well as other properties of the quantum transfer matrix are based to a large extent on numerical studies of the above Bethe ansatz equations (1.13).

Another aspect where numerical investigations and a deeper understanding of the solutions to the Bethe ansatz equations (1.13) are of importance is the observation of so-called quantum-classical crossover phenomena driven by temperature. At sufficiently high temperatures the first subleading eigenvalue of the quantum transfer matrix at $z = 1$ is real and unique. As the temperature sinks below a certain threshold, the next-leading eigenvalues at $z = 1$ form complex conjugate pairs resulting in incommensurate spatial oscillations of the correlations functions. The wavelength of these incommensurate oscillations is temperature dependent. This phenomenon has been investigated for the massless ferromagnetic regime ($-1 < \Delta \leqslant 0$) at a vanishing magnetic field ($h = 0$) in [6] and for the massless antiferromagnetic regime at a finite magnetic field ($h \geqslant 0$) in [7]. We will make contact with these investigations on the level of the spectrum of the quantum transfer matrix.

In light of the aforementioned points it is worthwhile to study alternative methods of deriving the spectrum, and in particular the largest eigenvalue, which lead to systems of equations simpler than the Bethe ansatz equations (1.13). The purpose of this paper is to diagonalize the quantum transfer matrix employing Baxter's idea of an auxiliary matrix known as Q-operator similar to what has been done in the classical six-vertex model [8, 9]. The eigenvalues of the Q-operator give the Q-function in (1.12) and we will derive a set of functional relations analogous to the ones first obtained in the context of conformal field theory [10] based on the existence of two linearly independent solutions to Baxter's TQ equation and

generalizations thereof. For a discussion of the analogous functional relations in the context of the eight and six-vertex model, we refer the reader to [11–14]. In particular, the case which we discuss here resembles the one of quasi-periodic boundary conditions or external electric fields treated in [13, 14]. In neither of the last mentioned papers explicit Q-operator constructions for the mentioned lattice models have been considered.

Concrete operator constructions of Q for the finite XXZ spin-chain have been investigated in [15, 16–18]. In particular, we will follow closely the construction for the twisted XXZ spin-chain given in [18] where the functional relations postulated in [13] have been derived in terms of concrete operators. By explicitly constructing Q we prove existence of the solutions to the aforementioned functional equations. A step which is still missing in the eight-vertex case [14].

1.1. Summary of the key results and identities

We will explicitly construct Q-operator solutions $Q^{\pm}$ for a generalization of Baxter's TQ-equation by employing the representation theory of quantum groups. The main results for $h \neq 0$ in (1.1) are novel identities for the spectrum of the quantum transfer matrix and its associated fusion hierarchy:

$$\tau^{(d-1)}(z) = \frac{q^{d(\alpha-S_A)}Q^+(zq^{-d})Q^-(zq^d) - q^{d(S_A-\alpha)}Q^+(zq^d)Q^-(zq^{-d})}{q^{\alpha-S_A} - q^{S_A-\alpha}}. \tag{1.14}$$

Here $\tau^{(d-1)}$ denotes the quantum transfer matrix of dimension d and for $d = 2$ one recovers the previously introduced quantum transfer matrix (1.2) up to a normalization factor which will be given in the text; see section 3 for details. For $d = 1$, the left-hand side of the above identity is explicitly known, thus resulting in a set of equations which allows one to compute the spectrum of $Q^{\pm}$. The latter equations imply the Bethe ansatz equations (1.13) but are *quadratic*; see the next paragraph. In contrast, the Bethe ansatz equations are of polynomial order N in the Bethe roots.

One of the main results in this paper is that the largest eigenvalue Λ_N of (1.2) can be expressed in terms of a *single* polynomial eigenvalue (I shall often denote eigenvalues and operators by the same symbol)

$$Q^+(z) = \sum_{k=0}^{n} e_k^+(-z)^k, \tag{1.15}$$

whose coefficients e_k^+ (with $e_0^+ = 1$) solve the following system of *quadratic* equations

$$e_n^+ \sum_{k+l=m} \binom{n}{k}\binom{n}{l}(wq)^{k-l} = \sum_{k+l=m} \frac{\sinh\left[\frac{\beta h}{2} - \mathrm{i}\gamma(k-l)\right]}{\sinh[\beta h/2]} e_k^+ e_{n-l}^+. \tag{1.16}$$

Here the summation convention in (1.16) is to be understood as follows. First fix the variable m in the allowed range $m = 1, \ldots, N-1$ and then sum in (1.16) over all possible values for k, l such that $k + l = m$. Thus, one obtains in total $N - 1$ coupled quadratic equations in the $n = N/2$ unknowns e_k^+. For real z, the largest eigenvalue of the quantum transfer matrix (1.2) is then given by

$$\Lambda_N(z; w) = \frac{\mathrm{e}^{\beta h}Q^+(zq^{-2})Q^-(zq^2) - \mathrm{e}^{-\beta h}Q^+(zq^2)Q^-(zq^{-2})}{\sinh[\beta h/2][(zwq-1)(z/wq-1)]^{N/2}}, \tag{1.17}$$

where Q^- is the reciprocal polynomial of Q^+, i.e.

$$Q^-(z) = \sum_{k=0}^{n} \frac{e_{n-k}^+}{e_n^+}(-z)^k = z^n Q^+(z^{-1})/e_n^+. \tag{1.18}$$

In the critical regime, $q \in \mathbb{S}^1$, the coefficients e_k^+ obey the additional constraint

$$\left(e_k^+\right)^* = e_{n-k}^+ / e_n^+. \tag{1.19}$$

There are in general many solutions to equations (1.16) (similar as there are multiple solutions to the Bethe ansatz equations) describing a subset of the spectrum of (1.2). The largest eigenvalue of the quantum transfer matrix Λ_N appears to be always among them; this has been numerically verified for $N = 2, 4, 6, 8, 10, 12, 14, 16$ [2] and for all of these cases the total number of solutions to (1.16) is found to be 2^n.

The identities (1.16), (1.17) and (1.18) are special cases of the generally valid expression (1.14) for $d = 1$ which yields the complete spectrum of the quantum transfer matrix; see equations (4.2) and (4.3) in the text. In particular, the polynomials $Q^{\pm}$ are in general independent. We discuss these identities in the context of higher spin quantum transfer matrices and the associated fusion hierarchy. This is motivated by the definition of a trace functional which might be relevant for the computation of correlation functions.

As mentioned above, the derivation of the main results is based on a concrete construction of the Q-operators whose eigenvalues yield the aforementioned polynomials $Q^{\pm}$. By abuse of notation operators and eigenvalues will often be denoted by the same symbol. The explicit operator construction establishes existence of the solutions to the various functional equations such as (1.16) for $h \neq 0$. At a vanishing magnetic field, $h = 0$ in (1.1), the identity (1.14) ceases to be true in general. However, the Q-operator construction can also be applied to $h = 0$ albeit one has then to restrict the deformation parameter q to a root of unity, $q^\ell = 1$, $\ell > 2$. For this special case, we argue that the quantum transfer matrix exhibits a loop algebra symmetry just as the classical six-vertex transfer matrix [20], albeit in a different representation.

1.2. Outline of the paper

The outline of the paper is as follows. In section 2 we connect the structure of the quantum transfer matrix to the representation theory of the quantum affine algebra $U_q(\widehat{sl}_2)$. In particular, we discuss a specific dual representation and the corresponding L-operator. This will yield the commutation relations between the quantum monodromy matrix elements corresponding to (1.2) and the Chevalley–Serre generators of $U_q(\widehat{sl}_2)$ which allows us to prove the loop algebra symmetry $U(\tilde{sl}_2)$ of the quantum transfer matrix at roots of unity and for a vanishing magnetic field. As a preparatory step for the discussion of the Q-operator we introduce the quantum fusion hierarchy, i.e., the higher spin analogues of the quantum transfer matrix.

In section 3 we construct the Q-operator for the quantum transfer matrix and discuss its properties and operator functional relations. The proofs can be found in appendices A and B. For the construction of the Q-operator one has carefully to distinguish between the case of generic q and q a root of unity. In the former case the auxiliary space of the Q-operator is infinite-dimensional and one needs to introduce a boundary parameter (the external magnetic field h) in order to ensure convergence. At a root of unity the auxiliary space is finite-dimensional and the construction of Q then also applies to the case $h = 0$. However, some of the functional relations which hold true at $h \neq 0$ then cease to be valid.

Section 4 is devoted to a special Q-operator functional equation, the Wronskian relation, which at a finite magnetic field $h > 0$ suffices to compute the spectrum of the quantum transfer matrix and implies the Bethe ansatz equations. At the end we discuss the special solutions (1.18) which contain the largest eigenvalue and are based on numerical evidence. We also make contact with the previously mentioned crossover phenomena.

Section 5 contains the conclusions.

[2] It appears that there is a difference between $n = N/2$ odd and even; compare with the footnote in [5], section 2.6. For n odd, the largest eigenvalue might have less than n Bethe roots. Nevertheless, in the cases $N = 2, 6, 10$ we have numercially verified that (1.16) and (1.17) still hold true.

2. The quantum transfer matrix and representation theory

As a preparatory step for the construction of the Q-operator for the quantum transfer matrix, let us first analyse the definition (1.2) from a representation theoretic point of view. This will enable us to define the corresponding L-operator from which the Q-operator will be built.

Recall that the six-vertex R-matrix is an intertwiner of the quantum affine algebra $U_q(\widehat{sl}_2)$ with respect to the tensor product of the two-dimensional evaluation representation. The quantum affine algebra $U_q(\widehat{sl}_2)$ is generated from the Chevalley–Serre elements subject to the relations

$$\begin{aligned} &q^{h_i}q^{h_j} = q^{h_j}q^{h_i}, \qquad && q^{h_i}e_jq^{-h_i} = q^{A_{ij}}e_j, \\ &q^{h_i}f_jq^{-h_i} = q^{-A_{ij}}f_j, \qquad && [e_i, f_j] = \delta_{ij}\frac{q^{h_i}-q^{-h_i}}{q-q^{-1}} \end{aligned} \tag{2.1}$$

and

$$x_i^3x_j - [3]_q x_i^2x_jx_i + [3]_q x_ix_jx_i^2 - x_jx_i^3 = 0, \qquad x = e, f. \tag{2.2}$$

Here the indices i, j take the values 0, 1 and A_{ij} is the Cartan matrix of $\widehat{sl}_2$. The evaluation homomorphism $ev_z : U_q(\widehat{sl}_2) \to U_q(sl_2)$ defined by

$$ev_z(e_0) = zf, \qquad ev_z(f_0) = z^{-1}e, \qquad ev_z(q^{h_0}) = q^{-h} \tag{2.3}$$

and

$$ev_z(e_1) = e, \qquad ev_z(f_1) = f, \qquad ev_z(q^{h_1}) = q^h. \tag{2.4}$$

An evaluation representation is now obtained by combining the evaluation homomorphism with any finite-dimensional representation of $U_q(sl_2)$, in particular we can choose the two-dimensional, spin $1/2$ representation in terms of Pauli matrices,

$$\pi(e) = \sigma^+, \qquad \pi(f) = \sigma^-, \qquad \pi(q^h) = q^{\sigma^z}. \tag{2.5}$$

The six-vertex R-matrix then intertwines the tensor product representation $\pi_z \otimes \pi_1$ with $\pi_z = \pi \circ ev_z$.

