Q-systems with boundary parameters

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Abstract

Q-systems provide an efficient way of solving Bethe equations. We formulate here Q-systems for both the isotropic and anisotropic open Heisenberg quantum spin-1/2 chains with diagonal boundary magnetic fields. We check these Q-systems using novel discrete Wronskian-type formulas (relating the fundamental Q-function and its dual) that involve the boundary parameters.

Keywords: boundary integrability, Bethe ansatz, duality, Wronskian

1. Introduction

An efficient way of solving rational Bethe equations for periodic models was introduced in 2016 by Marboe and Volin [1]. This so-called Q-system method, which is an outgrowth of a long line of research (see e.g. [2–4] and references therein), has already been exploited in various investigations, see e.g. [5–10]. This method was recently generalized [11] for the rank-1 case in two different directions: from rational to trigonometric, and from periodic to open boundary conditions. However, there the models with boundaries were restricted to ‘free’ boundary conditions, without any boundary parameters. In this paper, we show how to further generalize the rank-1 Q-system, so as to incorporate two arbitrary boundary parameters. To check the new Q-systems, we use novel discrete Wronskian-type formulas (relating the fundamental Q-function and its dual) that involve the boundary parameters.

We start with the simpler case of the isotropic open Heisenberg quantum spin-1/2 chain with boundary magnetic fields in section 2, and we then consider the anisotropic case in section 3. We end with a brief conclusion in section 4. If the boundary parameters are on a special manifold, then a separate treatment of the Bethe equations is required, which is presented in appendix A. The closed spin chain with diagonal twisted boundary conditions is briefly discussed in appendix B.

2. Rational case

We consider here the isotropic (XXX) open Heisenberg quantum spin-1/2 chain of length $N$ with boundary magnetic fields, whose Hamiltonian is given by
\[ H = \sum_{k=1}^{N-1} \vec{\sigma}_k \cdot \vec{\sigma}_{k+1} - \frac{1}{\beta^2} \sigma_1^z + \frac{1}{\alpha} \sigma_N^z, \]  

(2.1)

where \( \alpha \) and \( \beta \) are arbitrary parameters. This model is \( U(1) \) invariant

\[ [H, S^z] = 0, \quad S^z = \sum_{k=1}^{N} \frac{1}{2} \sigma^z. \]  

(2.2)

The special rational case considered in [11] corresponds to the limit where both \( \alpha \) and \( \beta \) tend to infinity, in which case the model becomes \( SU(2) \) invariant. We discuss the Bethe ansatz solution of this model in section 2.1, and we present corresponding \( Q \)-systems in section 2.2.

2.1. Bethe ansatz

We begin by briefly reviewing the algebraic Bethe ansatz solution of the model (2.1) in section 2.1.1. The dual Bethe equations and dual \( TQ \)-equations are presented in section 2.1.2. Starting from a \( Q \)-function, we show in section 2.1.3 how to construct the corresponding dual \( Q \)-function, which will be needed for our later discussion of the \( Q \)-system. We shall see that the \( Q \)-function and its dual are related by a novel Wronskian-type formula that involves the boundary parameters.

2.1.1. Algebraic Bethe ansatz. The algebraic Bethe ansatz solution of the model (2.1) was formulated by Sklyanin [12]. Following the notations in [11], we consider the \( R \)-matrix (solution of the Yang–Baxter equation) given by the \( 4 \times 4 \) matrix

\[ R(u) = \begin{pmatrix} u - \frac{i}{2} & 0 \\ 0 & u + \frac{i}{2} \end{pmatrix} I + iP, \]  

(2.3)

where \( P \) is the permutation matrix and \( I \) is the identity matrix. We define the monodromy matrices

\[ \mathcal{M}_0(u) = R_{01}(u) R_{02}(u) \ldots R_{0N}(u), \]

\[ \hat{\mathcal{M}}_0(u) = R_{0N}(u) \ldots R_{02}(u) R_{01}(u). \]  

(2.4)

We consider the \( K \)-matrices (solutions of boundary Yang–Baxter equations) given by the diagonal \( 2 \times 2 \) matrices

\[ K_{0}(u) = \text{diag}(i \left( \alpha - \frac{1}{2} \right) + u, i \left( \alpha + \frac{1}{2} \right) - u), \]

\[ K_{L}(u) = \text{diag}(i \left( \beta - \frac{1}{2} \right) - u, i \left( \beta + \frac{1}{2} \right) + u), \]  

(2.5)

which evidently depend on the boundary parameters \( \alpha \) and \( \beta \), respectively. The transfer matrix \( T(u) = T(u; \alpha, \beta) \) is given by [12]

\[ T(u) = \text{tr}_0 U_0(u), \quad U_0(u) = \mathcal{K}_0(u) \mathcal{M}_0(u) \mathcal{K}_L(u) \hat{\mathcal{M}}_0(u). \]  

(2.6)

1 If we require \( H \) to be Hermitian, then \( \alpha \) and \( \beta \) must be real.

2 The coordinate Bethe ansatz solution was found in [13, 14]. For an introduction to algebraic Bethe ansatz, see e.g. [15].
which has the commutativity property
\[ [\mathcal{T}(u), \mathcal{T}(v)] = 0 \] (2.7)
and satisfies \( \mathcal{T}(-u) = \mathcal{T}(u) \). The Hamiltonian (2.1) is equal to \( \frac{1}{2\alpha(u)} \left. \frac{d^2}{du^2} \mathcal{T}(u) \right|_{u=i/2} \), up to an additive constant. If either of the boundary parameters vanishes, then a local integrable Hamiltonian can be obtained from the second derivative of the transfer matrix at \( u = i/2 \).

