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An inhomogeneous $T$-$Q$ equation for the open XXX chain with general boundary terms: completeness and arbitrary spin

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Abstract
An inhomogeneous $T$-$Q$ equation has recently been proposed by Cao, Yang, Shi and Wang for the open spin-1/2 XXX chain with general (nondiagonal) boundary terms. We argue that a simplified version of this equation describes all the eigenvalues of the transfer matrix of this model. We also propose a generating function for the inhomogeneous $T$-$Q$ equations of arbitrary spin.

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1. Introduction

The open spin-1/2 XXZ quantum spin chain with general (nondiagonal) boundary terms has long been known to be integrable [1–3]. Nevertheless, the Bethe ansatz solution of this model has remained elusive. One of the difficulties is that a reference state (simple eigenstate of the transfer matrix) is not available.

Another (perhaps related) difficulty concerns the so-called Baxter $T$-$Q$ equation. For the periodic spin-1/2 XXX chain, given an eigenvalue $T$ of the transfer matrix (which is a polynomial function of the spectral parameter), the $T$-$Q$ equation is a homogeneous linear second-order finite-difference equation for $Q$, which is also a polynomial function of the spectral parameter. However, for the corresponding open chain with general boundary terms, the asymptotic behavior of $T$ for large values of the spectral parameter is not compatible with both (i) a conventional (homogeneous) $T$-$Q$ equation and (ii) $Q$-functions that are polynomial functions of the spectral parameter (see e.g. [11]).

An important advance was recently made by Cao, Yang, Shi and Wang (CYSW) [12, 13] (see also [14, 15]), who proposed to use instead an inhomogeneous $T$-$Q$ equation. Although the inhomogeneous term in the $T$-$Q$ equation gives rise to an unconventional term in the Bethe

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1 Solutions have been known for various special cases, such as diagonal boundary terms [1, 4–6] and nondiagonal boundary terms whose boundary parameters obey certain constraints [7–10].
equations, it overcomes the difficulty of reconciling the asymptotic behavior of $T$ with $Q$’s that are polynomial functions of the spectral parameter.

Several interesting questions about this approach remain to be addressed, and in this note we focus on two of them: the completeness of the proposed solution, and the generalization to higher spin. For simplicity, we restrict to the isotropic (XXX) chain. After briefly reviewing in section 2 the solution proposed by CYSW [12], we argue in section 3 that a simplified version of their solution is already complete. Hence, every eigenvalue of the transfer matrix can be characterized by a set of Bethe roots. In section 4, we formulate the inhomogeneous $T$-$Q$ equation for an auxiliary space of arbitrary spin. We briefly summarize our conclusions and mention some outstanding problems in section 5.

2. The CYSW solution

Following [12], we consider an open spin-1/2 XXX chain of length $N$, with the Hamiltonian

$$H = \sum_{n=1}^{N-1} \sigma_n \cdot \sigma_{n+1} + \frac{1}{q}(\sigma_1^x + \xi \sigma_1^y) + \frac{1}{p}\sigma_N^y,$$

where $p$, $q$, $\xi$ are arbitrary boundary parameters. The corresponding transfer matrix is given by

$$T(u) = \text{tr}_0 K_0^+(u) T_0(u) K_0^-(u),$$

where the monodromy matrices are given by

$$T_0(u) = R_{01}(u) \cdots R_{0N}(u), \quad \hat{T}_0(u) = R_{0N}(u) \cdots R_{01}(u).$$

The $R$-matrix is an $SU(2)$-invariant solution of the Yang–Baxter equation given by

$$R(u) = u + \mathcal{P},$$

where $\mathcal{P}$ is the permutation matrix; and the $K$-matrices are corresponding solutions of the boundary Yang–Baxter equations given by [2, 3]

$$K^-(u) = \begin{pmatrix} p+u & 0 \\ 0 & p-u \end{pmatrix}, \quad K^+(u) = \begin{pmatrix} q+u+1 & \xi(u+1) \\ \xi(u+1) & q-u-1 \end{pmatrix}.$$ (5)

The transfer matrix has the commutativity property $[T(u), T(v)] = 0$, and is therefore the generating function of a family of commuting operators, among which is the Hamiltonian (1).