Given any representation $\rho : U_q(\widehat{sl}_2) \to \operatorname{End} V$ over some finite-dimensional vector space V, we define the following representation over its dual space V^*:

$$\begin{aligned} &\rho^* : U_q(\widehat{sl}_2) \to \operatorname{End} V^*, \qquad && \langle \rho^*(x)v^*, w\rangle := \langle v^*, \rho(\gamma^{-1}(x))w\rangle, \\ &x \in U_q(\widehat{sl}_2), \qquad && w \in V. \end{aligned} \tag{2.6}$$

Here γ is the antipode which is defined on the Chevalley–Serre generators as follows:

$$\gamma(e_i) = -q^{-h_i}e_i, \qquad \gamma(f_i) = -f_iq^{h_i}, \qquad \gamma(q^{\pm h_i}) = q^{\mp h_i} \tag{2.7}$$

$$\gamma^{-1}(e_i) = -e_iq^{-h_i}, \qquad \gamma^{-1}(f_i) = -q^{h_i}f_i, \qquad \gamma^{-1}(q^{\pm h_i}) = q^{\mp h_i}. \tag{2.8}$$

If we canonically identify V^* with V, the representation ρ^* in terms of matrices is simply given by

$$\rho^*(x) = (\rho(\gamma^{-1}(x)))^t, \qquad x \in U_q(\widehat{sl}_2) \tag{2.9}$$

with t denoting the transpose. Note that definition (2.7) is compatible with the following choice for the coproduct:

$$\Delta(e_i) = e_i \otimes 1 + q^{h_i} \otimes e_i, \qquad \Delta(f_i) = f_i \otimes q^{-h_i} + 1 \otimes f_i, \qquad \Delta(q^{h_i}) = q^{h_i} \otimes q^{h_i}. \tag{2.10}$$

Setting $\rho = \pi_1 = \pi \circ ev_{z=1}$, the two-dimensional evaluation module, we are interested in finding the intertwiner

$$L^*(z)\Delta^*(x) = \Delta^*_{\mathrm{op}}(x)L^*(z), \qquad x \in U_q(\widehat{sl}_2) \tag{2.11}$$

with

$$\Delta^* = (ev_z \otimes \pi_1^*)\Delta \qquad \text{and} \qquad L^*(z) \in U_q(sl_2) \otimes \mathrm{End}\, V^*. \tag{2.12}$$

Here we have restricted ourselves to evaluation representations from which all irreducible finite-dimensional representations of the affine quantum group $U_q(\widehat{sl}_2)$ can be obtained. Explicitly, the coproduct relations for the Chevalley generators read

$$\Delta^*(e_1) = e \otimes 1 - q^{1+h} \otimes \sigma^-, \qquad \Delta^*_{\mathrm{op}}(e_1) = e \otimes q^{-\sigma^z} - q1 \otimes \sigma^-, \tag{2.13}$$

$$\Delta^*(f_1) = f \otimes q^{\sigma^z} - q^{-1}1 \otimes \sigma^+, \qquad \Delta^*_{\mathrm{op}}(f_1) = f \otimes 1 - q^{-1-h} \otimes \sigma^+, \tag{2.14}$$

and

$$\Delta^*(e_0) = zf \otimes 1 - q^{1-h} \otimes \sigma^+, \qquad \Delta^*_{\mathrm{op}}(e_0) = zf \otimes q^{\sigma^z} - q1 \otimes \sigma^+, \tag{2.15}$$

$$\Delta^*(f_0) = z^{-1}e \otimes q^{-\sigma^z} - q^{-1}1 \otimes \sigma^-, \qquad \Delta^*_{\mathrm{op}}(f_0) = z^{-1}e \otimes 1 - q^{-1-h} \otimes \sigma^-. \tag{2.16}$$

In addition, let us state the expressions for the generators in the dual evaluation representation of spin $1/2$:

$$\pi_1^*(e_1) = -(\sigma^+ q^{-\sigma^z})^t = -q\sigma^-, \qquad \pi_1^*(f_1) = -(q^{\sigma^z}\sigma^-)^t = -q^{-1}\sigma^+, \tag{2.17}$$

$$\pi_1^*(e_0) = -(\sigma^- q^{\sigma^z})^t = -q\sigma^+, \qquad \pi_1^*(f_0) = -(q^{-\sigma^z}\sigma^+)^t = -q^{-1}\sigma^-. \tag{2.18}$$

We will see below that the intertwiner (2.11) specializes to the R-matrix used in the definition of the quantum transfer matrix (1.2). Solving the above intertwining condition (2.11) for an evaluation module with central charge zero, i.e. $q^{h_0} = q^{-h_1}$, we find

$$L^*(z) = \begin{pmatrix} zq^{-\frac{h+1}{2}} - q^{\frac{h+1}{2}} & (q^{-1}-q)eq^{-\frac{h+1}{2}} \\ z(q^{-1}-q)q^{\frac{h+1}{2}}f & zq^{\frac{h-1}{2}} - q^{-\frac{h-1}{2}} \end{pmatrix}. \tag{2.19}$$

For comparison and in order to keep this article self-contained recall that the conventional L-operator, where π_1^* is replaced by π_1 in (2.12), reads

$$L(z) = \begin{pmatrix} zq^{\frac{h+1}{2}} - q^{-\frac{h+1}{2}} & z(q-q^{-1})q^{\frac{h+1}{2}}f \\ (q-q^{-1})eq^{-\frac{h+1}{2}} & zq^{-\frac{h-1}{2}} - q^{\frac{h-1}{2}} \end{pmatrix}. \tag{2.20}$$

Note that we slightly deviate from standard conventions here be decomposing the L-operators over one factor space V in quantum space $V^{\otimes M}$. The matrix elements of L, L^* act in the so-called auxiliary space which is as of yet undetermined. Note further that in light of the following identity for the universal R-matrix, $(1 \otimes \gamma^{-1})\boldsymbol{R} = \boldsymbol{R}^{-1}$, it would be more natural to use $-z^{-1}L^*(z)$ as intertwiner for the dual representation π^*. However, we wish for later purposes to keep the L^*-operator polynomial in z instead of z^{-1}.

Evaluating the intertwiner (2.19) in the two-dimensional spin $1/2$ representation (2.5) yields

$$R^*(z) := \frac{(\pi \otimes 1)L^*(z)}{zq^{-1}-q} = [R_{21}(z^{-1})]^{1\otimes t} = \begin{pmatrix} a_{z^{-1}} & 0 & 0 & c'_{z^{-1}} \\ 0 & b_{z^{-1}} & 0 & 0 \\ 0 & 0 & b_{z^{-1}} & 0 \\ c_{z^{-1}} & 0 & 0 & a_{z^{-1}} \end{pmatrix}, \tag{2.21}$$

which is one of the R-matrices used in the definition of the quantum transfer matrix (1.2). Thus, we conclude that one lattice row associated with the monodromy matrix of the quantum transfer matrix corresponds to the following quantum group module:

$$\pi_z \otimes \mathfrak{M}_w^{(N)}, \qquad \mathfrak{M}_w^{(N)} = \underbrace{\pi_w^* \otimes \pi_{w^{-1}} \cdots \otimes \pi_w^* \otimes \pi_{w^{-1}}}_{N}. \tag{2.22}$$

From this we immediately deduce that the quantum transfer matrix $\tau(z; w)$ block decomposes with respect to the following alternating spin operator,

$$[\tau(z; w), S_A] = 0, \qquad S_A := \frac{1}{2}\sum_{k=1}^{N}(-)^k \sigma_k^z, \tag{2.23}$$

since the quantum monodromy matrix (decomposed over the auxiliary space)

$$R_{0N}(zw)R^{t_{N-1}}_{(N-1)0}(w/z)\cdots R_{02}(zw)R^{t_1}_{10}(w/z) = \begin{pmatrix} A(z) & B(z) \\ C(z) & D(z) \end{pmatrix} \tag{2.24}$$

is an intertwiner with respect to the tensor product (2.22). More generally, we have

$$\begin{aligned} &[A, q^{H_1}] = [D, q^{H_1}] = 0, && q^{H_1} B q^{-H_1} = q^{-2} B, \\ &q^{H_1} C q^{-H_1} = q^2 C, && q^{H_1} = q^{2S_A}. \end{aligned} \tag{2.25}$$

Denoting the Chevalley–Serre generators acting in quantum space (2.22) by capital letters, $\{E_1, E_0, F_1, F_0, H_0 = -H_1\}$, one finds the analogous commutation relations as in the classical case; see equations (14), (15) in [21]. The difference between the relations for the classical and the quantum transfer matrix is purely in the explicit form of the quantum group generators which is fixed through the identification of the quantum group module $\mathfrak{M}_w^{(N)}$ in (2.22). For instance, employing (2.10) and (2.5), (2.17) one has

$$E_1 = \sum_{k=1}^{N} \varepsilon_k q^{\frac{1-\varepsilon_k}{2}} \left(\prod_{j<k} q^{\varepsilon_j \sigma_j^z}\right) \sigma_k^{\varepsilon_k}, \qquad \varepsilon_k = (-1)^k \tag{2.26}$$

$$F_1 = \sum_{k=1}^{N} \varepsilon_k q^{\frac{\varepsilon_k - 1}{2}} \sigma_k^{-\varepsilon_k} \left(\prod_{j>k} q^{-\varepsilon_j \sigma_j^z}\right), \tag{2.27}$$

and so forth. Following the same line of argument as presented in [21] (cf equations (23), (24) therein) one then proves that for zero magnetic field $h = 0$ and q being a primitive root of unity of order ℓ the quantum transfer matrix (1.2) enjoys a loop algebra symmetry $U(\widetilde{sl}_2)$ in the sectors

$$2S_A = 0 \bmod \ell. \tag{2.28}$$

The Chevalley–Serre generators of the loop algebra $U(\widetilde{sl}_2)$ are obtained from the restricted quantum group (compare with the discussion in [22]) via taking the following limit from generic q' to the root of unity value q:

$$\begin{aligned} &q^\ell = 1: && E_1^{(\ell')} := \lim_{q' \to q} E_1^{\ell'} \big/ [\ell']_{q'}!, \\ &[x]_q := \frac{q^x - q^{-x}}{q - q^{-1}}, && \ell' = \begin{cases} \ell, & \text{if } \ell \text{ is odd} \\ \ell/2, & \text{if } \ell \text{ is even.} \end{cases} \end{aligned}$$

Analogous expressions hold for the remaining generators. All of the Chevalley–Serre generators, $\{E_1^{(\ell')}, E_0^{(\ell')}, F_1^{(\ell')}, F_0^{(\ell')}\}$, (anti)commute in the commensurate sectors (2.28) with the quantum transfer matrix, e.g.,

$$\tau(z;w)E_1^{(\ell')} = q^{\ell'}E_1^{(\ell')}\tau(z;w) \qquad \text{for} \quad h=0, \qquad q^{\ell}=1 \quad \text{and} \quad 2S_A = 0 \bmod \ell. \tag{2.29}$$

This result for the quantum transfer matrix is analogous to the loop symmetry of the classical transfer matrix first discovered in [20], albeit via a different proof.