In order to construct eigenstates of the transfer matrix, we define the operators \( \mathcal{A}(u) \), \( \mathcal{B}(u) \), \( \mathcal{C}(u) \), \( \mathcal{D}(u) \) from \( \mathbb{U}_0(u) \) (2.6) as follows\(^3\):
\[ \mathbb{U}_0(u) = \left( \begin{array}{ccc} \delta_0(u) \mathcal{A}(u) \\ \mathcal{C}(u) \\ \delta_1(u) \mathcal{D}(u) + \delta_2(u) \mathcal{A}(u) \end{array} \right), \] (2.8)
with
\[ \delta_0(u) = \frac{u - i \left( \beta - \frac{1}{2} \right)}{u - i \left( \beta + \frac{1}{2} \right)}, \quad \delta_1(u) = \frac{u - i}{u}, \quad \delta_2(u) = -\frac{i \left( u + i \beta + \frac{1}{2} \right)}{2u \left( u - i \left( \beta + \frac{1}{2} \right) \right)}. \] (2.9)

Choosing the reference state
\[ |0\rangle = \left( \begin{array}{c} 1 \\ 0 \end{array} \right)^{\otimes N}, \] (2.10)
the Bethe states are defined by
\[ |u_1, \ldots, u_M\rangle = \prod_{k=1}^M \mathcal{B}(u_k)|0\rangle. \] (2.11)
These states are eigenstates of the transfer matrix \( \mathcal{T}(u) \) with eigenvalues \( T(u) \)
\[ \mathcal{T}(u)|u_1, \ldots , u_M\rangle = T(u)|u_1, \ldots , u_M\rangle, \] (2.12)
provided that \( \{u_1, \ldots, u_M\} \) are admissible solutions of the Bethe equations\(^4\):
\[ \frac{g(u_j - \frac{1}{2})}{f(u_j + \frac{1}{2})} \frac{u_j + i}{u_j - \frac{1}{2}} = \prod_{k=1, k \neq j}^M \frac{u_j - u_k + i}{u_j - u_k - i} \frac{(u_j + u_k + i)}{(u_j + u_k - i)}, \] (2.13)
where we have introduced the functions \( f(u) \) and \( g(u) \) defined by
\[ f(u) = (u - i\alpha)(u + i\beta), \quad g(u) = f(-u) = (u + i\alpha)(u - i\beta), \] (2.14)
which will play an important role in the following. The eigenvalues \( T(u) \) (which are necessarily polynomials in \( u^2 \)) are given by the \( TQ \)-equation
\[ -u T(u) Q(u) = (u^+)^{2N+1} g^-(u) Q^- (u) + (u^-)^{2N+1} f^+(u) Q^+(u), \] (2.15)
\(^3\)This construction is similar to, but not the same as, the one in [12].
\(^4\)Some solutions of the Bethe equations do not correspond to eigenvalues and eigenvectors of the transfer matrix. Examples include solutions with repeated Bethe roots; and, since the spin chain is open, solutions with the Bethe roots 0 or \( \pm i/2 \), see [11] and references therein. Here we call admissible those solutions of the Bethe equations that do correspond to genuine eigenvalues and eigenvectors of the transfer matrix.
where \( Q(u) \) is also a polynomial in \( u^2 \) defined by
\[
Q(u) = \prod_{k=1}^{M} (u - u_k)(u + u_k),
\]
(2.16)
and we use the standard notation \( F^\pm(u) = F(u \pm \frac{i}{2}) \) for any function \( F(u) \). For generic values of the boundary parameters, the transfer-matrix eigenvalues \( T(u) \) are not degenerate. For the special case \( \alpha - \beta = 1 \), the functions in (2.14) satisfy \( f^+ = g^- \), and the Bethe equation (2.13) must be slightly modified. This special case is discussed further in appendix A.

2.1.2. Duality. We observe that the transfer matrix is not invariant under charge conjugation \( C = (\sigma_x^+) \otimes N \); indeed, the boundary parameters become negated
\[
C T(u; \alpha, \beta) C = T(u; -\alpha, -\beta).
\]
(2.17)
Similarly, the \( B \) and \( C \) operators are related by
\[
C B(u; \alpha, \beta) C = C(u; -\alpha, -\beta).
\]
(2.18)
A given eigenstate of the transfer matrix with eigenvalue \( T(u) \) can be represented either by a Bethe state (2.11), or by a corresponding ‘dual’ Bethe state
\[
|\tilde{u}_1, \ldots, \tilde{u}_{\tilde{M}}\rangle = \prod_{k=1}^{\tilde{M}} C(\tilde{u}_k)|\tilde{0}\rangle
\]
(2.19)
constructed with the ‘dual’ reference state
\[
|\tilde{0}\rangle = C|0\rangle = \left( \begin{array}{c} 0 \\ 1 \end{array} \right) \otimes^N.
\]
(2.20)
Hence, the dual Bethe state satisfies
\[
\mathcal{T}(u)|\tilde{u}_1, \ldots, \tilde{u}_{\tilde{M}}\rangle = T(u)|\tilde{u}_1, \ldots, \tilde{u}_{\tilde{M}}\rangle,
\]
(2.21)
where \{\tilde{u}_1, \ldots, \tilde{u}_{\tilde{M}}\} satisfy the ‘dual’ Bethe equations\(^5\)
\[
f\left(\tilde{u}_j - \frac{i}{2}\right)\left(\tilde{u}_j + \frac{i}{2}\right)^{2N} = \prod_{k=1, k \neq j}^{\tilde{M}} \frac{\left(\tilde{u}_j - \tilde{u}_k + i\right)\left(\tilde{u}_j + \tilde{u}_k + i\right)}{\left(\tilde{u}_j - \tilde{u}_k - i\right)\left(\tilde{u}_j + \tilde{u}_k - i\right)},
\]
(2.22)
In terms of the dual Bethe roots, the eigenvalues \( T(u) \) are given by a ‘dual’ \( TQ \)-equation
\[
-u T(u) P(u) = (u^+)^{2N+1} f^+(u) P^{--}(u) + (u^-)^{2N+1} g^+(u) P^{++}(u),
\]
(2.23)
where \( P(u) \) is the corresponding ‘dual’ \( Q \)-function\(^6\)
\[
P(u) \propto \prod_{k=1}^{\tilde{M}} (u - \tilde{u}_k)(u + \tilde{u}_k).
\]
(2.24)
\(^5\)This fact was already noticed in [12].
\(^6\)We do not specify the overall constant in (2.24), which will be specified in (2.29) below.
The symbol $\propto$ used here and below denotes proportionality, i.e. equality up to a constant. The Bethe equation (2.13) and their duals (2.22), and similarly the $TQ$ equations (2.15) and (2.23), are related [as follows from (2.18)] by $\alpha \mapsto -\alpha$ and $\beta \mapsto -\beta$, together with $u_j \mapsto \bar{u}_j$. The fact that the Bethe equations and $TQ$-equation are not self-dual is a new feature of this problem. Indeed, for the periodic closed chain and for the $SU(2)$-invariant open chain considered earlier [11], the Bethe equations and $TQ$-equation are self-dual in this sense.

