Spin-$\frac{1}{2}$ XYZ model revisit: general solutions via off-diagonal Bethe ansatz

Junpeng Cao$^{a,b}$, Wen-Li Yang$^{c,d,1}$, Kangjie Shi$^c$ and Yupeng Wang$^{a,b,2}$

$^a$Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

$^b$Collaborative Innovation Center of Quantum Matter, Beijing, China

$^c$Institute of Modern Physics, Northwest University, Xian 710069, China

$^d$Beijing Center for Mathematics and Information Interdisciplinary Sciences, Beijing, 100048, China

Abstract

The spin-$\frac{1}{2}$ XYZ model with periodic boundary and anti-periodic boundary conditions are studied via the off-diagonal Bethe ansatz method. General spectrum of the Hamiltonian for each condition is derived by constructing an extended T-Q ansatz which allows us to treat both even $N$ and odd $N$ cases in an unified framework.

PACS: 75.10.Pq, 03.65.Vf, 71.10.Pm

Keywords: Spin chain; Reflection equation; Bethe Ansatz; T-Q relation

---

$^1$Corresponding author: wlyang@nwu.edu.cn

$^2$Corresponding author: yupeng@iphy.ac.cn
1 Introduction

The spin-$\frac{1}{2}$ XYZ model is a typical model in statistical physics, one-dimensional magnetism and the quantum communication. The first exact solution of the model with periodic boundary condition was derived by Baxter [1, 2, 3, 4] based on its intrinsic relationship to the classical two-dimensional eight-vertex model. In his famous series works, the fundamental equation (the so called Yang-Baxter equation [5, 6, 7]) and the T-Q method were proposed. Subsequently, Takhtadzhan and Faddeev [8] resolved the model by the algebraic Bethe ansatz method [9, 10]. In both Baxter’s method and Takhtadzhan and Faddeev’s method, a local gauge transformation has played a very important role in making it possible to obtain a proper local vacuum state (or reference state) on which the conventional Bethe ansatz analysis can be applied. However, such a proper local state is so far only available for even number of sites. In fact, for the odd site number case such a proper local state is still missing. This gives rise to a longstanding problem for exact solutions of the XYZ model of the odd number of sites with periodic boundary condition. The obstacle for applying those methods to the latter case lies in the absence of a proper local vacuum in the usual Bethe ansatz methods, which is a common feature of the integrable models without $U(1)$ symmetry and has been a very important and difficult issue in the field.

In this paper, we revisit the XYZ model by employing the off-diagonal Bethe ansatz method proposed recently by the present authors [11, 12, 13]. The Hamiltonian of the XYZ spin chain is

$$H = \frac{1}{2} \sum_{n=1}^{N} (J_x \sigma_n^x \sigma_{n+1}^x + J_y \sigma_n^y \sigma_{n+1}^y + J_z \sigma_n^z \sigma_{n+1}^z).$$

(1.1)

The coupling constants are expressed in terms of some elliptic function

$$J_x = e^{i\pi \sigma(\eta + \frac{1}{2})}, \quad J_y = e^{i\pi \sigma(\eta + \frac{1+i\tau}{2})}, \quad J_z = \frac{\sigma(\eta + \frac{1}{2})}{\sigma(\frac{1}{2})},$$

(1.2)

with the elliptic function $\sigma(u)$ defined by (2.2) below and $\sigma^x, \sigma^y, \sigma^z$ are the usual Pauli matrices. The Hamiltonian with periodic boundary condition

$$\sigma_{N+1}^x = \sigma_1^x, \quad \sigma_{N+1}^y = \sigma_1^y, \quad \sigma_{N+1}^z = \sigma_1^z,$$

(1.3)

and anti-periodic boundary condition (or the quantum topological spin ring [11])

$$\sigma_{N+1}^x = \sigma_1^x, \quad \sigma_{N+1}^y = -\sigma_1^y, \quad \sigma_{N+1}^z = -\sigma_1^z.$$

(1.4)
both are integrable. General spectrum of the Hamiltonian with the boundary conditions are obtained by constructing an extended T-Q ansatz which allows us to treat both even \( N \) and odd \( N \) cases in an unified framework.

The paper is organized as follows. Section 2 serves as an introduction of our notations and some basic ingredients. After briefly describing the inhomogeneous XYZ spin chains with periodic boundary conditions, we derive the operator product identities of the transfer matrices at some special points of the spectral parameter. In Section 3, the T-Q ansatz for the eigenvalues of the transfer matrix and the corresponding Bethe ansatz equations (BAEs) of the model with both even \( N \) and odd \( N \) cases are constructed based on the operator product identities of the transfer matrix and its quasi-periodic properties. Section 4 is attributed to the exact solution of the XYZ spin chain with the antiperiodic boundary condition. In Section 5, we summarize our results and give some discussions. Some useful identities of elliptic functions are listed in Appendix A.