2.1. Transformation under spin reversal

In order to show the existence of two independent solutions to the TQ-equation, we discuss the behaviour of the quantum transfer matrix under spin-reversal. From the elementary identities

$$\begin{aligned}(1\otimes\sigma^x)R(z)(1\otimes\sigma^x) &= \big(\sigma^x\otimes z^{-\frac{\sigma^z}{2}}\big)R(z)\big(\sigma^x\otimes z^{\frac{\sigma^z}{2}}\big)\\ (1\otimes\sigma^x)R^*(z)(1\otimes\sigma^x) &= \big(\sigma^x\otimes z^{\frac{\sigma^z}{2}}\big)R^*(z)\big(\sigma^x\otimes z^{-\frac{\sigma^z}{2}}\big),\end{aligned}$$

we infer that the quantum transfer matrix (1.2) transforms as

$$w^{S^z}\mathfrak{R}\tau_\alpha(z;w)w^{S^z}\mathfrak{R} = \tau_{-\alpha}(z;w) \tag{2.30}$$

under the involution $w^{S^z}\mathfrak{R}$ with

$$\mathfrak{R} = \prod_{j=1}^{N}\sigma_j^x \qquad \text{and} \qquad S^z = \frac{1}{2}\sum_{j=1}^{N}\sigma_j^z. \tag{2.31}$$

In addition, the quantum transfer matrix obeys another identity. First we observe that the following equations for the Boltzmann weights (1.5) hold true:

$$a_{z^{-1}} = 1, \qquad b_{z^{-1}} = 1/b_{zq^{-2}}, \qquad c_{z^{-1}} = -qc'_{zq^{-2}}/b_{zq^{-2}}, \qquad c'_{z^{-1}} = -q^{-1}c_{zq^{-2}}/b_{zq^{-2}}. \tag{2.32}$$

Employing the identities

$$\begin{aligned}R(z^{-1}) &= \frac{1}{b_{zq^{-2}}}\big(\sigma^x\otimes(-q)^{-\frac{\sigma^z}{2}}\big)R(zq^{-2})^{1\otimes t}\big(\sigma^x\otimes(-q)^{\frac{\sigma^z}{2}}\big)\\ R^*(z^{-1}) &= \frac{1}{b_{z^{-1}q^{-2}}}\big(\sigma^x\otimes(-q)^{\frac{\sigma^z}{2}}\big)R^*(zq^2)^{1\otimes t}\big(\sigma^x\otimes(-q)^{-\frac{\sigma^z}{2}}\big),\end{aligned}$$

we then easily find the expression for the transpose of the quantum transfer matrix,

$$\begin{aligned}\tau_{-\alpha}(z^{-1},w^{-1}) &= \operatorname*{Tr}_0 q^{-\alpha\sigma^z\otimes 1}R_{0N}(z^{-1}w^{-1})R^*_{0N-1}(w/z)\cdots R_{02}(z^{-1}w^{-1})R^*_{01}(w/z)\\ &= \frac{\tau_\alpha(z,wq^{-2})^t}{b^n_{zwq^{-2}}b^n_{wq^{-2}/z}},\end{aligned} \tag{2.33}$$

where we have used that $[S_A,\tau_\alpha(z,w)]=0$.

2.2. The quantum fusion hierarchy

The quantum transfer matrix (1.2) commutes with an infinite family of higher spin transfer matrices. In close analogy with the classical six-vertex model one defines for $d\in\mathbb{N}$ the following family of transfer matrices[3],

$$\tau^{(d-1)}(z;w) = \operatorname*{Tr}_{\pi^{(d-1)}} q^{\alpha h\otimes 1}L_N(zw)L^*_{N-1}(z/w)\cdots L_2(zw)L^*_1(z/w), \qquad q^\alpha = \mathrm{e}^{\frac{h\beta}{2}}, \tag{2.34}$$

[3] In the following we shall often suppress the explicit dependence on the temperature parameter w.

where the representation in auxiliary space has been replaced by the spin $(d-1)/2$ evaluation module $\pi^{(d-1)}$,

$$\begin{aligned}&\pi^{(d-1)}(e)|k\rangle = [d-k]_q|k-1\rangle, \qquad \pi^{(d-1)}(f)|k\rangle = [k+1]_q|k+1\rangle,\\ &\pi^{(d-1)}(q^h)|k\rangle = q^{d-2k-1}|k\rangle.\end{aligned} \tag{2.35}$$

The index k labelling the basis vectors of the representation takes values in the set $k = 0, 1, 2, \ldots, d-1$ and we set $e|0\rangle = f|d-1\rangle = 0$. Our motivation for introducing (2.34) is twofold. They are natural objects to consider from a representation theoretic point of view and we will encounter them when deriving functional relations for the Q-operator in the subsequent section. The other reason is their extension to complex dimension $d \in \mathbb{C}$ which is closely related to the trace functional used in recent formulations for correlation functions [19].

Setting $d = 2$ we identify $\pi^{(1)} \equiv \pi$ in (2.5) and recover the quantum transfer matrix via the relation

$$\tau(z;w) = \frac{(-z/w)^{-n}\tau^{(1)}(z;w)}{(zwq-q^{-1})^n(wq/z-q^{-1})^n} = \frac{\tau^{(1)}(z;w)}{(zwq-q^{-1})^n(z/wq-q)^n}. \tag{2.36}$$

The spin 0 representation yields the quantum determinant,

$$\begin{aligned}\tau^{(0)}(z;w) &= \left(zwq^{\frac{1}{2}} - q^{-\frac{1}{2}}\right)^n \left(zq^{-\frac{1}{2}}/w - q^{\frac{1}{2}}\right)^n \\ &= (zw-q^{-1})^n(z/w-q)^n = (zwq-1)^n(z/wq-1)^n.\end{aligned} \tag{2.37}$$

Similar to the classical six-vertex model, the higher-spin quantum transfer matrices $\tau^{(d)}$ satisfy a functional relation known as the fusion hierarchy,

$$\tau^{(d-1)}(zq^d)\tau^{(1)}(z) = \tau^{(0)}(zq^{-1})\tau^{(d-2)}(zq^{d+1}) + \tau^{(0)}(zq)\tau^{(d)}(zq^{d-1}), \tag{2.38}$$

which is a corollary of the decomposition of the tensor product $\pi^{(d-1)}_{zq^d} \otimes \pi^{(1)}_z$ described by the exact sequence

$$0 \to \pi^{(d-2)}_{zq^{d+1}} \overset{\iota}{\hookrightarrow} \pi^{(d-1)}_{zq^d} \otimes \pi^{(1)}_z \overset{p}{\to} \pi^{(d)}_{zq^{d-1}} \to 0. \tag{2.39}$$

Since the auxiliary spaces in the quantum transfer matrices are the same as in the classical case, we can use the same representation theoretic results to derive all relevant functional relations. What changes in the transition from 'classical' to 'quantum' are the coefficient functions which appear in the respective functional equation. For instance, the coefficients $\tau^{(0)}(zq^{-1})$, $\tau^{(0)}(zq)$ follow from the identities

$$\begin{aligned}&(\pi^{(d-1)} \otimes 1)L_{13}(zq^d)R_{23}(z)(\iota \otimes 1) = (z-1)(\iota \otimes 1)(\pi^{(d-2)} \otimes 1)L(zq^{d+1})\\ &(p \otimes 1)(\pi^{(d-1)} \otimes 1)L_{13}(zq^d)R_{23}(z) = (zq-q^{-1})(\pi^{(d)} \otimes 1)L(zq^{d-1})(p \otimes 1)\end{aligned} \tag{2.40}$$

and

$$\begin{aligned}&(\pi^{(d-1)} \otimes 1)L^*_{13}(zq^d)R^*_{23}(z)(\iota \otimes 1) = (z^{-1}q-q^{-1})(\iota \otimes 1)(\pi^{(d-2)} \otimes 1)L^*(zq^{d+1})\\ &(p \otimes 1)(\pi^{(d-1)} \otimes 1)L^*_{13}(zq^d)R_{23}(z) = (z^{-1}-1)(\pi^{(d)} \otimes 1)L^*(zq^{d-1})(p \otimes 1)\end{aligned} \tag{2.41}$$

where the maps

$$\iota : |k\rangle \hookrightarrow [d-k-1]_q|k\rangle \otimes |1\rangle - q^{d-k-1}[k+1]_q|k+1\rangle \otimes |0\rangle \tag{2.42}$$

and

$$p : \frac{[d]}{[d-k]}|k\rangle \otimes |0\rangle \to |k\rangle \tag{2.43}$$

are the inclusion and projection map in the exact sequence (2.39).