2.1.3. Wronskian-type formula. We now show that $Q(u)$ and $P(u)$ (the dual $Q$-function) satisfy a Wronskian-type formula, which will be needed in section 2.2. The result is similar to the one for the periodic closed chain [16]; however, there are some interesting new features, since the $TQ$-equation is no longer self-dual.

We begin by multiplying both sides of the $TQ$-equation (2.15) by $P$, 

$$-u T Q P = (u^+)^{2N+1} g^- Q^- P + (u^-)^{2N+1} f^+ Q^+ P; \quad (2.25)$$

and multiplying both sides of the dual $TQ$-equation (2.23) by $Q$, 

$$-u T Q P = (u^+)^{2N+1} f^- P^- Q + (u^-)^{2N+1} g^+ P^+ Q. \quad (2.26)$$

Subtracting these two equations, we obtain 

$$0 = (u^+)^{2N+1} W^- - (u^-)^{2N+1} W^+, \quad (2.27)$$

where we have introduced the function $W(u)$ defined by 

$$W = g^+ P^+ Q^- - f^- P^- Q^+. \quad (2.28)$$

We regard (2.27) as a functional equation for $W$, which has the solution $W \propto u^{2N+1}$. Since the proportionality constant is generically nonzero (exceptions can occur on the special manifold $\alpha - \beta = \pm 1$, see (A.5)), we normalize $P$ so that the constant is 1. We conclude that 

$$g^+ P^+ Q^- - f^- P^- Q^+ = u Q_{0,0}, \quad (2.29)$$

where we have set 

$$Q_{0,0}(u) = u^{2N} \quad (2.30)$$

in anticipation of a notation that will be introduced in section 2.2. The result (2.29) is an important discrete Wronskian-type formula relating $Q$ and $P$, which interestingly is ‘deformed’ by the functions $f$ and $g$ (2.14). Note that 

$$M + \tilde{M} = N, \quad (2.31)$$

where $2M$ and $2\tilde{M}$ are the degrees of $Q$ and $P$, respectively. We also note that by using (2.29) to eliminate $(u^+)^{2N+1}$ from the $TQ$-equation (2.15), we obtain 

$$-u T = g^+ g^- P^{++} Q^{--} - f^+ f^- P^{--} Q^{++}, \quad (2.32)$$

which is a deformation of another well-known result [16].

Let us pause to underscore the new insight that this problem has revealed. In the context of quantum integrability, the discrete Wronskian (or Casoratian) formula has generally been regarded (see e.g. [16]) as a relation between two solutions of the same finite-difference $TQ$-equation. However, we now recognize this to be an exceptional situation, which occurs when
the $TQ$-equation is self-dual. We should instead regard the Wronskian formula as a relation between a solution of the $TQ$-equation and a solution of the dual $TQ$-equation; and these two $TQ$-equations are generally not the same\textsuperscript{7}.

For the periodic chain, it was proved in [17, 18] that polynomiality of $P(u)$ is equivalent to the admissibility of the solution \{u\textsubscript{1}, \ldots, u\textsubscript{M}\} of the Bethe equations. We conjecture that a similar result is true for the open spin chain with diagonal boundary fields; namely, only those solutions \{u\textsubscript{1}, \ldots, u\textsubscript{M}\} of the Bethe equation (2.13) for which there exist corresponding solutions \{u\textsubscript{1}, \ldots, u\textsubscript{M}\} of the dual Bethe equation (2.22) such that the Wronskian formula (2.29) is satisfied are admissible.

### 2.2. Q-systems

We now look for a $Q$-system for the Bethe equation (2.13). Surprisingly, the answer is not unique; and we present two such $Q$-systems. For both systems, we take [as anticipated in (2.30)]

$$Q_{0,0}(u) = u^{2N},$$

and we identify $Q_{1,0}(u)$ as the fundamental $Q$-function (2.16)

$$Q_{1,0}(u) = Q(u) = \prod_{k=1}^{M} (u - u_{k})(u + u_{k}) = \sum_{k=0}^{M-1} c_{k} u^{2k} + u^{2M},$$

For the rank-1 case that we consider in this paper, there are only two nontrivial sets of $Q$-functions, namely, $Q_{0,0}(u)$ and $Q_{1,0}(u)$. Our two $Q$-systems are distinguished by which of these two sets of $Q$-functions are ‘deformed’ by the functions $f$ and $g$ defined in (2.14). We consider these systems separately in sections 2.2.1 and 2.2.2.

#### 2.2.1. Deforming $Q_{1,n}$

We begin by considering the following $Q$-system

$$u Q_{1,n} \propto f^{(-n-1)} Q_{1,n-1}^{+} - g^{(n-1)} Q_{1,n-1}^{-}, \quad n = 1, 2, \ldots,$$

$$u Q_{0,n} Q_{1,n-1} \propto Q_{1,n}^{+} Q_{0,n-1}^{+} - Q_{1,n}^{-} Q_{0,n-1}^{-}, \quad n = 1, 2, \ldots,$$

where we use the notation $F^{(n)}(u) = F(u + \frac{n}{2})$, and we remind the reader that the functions $f$ and $g$ are defined in (2.14). Comparing with the corresponding $Q$-system in [11], we see that only the relations for $Q_{1,n}$ are deformed by $f$ and $g$. We claim that all of these $Q$-functions are polynomials if and only if \{u\textsubscript{1}, \ldots, u\textsubscript{M}\} (given by zeros of $Q_{1,0}(u)$) is an admissible solution of the Bethe equation (2.13).

As a preliminary check of this $Q$-system, let us verify that it leads to the Bethe equations. We see appendix B.