2 Transfer matrix

Let us fix a generic complex number \( \tau \) such that \( \text{Im}(\tau) > 0 \) and a generic complex number \( \eta \). Introduce the following elliptic functions

\[
\theta \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} (u, \tau) = \sum_{m=-\infty}^{\infty} \exp \left\{ i\pi \left[ (m + a_1)^2 \tau + 2(m + a_1)(u + a_2) \right] \right\},
\]

(2.1)

\[
\sigma(u) = \theta \left[ \frac{1}{a_1} \right] (u, \tau), \quad \zeta(u) = \frac{\partial}{\partial u} \{ \ln \sigma(u) \}.
\]

(2.2)

Among them the \( \sigma \)-function satisfies the following identity:

\[
\sigma(u + x)\sigma(u - x)\sigma(v + y)\sigma(v - y) - \sigma(u + y)\sigma(u - y)\sigma(v + x)\sigma(v - x)
\]

\[
= \sigma(u + v)\sigma(u - v)\sigma(x + y)\sigma(x - y),
\]

(2.3)

which will be useful in deriving equations in the following.

The well-known eight-vertex model R-matrix \( R(u) \in \text{End}(\mathbb{C}^2 \otimes \mathbb{C}^2) \) is given by

\[
R(u) = \begin{pmatrix} \alpha(u) & \delta(u) \\ \beta(u) & \gamma(u) \\ \gamma(u) & \beta(u) \\ \delta(u) & \alpha(u) \end{pmatrix}.
\]

(2.4)
The non-vanishing matrix elements are [7]

\[
\begin{align*}
\alpha(u) &= \frac{\theta \left[ \frac{1}{2}, u, 2\tau \right] \theta \left[ \frac{1}{2}, u + \eta, 2\tau \right]}{\theta \left[ \frac{1}{2}, 0, 0 \right] \theta \left[ \frac{1}{2}, 0, \eta, 2\tau \right]}, \\
\beta(u) &= \frac{\theta \left[ \frac{1}{2}, u, 2\tau \right] \theta \left[ \frac{1}{2}, u + \eta, 2\tau \right]}{\theta \left[ \frac{1}{2}, 0, 0 \right] \theta \left[ \frac{1}{2}, 0, \eta, 2\tau \right]}, \\
\gamma(u) &= \frac{\theta \left[ \frac{1}{2}, u, 2\tau \right] \theta \left[ \frac{1}{2}, u + \eta, 2\tau \right]}{\theta \left[ \frac{1}{2}, 0, 0 \right] \theta \left[ \frac{1}{2}, 0, \eta, 2\tau \right]}, \\
\delta(u) &= \frac{\theta \left[ \frac{1}{2}, u, 2\tau \right] \theta \left[ \frac{1}{2}, u + \eta, 2\tau \right]}{\theta \left[ \frac{1}{2}, 0, 0 \right] \theta \left[ \frac{1}{2}, 0, \eta, 2\tau \right]}.
\end{align*}
\] (2.5)

Here \( u \) is the spectral parameter and \( \eta \) is the so-called crossing parameter. In addition to the quantum Yang-Baxter equation,

\[
R_{12}(u_1 - u_2)R_{13}(u_1 - u_3)R_{23}(u_2 - u_3) = R_{23}(u_2 - u_3)R_{13}(u_1 - u_3)R_{12}(u_1 - u_2),
\] (2.6)

the R-matrix also satisfies the following properties:

- Initial condition: \( R_{12}(0) = P_{12} \),
- Unitarity relation: \( R_{12}(u)R_{21}(-u) = -\xi(u)\text{id}, \quad \xi(u) = \frac{\sigma(u - \eta)\sigma(u + \eta)}{\sigma(\eta)\sigma(\eta)} \),
- Crossing relation: \( R_{12}(u) = V_1 R_{12}^t(-u - \eta)V_1, \quad V = -i\sigma_y \),
- PT-symmetry: \( R_{12}(u) = R_{21}(u) = R_{12}^{t_1 t_2}(u) \),
- \( Z_2 \)-symmetry: \( \sigma_i^1 \sigma_i^2 R_{1,2}(u) = R_{1,2}(u)\sigma_i^1 \sigma_i^2 \), for \( i = x, y, z \),
- Antisymmetry: \( R_{12}(-\eta) = -(1 - P) = -2P^{(-)} \).