3. Explicit construction of a quantum Q-operator

After outlining the derivation of (2.38), we now turn to the Q-operator and apply the same strategy as in the case of the fusion hierarchy. The main difference lies in the fact that for the definition of the Q-operator we need to introduce an *infinite*-dimensional evaluation module when q is generic (i.e. not a root of unity) [15, 16]:

$$\begin{aligned}&\rho^+(e_0)|k\rangle = z|k+1\rangle, \qquad \rho^+\big(q^{\frac{h_1}{2}}\big)|k\rangle = \rho^+\big(q^{-\frac{h_0}{2}}\big)|k\rangle = r^{\frac{1}{2}}q^{-k-1/2}|k\rangle,\\ &\rho^+(e_1)|k\rangle = \frac{s+1-q^{2k}-sq^{-2k}}{(q-q^{-1})^2}|k-1\rangle, \qquad \rho^+(e_1)|0\rangle = 0, \qquad r,s,z\in\mathbb{C}.\end{aligned} \tag{3.1}$$

Here s, r are free parameters characterizing the representation and z denotes the spectral variable as before. As long as r, s are independent (3.1) defines a representation of the upper Borel subalgebra but extends to the whole affine algebra once we set $r = s^{1/2}$. In connection with spin-reversal, one also encounters the module

$$\rho^- := \rho^+ \circ \omega \qquad \text{with} \quad \big\{e_1, e_0, q^{\frac{h_1}{2}}, q^{\frac{h_0}{2}}\big\} \overset{\omega}{\to} \big\{e_0, e_1, q^{\frac{h_0}{2}}, q^{\frac{h_1}{2}}\big\}. \tag{3.2}$$

Note that in the limit $s \to 0$ we recover the q-oscillator representations used in [10]. In the case that q is a primitive root of unity of order ℓ we truncate the evaluation module ρ^+ by imposing the condition (compare with [17])

$$q^\ell = 1: \quad \rho^+(e_0)|\ell' - 1\rangle = 0, \quad \ell' = \begin{cases}\ell, & \text{if } \ell \text{ is odd}\\ \ell/2, & \text{if } \ell \text{ is even}\end{cases}. \tag{3.3}$$

The intertwiner corresponding to the quantum group module $\rho^+ \otimes \pi_1$ has been computed previously [15, 16] and reads

$$\mathfrak{L}(z) = \begin{pmatrix} z\frac{s}{r}q^{\frac{h_1+1}{2}} - q^{-\frac{h_1+1}{2}} & (q-q^{-1})q^{\frac{h_1+1}{2}}e_0\\ (q-q^{-1})e_1q^{-\frac{h_1+1}{2}} & zrq^{-\frac{h_1-1}{2}} - q^{\frac{h_1-1}{2}}\end{pmatrix} \in U_q(\widehat{sl}_2)\otimes \operatorname{End} V. \tag{3.4}$$

In order to define a Q-operator for the quantum transfer matrix we now need to compute the intertwiner corresponding to the module $\rho^+ \otimes \pi_1^*$. The result is

$$\mathfrak{L}^*(z) = \begin{pmatrix} zrq^{-\frac{h_1+1}{2}} - q^{\frac{h_1+1}{2}} & (q^{-1}-q)e_1q^{-\frac{h_1+1}{2}}\\ (q^{-1}-q)q^{\frac{h_1+1}{2}}e_0 & z\frac{s}{r}q^{\frac{h_1-1}{2}} - q^{-\frac{h_1-1}{2}}\end{pmatrix} \in U_q(\widehat{sl}_2)\otimes \operatorname{End} V^*. \tag{3.5}$$

The last expression is derived from the coproduct relations

$$\begin{aligned}&(1\otimes\pi_1^*)\Delta(e_1) = e_1\otimes 1 - q^{1+h_1}\otimes\sigma^-, \qquad (1\otimes\pi_1^*)\Delta_{\mathrm{op}}(e_1) = e_1\otimes q^{-\sigma^z} - q1\otimes\sigma^-,\\ &(1\otimes\pi_1^*)\Delta(e_0) = e_0\otimes 1 - q^{1+h_0}\otimes\sigma^+, \qquad (1\otimes\pi_1^*)\Delta_{\mathrm{op}}(e_0) = e_0\otimes q^{\sigma^z} - q1\otimes\sigma^+.\end{aligned} \tag{3.6}$$

We define for $r = 1$ in ρ^+ the operator

$$Q(z;s) = \operatorname*{Tr}_{\rho^+} q^{\alpha h_1\otimes 1}\mathfrak{L}_N(zw)\mathfrak{L}^*_{N-1}(z/w)\cdots\mathfrak{L}_2(zw)\mathfrak{L}^*_1(z/w), \qquad q^\alpha = \mathrm{e}^{\beta h/2}, \tag{3.7}$$

where we have normalized (3.5) such that Q is polynomial in the spectral parameter z. The specialization to $r = 1$ can be imposed without any loss of generality due to the identity

$$Q(z;r,s) = r^{\alpha - S_A}Q(z;r=1,s). \tag{3.8}$$

Having stated the explicit definition of the Q-operator we now turn to its properties and the functional relations it satisfies. Since the auxiliary spaces of the quantum transfer matrix and the Q-operator are the same as in the conventional, classical six-vertex model the proofs for the statements made below follow closely the line of argument presented previously in [16–18]. I shall therefore omit the proofs from the main text and refer the reader to the appendix for further details.

3.1. Operator factorization

One important result is that the Q-operator factorizes into simpler operators as follows (we still assume $\alpha \neq 0$):

$$Q(z;s) = Q(0;s)Q^{+}(z)Q^{-}(zs), \tag{3.9}$$

where we define

$$Q^{+}(z) := \lim_{s\to 0} Q(0;s)^{-1}Q(z;s) \tag{3.10}$$

and

$$Q^{-}(z) := \lim_{s\to\infty} Q(0;s)^{-1}Q(z/s;s). \tag{3.11}$$

Note that both operator limits are well defined and can be taken directly in (3.4) and (3.5) by noting that the off-diagonal elements of $\mathfrak{L}$, $\mathfrak{L}^*$ always occur in pairs in the matrix elements of the Q-operator. Moreover, the normalization factor $Q(0;s)$ at $z=0$ is independent of s and easily computed to be

$$\lim_{z\to 0} Q(z;s) = \operatorname*{Tr}_{\rho^+} q^{(\alpha-S_A)h_1} = \begin{cases} \dfrac{1}{q^{\alpha-S_A}-q^{S_A-\alpha}}, & q \text{ generic} \\ \dfrac{1-q^{2\ell(S_A-\alpha)}}{q^{\alpha-S_A}-q^{S_A-\alpha}}, & q^{\ell}=\pm 1. \end{cases} \tag{3.12}$$

The identity (3.12) for generic q has to be understood as analytic continuation from the region of convergence. Note that the point $\alpha = 0$, i.e. vanishing magnetic field $h = 0$, remains singular. This can be understood from the construction of the Q-operator since for generic q the auxiliary space given by the representation (3.1) is infinite-dimensional and twisted boundary conditions with an appropriate choice of α are needed to ensure that the trace in (3.7) is well defined; compare with the discussion in [16].

The operators $Q^{\pm}$ can be related to each other by employing the following transformation:

$$Q(z^{-1},w^{-1};s) = z^{-N}s^{\frac{N}{2}+S_A}(w/q)^{-S^z}\mathfrak{R}Q(z/s,wq^{-2};s)^{t}\mathfrak{R}(w/q)^{S^z}. \tag{3.13}$$

Here the operators S^z, $\mathfrak{R}$ have been introduced earlier in (2.31) and use has been made of the identities

$$\mathfrak{L}(z^{-1}) = -z^{-1}q\big(1\otimes\big(-\tfrac{z}{sq}\big)^{-\sigma^z}\sigma^x\big)\mathfrak{L}(zq^{-2}/s)^{1\otimes t}\big(1\otimes\sigma^x\big(-\tfrac{z}{sq}\big)^{\sigma^z}\big)s^{\frac{1+\sigma^z}{2}}$$

$$\mathfrak{L}^*(z^{-1}) = -z^{-1}q^{-1}\big(1\otimes\big(-\tfrac{zq}{s}\big)^{\sigma^z}\sigma^x\big)\mathfrak{L}^*(zq^2/s)^{1\otimes t}\big(1\otimes\sigma^x\big(-\tfrac{zq}{s}\big)^{-\sigma^z}\big)s^{\frac{1-\sigma^z}{2}}.$$

The identity (3.13) then allows one to determine the maximal polynomial degree of both operators, since up to an unimportant normalization constant we must have

$$Q^{-}(z,w) \propto z^{\frac{N}{2}+S_A}(wq)^{S^Z}\mathfrak{R}Q^{+}(z^{-1},w^{-1}q^{-2})^{t}\mathfrak{R}(wq)^{-S^Z}. \tag{3.14}$$

Note that the action of the spin-reversal operator relates Q^{-} to the representation (3.2). Both operators $Q^{\pm}$ have polynomial eigenvalues w.r.t. the spectral variable z and these eigenvalues, which shall be denoted by the same symbol as the operators, coincide with the polynomials mentioned in the introduction,

$$Q^{\pm}(z) = \prod_{k=1}^{n_{\pm}}(1-x_k^{\pm}z) = \sum_{k=0}^{n_{\pm}} e_k^{\pm}(-z)^k, \qquad n_{\pm} = n \mp S_A. \tag{3.15}$$

As we will see below, the polynomial roots $x_k^{\pm}$ are two sets of Bethe roots. They can be (numerically) computed by employing a number of functional relations which are satisfied by the Q-operator.

3.2. Operator functional relations

The best known functional relation is the generalization of Baxter's TQ-equation for the six-vertex model. This equation is obtained in the present construction for the Q-operator (which differs from Baxter's approach) by first deriving the functional relation

$$Q(z;s)\tau^{(1)}(z) = q^{\alpha-S_A}\tau^{(0)}(zq)Q(zq^{-2};sq^2) + q^{S_A-\alpha}\tau^{(0)}(zq^{-1})Q(zq^2;sq^{-2}) \tag{3.16}$$

which is a direct consequence of the following decomposition of the tensor product of representations, $\rho^+(z;r,s)\otimes\pi_z$, described by the exact sequence [15, 16]

$$0 \to \rho^+(zq^2;rq^{-1},sq^{-2}) \hookrightarrow \rho^+(z;r,s)\otimes\pi_z \to \rho^+(zq^{-2},rq,sq^2) \to 0. \tag{3.17}$$

Here $\tau^{(0)}$ is the quantum determinant introduced in (2.37). The above decomposition holds for the upper Borel algebra of $U_q(\widehat{sl}_2)$ but extends to the whole algebra under the previously mentioned specialization $r = s^{1/2}$. Taking the limit $s \to 0$ employing (3.10), we obtain the TQ-equation,

$$Q^+(z)\tau^{(1)}(z) = q^{\alpha-S_A}\tau^{(0)}(zq)Q^+(zq^{-2}) + q^{S_A-\alpha}\tau^{(0)}(zq^{-1})Q^+(zq^2). \tag{3.18}$$

A similar relation holds for Q^- when employing the transformations (2.30), (2.33) and (3.13). The TQ equation holds true also for a vanishing external magnetic field, i.e. $\alpha = 0$.