\textsuperscript{7}In fact, the $TQ$-equation (2.15) has only one polynomial solution, instead of two. This can be understood heuristically from the fact that, in contrast with [16], here there is no notion of ‘equator’; due to the absence of $SU(2)$ symmetry, it is necessary to include values of $M$ (the number of Bethe roots) up to $N$, instead of $N/2$. Indeed, a second solution of (2.15) is $P = UP$, where $U$ satisfies $U^{2} = \frac{1}{2}$, which has a solution in terms of products of gamma functions

$$U(u) = \Gamma \left(ia + \frac{1}{2} + \alpha\right) \Gamma \left(-ia + \frac{1}{2} + \alpha\right) \Gamma \left(ia + \frac{1}{2} - \beta\right) \Gamma \left(-ia + \frac{1}{2} - \beta\right),$$

see appendix B.
equation (2.13). Equation (2.35) with \( n = 1 \) reads

\[
\begin{align*}
  u \, Q_{1,1}(u) &\propto f(u) \, Q_{1,0}^+(u) - g(u) \, Q_{1,0}^-(u), \\
  u \, Q_{0,1}(u) &\propto Q_{1,0}^+(u) \, Q_{0,0}(u) - Q_{1,1}(u) \, Q_{0,0}^+(u).
\end{align*}
\]

Performing in (2.36) the shifts \( u \mapsto u \pm \frac{i}{2} \) and evaluating at a Bethe root \( u = u_j \), we obtain

\[
\left( u_j + \frac{i}{2} \right) Q_{1,1}^+(u_j) \propto f^+(u_j) \, Q^{++}(u_j), \quad \left( u_j - \frac{i}{2} \right) Q_{1,1}^-(u_j) \propto -g^-(u_j) \, Q^{--}(u_j),
\]

since \( Q(u_j) = 0 \). Evaluating (2.37) at \( u = u_j \) gives

\[
Q_{1,1}^+(u_j) \, Q_{0,0}^+(u_j) = Q_{1,1}^-(u_j) \, Q_{0,0}^+(u_j).
\]

Finally, substituting (2.38) into (2.39), we indeed arrive at the Bethe equation (2.13). We have also verified numerically for small values of \( N \) that this \( Q \)-system reproduces the complete spectrum of the transfer matrix.

We can solve the \( Q \)-system (2.35) in terms of \( Q(u) \) and a function \( P(u) \) defined by the Wronskian-type formula (2.29). Indeed, we find that this system is solved by\(^8\)

\[
Q_{1,n} \propto D^n Q ,
\]

\[
u \, Q_{0,n} \propto g^n (D^n P)^+ (D^n Q)^- - f^{[-n]} (D^n P)^- (D^n Q)^+ ,
\]

where, as in [11], \( D^n P \) is defined by

\[
D^n P = \frac{1}{u} \left[ (D^{n-1} P)^+ - (D^{n-1} P)^- \right], \quad n = 1, 2, \ldots ,
\]

(2.41) and we now define \( D^n Q \) by

\[
D^n Q = \frac{1}{u} \left[ f^{[-(n-1)]} (D^{n-1} Q)^+ - g^{[n-1]} (D^{n-1} Q)^- \right], \quad n = 1, 2, \ldots .
\]

(2.42) Note that the expression for \( D^n P \) (2.41) is not deformed, while the expression for \( D^n Q \) (2.42) is deformed by \( f \) and \( g \). The solution (2.40) shows that polynomiality of \( P(u) \) is equivalent to polynomiality of all the \( Q \)-functions. Since polynomiality of \( P(u) \) is equivalent to the admissibility of the solution \( \{ u_1, \ldots , u_M \} \) (see section 2.1.3), we conclude that (2.35) is indeed a \( Q \)-system for the model (2.1).

2.2.2. Deforming \( Q_{0,n} \). We now consider a different \( Q \)-system

\[
\begin{align*}
  u \, Q_{1,n} \propto Q_{1,n-1}^+ - Q_{1,n-1}^- , \quad n = 1, 2, \ldots , \\
  u \, Q_{0,n} \propto Q_{1,n}^+ \, Q_{0,n-1}^+ - g^{[n]} Q_{1,n}^- \, Q_{0,n-1}^- , \quad n = 1, 2, \ldots ,
\end{align*}
\]

(2.43) where now the relations for \( Q_{1,n} \) are deformed by \( f \) and \( g \). We again claim that all the \( Q \)-functions are polynomials if and only if \( \{ u_1, \ldots , u_M \} \) is an admissible solution of the Bethe equations (2.13).

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\(^8\) Somewhat similar formulas have been known in the context of supersymmetric spin chains [19, 20].
Let us begin by verifying that this $Q$-system also leads to the Bethe equations (2.13). Equation (2.43) with $n = 1$ reads
\[ u Q_{1,1} (u) \propto Q_{1,0} (u) - Q_{0,0} (u), \tag{2.44} \]
\[ u Q_{0,1} (u) Q_{1,0} (u) \propto f^+ (u) Q_{1,1} (u) Q_{0,0} (u) - g^- (u) Q_{1,1} (u) Q_{0,0} (u). \tag{2.45} \]
Performing in (2.44) the shifts $u \mapsto u \pm i \frac{1}{2}$ and evaluating at a Bethe root $u = u_j$, we obtain
\[ \left( u_j + i \frac{1}{2} \right) Q_{1,1}^+ (u_j) \propto Q^{++} (u_j), \quad \left( u_j - i \frac{1}{2} \right) Q_{1,1}^- (u_j) \propto Q^{--} (u_j). \tag{2.46} \]
Evaluating (2.45) at $u = u_j$ gives
\[ f^+ (u_j) Q_{1,1}^+ (u_j) Q_{0,0}^- (u_j) = g^- (u_j) Q_{1,1}^- (u_j) Q_{0,0}^+ (u_j). \tag{2.47} \]
Finally, substituting (2.46) into (2.47), we again arrive at the Bethe equation (2.13). We have also verified numerically for small values of $N$ that this $Q$-system reproduces the complete spectrum of the transfer matrix.

We can also solve the $Q$-system (2.43) in terms of $Q(u)$ and a function $P(u)$ defined by the Wronskian-type formula (2.29). Indeed, we find that this system is solved by
\[ Q_{1,n} \propto D^n P, \]
\[ u Q_{0,n} \propto g^{[n]} (D^n P)^+ (D^n Q)^- - f^{[n]} (D^n P)^- (D^n Q)^+, \tag{2.48} \]
where $D^n P$ is now defined by
\[ D^n P = \frac{1}{u} \left[ g^{[-n-1]} (D^{n-1} P)^+ - f^{-[n]} (D^{n-1} P)^- \right], \quad n = 1, 2, \ldots, \tag{2.49} \]
while $D^n Q$ is defined by
\[ D^n Q = \frac{1}{u} \left[ (D^{n-1} Q)^+ - (D^{n-1} Q)^- \right] \quad n = 1, 2, \ldots. \tag{2.50} \]
Note that now the expression for $D^n P$ (2.49) is deformed, while the expression for $D^n Q$ (2.50) is not deformed. The solution (2.48) shows that polynomiality of $P(u)$ is equivalent to polynomiality of all the $Q$-functions, hence (2.43) is also a $Q$-system for the model (2.1).