CYSW proposed the following inhomogeneous $T$-$Q$ equation:

$$\Lambda^{(\pm)}(u) Q^{(\pm)}(u) Q^{(\pm)}_1(u) Q^{(\pm)}_2(u) = \tilde{a}^{(\pm)}(u) Q^{(\pm)}(u-1) Q^{(\pm)}_1(u-1) Q^{(\pm)}_2(u)$$

$$+ 2(1 - \sqrt{1 + \xi^2}) (u(u+1))^{2N+1}.$$

where

$$\tilde{a}^{(\pm)}(u) = \frac{2u + 2}{2u + 1} (u \pm p)(\sqrt{1 + \xi^2}u \pm q)(u+1)^{2N}, \quad \tilde{a}^{(\pm)}(u) = \tilde{a}^{(\pm)}(-u - 1),$$ (7)

2 The most general boundary terms would consist of $\sigma_n^x$, $\sigma_n^y$, $\sigma_n^z$, $\sigma_n^x$, $\sigma_n^y$, $\sigma_n^z$, each with independent boundary parameters as coefficients. However, $\sigma_n^x$ and $\sigma_n^y$ can be eliminated by a global $SU(2)$ rotation, and $\sigma_n^z$ can easily be accommodated by using a non-symmetric generalization of the matrix $K^+(u)$ in equation (5).

3 For simplicity, we set to zero the inhomogeneity parameters $\theta_1, \ldots, \theta_N$ appearing in [12].
and $\Lambda^{(\pm)}(u)$ are the eigenvalues of the transfer matrix (2). Moreover, the $Q$ are polynomial functions of $u$ given by

$$Q^{(\pm)}(u) = \prod_{j=1}^{N-2M} \left( u - \lambda_j^{(\pm)} \right) \left( u + \lambda_j^{(\pm)} + 1 \right),$$

$$Q^{(\pm)}_1(u) = \prod_{j=1}^{M} \left( u - \mu_j^{(\pm)} \right) \left( u + \nu_j^{(\pm)} + 1 \right),$$

$$Q^{(\pm)}_2(u) = \prod_{j=1}^{M} \left( u - \nu_j^{(\pm)} \right) \left( u + \mu_j^{(\pm)} + 1 \right),$$

where $M = 0, \ldots, \left\lfloor \frac{N}{2} \right\rfloor$. The key feature is the final (inhomogeneous) term in (6), which is absent if the Hamiltonian (1) has only diagonal boundary terms ($\xi = 0$). As usual, the Bethe equations follow from the $T$-$Q$ equation and the requirement that the eigenvalues of the transfer matrix cannot have poles. The eigenvalues of the Hamiltonian are given in terms of the Bethe roots (zeros of $Q$-functions) by

$$E^{(\pm)} = 2 \sum_{j=1}^{N-2M} \frac{1}{\lambda_j^{(\pm)} (\lambda_j^{(\pm)} + 1)} + 2 \sum_{j=1}^{M} \left( \frac{1}{\nu_j^{(\pm)}} - \frac{1}{\mu_j^{(\pm)} + 1} \right) + c. \quad (9)$$

3. Completeness

An important question is whether this solution is complete; i.e., whether every eigenvalue of the transfer matrix (2) can be expressed in the form (6). CYSW conjectured [12] that completeness is achieved by taking $M = \frac{N}{2}$ for $N$ even ($M = \frac{N+1}{2}$ for $N$ odd) in (8), and by also considering both signs ($\pm$) in equations (6)–(9), as in [9].

We conjecture that the situation is considerably simpler: it is enough to take $M = 0$ in (8), and consider just one sign (say, $+$) in equations (6)–(9). In other words, we claim that completeness can be achieved (for any value of $N$) with the following linear $T$-$Q$ equation:

$$\Lambda(u)Q(u) = \tilde{a}(u)Q(u-1) + \tilde{d}(u)Q(u+1) + 2 \left( 1 - \sqrt{1 + \xi^2} \right) (u(u+1))^{2N+1}, \quad (10)$$

where

$$\tilde{a}(u) = \frac{2u+2}{2u+1} (u+p) \left( \sqrt{1 + \xi^2} u + q \right) (u+1)^{2N}, \quad \tilde{d}(u) = \tilde{a}(-u-1), \quad (11)$$

and

$$Q(u) = \prod_{j=1}^{N} \left( u - \lambda_j \right) \left( u + \lambda_j + 1 \right). \quad (12)$$

The eigenvalues of the Hamiltonian (1) are then given by

$$E = 2 \sum_{j=1}^{N} \frac{1}{\lambda_j (\lambda_j + 1)} + c, \quad (13)$$

where $c = N - 1 + \frac{1}{p} + \frac{\sqrt{1+\xi^2}}{q}$.