Here \( R_{21}(u) = P_{12}R_{12}(u)P_{12} \) with \( P_{12} \) being the usual permutation operator and \( t_i \) denotes transposition in the \( i \)-th space. Throughout this paper we adopt the standard notations: for any matrix \( A \in \text{End}(\mathbb{C}^2) \), \( A_j \) is an embedding operator in the tensor space \( \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \cdots \), which acts as \( A \) on the \( j \)-th space and as identity on the other factor spaces; \( R_{ij}(u) \) is an embedding operator of R-matrix in the tensor space, which acts as identity on the factor spaces except for the \( i \)-th and \( j \)-th ones.

Let us introduce the monodromy matrix

\[
T_0(u) = R_{0N}(u - \theta_N) \ldots R_{01}(u - \theta_1),
\] (2.13)

where \( \{\theta_j\}_{j = 1, \cdots, N} \) are generic free complex parameters which are usually called as inhomogeneous parameters. The transfer matrix \( t(u) \) of the inhomogeneous XYZ chain with
periodic boundary condition is given by [7]

\[ t(u) = t r_0 \{ T_0(u) \}, \quad (2.14) \]

\( t r_0 \) denotes trace over the “auxiliary space” 0. The Hamiltonian (1.1) with the periodic boundary condition is given by

\[ H = \frac{\sigma(\eta)}{\sigma'(0)} \left\{ \frac{\partial \ln t(u)}{\partial u} \bigg|_{u=0,\theta_j=0} - \frac{1}{2} N \zeta(\eta) \right\}, \quad (2.15) \]

where \( \sigma'(0) = \frac{\partial}{\partial u} \sigma(u) \bigg|_{u=0} \) and \( \zeta(u) = \frac{\partial}{\partial u} \ln \sigma(u) \). It is remarked that the identities (A.1)-(A.4) are very useful in deriving the coupling constants \( J_x, J_y \) and \( J_z \) given by (1.2). The QYBE (2.6) leads to the fact that the transfer matrices with different spectral parameters commute with each other [10]: \([t(u), t(v)] = 0\). Then \( t(u) \) serves as the generating functional of the conserved quantities of the corresponding system, which ensures the integrability of the (inhomogeneous) XYZ spin chain described by the Hamiltonian (1.1) with the periodic boundary condition.

Let us evaluate the transfer matrix of the closed chain at some special points. The initial condition of the R-matrix: \( R_{12}(0) = P_{12} \) implies that

\[ t(\theta_j) = R_{j j-1}(\theta_j - \theta_{j-1}) \ldots R_{j 1}(\theta_j - \theta_1) \times R_{j N}(\theta_j - \theta_N) \ldots R_{j j+1}(\theta_j - \theta_{j+1}). \quad (2.16) \]

The crossing relation equation (2.9) enables one to have

\[ t(\theta_j - \eta) = (-1)^N R_{j j+1}(\theta_j + \theta_{j+1}) \ldots R_{j N}(\theta_j + \theta_N) \times R_{j 1}(\theta_j + \theta_1) \ldots R_{j j-1}(\theta_j + \theta_{j-1}). \]

Then the unitary relation (2.8) leads to the following operator identity (which was also obtained previously in [14] by quantum separation of variables method)

\[ t(\theta_j)t(\theta_j - \eta) = \Delta_q(\theta_j), \quad j = 1, \ldots, N. \quad (2.17) \]

For generic values of \( \{\theta_j\} \), the quantum determinant of the monodromy matrix \( T(u) \) is proportional to the identity operator

\[ \Delta_q(u) = a(u)d(u - \eta) \times \text{id}, \quad (2.18) \]

\[ a(u) = \prod_{i=1}^{N} \frac{\sigma(u - \theta_i + \eta)}{\sigma(\eta)}, \quad d(u) = a(u - \eta) = \prod_{i=1}^{N} \frac{\sigma(u - \theta_i)}{\sigma(\eta)}. \quad (2.19) \]
Using the unitary relation (2.8) and explicit expressions (2.16) of the transfer matrix at special points, one may derive the following operator identity [15, 16]:

\[ \prod_{j=1}^{N} t(\theta_j) = \prod_{j=1}^{N} a(\theta_j) \times \text{id.} \quad (2.20) \]