3. Trigonometric case

We now consider the anisotropic (XXZ) open Heisenberg quantum spin-1/2 chain of length $N$ with anisotropy parameter $\eta$ and with diagonal boundary magnetic fields, whose Hamiltonian is given by
\[ H = \sum_{k=1}^{N-1} \left[ \sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \cosh(\eta) \sigma_k^z \sigma_{k+1}^z \right] - \sinh(\eta) \coth(\beta \eta) \sigma_1^z + \sinh(\eta) \coth(\alpha \eta) \sigma_N^z, \tag{3.1} \]
where $\alpha$ and $\beta$ are arbitrary parameters. This model reduces to the isotropic model (2.1) in the limit $\eta \to 0$, and, like the latter, is $U(1)$ invariant (2.2). The special trigonometric case considered in [11] corresponds to the limit where both $\alpha$ and $\beta$ tend to infinity, in which case the model becomes $U_q(su(2))$ invariant. We first discuss the Bethe ansatz solution of this model in section 3.1, and we then present corresponding $Q$-systems in section 3.2.

3.1. Bethe ansatz

The algebraic Bethe ansatz solution of the anisotropic model (3.1) is similar to the one for its isotropic limit (2.1) discussed in section 2.1. Hence, we present only the salient formulas.

The $R$-matrix is now given by

$$
\mathbb{R}(u) = \begin{pmatrix}
\sinh \left( u + \frac{\eta}{2} \right) & 0 & 0 & 0 \\
0 & \sinh \left( u - \frac{\eta}{2} \right) & \sinh(\eta) & 0 \\
0 & \sinh(\eta) & \sinh \left( u - \frac{\eta}{2} \right) & 0 \\
0 & 0 & 0 & \sinh \left( u + \frac{\eta}{2} \right)
\end{pmatrix},
$$

(3.2)

and the $K$-matrices are given by

$$
\mathbb{K}^L(u) = \text{diag} \left( \sinh \left( \eta \left( \alpha - \frac{1}{2} \right) + u \right), \sinh \left( \eta \left( \alpha + \frac{1}{2} \right) - u \right) \right),
$$

$$
\mathbb{K}^R(u) = \text{diag} \left( \sinh \left( \eta \left( \beta - \frac{1}{2} \right) - u \right), \sinh \left( \eta \left( \beta + \frac{1}{2} \right) + u \right) \right).
$$

(3.3)

These matrices reduce to (2.3) and (2.5), respectively, by setting $u \mapsto \epsilon u$, $\eta \mapsto i \epsilon$ and letting $\epsilon \to 0$. The Hamiltonian (3.1) is proportional to $\frac{d \mathbb{R}(u)}{du} \bigg|_{u=\eta/2}$, up to an additive constant.

The Bethe equations are now given by

$$
g(u_j - \frac{\eta}{2}) \left( \frac{\sinh \left( u_j + \frac{\eta}{2} \right)}{\sinh \left( u_j - \frac{\eta}{2} \right)} \right)^{2N} = \prod_{k=1,k \neq j}^{M} \frac{\sinh \left( u_j - u_k + \eta \right) \sinh \left( u_j + u_k + \eta \right)}{\sinh \left( u_j - u_k - \eta \right) \sinh \left( u_j + u_k - \eta \right)},
$$

$$
j = 1, \ldots, M, \quad M = 0, \ldots, N,
$$

(3.4)

where the functions $f(u)$ and $g(u)$ are now given by

$$
f(u) = \sinh(u - \eta \alpha) \sinh(u + \eta \beta), \quad g(u) = f(-u) = \sinh(u + \eta \alpha) \sinh(u - \eta \beta),
$$

(3.5)

cf (2.13) and (2.14). The $TQ$-equation becomes

$$
- \sinh(2u) T(u) Q(u) = \sinh(2u + \eta) \sinh^{2N} \left( u + \frac{\eta}{2} \right) g^-(u) Q^- (u)
$$

$$
+ \sinh(2u - \eta) \sinh^{2N} \left( u - \frac{\eta}{2} \right) f^+(u) Q^+ (u),
$$

(3.6)
with

\[ Q(u) = \prod_{k=1}^{M} \sinh(u - u_k) \sinh(u + u_k), \] (3.7)

where we now use the notation \( F^\pm(u) = F(u \pm \frac{\eta}{2}) \), cf (2.15) and (2.16). The \( Q \)-function is a polynomial in \( t^2 \) and \( t^{-2} \), where \( t = e^u \).

The dual Bethe equations are now given by

\[ f(\tilde{u}_j - \frac{\eta}{2}) \left( \frac{\sinh(\tilde{u}_j + \frac{\eta}{2})}{\sinh(\tilde{u}_j - \frac{\eta}{2})} \right)^{2N} = \prod_{k=1,k\neq j}^M \frac{\sinh(\tilde{u}_j - \tilde{u}_k + \eta)}{\sinh(\tilde{u}_j - \tilde{u}_k - \eta)} \sinh(\tilde{u}_j + \tilde{u}_k + \eta), \]

\[ j = 1, \ldots, M, \quad M = 0, \ldots, N, \] (3.8)

and the dual \( TQ \)-equation is

\[ -\sinh(2u) \, T(u) \, P(u) = \sinh(2u + \eta) \sinh^{2N} \left( u + \frac{\eta}{2} \right) f^{-} (u) \, P^{-} (u) + \sinh(2u - \eta) \sinh^{2N} \left( u - \frac{\eta}{2} \right) g^{+} (u) \, P^{+} (u), \] (3.9)

where \( P(u) \) is the corresponding dual \( Q \)-function

\[ P(u) \propto \prod_{k=1}^{M} \sinh(u - \tilde{u}_k) \sinh(u + \tilde{u}_k), \] (3.10)

cf (2.22)–(2.24). Finally, the Wronskian-type relation becomes

\[ g \, P^{+} \, Q^{-} - f \, P^{-} \, Q^{+} = \sinh(2u) \, Q_{0,0}, \] (3.11)

where \( Q_{0,0}(u) \) is given by (3.12), cf (2.32). As in the rational case, more care is required when the boundary parameters lie on the special manifold \( \alpha - \beta = \pm 1 \).