If the magnetic field is nonzero, however, there is another identity which makes use of both solutions $Q^\pm$ and on which we will focus. It yields a simple expression for all elements in the fusion hierarchy in terms of $Q^\pm$,

$$\tau^{(d-1)}(z) = \frac{q^{d(\alpha-S_A)}Q^+(zq^{-d})Q^-(zq^d) - q^{d(S_A-\alpha)}Q^+(zq^d)Q^-(zq^{-d})}{q^{\alpha-S_A}-q^{S_A-\alpha}}. \tag{3.19}$$

For the derivation see appendix A. The last expression can even be analytically continued to complex dimension d if one wishes to make contact with the trace functional introduced in the context of correlation functions for the infinite XXZ spin-chain. Here we shall not pursue this aspect further but refer the reader to [19] and references therein; see also [18].

4. The Wronskian relation

Note that when setting $d = 1$ in (3.19) the left-hand side of the above equation is explicitly known and we arrive at

$$(zwq-1)^n(z/wq-1)^n = \frac{q^{\alpha-S_A}Q^+(zq^{-1})Q^-(zq) - q^{S_A-\alpha}Q^+(zq)Q^-(zq^{-1})}{q^{\alpha-S_A}-q^{S_A-\alpha}}. \tag{4.1}$$

This functional relation, which is the discrete analogue of a Wronskian in the theory of second-order differential equations, can therefore be employed to compute the eigenvalues of $Q^\pm$. It is this observation which we will investigate further in the remainder of this paper.

4.1. System of quadratic equations

Expanding the Wronskian relation (4.1) with respect to the spectral parameter z yields the following system of N-quadratic equations for the unknown coefficients $e_k^\pm$ which are the elementary symmetric polynomials in the Bethe roots,

$$\sum_{k+l=m}\binom{n}{k}\binom{n}{l}(wq)^{k-l} = \sum_{k+l=m}\frac{q^{\alpha-S_A-k+l}-q^{S_A-\alpha+k-l}}{q^{\alpha-S_A}-q^{S_A-\alpha}}e_k^+e_l^-. \tag{4.2}$$

It should be emphasized once more that this set of equations contains for $\alpha \neq 0$ all the necessary information about the spectrum of the quantum transfer matrix as well as the higher

spin transfer matrices. Recall that N is the Trotter number, $w = \mathrm{e}^{-\beta'/N} = \exp\big(-\frac{\beta(q-q^{-1})}{N}\big)$ contains the temperature variable and $q^\alpha = \mathrm{e}^{h\beta/2}$, the external magnetic field. Setting now $n = 2$ in (3.19), the eigenvalues of the quantum transfer matrix (1.2) are obtained from the identity

$$\tau(z;w) = \frac{q^{2(\alpha-S_A)}Q^+(zq^{-2})Q^-(zq^2) - q^{2(S_A-\alpha)}Q^+(zq^2)Q^-(zq^{-2})}{(q^{\alpha-S_A}-q^{S_A-\alpha})(zwq-q^{-1})^n(z/wq-q)^n}. \tag{4.3}$$

Equations (4.2) and (4.3) are the aforementioned generalizations of the identities (1.16) and (1.17) in the introduction.

4.1.1. The Bethe ansatz equations. Having identified (4.2) as the key relation in describing the spectrum of the quantum transfer matrix for finite N, we need to discuss the relation with the Bethe ansatz equations which are usually considered to be the fundamental set of identities for discussing the spectrum. Starting from the quantum Wronskian we set

$$z = q/x_i^+\colon \quad \frac{-q^{S_A-\alpha}Q^+\big(q^2/x_i^+\big)Q^-\big(1/x_i^+\big)}{q^{\alpha-S_A}-q^{S_A-\alpha}} = \big(wq^2/x_i^+ - 1\big)^n\big(1/wx_i^+ - 1\big)^n$$

$$z = q^{-1}/x_i^+\colon \quad \frac{q^{\alpha-S_A}Q^+\big(q^{-2}/x_i^+\big)Q^-\big(1/x_i^+\big)}{q^{\alpha-S_A}-q^{S_A-\alpha}} = \big(w/x_i^+ - 1\big)^n\big(q^{-2}/wx_i^+ - 1\big)^n$$

and obtain

$$-q^{-2\alpha}\prod_{j=1}^{n_+}\frac{x_j^+q/x_i^+ - q^{-1}}{x_j^+q^{-1}/x_i^+ - q} = \left(\frac{wq - x_i^+q^{-1}}{q^{-1}-wx_i^+q}\right)^n\left(\frac{1-wx_i^+}{w-x_i^+}\right)^n. \tag{4.4}$$

The last equation is one among the n_+ Bethe ansatz equations as they can be found, for instance, in [3]; see equations (29) and (30). To facilitate the comparison note that under the parametrization

$$x_i = \mathrm{e}^{\gamma\lambda_i}, \qquad q = \mathrm{e}^{\mathrm{i}\gamma}, \qquad w = \mathrm{e}^{-\mathrm{i}\gamma\tau} = \mathrm{e}^{-(q-q^{-1})\beta/N}, \qquad q^{2\alpha} = \mathrm{e}^{\beta h}$$

the Bethe ansatz equations are rewritten as

$$\begin{aligned}\frac{\phi(\lambda_j+\mathrm{i})}{\phi(\lambda_j-\mathrm{i})} &:= \frac{\sinh^{\frac{N}{2}}\frac{\gamma}{2}(\lambda_j-\mathrm{i}\tau+2\mathrm{i})\sinh^{\frac{N}{2}}\frac{\gamma}{2}(\lambda_j+\mathrm{i}\tau)}{\sinh^{\frac{N}{2}}\frac{\gamma}{2}(\lambda_j+\mathrm{i}\tau-2\mathrm{i})\sinh^{\frac{N}{2}}\frac{\gamma}{2}(\lambda_j-\mathrm{i}\tau)}\\ &= -\mathrm{e}^{\beta h}\prod_{k=1}^{n_+}\frac{\sinh\frac{\gamma}{2}(\lambda_j-\lambda_k+2\mathrm{i})}{\sinh\frac{\gamma}{2}(\lambda_j-\lambda_k-2\mathrm{i})} =: -\mathrm{e}^{\beta h}\frac{\mathcal{Q}(\lambda_j+2\mathrm{i})}{\mathcal{Q}(\lambda_j-2\mathrm{i})}\end{aligned}$$

which is the notation used in [3]. From this we infer that the Wronskian relation (4.1) implies the Bethe ansatz equations, the converse is not true. Note that Q^- yields another set of Bethe roots, which in terms of the algebraic Bethe ansatz (see the appendix) allow one to construct the eigenvector from the lowest (instead of the highest) weight vector.

4.2. Special solutions in the $S_A = 0$ sector

As pointed out earlier, the quantum transfer matrix block decomposes with respect to the alternating spin-operator S_A. In particular, the largest eigenvalue Λ_N appears to be in the $S_A = 0$ sector. Since $\lim_{N\to\infty}\Lambda_N$ yields the partition function (1.3) in the thermodynamic limit its corresponding solutions to (4.2) are of particular, physical interest.

Quite generally, we infer from (4.1) that there are certain symmetries among the solutions to the Wronskian relation, for instance when replacing $z \to z^{-1}$. It is then natural to assume

that some solutions are invariant under these transformations, especially when they belong to non-degenerate or distinguished eigenvalues such as Λ_N. Thus, one would expect that there is a subset of solutions for which

$$Q^{\pm}(z) = \prod_{i=1}^{n} \left(1 - z/x_i^{\mp}\right) \tag{4.5}$$

holds. That is, $Q^{\pm}$ are the inverse or reciprocal polynomial of each other. In fact, one verifies numerically for Trotter numbers up to 16 that in the $S_A = 0$ sector there are always 2^n such 'special' solutions (for q real or on the unit circle) and that among this set of solutions is the one describing the largest eigenvalue of the quantum transfer matrix. Conjecturing this to be true for all N one can then halve the number of variables in (4.2) arriving at the result (1.16), (1.17) stated in the introduction. A similar observation has been made previously for the twisted XXX spin-chain; see section 5.1 in [23].

Provided that q (and therefore $w = \exp[-(q - q^{-1})\beta/N]$) lies on the unit circle there is another obvious 'symmetry' of (4.1), complex conjugation. In fact, one finds for $S_A = 0$ that there exist solutions $Q^{\pm}$ invariant under this transformation, i.e. obeying the additional restriction

$$Q^{\pm}(z) = \prod_{i=1}^{n} \left(1 - \left(x_i^{\mp}\right)^* z\right), \qquad z \in \mathbb{R}. \tag{4.6}$$

In terms of the elementary symmetric polynomials $e_k^{\pm}$ the restrictions (4.5) and (4.6) correspond to the identities

$$e_k^{\pm} = e_{n-k}^{\mp}/e_n^{\mp} \tag{4.7}$$

and

$$e_k^{\pm} = \left(e_k^{\mp}\right)^*, \tag{4.8}$$

respectively. Whether these solutions persist for Trotter numbers $N > 16$ needs to be investigated numerically. We leave this to future work.

4.3. Quantum-classical crossover

In this section we are going to discuss the quantum-classical crossover observed in [6, 7] in terms of solutions to the quantum Wronskian (4.2) and the 'symmetries' (4.7), (4.8). Recall that the crossover manifests itself in a change of the next-leading eigenvalue of the quantum transfer matrix. At high temperatures there is a single real eigenvalue (classical regime) while beneath a certain threshold temperature the next-leading eigenvalues consists of a pair (or pairs) of complex eigenvalues (quantum regime)[4]. In terms of the corresponding $Q^{\pm}$ eigenvalues this transition manifests itself in breaking one of the symmetries (4.5) and (4.6) or both. In contrast, the leading eigenvalue, which is always real and positive for the cases we discuss, always possesses both symmetries. We now give several examples based on numerical computations with Mathematica 5.2 and standard machine precision.

4.3.1. Parameter values: $\Delta = 1/2, h = 0.6, N = 12$. Let us first consider the antiferromagnetic regime of the XXZ spin-chain setting $q = \exp i\pi/3$ following [7].