This conjecture is supported by numerical evidence for chains of small length. Indeed, for generic values of the boundary parameters and $N = 2, \ldots, 8$, we have determined (following the method described in [9]) the set of Bethe roots $\{\lambda_1, \ldots, \lambda_N\}$ that characterize each of the $2^N$ eigenvalues via equations (10)–(12). As a check, we have verified that the energies
computed using (13) coincide with those obtained by direct diagonalization of the Hamiltonian (1). Sample results for \( N = 3 \) and \( N = 4 \) are presented in tables 1 and 2, respectively.

We have also numerically verified completeness using instead the \( T-Q \) equation (6) with \( M = 1 \) and again with just one sign (say, \( + \)) for \( N = 2, 3 \). However, that equation is nonlinear in the \( Q \)’s, and is therefore significantly more complicated than (10), which is linear in \( Q \).

4. Higher spin

The transfer matrix (2) is constructed by tracing over a spin-1/2 (i.e., two-dimensional) auxiliary space. Using the fusion procedure [16], open-chain transfer matrices \( T_{1,s}(u) \) corresponding to auxiliary spaces of arbitrary spin \( s/2 \) \( (s = 1, 2, \ldots) \) can be constructed [17–19]. These transfer matrices (and therefore their eigenvalues) obey the Hirota equation (see e.g. [20] and references therein)\(^4\)

\[
T_{1,s}^{-1} T_{1,s'} = T_{2,s} + T_{1,s+1} T_{1,s-1}, \quad s = 1, 2, \ldots \tag{14}
\]

\(^4\) We follow the notation in [20] such that, for any function \( f(u) \), \( f^\pm = f(u \pm \frac{1}{2}) \) and \( f^{\pm n} = f(u \pm \frac{3n}{2}) \). Also, \( T_{s}(u) \) denotes the transfer matrix whose auxiliary space is in the representation of the symmetry group (here \( SU(2) \)) given by the rectangular Young tableau with \( a \) rows and \( s \) columns.
where $T_{2,s}$ satisfies
\[ T_{2,s}^+T_{2,s}^{-} = T_{2,s+1}T_{2,s-1}, \tag{15} \]
and $T_{2,0} = 1$.

For the special case of diagonal boundary terms ($\xi = 0$), the eigenvalues of $T_{1,s}$ (which by abuse of notation we henceforth denote by the same symbol) satisfy simple homogeneous $T$-$Q$ relations, which can be compactly formulated in terms of the following generating functional\footnote{The eigenvalues of the corresponding closed-chain transfer matrices have essentially the same structure. Hence, the generating function (16) has presumably already appeared in the literature, but we have not been able to find the reference.}:
\[ \mathcal{W}_{\text{diag}} \equiv (1 - DDB)^{-1}(1 - DAD)^{-1} = \sum_{s=0}^{\infty} D'D'T_{1,s}D^s, \tag{16} \]

where
\[ A = d\frac{Q^{[-2]}}{Q}, \quad B = d\frac{Q^{[+2]}}{Q}, \tag{17} \]
and $D = e^{-i\phi}$ implying that $Df = f^{-D}$. For example, by expanding both sides of (16), one easily obtains
\[ T_{1,0} = 1, \tag{18} \]
\[ T_{1,1} = A + B = d\frac{Q^{[-2]}}{Q} + d\frac{Q^{[+2]}}{Q}, \tag{19} \]
\[ T_{1,2} = A^+A^- + A^-B^+ + B^+B^- = d\frac{Q^{[-3]}}{Q^+} + d\frac{Q^{[+3]}}{Q^+Q} + d^+d^- \frac{Q^{[-3]}}{Q^+Q}. \tag{20} \]

Equation (19) is a rewriting of the fundamental (spin-1/2) $T$-$Q$ equation (10), while (20) is the spin-1 $T$-$Q$ equation. These transfer matrix eigenvalues satisfy the Hirota equation (14) with
\[ T_{2,s} = \prod_{k=-\infty}^{\infty} A^{[2k+1]}B^{[-2k-1]} = \prod_{k=-\infty}^{\infty} d^{[2k+1]}\tilde{d}^{-[2k-1]}, \tag{21} \]
which is independent of $Q$.