3.2. \( Q \)-systems

We now look for a \( Q \)-system for the Bethe equation (3.4). As in the rational case, we find two such systems. For both systems, we take

\[ Q_{0,0}(u) = \sinh^{2N}(u), \] (3.12)

and we identify \( Q_{1,0}(u) \) as the fundamental \( Q \)-function (3.7)

\[ Q_{1,0} (u) = Q(u) = \sum_{k=0}^{M-1} c_k \left( e^{2ak} + e^{-2ak} \right) + e^{2aM} + e^{-2aM}. \] (3.13)

We present the two \( Q \)-systems separately in sections 3.2.1 and 3.2.2.

3.2.1. Deforming \( Q_{1,n} \). We begin by considering the following \( Q \)-system

\[ \sinh(2u) \, Q_{1,n} \propto f^{\pm(n-1)} \, Q_{1,n-1}^{\pm} - g^{\pm(n-1)} \, Q_{1,n-1}^{\pm}, \quad n = 1, 2, \ldots, \]

\[ \sinh(2u) \, Q_{0,n} \propto Q_{1,n}^{\pm} \, Q_{0,n-1}^{\pm} - Q_{1,n}^{\pm} \, Q_{0,n-1}^{\pm}, \quad n = 1, 2, \ldots, \] (3.14)
where now $F^{[n]}(u) = F(u + \frac{n}{2})$, and the functions $f$ and $g$ are defined in (3.5). As in (2.35), the relations for $Q_{1,n}$ are deformed by $f$ and $g$. All the $Q$-functions must now be polynomials in $t^2$ and $t^2$, where $t = e^u$.

By repeating the steps (2.45)–(2.47), one can easily verify that the $Q$-system (3.14) indeed leads to the Bethe equation (3.4). We have also verified numerically for small values of $N$ that this $Q$-system reproduces the complete spectrum of the transfer matrix.

We can solve the $Q$-system (3.14) in terms of $Q(u)$ and a function $P(u)$ defined by the Wronskian-type formula (3.11). Indeed, we find that this system is solved by

$$Q_{1,n} \propto D^n Q,$$

$$\sinh(2u) Q_{0,n} \propto g^{[n]} (D^n P)^+(D^n Q)^- - f^{[n]} (D^n P)^-(D^n Q)^+, \quad n = 1, 2, \ldots ,$$

(3.15)

where, similarly to [11], $D^n P$ is defined by

$$D^n P = \frac{1}{\sinh(2u)} \left[ (D^{n-1} P)^+ - (D^{n-1} P)^- \right], \quad n = 1, 2, \ldots ,$$

(3.16)

and we now define $D^n Q$ by

$$D^n Q = \frac{1}{\sinh(2u)} \left[ f^{[n]} (D^{n-1} Q)^+ - g^{[n]} (D^{n-1} Q)^- \right], \quad n = 1, 2, \ldots .$$

(3.17)

The solution (3.15) shows that polynomiality (in $t^2$ and $t^2$) of $P(u)$ is equivalent to polynomiality of all the $Q$-functions, hence (3.14) is indeed a $Q$-system for the model (3.1).

3.2.2. Deforming $Q_{0,n}$. We now consider a different $Q$-system

$$\sinh(2u) Q_{1,n} \propto Q_{1,n-1}^+ - Q_{1,n-1}^- , \quad n = 1, 2, \ldots ,$$

$$\sinh(2u) Q_{0,n} Q_{0,n-1}^+ - f^{[n]} Q_{0,n}^+ Q_{0,n-1}^- - g^{[n]} Q_{0,n}^- Q_{0,n-1}^+ , \quad n = 1, 2, \ldots .$$

(3.18)

where now the relations for $Q_{0,n}$ are deformed by $f$ and $g$. Again, all the $Q$-functions must be polynomials in $t^2$ and $t^2$, where $t = e^u$.

By repeating the steps (2.45)–(2.47), we verify that this $Q$-system also leads to the Bethe equation (2.13). We have also verified numerically for small values of $N$ that this $Q$-system reproduces the complete spectrum of the transfer matrix.

We can also solve the $Q$-system (3.18) in terms of $Q(u)$ and a function $P(u)$ defined by the Wronskian-type relation (3.11). Indeed, we find that this system is solved by

$$Q_{1,n} \propto D^n Q,$$

$$\sinh(2u) Q_{0,n} \propto g^{[n]} (D^n P)^+(D^n Q)^- - f^{[n]} (D^n P)^-(D^n Q)^+, \quad n = 1, 2, \ldots ,$$

(3.19)

where $D^n P$ is now defined by

$$D^n P = \frac{1}{\sinh(2u)} \left[ g^{[n-1]} (D^{n-1} P)^+ - f^{[n-1]} (D^{n-1} P)^- \right], \quad n = 1, 2, \ldots ,$$

(3.20)
while $D^nQ$ is defined by
\[
D^nQ = \frac{1}{\sinh(2u)} \left[ (D^{n-1}Q)^+ - (D^{n-1}Q)^- \right] \quad n = 1, 2, \ldots \tag{3.21}
\]

The solution (3.19) shows that polynomiality (in $t^2$ and $t^{-2}$) of $P(u)$ is equivalent to polynomiality of all the $Q$-functions, hence (3.18) is also a $Q$-system for the model (3.1).

4. Conclusions

We have shown that boundary parameters can be introduced in rank-1 $Q$-systems, for both the rational (2.35) and (2.43) and trigonometric (3.14) and (3.18) cases. We have also found novel Wronskian-type formulas involving the boundary parameters (2.29) and (3.11). More generally, we have recognized that such Wronskian formulas should be understood as relations between a solution of the $TQ$-equation and a solution of the dual $TQ$-equation; and that these two $TQ$-equations are generally not the same. We expect that these results will have applications to various integrable boundary problems in AdS/CFT and statistical mechanics, as has already occurred for integrable periodic problems [5–10].