The quasi-periodicity of the elliptic functions \( \sigma \)-function

\[ \sigma(u + \tau) = -e^{-2i\pi(u + \frac{\eta}{2})}\sigma(u), \quad \sigma(u + 1) = -\sigma(u), \]

allow one to derive the quasi-periodic properties of the R-matrix

\[ R_{12}(u + 1) = -\sigma_1^x R_{12}(u)\sigma_1^x, \]
\[ R_{12}(u + \tau) = -e^{-2i\pi(u + \frac{\eta}{2})}\sigma_1^x R_{12}(u)\sigma_1^x. \]

The above relations imply that the transfer matrix \( t(u) \) also satisfies the following quasi-periodic properties

\[ t(u + \tau) = (-1)^Ne^{-2i\pi(Nu + N\frac{\eta}{2} - \sum_{j=1}^{N}\theta_j)}t(u), \quad (2.21) \]
\[ t(u + 1) = (-1)^N t(u). \quad (2.22) \]

In the next section we shall show that the above quasi-periodic properties and the very relation (2.17) and (2.20) allow us to determine the spectrum \( \Lambda(u) \) of the transfer matrix \( t(u) \) given by (2.14).

### 3 Functional relations and the T-Q relation

The commutativity of the transfer matrices with different spectrum implies that they have common eigenstates. Let \( |\Psi\rangle \) be an eigenstate of \( t(u) \), which does not depend upon \( u \), with the eigenvalue \( \Lambda(u) \), i.e.,

\[ t(u)|\Psi\rangle = \Lambda(u)|\Psi\rangle. \]

The analyticity of the R-matrix implies the following analytic property of eigenvalue \( \Lambda(u) \) of the transfer matrix:

\[ \Lambda(u) \text{ is an entire function of } u. \quad (3.1) \]
The quasi-periodic properties of the transfer matrix \( (2.21) \) and \( (2.22) \) enable us to derive that the corresponding eigenvalue \( \Lambda(u) \) also has the following quasi-periodic properties:

\[
\Lambda(u + 1) = (-1)^N \Lambda(u), \tag{3.2}
\]

\[
\Lambda(u + \tau) = (-1)^N e^{-2\pi i (Nu + N(\frac{\pi}{2}) - \sum_{j=1}^{N} \theta_j)} \Lambda(u). \tag{3.3}
\]

The analytic property \( (3.1) \) and the quasi-periodic properties \( (3.2) - (3.3) \) of the eigenvalue \( \Lambda(u) \) indicate that \( \Lambda(u) \), as a function of \( u \), is an elliptic polynomial of degree \( N \). Moreover, the very operator identity \( (2.17) \) and \( (2.20) \) lead to that the corresponding eigenvalue \( \Lambda(u) \) satisfies the following relation

\[
\Lambda(\theta_j) \Lambda(\theta_j - \eta) = a(\theta_j) d(\theta_j - \eta), \quad j = 1, \ldots, N, \tag{3.4}
\]

\[
\prod_{j=1}^{N} \Lambda(\theta_j) = \prod_{j=1}^{N} a(\theta_j). \tag{3.5}
\]

The above equations \( (3.1) - (3.5) \) can determine the function \( \Lambda(u) \). We can construct the solution of these equations in terms of a generalized T-Q relation (cf. [7])

\[
\Lambda(u) = e^{2\pi i l_1 u + i\phi} a(u) \frac{Q_1(u - \eta)}{Q_2(u)} + e^{-2\pi i l_1 (u + \eta) - i\phi} d(u) \frac{Q_2(u + \eta)}{Q_1(u)}
+ c \frac{\sigma^n(u + \frac{\eta}{2}) a(u) d(u)}{\sigma^n(\eta) Q_1(u) Q_2(u)}. \tag{3.6}
\]

where \( l_1 \) is a certain integer, and \( M \) and \( n \) are two non-negative integers which satisfy the following relation

\[
N + n = 2M. \tag{3.7}
\]

It is remarked that \( n \) is even if \( N \) is even, while \( n \) is odd if \( N \) is odd. The functions \( Q_1(u) \) and \( Q_2(u) \) are parameterized by \( 2M \) unequal parameters \( \{\mu_j|j = 1, \ldots, M\} \) and \( \{\nu_j|j = 1, \ldots, M\} \) as follows,

\[
Q_1(u) = \prod_{j=1}^{M} \frac{\sigma(u - \mu_j)}{\sigma(\eta)}, \quad Q_2(u) = \prod_{j=1}^{M} \frac{\sigma(u - \nu_j)}{\sigma(\eta)}. \tag{3.8}
\]