[4] At finite Trotter numbers N there is a third temperature regime in which the behaviour changes once more. However, the corresponding transition temperature appears to approach zero as $N \to \infty$, whence we shall not discuss this regime here; see [6] for details.

A concrete numerical value for the crossover temperature has not been stated in [7]. However, the present numerical computations indicate that the crossover occurs in the interval $1.25 < \beta < 1.27$. For Trotter number $N = 12$, we find that the leading and next-leading eigenvalue of the quantum transfer matrix are in the $S_A = 0$ sector which has dimension 924. The two leading eigenvalues of the quantum transfer matrix at $\beta = 1.25$ and $z = 1$ are stated in table 1; see also table C.1 in the appendix for further subleading eigenvalues.

Table 1.

β	Λ_0	Λ_1
1.25	4.310 31	−1.137 95

Upon numerically solving the Wronskian relation (4.2), we find that the leading as well as the next-leading eigenvalue possess both symmetries (4.5), (4.6), i.e. for $z \in \mathbb{R}$ we have

$$Q_1^+(z) = z^n Q_1^-(z^{-1})/e_6^- = z^n \big[Q_1^+(z^{-1})/e_6^+\big]^*. \tag{4.9}$$

The analogous identities hold for the leading eigenvalue as mentioned earlier. The corresponding roots are listed in table 2.

Table 2.

$\beta = 1.25$	Q_0^+	Q_1^+
$-\gamma^{-1}\ln x_1$	−0.554 408 − 0.095 3871i	−1.986 93i
$-\gamma^{-1}\ln x_2$	0.554 408 − 0.0953 871i	0.043 1929i
$-\gamma^{-1}\ln x_3$	−0.167 918 − 0.016 9269i	−0.212 289 + 0.041 1305i
$-\gamma^{-1}\ln x_4$	0.167 918 − 0.016 9269i	0.212 289 + 0.041 1305i
$-\gamma^{-1}\ln x_5$	−0.045 5171 − 0.009 333 47i	−0.071 9618 + 0.036 3293i
$-\gamma^{-1}\ln x_6$	0.045 5171 − 0.009 333 47i	0.071 9618 + 0.036 3293i

The root distribution of Q_1^+ shows the appearance of an approximate one-string located on the imaginary axis in accordance with the findings in [7].

As the temperature is decreased the behaviour changes and we find a complex conjugate pair of next-leading eigenvalues; see table 3 and table C.2 in the appendix.

Table 3.

β	Λ_0	$\lvert\Lambda_{1,2}/\Lambda_0\rvert$	$\arg \Lambda_{1,2}/\Lambda_0$
1.27	4.38649	0.255461	$\mp$3.10797

The corresponding eigenvalues of the $Q^{\pm}$-operators are related via

$$Q_1^+(z) = z^6 Q_1^-(z^{-1})/e_6^{(1),-} = z^6\big[Q_2^+(z^{-1})/e_6^{(2),+}\big]^* = Q_2^-(z)^*, \qquad z \in \mathbb{R}. \tag{4.10}$$

Here $e_6^{(1),-}$, $e_6^{(2),+}$ denote the elementary symmetric polynomials of degree 6 in the roots of Q_1^- and Q_2^+, respectively. Thus, we have 'lost' the symmetry (4.6) and according to (3.19) the corresponding quantum transfer matrix eigenvalue ceases to be real. The root distribution is given in table 4.

Table 4.

$\beta = 1.27$	Q_0^+	Q_1^+
$-\gamma^{-1} \ln x_1$	$-0.561\,107 - 0.097\,5509\mathrm{i}$	$0.070\,5891 - 1.8782\mathrm{i}$
$-\gamma^{-1} \ln x_2$	$0.561\,107 - 0.097\,5509\mathrm{i}$	$0.070\,359 + 0.122\,035\mathrm{i}$
$-\gamma^{-1} \ln x_3$	$-0.170\,463 - 0.017\,425\mathrm{i}$	$-0.202\,551 + 0.028\,7092\mathrm{i}$
$-\gamma^{-1} \ln x_4$	$0.170\,463 - 0.017\,425\mathrm{i}$	$0.190\,885 + 0.049\,1244\mathrm{i}$
$-\gamma^{-1} \ln x_5$	$-0.046\,2239 - 0.009\,617\,32\mathrm{i}$	$-0.059\,2975 + 0.022\,7741\mathrm{i}$
$-\gamma^{-1} \ln x_6$	$0.046\,2239 - 0.009\,617\,32\mathrm{i}$	$0.039\,8655 + 0.029\,0445\mathrm{i}$

From the data we see that the one-string contribution has now moved away from the imaginary axis.

4.3.2. Parameter values: $\Delta = -1/2, h = 0.6, N = 12$. We now turn to the attractive regime setting $q = \exp 2\pi\mathrm{i}/3$ and choose a finite magnetic field value, $h = 0.6$. Note that this case is not investigated in [6] or [7]. However, we adopt the values in [6] given for the transition temperatures at $h = 0$ and find in the classical regime that the next-leading eigenvalue of the quantum transfer matrix at $z = 1$ is indeed unique and real; compare with table 5 and table C.3 in the appendix.

Table 5.

β^{-1}	Λ_0	Λ_1
0.362	3.283 05	0.639 32

Solving the Wronskian relation (4.2) we find that the corresponding eigenvalues of the $Q^{\pm}$-operators for the next-leading eigenvalue possess again the symmetries,

$$Q_1^-(z) = z^6 Q_1^+(z^{-1}) \big/ e_6^+ = Q_1^+(z)^*, \qquad z \in \mathbb{R}. \tag{4.11}$$

The corresponding roots are displayed in table 6.

Table 6.

$\beta^{-1} = 0.362$	Q_0^+	Q_1^+
$-\gamma^{-1} \ln x_1^+$	$-0.457\,174 - 0.263\,584\mathrm{i}$	$1.481\,73\mathrm{i}$
$-\gamma^{-1} \ln x_2^+$	$0.457\,174 - 0.263\,584\mathrm{i}$	$-0.034\,7615\mathrm{i}$
$-\gamma^{-1} \ln x_3^+$	$-0.170\,624 - 0.066\,3904\mathrm{i}$	$-0.326\,099 - 0.174\,081\mathrm{i}$
$-\gamma^{-1} \ln x_4^+$	$0.170\,624 - 0.066\,3904\mathrm{i}$	$0.326\,099 - 0.174\,081\mathrm{i}$
$-\gamma^{-1} \ln x_5^+$	$-0.047\,8432 - 0.038\,8699\mathrm{i}$	$-0.111\,579 - 0.047\,8781\mathrm{i}$
$-\gamma^{-1} \ln x_6^+$	$0.047\,8432 - 0.038\,8699\mathrm{i}$	$0.111\,579 - 0.047\,8781\mathrm{i}$

In the 'quantum regime' there are now four next-leading eigenvalues of the quantum transfer matrix at $z = 1$ whose modulus is the same but which differ by a phase, see table 7 and table C.4 in the appendix.

Table 7.

β^{-1}	Λ_0	$\lvert\Lambda_{1-4}/\Lambda_0\rvert$	$\arg \Lambda_{1,2}$	$\arg \Lambda_{3,4}$
0.227 82901	5.747 01	0.2387	−0.221 125	0.221 125

Again the temperature value is taken from [6]. The corresponding eigenvalues of the $Q^{\pm}$-operators are related to each other via the transformations ($z \in \mathbb{R}$)

$$Q_1^{\pm}(z) = z^6 Q_2^{\mp}(z^{-1})/e_6^{(2),+} = Q_3^{\mp}(z)^* = z^6\big[Q_4^{\mp}(z^{-1})/e_6^{(4),+}\big]^*. \tag{4.12}$$

Thus, in this case neither of the symmetries (4.5), (4.6) hold for the next-leading contribution and we obtain a twofold degenerate pair of complex eigenvalues. For the roots corresponding to the leading eigenvalue, see table 8.

Table 8.

$\beta^{-1} = 0.227\,829\,01$	$Q_0^{\pm}$
$-\gamma^{-1}\ln x_1^{\pm}$	$-0.535\,996 \mp 0.432\,308\mathrm{i}$
$-\gamma^{-1}\ln x_2^{\pm}$	$0.535\,996 \mp 0.432\,308\mathrm{i}$
$-\gamma^{-1}\ln x_3^{\pm}$	$-0.237\,71 \mp 0.149\,665\mathrm{i}$
$-\gamma^{-1}\ln x_4^{\pm}$	$0.237\,71 \mp 0.149\,665\mathrm{i}$
$-\gamma^{-1}\ln x_5^{\pm}$	$-0.069\,6051 \mp 0.095\,3902\mathrm{i}$
$-\gamma^{-1}\ln x_6^{\pm}$	$0.069\,6051 \mp 0.095\,3902\mathrm{i}$

and for the next leading eigenvalue one finds the results given in table 9.

Table 9.

$\beta^{-1} = 0.227\,829\,01$	Q_1^{+}	Q_1^{-}
$-\gamma^{-1}\ln x_1^{\pm}$	$0.252\,524 + 1.397\,97\mathrm{i}$	$0.202\,223 + 1.392\,11\mathrm{i}$
$-\gamma^{-1}\ln x_2^{\pm}$	$-0.462\,546 - 0.371\,296\mathrm{i}$	$-0.440\,937 + 0.409\,25\mathrm{i}$
$-\gamma^{-1}\ln x_3^{\pm}$	$-0.193\,085 - 0.124\,993\mathrm{i}$	$-0.186\,694 + 0.147\,141\mathrm{i}$
$-\gamma^{-1}\ln x_4^{\pm}$	$-0.025\,5607 - 0.085\,4029\mathrm{i}$	$-0.025\,7797 + 0.106\,308\mathrm{i}$
$-\gamma^{-1}\ln x_5^{\pm}$	$0.133\,642 - 0.102\,75\mathrm{i}$	$0.123\,314 + 0.131\,733\mathrm{i}$
$-\gamma^{-1}\ln x_6^{\pm}$	$0.362\,16 - 0.278\,72\mathrm{i}$	$0.260\,739 + 0.3786\,46\mathrm{i}$

Note that some of the roots of $Q_1^{\pm}$ lie close to each other or their complex conjugates, this might signal the restoration of one or both of the symmetries (4.5), (4.6) at higher temperatures. To confirm this further numerical calculations are needed which are beyond the intended scope of this paper.