For the general case of nondiagonal boundary terms, we propose the following generating function for the inhomogeneous $T$-$Q$ equations:
\[ \mathcal{W} \equiv [1 - D(A + B + C)D + DAD^2BD]^{-1} = \sum_{s=0}^{\infty} D'T_{1,s}D^s, \tag{22} \]
where $A$ and $B$ are again given by (17), and $C$ is given by
\[ C = \frac{\Delta}{Q}, \tag{23} \]
where $\Delta$ is the inhomogeneous term in the $T$-$Q$ equation (10)
\[ \Delta = 2(1 - \sqrt{1 + \xi^2})(u(u + 1))^{2N+1}. \tag{24} \]

Our proposal (22) for the generating function passes several nontrivial checks. First, for the special case of diagonal boundary terms ($C = 0$), it correctly reduces to the previous result (16):
\[ \mathcal{W}|_{C=0} = [1 - D(A + B)D + DAD^2BD]^{-1} \\
= [(1 - DAD)(1 - DBD)]^{-1} \\
= (1 - DBD)^{-1} = \mathcal{W}_{\text{diag}}. \tag{25} \]
Moreover, by expanding both sides of (22), we obtain
\[ T_{1,0} = 1, \]  
\[ T_{1,1} = A + B + C = a \frac{Q^{[1]}}{Q} + b \frac{Q^{[2]}}{Q} + \Delta, \]  
\[ T_{1,2} = A^+A^- + A^-B^+ + B^+B^- + C^+(A^- + B^-) + C^- (A^+ + B^+) + C^+ C^-, \]  
(26)  
(27)  
(28)

Equation (27) is a rewriting of the \( T-Q \) equation (10), and (28) is our result for the spin-1 inhomogeneous \( T-Q \) equation. We have explicitly verified that this expression for \( T_{1,2} \) (and similarly for \( T_{1,s} \) up to \( s = 4 \)) satisfies the Hirota equation (14), where \( T_{2,s} \) is again given by (21).

Notice that the inhomogeneous \( T-Q \) equation for spin-1 (28) has 8 terms (once all the products are expanded), while its homogeneous counterpart (20) has only 3. We find that the number of terms \( n_s \) in the inhomogeneous \( T_{1,s} \) is given by the following generating function:

\[ w = (1 - 3x + x^2)^{-1} = 1 + 3x + 8x^2 + 21x^3 + \cdots = \sum_{n=0}^{\infty} n_s x^n. \]  
(29)

As yet another check of the generating function \( \mathcal{W} \) (22), we observe that it reduces to \( w \) (29) in the character limit \( DAD = DBD = DCD \equiv x \).

5. Conclusion

We have argued that a simplified version of the CYSW \( T-Q \) equation, namely (10), describes all the eigenvalues of the transfer matrix of the open spin-1/2 XXX chain with general boundary terms. We hope that it, together with the corresponding Bethe equations, can now be used to investigate the thermodynamic limit of this model. Due to the presence of several boundary parameters, we expect that this model has a rich phase structure. This solution may have many other applications, such as the brane–antibrane system in AdS/CFT [21].

We have also proposed a generating function (22) for the inhomogeneous \( T-Q \) equations of arbitrary spin \( s/2, s = 1, 2, \ldots \). These equations differ significantly from their familiar homogeneous counterparts, and may be useful in more formal investigations of the model.

It should be possible to generalize this work to anisotropic spin chains [13], and to integrable spin chains with bulk symmetry algebras of higher rank.

We have focused here only on the eigenvalues of the model’s transfer matrix. For a recent discussion of also the eigenvectors, see [22] and references therein.

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