For the rational case, operators whose eigenvalues are given by $Q(u)$ and $P(u)$ have been constructed in [21], called there $Q_+$ and $Q_-$. It would be interesting to prove the Wronskian-type formula (2.35) directly for the corresponding operators. These operators should provide, through (2.40) and (2.48), realizations of $Q$-operators satisfying the $Q$-systems (2.35) and (2.43), respectively. Trigonometric generalizations of these operators have been considered in [22].

We have restricted our attention here to cases with diagonal $K$-matrices (2.5) and (3.3). It would be very interesting if these results could be further generalized to cases with non-diagonal $K$-matrices [23, 24], where the Bethe equations are significantly more complicated [25–27]. It would also be interesting to consider generalizations to rank higher than one. Indeed, perhaps we can now speculate that all integrable problems can be reformulated as $Q$-systems.

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Appendix A. The special manifold $\alpha - \beta = \pm 1$

The Bethe equation (2.13) or dual Bethe equation (2.22) become modified if the boundary parameters $\alpha$ and $\beta$ are on the special manifold $\alpha - \beta = \pm 1$. We consider separately the cases $\alpha - \beta = 1$ and $\alpha - \beta = -1$.

A.1. The case $\alpha - \beta = 1$

We first consider the case when the boundary parameters satisfy $\alpha - \beta = 1$. For definiteness, we set $\beta = \alpha - 1$, with $\alpha$ a free parameter. For this case, since the functions in (2.14) satisfy
$f^+ = g^-$, the Bethe equations are no longer given by (2.13); instead, they are

$$f \left( u_j + \frac{i}{2} \right) \left[ \left( \frac{u_j + i}{u_j - \frac{i}{2}} \right)^{2N} - \prod_{k=1, k \neq j}^{M} \left( \frac{u_j - u_k + i}{u_j - u_k - i} \right) \right] = 0,$$

$$j = 1, \ldots, M, \quad M = 0, \ldots, N. \quad (A.1)$$

Indeed, (A.1) are the conditions for the rhs of the $TQ$-equation (2.15) to vanish when $f^+ = g^-$ and $u = u_j$. In other words, a Bethe root $u_j$ must obey either $f(u_j + \frac{i}{2}) = 0$, i.e.

$$u_j = \pm i \left( \alpha - \frac{1}{2} \right), \quad (A.2)$$

or

$$\left( \frac{u_j + i}{u_j - \frac{i}{2}} \right)^{2N} = \prod_{k=1, k \neq j}^{M} \left( \frac{u_j - u_k + i}{u_j - u_k - i} \right) \left( \frac{u_j + u_k + i}{u_j + u_k - i} \right). \quad (A.3)$$

A similar example has been discussed in appendix B.3 of [28]. Since $f^- \neq g^+$, the dual Bethe equations for this case are still given by (2.22).

Since Bethe roots are not repeated, there are only two possible classes of configurations of Bethe roots $\mathcal{S} = \{u_1, \ldots, u_M\}$:

- class I $\mathcal{S}$ contains one Bethe root of the form (A.2)
- class II $\mathcal{S}$ does not contain any Bethe roots of the form (A.2)

Let us first consider class I. Since the corresponding $Q$-function vanishes at $u = i(\alpha - \frac{1}{2})$, $Q(u)$ must contain $f^+(u)$ as one of its factors. We conjecture that

$$Q(u) = f^+(u) P(u) \quad (\text{class I}), \quad (A.4)$$

where $P(u)$ is the dual $Q$-function. Indeed, by substituting (A.4) into the $TQ$-equation (2.15), and making use of the fact $f^+ = g^-$, we obtain the dual $TQ$-equation (2.23). Moreover, we have verified (A.4) numerically for several examples. It follows from (A.4) and $f^+ = g^-$ that the Wronskian vanishes

$$g^{P^+} Q^- - f^+ P^- Q^+ = 0 \quad (\text{class I}). \quad (A.5)$$

For class II, all the Bethe roots satisfy (A.3), which are the Bethe equations for the $SU(2)$-invariant model (see e.g. [11]).

### A.2. The case $\alpha - \beta = -1$

Let us now consider the case when the boundary parameters satisfy $\alpha - \beta = -1$. For definiteness, we set $\beta = \alpha + 1$, with $\alpha$ a free parameter. Since $f^+ \neq g^-$, the Bethe equations are still given by (2.13). However, now $f^- = g^+$; hence, the dual Bethe equations are no longer given by (2.22), and are instead given by

$$f \left( \tilde{u}_j - \frac{i}{2} \right) \left[ \left( \frac{\tilde{u}_j + i}{\tilde{u}_j - \frac{i}{2}} \right)^{2\tilde{M}} - \prod_{k=1, k \neq j}^{\tilde{M}} \left( \frac{\tilde{u}_j - \tilde{u}_k + i}{\tilde{u}_j - \tilde{u}_k - i} \right) \right] = 0,$$

$$j = 1, \ldots, \tilde{M}, \quad \tilde{M} = 0, \ldots, N. \quad (A.6)$$
These are the conditions for the rhs of the dual $TQ$-equation (2.23) to vanish when $f^- = g^+$ and $u = \tilde{u}_j$. Hence, a dual Bethe root $\tilde{u}_j$ must obey either $f(\tilde{u}_j - i) = 0$, i.e.

\[ \tilde{u}_j = \pm i \left( \alpha + \frac{1}{2} \right), \] (A.7)

or

\[ \left( \frac{\tilde{u}_j + \frac{1}{2}}{\tilde{u}_j - \frac{1}{2}} \right)^{2N} = \prod_{k=1; k \neq j}^{\tilde{m}} \frac{\tilde{u}_j - \tilde{u}_k + i}{\tilde{u}_j - \tilde{u}_k - i} \frac{\tilde{u}_j + \tilde{u}_k + i}{\tilde{u}_j + \tilde{u}_k - i}. \] (A.8)

There are two classes of configurations of dual Bethe roots $\tilde{S} = \{ \tilde{u}_1, \ldots, \tilde{u}_\tilde{m} \}$:

- class I $\tilde{S}$ contains one dual Bethe root of the form (A.7)
- class II $\tilde{S}$ does not contain any dual Bethe roots of the form (A.7)

For class I, since the dual $Q$-function vanishes at $u = i(\alpha + \frac{1}{2})$, $P(u)$ must contain $f^-$ as one of its factors. We conjecture that

\[ P(u) = f^-(u) Q(u) \] (class I).