4.3.3. Parameter values: $\Delta = -1/2, h = 0, N = 12$. For completeness we state here also numerical results for the case of vanishing magnetic field $h = 0$ ($\alpha = 0$) and $q = \exp 2\pi\mathrm{i}/3$. This is the case investigated in [6]. Note that as mentioned earlier the Wronskian ceases to hold for vanishing magnetic field and one now has to rely on diagonalizing the Q-operator (3.7) directly or employ the TQ-equation (3.18). According to the present computations the numerical data for the subleading eigenvalues in [6] are missing some of the quantum transfer matrix eigenvalues at $z = 1$ or state some of the multiplicities incorrectly. We therefore present in the appendix the numerical data for the first 20 eigenvalues as reference; see tables C.5 and C.6. For the leading and next-leading eigenvalues the present results (tables 10 and 11) agree with those in [6] (see table V and IV therein)

Table 10.

β^{-1}	Λ_0	Λ_1/Λ_0
0.362	2.679 57	0.186 218

Table 11.

β^{-1}	Λ_0	$\lvert\Lambda_{1-4}/\Lambda_0\rvert$	$\arg\Lambda_{1,2}$	$\arg\Lambda_{3,4}$
0.227 829 01	4.1737	0.238 817	-1.1555×10^{-4}	1.1555×10^{-4}

and in order to make contact with our previous discussion at $h \neq 0$ we compute here the corresponding Q^+ eigenvalues. These results are new and are not contained in [6].

For the regime above the crossover temperature there is a unique real next-leading eigenvalue and we find for the corresponding Q^+-eigenvalue the root distribution stated in table 12.

Table 12.

$\beta^{-1} = 0.362$	Q_0^+	Q_1^+
$-\gamma^{-1}\ln x_1$	0.581 829	0
$-\gamma^{-1}\ln x_2$	−0.581 829	1.5i
$-\gamma^{-1}\ln x_3$	0.183 537	0.408 961
$-\gamma^{-1}\ln x_4$	−0.183 537	−0.408 961
$-\gamma^{-1}\ln x_5$	0.049 9902	0.117 835
$-\gamma^{-1}\ln x_6$	−0.049 9902	−0.117 835

As the temperature sinks below the threshold value for the crossover the next-leading eigenvalues consist now of two pairs of complex eigenvalues. Similar to our previous discussion for $h \neq 0$ we find that the corresponding four eigenvalues of the Q-operator are related via

$$Q_1^+(z) = -z^6 Q_2^+(z^{-1}) = Q_3^+(z)^* = -z^6\big[Q_4^+(z^{-1})\big]^*, \qquad z \in \mathbb{R}. \tag{4.13}$$

Note that $Q^+ = Q^-$ and $e_6^+ = -1$ for all four eigenvalues in this instance. The corresponding root distribution for the leading and next-leading eigenvalue are listed in table 13.

Table 13.

$\beta^{-1} = 0.22782901$	Q_0^+	Q_1^+
$-\gamma^{-1}\ln x_1$	0.801 415	$0.0334\,987 - 6.085\,86\times10^{-6}$i
$-\gamma^{-1}\ln x_2$	−0.801 415	−0.310 075 − 1.499 93i
$-\gamma^{-1}\ln x_3$	0.279 83	0.713 681 − 0.000 011 2598i
$-\gamma^{-1}\ln x_4$	−0.279 83	−0.523 847 − 0.000 037 0802i
$-\gamma^{-1}\ln x_5$	0.077 5136	$0.229\,102 - 6.598\,57\times10^{-6}$i
$-\gamma^{-1}\ln x_6$	−0.077 5136	$-0.142\,361 - 9.809\,82\times10^{-6}$i

As some of the numerical values are quite small for the next leading eigenvalue we list for this example also the values of the symmetric elementary polynomials e_k^+ as additional reference; see table 14.

Table 14.

$\beta^{-1} = 0.227\,829\,01$	Q_0^+	Q_1^+
e_1	9.92391	4.203 98 + 0.000 570 062i
e_2	32.0512	0.958 515 + 0.002 188 51i
e_3	46.2876	−12.947 + 0.002 864 54i
e_4	32.0512	−17.3613 + 0.001 501 62i
e_5	9.923 91	−7.700 27 + 0.000 259 803i
e_6	1.0	−1.0

5. Conclusions and outlook

In this paper Baxter's Q-operator has been constructed for the quantum transfer matrix of the XXZ spin-chain. The main motivation has been to derive equations which allow one to describe the spectrum of the quantum transfer matrix and are simpler than the previously known Bethe ansatz equations. For a non-vanishing external magnetic field this is indeed possible and the order of the equations can be reduced from N (Bethe ansatz equations (4.4)) to order two (the Wronskian relation (4.2)) which is a great simplification for numerical computations. Of particular interest is the largest eigenvalue of the quantum transfer matrix which in the thermodynamic limit (i.e. the physical system size L tends to infinity) contains all the relevant finite temperature behaviour of the spin-chain. For this eigenvalue we observed further simplifications in its polynomial structure which lead to a reduction of the number of variables by a factor two. The latter observation is based on symmetries of the Wronskian relation (4.1) and numerical computations which were carried out up to the Trotter number $N = 16$. To go beyond this bound requires more extensive numerical computations which are planned to be carried out in future work. In this context we also touched upon the previously observed quantum-classical crossover [6, 7] and demonstrated for a few examples that the new identities for the spectrum of the quantum transfer matrix at a finite magnetic field allow for an efficient numerical investigation of the corresponding Q-eigenvalues and Bethe root distributions. In addition, we interpreted the crossover in terms of polynomial dependencies between the eigenvalues of the $Q^{\pm}$-operators. Further investigations are needed also here to confirm the findings for $N \gg 1$.

An aspect which has been omitted from the present work is the derivation of integral equations similar to those nonlinear integral equations which have been previously obtained on the basis of the Bethe ansatz equations for the *quantum* transfer matrix; see, e.g., [3] and references therein. The basis for such a derivation is numerical evidence for the distribution of the Bethe roots in the large Trotter number limit, $N \to \infty$. For this reason the discussion of integral equations and their connection with the thermodynamic Bethe ansatz [26] are postponed until the necessary numerical data have been obtained.

For a vanishing magnetic field the Wronskian relation ceases to be valid, but in the text it was shown that at roots of unity one might be able to employ the same loop algebra symmetry as the one which exists for the six-vertex model. This might possibly help to reduce the order of equations or simplify the computation of the spectrum of the quantum transfer matrix.

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Appendix A. Properties of Q for generic q

For comparison with the line of argument for the classical six-vertex model, the reader might wish to consult [16]. The line of argument closely follows the exposition given there.

A.1. The fusion hierarchy in terms of Q

Setting the free parameter s in ρ^+ to the special value $s = q^{2d}, d = 1, 2, \ldots$, one derives the following identities by restricting the $\mathfrak{L}$ and $\mathfrak{L}^*$-operator given in (3.4) and (3.5) to the

subspaces $V_{<d} = \mathrm{span}\{|k\rangle\}_{k=0}^{d-1}$ and $V_{\geqslant d} = \mathrm{span}\{|k\rangle\}_{k=d}^{\infty}$,

$$s = q^{2d} : \mathfrak{L}^*(z)|_{V_{<d}} = q^d\big(1 \otimes q^{\frac{d}{2}\sigma^z}\big) L^{*(d-1)}(zq^d)\big(1 \otimes q^{-d\sigma^z}\big) \tag{A.1}$$

$$s = q^{2d} : \mathfrak{L}^*(z)|_{V_{\geqslant d}} = q^{2d}(1 \otimes q^{d\sigma^z})\mathfrak{L}^*(zq^{2d}; s \to q^{-2d})\big(1 \otimes q^{-2d\sigma^z}\big). \tag{A.2}$$

Employing that by construction the Q-operator commutes with the alternating spin-operator, $[Q, S_A] = 0$, one deduces from these last two equations the following identity for the higher spin quantum transfer matrices,

$$\tau^{(d-1)}(z) = q^{d(\alpha - S_A)} Q(zq^{-d}; s = q^{2d}) - q^{d(S_A - \alpha)} Q(zq^d; s = q^{-2d}). \tag{A.3}$$

Below we will see that this relation can be simplified further due to a factorization of the Q-operator into two parts.

A.2. Algebraic Bethe ansatz computation

In order to obtain the eigenvalues we apply the algebraic Bethe ansatz for the quantum transfer matrix (see, e.g., [5]) and compute the action of Q on a Bethe state. Denote by $\{\uparrow, \downarrow\}$ by the orthogonal basis in $\mathbb{C}^2$ and consider the reference state

$$|0\rangle = \downarrow \otimes \uparrow \cdots \otimes \downarrow \otimes \uparrow. \tag{A.4}$$

Let $\{A, B, C, D\}$ be the matrix elements of the quantum monodromy matrix (2.24); then a Bethe state is given by

$$\big|x_1^+, \ldots, x_{n_+}^+\big\rangle := B\big(1/x_1^+\big) \cdots B\big(1/x_{n_+}^+\big)|0\rangle$$

with $\{x_1^+, \ldots, x_{n_+}^+\}$ being a solution to the Bethe ansatz equations (4.4). Since the auxiliary space of the quantum transfer matrix (1.2) and Q-operator (3.7) are the same as in the ordinary case of the classical six-vertex transfer matrix with quasi-periodic boundary conditions the results from [16] apply. Using the commutation relations between the matrix elements A, B, C, D and those of the monodromy matrix of the Q-operator,

$$\boldsymbol{Q}_{k,l}(z; s) := \langle k|q^{\alpha h_1 \otimes 1}\mathfrak{L}_N(zw)\mathfrak{L}^*_{N-1}(z/w)\cdots\mathfrak{L}_2(zw)\mathfrak{L}^*_1(z/w)|l\rangle, \tag{A.5}$$

detailed in [16], we obtain

$$Q(z; s)\big|x_1^+, \ldots, x_{n_+}^+\big\rangle = \left\{\sum_{k=0}^{\infty}\langle 0|\boldsymbol{Q}_{kk}(z; s)|0\rangle \prod_{j=1}^{n_+} \frac{\langle k+1|\mathfrak{a}_j|k+1\rangle\langle k|\mathfrak{d}_j|k\rangle - \langle k|\mathfrak{c}_j\mathfrak{b}_j|k\rangle}{\langle k+1|\mathfrak{a}_j|k+1\rangle\langle k|\mathfrak{a}_j|k\rangle}\right\} \times \big|x_1^+, \ldots, x_{n_+}^+\big\rangle.$$

Here we have introduce the abbreviations

$$\mathfrak{L}\big(zx_j^+\big) = \begin{pmatrix} \mathfrak{a}_j & \mathfrak{b}_j \\ \mathfrak{c}_j & \mathfrak{d}_j \end{pmatrix} \tag{A.6}$$

for the matrix elements of the $\mathfrak{L}$-operator. Inserting the explicit expressions for the latter which can be read off from (3.4), one arrives at

$$\begin{aligned} Q(z; s)\big|x_1^+, \ldots, x_{n_+}^+\big\rangle &= \left\{\sum_{k=0}^{\infty}\langle 0|\boldsymbol{Q}_{kk}(z; s)|0\rangle \prod_{j=1}^{n_+} \frac{q^{-2k-1}\big(1 - zx_j^+\big)\big(1 - zsx_j^+\big)}{\big(1 - zsq^{-2k}x_j^+\big)\big(1 - zsq^{-2k-2}x_j^+\big)}\right\} \\ &\quad \times \big|x_1^+, \ldots, x_{n_+}^+\big\rangle \\ &= q^{S_A - \alpha}Q^+(z)Q^+(zs)\sum_{k=0}^{\infty}\frac{q^{2k(S_A-\alpha)}\tau^{(0)}(zsq^{-2k-1})}{Q^+(zsq^{-2k})Q^+(zsq^{-2k-2})}\big|x_1^+, \ldots, x_{n_+}^+\big\rangle. \end{aligned}$$

In the last line we have used the definition of Q^+ as a polynomial (3.15) and

$$\langle 0|\boldsymbol{Q}_{kk}(z;s)|0\rangle = q^{(n-\alpha)(2k+1)}[(zwsq^{-2k}-1)(zsq^{-2k-2}/w-1)]^n.$$

Taking the limit $s \to 0$ in order to fix the normalization constant we deduce from this expression the following formula for Q^-,

$$Q^-(z) = Q^+(z)\sum_{k=0}^{\infty}\frac{q^{2k(S_A-\alpha)}\tau^{(0)}(zq^{-2k-1})}{Q^+(zq^{-2k})Q^+(zq^{-2k-2})}. \tag{A.7}$$

Note that in [16] the vanishing of the unwanted terms in the Bethe ansatz has only been verified for $n_+ = 1, 2, 3$, since the algebraic Bethe ansatz computation is more involved than in the case of the transfer matrix due to the infinite-dimensional auxiliary space of the Q-operator. However, the result for the spectrum coincides with the one found at roots of unity and the eigenvalues satisfy all aforementioned functional relations for the Q-operator, which have been derived by different means. We shall take this as sufficient evidence that the algebraic Bethe ansatz computation presented above holds also true for $n_+ > 3$.

Appendix B. Properties of Q when q is a root of unity

Let us now turn to the case when q is a primitive root of unity of order ℓ.

B.1. Functional relations for the fusion hierarchy

The evaluation module ρ^+ is now finite-dimensional according to (3.3). For analysing the spectrum of Q we now rely on a functional relation derived in [17]. To connect with the discussion therein, we set $r = \mu^{-1}$ and $s = \mu^{-2}$ in (3.1) and obtain the evaluation representation π_z^μ specified in equation (15), (16) of [17]. Thus, in the following we refer to $\rho^+(r = \mu^{-1}, s = \mu^{-2})$ as π_z^μ. Then the following short exact sequence holds (see equations (52), (53) in [17]),

$$0 \to \pi^{\mu\nu q}_{\mu q} \to \pi^{\mu}_{\mu\nu q^2}\otimes\pi^{\nu}_{1} \to \pi^{\mu\nu q^{-\ell'+1}}_{\mu q^{-\ell'+1}}\otimes\pi^{(\ell'-2)}_{\nu q^{\ell'+1}} \to 0. \tag{B.1}$$

Here $\pi_z^{(\ell'-2)}$ is the evaluation representation of spin $(\ell'-1)/2$. As before this decomposition of the tensor product of representations implies a functional relation, but this time it involves a product of two Q-operators with different values for the free parameters entering (3.1). Setting $s = \mu^{-2}$ and $t = \nu^{-2}$ this functional relation reads

$$Q(zq^2/s;s)Q(z;t) = q^{S_A-\alpha}Q(zq^2/s;stq^{-2})[\tau^{(0)}(zq) + q^{\ell'(S_A-\alpha)}\tau^{(\ell'-2)}(zq^{\ell'+1})], \tag{B.2}$$

compare with equation (46) in [18]. Assume that $[Q(z_1;s_1), Q(z_2;s_2)] = 0$ for arbitrary pairs $z_{1,2}, s_{1,2} \in \mathbb{C}$. This has been proved for $\ell = 3, 4, 6$ by explicitly constructing the corresponding intertwiner for $\rho^+(z_1,s_1)\otimes\rho^+(z_2;s_2)$ [24, 25]. Thus, the eigenvalues of $Q(z;s)$ must be polynomial in z (and s), their most general form being

$$Q(z;s) = \frac{1-q^{2\ell'(S_A-\alpha)}}{q^{\alpha-S_A}-q^{S_A-\alpha}}\prod_{j=1}^{k}(1-zx_j)\prod_{j=1}^{N-k}(1-zy_j(s)).$$

Here we have taken the limit $z \to 0$ to fix the normalization constant,

$$\lim_{z\to 0}Q(z;s) = \operatorname*{Tr}_{\rho^+} q^{(\alpha-S_A)h_1}. \tag{B.3}$$

We assume that the roots $x_j = x_j^+$ are independent of s while the y_j's depend on it allowing for the possibilities that either $k = 0$ or $k = N$. Inserting this general expression for the eigenvalue into (B.2), one deduces that the roots $y_j(s)$ can only depend linearly on s, i.e.

$y_j(s) = x_j^- s$ for some x_j^-. This implies the factorization (3.9) in the text. Furthermore, we infer from (3.13) that $k = N/2 - S_A$ in each fixed S_A sector.

Appendix C. Crossover: numerical results for the leading eigenvalues

To enable the reader to compare with the numerical results in section 4 of the main text, the following tables list the results obtained via direct diagonalization of the quantum transfer matrix (1.2).

C.1. Parameter values: $\Delta = 1/2, h = 0.6, N = 12$

Leading eigenvalues of the quantum transfer matrix (1.2) at $z = 1$ in the antiferromagnetic regime and finite magnetic field. The index j labels the subleading eigenvalues and indicates the multiplicities.

Table C.1. $\beta = 1.25\Lambda_0 = 4.310\,306\,992\,327\,662$

j	$\lvert\Lambda_j/\Lambda_0\rvert$	$\arg \Lambda_j/\Lambda_0$
1	0.264 007	π
2	0.238 494	π
3, 4	0.178 743	0
5, 6	0.098 3347	π
7, 8	0.060 5388	0
9, 10	0.060 4633	π
11	0.056 6445	0
12, 13	0.052 6504	0
14	0.034 5386	π
15, 16	0.034 0711	π
17, 18	0.025 0504	π
19, 20	0.020 9289	0

Table C.2. $\beta = 1.27\Lambda_0 = 4.386\,491\,865\,710\,346$

j	$\lvert\Lambda_j/\Lambda_0\rvert$	$\arg \Lambda_j/\Lambda_0$
1, 2	0.255 461	$\pm$ 3.10797
3, 4	0.182 32	0
5, 6	0.099 9678	π
7,8	0.062 3182	π
9, 10	0.061 8773	0
11	0.058 2046	0
12, 13	0.054 083	0
14	0.035 4927	π
15,16	0.034 659	π
17,18	0.025 8057	π
19,20	0.021 5638	0

C.2. Parameter values: $\Delta = -1/2, h = 0.6, N = 12$

Leading eigenvalues of the quantum transfer matrix (1.2) at $z = 1$ for the stated parameters. Compare with section 4.

Table C.3. $\beta^{-1} = 0.362\ \Lambda_0 = 3.283\,047\,854\,941\,951$

j	$\lvert\Lambda_j/\Lambda_0\rvert$	$\arg \Lambda_j/\Lambda_0$
1	0.194 734	0
2-5	0.177 083	±0.589 88
6,7	0.113 666	±2.004 09
8,9	0.085 3754	0
10-13	0.084 9442	±0.736 87
14-17	0.046 6159	±2.137 06
18,19	0.044 6591	0
20	0.035 0166	0
21-24	0.030 9993	±0.013 7908

Table C.4. $\beta^{-1} = 0.227\,829\,01\ \Lambda_0 = 5.747\,005\,236\,172\,5825$

j	$\lvert\Lambda_j/\Lambda_0\rvert$	$\arg \Lambda_j/\Lambda_0$
1-4	0.2387	±0.221 125
5	0.200 083	0
6,7	0.192 645	±1.7485
8-11	0.141 971	± 0.441 855
12,13	0.140 684	0
14,15	0.099 414	0
16-19	0.085 2877	±1.73
20-23	0.065 09	±0.095 19

C.3. Parameter values: $\Delta = -1/2, h = 0, N = 12$

The following data can be compared against the results listed in tables IV and V of reference [6]. As mentioned in section 4, there are additional eigenvalues and different multiplicities in comparison with the data presented in [6] for the computation of correlation functions. The data missing from tables IV and V are highlighted in *italic* in tables C.5 and C.6.

Table C.5. $\beta^{-1} = 0.362\ \Lambda_0 = 2.679\,572\,704\,141\,509$

j	$\lvert\Lambda_j/\Lambda_0\rvert$	$\arg \Lambda_j/\Lambda_0$
1	0.186 218	0
2-5	0.185 895	±0.596 836
6-9	0.086 3447	±0.769 169
10,11	*0.085 0952*	π
12,13	*0.081 37*	*0*
14,15	*0.042 843*	*0*
16	*0.038 1078*	*0*
17,18	*0.033 2116*	*±1.973 97*
19-22	0.027 5197	π
23-26	0.026 8943	±0.745 11

Table C.6. $\beta^{-1} = 0.227\,829\,01\Lambda_0 = 4.173\,697\,553\,454\,863$

j	$\lvert\Lambda_j/\Lambda_0\rvert$	$\arg\Lambda_j/\Lambda_0$
1-4	0.238 817	±0.000 115 55
5,6	*0.181 564*	π
7	0.177 917	0
8-11	0.134 718	±0.457 658
12,13	*0.131 249*	*0*
14,15	0.090 3746	0
16-19	*0.064 1918*	π
20,21	0.056 0389	±0.766 974
22-25	0.0455 845	0

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