Indeed, by substituting (A.9) into the dual $TQ$-equation (2.23), and making use of $f^- = g^+$, we obtain the $TQ$-equation (2.15). It follows that the Wronskian vanishes, as in (A.5).

### Appendix B. Transformations of $TQ$-equations and Wronskian relations

The open spin chain with diagonal boundary fields considered in this paper is not the first example of a model whose $TQ$-equation and its dual are not the same, and whose Wronskian relation does not have the ordinary form. Indeed, the closed chain with diagonal twisted boundary conditions has long been known to also have these features. Interestingly, for the latter model, it has also been known that there is a transformation that brings both the $TQ$-equation and its dual to the same ordinary form; and that there is a transformation that brings the Wronskian relation to the ordinary form. The price for obtaining the ordinary formulas is that the transformed functions ($Q$ and/or $P$) are no longer polynomial. We briefly review these results in section B.1, and we then consider corresponding transformations for the open chain in section B.2.

#### B.1. Twisted boundary conditions

For the closed spin chain with diagonal twisted boundary conditions, the transfer matrix is given by

\[ T(u) = tr_0 \mathbb{F}_0 \mathbb{M}_0 (u), \quad \mathbb{F} = \text{diag} \left( e^{i \frac{\phi}{2}}, e^{i \frac{\phi}{2}} \right), \] (B.1)

where $\phi$ is a constant ($u$-independent) twist angle. As is well known, the corresponding $TQ$-equation is given by

\[ TQ = e^{-i \frac{\phi}{2}} (u^+)^N Q^- + e^{i \frac{\phi}{2}} (u^-)^N Q^+, \] (B.2)

the dual $TQ$-equation is given by

\[ TP = e^{i \frac{\phi}{2}} (u^+)^N P^- + e^{-i \frac{\phi}{2}} (u^-)^N P^+, \] (B.3)
while the discrete Wronskian relation is given by
\[ e^{-\frac{i}{\tau} P^+ Q^-} - e^{i\frac{\tau}{2}} P^- Q^+ = u^N. \] (B.4)

Both \( P(u) \) and \( Q(u) \) are polynomials in \( u \). As in the case of the open chain with diagonal boundary fields discussed in sections 2.1.2 and 2.1.3, the \( TQ \)-equation (B.2) is not the same as the dual \( TQ \)-equation (B.3), and the Wronskian relation (B.4) is not the ordinary one. Nevertheless, as is also well known, it is possible to transform \( P \) and \( Q \) so that both transformed functions obey the same ordinary \( TQ \)-equation. Alternatively, by transforming only \( P \), it is possible to bring the Wronskian relation to the ordinary form.

Indeed, in terms of the transformed functions
\[ Q'(u) = e^{\frac{\tau}{2}} Q(u), \quad P'(u) = e^{-\frac{\tau}{2}} P(u), \] (B.5)
the \( TQ \)-equation and its dual both take the same ordinary form
\[ T Q' = (u^+)N Q'^-- + (u^-)N Q'^+, \]
\[ T P' = (u^+)N P'^-- + (u^-)N P'^+, \] (B.6)
except that \( Q' \) and \( P' \) are not polynomials.

Alternatively, one can transform only \( P \)
\[ P''(u) = e^{-iu_0} P(u), \] (B.7)
in which case the Wronskian relation takes the ordinary form
\[ P''+ Q^- - P''- Q^+ = e^{-iu_0} u^N, \] (B.8)
i.e. with trivial coefficients on the lhs, but \( P'' \) is not a polynomial.

**B.2. The open chain revisited**

Returning to the open spin chain, it is natural to ask whether transformations analogous to (B.5) and (B.7) can be found to bring the \( TQ \)-equations (2.15) and (2.23) to the same more-ordinary form, and to bring the Wronskian relation (2.29) to a more ordinary form, respectively. As we shall see, only the latter is possible.

We begin by defining, in analogy with (B.5), the new \( Q \)-function
\[ Q'(u) = S(u) Q(u), \] (B.9)
and we look for a function \( S(u) \) that brings the \( TQ \)-equation to a more ordinary form. To this end, we multiply both sides of the \( TQ \)-equation (2.15) by \( S \), and we demand that it have the same form as for the \( SU(2) \)-invariant open chain [11]
\[ -u T Q' = (u^+)2N+1 Q'^- - (u^-)2N+1 Q'^+, \] (B.10)
which requires that the function \( S \) satisfy
\[ S'^- = g^- S, \] (B.11)
\[ S'^+ = f^+ S. \] (B.12)
However, performing a + shift of (B.11) and − shift of (B.12), we obtain the relations

\[
S^- = g S^+,
\]
\[
S^+ = f S^-,
\] (B.13)

which imply the consistency condition \(fg = 1\), which is not satisfied. (Recall that \(f\) and \(g\) are given by (2.14).) We conclude that it is not possible to bring the \(TQ\)-equation (2.15) to the more ordinary form (B.10) by the transformation (B.9), and similarly for the dual \(TQ\)-equation (2.23).

We finally consider, in analogy with (B.7), the new \(P\)-function

\[
P''(u) = V(u) P(u),
\] (B.14)

and we look for a function \(V(u)\) that brings the Wronskian relation to a more ordinary form. To this end, we multiply both sides of the Wronskian relation (2.29) by \(V\), and we demand that it take the form

\[
P''^+ Q^- - P''^- Q^+ = u V Q_{0,0},
\] (B.15)

which requires that \(P''\) satisfy

\[
P''^+ = g V P^+,
\]
\[
P''^- = f V P^-.
\] (B.16) (B.17)

Performing a − shift of (B.16) and + shift of (B.17), we obtain the relations

\[
P' = g^- V^- P,
\]
\[
P' = f^+ V^+ P,
\] (B.18)

which imply that \(V(u)\) must satisfy the functional relation

\[
\frac{V^+}{V^-} = \frac{g^-}{f^+},
\] (B.19)

which has a solution in terms of products of gamma functions

\[
V(u) = \Gamma(iu + \alpha) \Gamma(-iu + \alpha) \Gamma(iu - \beta) \Gamma(-iu - \beta).
\] (B.20)

We conclude that the transformation (B.14) with \(V(u)\) given by (B.20) indeed brings the Wronskian relation (2.29) to the more ordinary form (B.15), where however \(P''(u)\) is not polynomial.
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