In order that the function \( (3.6) \) becomes the solution of equations \( (3.1) - (3.4) \), the \( 2M + 2 \) parameters should satisfy the following \( 2M + 2 \) equations (required by the regularity of \( \Lambda(u) \),
i.e., an elliptic polynomial of degree $N$)
\[
\frac{N}{2} - M)\eta - \sum_{j=1}^{M}(\mu_j - \nu_j) = l_1\tau + m_1, \quad l_1, m_1 \in \mathbb{Z}, \tag{3.9}
\]
\[
M\eta - \sum_{l=1}^{N}\theta_l + \sum_{j=1}^{M}(\mu_j + \nu_j) = m_2, \quad m_2 \in \mathbb{Z}, \tag{3.10}
\]
\[
c e^{2\pi i(l_1\mu_j + l_1\eta - \phi)}\sigma^n(\mu_j + \frac{\eta}{2}) a(\mu_j) = -Q_2(\mu_j)Q_2(\mu_j + \eta), \tag{3.11}
\]
\[
c e^{-2\pi i\nu_j - i\phi}\sigma^n(\nu_j + \frac{\eta}{2}) d(\nu_j) = -Q_1(\nu_j)Q_1(\nu_j - \eta). \tag{3.12}
\]

The equations (3.11) and (3.12) ensure that the function (3.6) is an entire function of $u$, namely, the function satisfies (3.1). The equations (3.9) and (3.10) imply that the function (3.6) has the same quasi-periodic properties as (3.2)-(3.3). Notice the fact that $\sigma(0) = 0$, we can evaluate the function (3.6) at points $\theta_j$ and $\theta_j - \eta$ respectively,
\[
\Lambda(\theta_j) = e^{2\pi i l_1\theta_j - i\phi} a(\theta_j) \frac{Q_1(\theta_j - \eta)}{Q_2(\theta_j)}, \quad j = 1, \ldots, N, \tag{3.13}
\]
\[
\Lambda(\theta_j - \eta) = e^{-2\pi i l_1\theta_j - i\phi} d(\theta_j - \eta) \frac{Q_2(\theta_j)}{Q_1(\theta_j - \eta)}, \quad j = 1, \ldots, N,
\]
which yields that
\[
\Lambda(\theta_j)\Lambda(\theta_j - \eta) = a(\theta_j)d(\theta_j - \eta), \quad j = 1, \ldots, N.
\]

This implies that the function (3.6) indeed satisfied (3.1) - (3.4) provided that the the $2M + 2$ parameters $\phi, c, \{\mu_j\}$ and $\{\nu_j\}$ satisfy the associated Bethe ansatz equations (BAEs) (3.9)-(3.12). Finally we conclude that the function (3.6) indeed satisfies (3.1) - (3.5) and gives the eigenvalue of the transfer matrix of the inhomogeneous XYZ model with periodic boundary condition, provided that the the $2M + 2$ parameters $\phi, c, \{\mu_j\}$ and $\{\nu_j\}$ satisfy the associated Bethe ansatz equations (BAEs) (3.9)-(3.12) and the selection rule (3.5).

Taking the homogeneous limit $\theta_j \to 0$, we have that the eigenvalue $\Lambda(u)$ of the transfer matrix of the XYZ spin chain with the periodic boundary condition can be given by
\[
\Lambda(u) = e^{2\pi i l_1 u + i\phi} \frac{\sigma^N(u + \eta)}{\sigma^N(\eta)} \frac{Q_1(u - \eta)}{Q_2(u)} + e^{-2\pi i l_1 (u + \eta) - i\phi} \frac{\sigma^N(u)}{\sigma^N(\eta)} \frac{Q_2(u + \eta)}{Q_1(u)}
\]
\[
+ \frac{c\sigma^N(u + \frac{\eta}{2})}{\sigma^N(\eta)Q_1(u)Q_2(u)} \frac{\sigma^N(u + \eta)\sigma^N(u)}{\sigma^N(\eta)\sigma^N(\eta)}, \tag{3.14}
\]

8
where $l_1$ is a certain integer, the functions $Q_1(u)$ and $Q_2(u)$ are given by (3.8). Here the $2M + 2$ parameters $c, \phi, \{\mu_j\}$ and $\{\nu_j\}$ satisfy the following BAEs

\[
\frac{N}{2} - M\eta - \sum_{j=1}^{M}(\mu_j - \nu_j) = l_1\tau + m_1, \quad l_1, m_1 \in \mathbb{Z}, \tag{3.15}
\]
\[
M\eta + \sum_{j=1}^{M}(\mu_j + \nu_j) = m_2, \quad m_2 \in \mathbb{Z}, \tag{3.16}
\]
\[
\frac{c e^{2i\pi(l_1\mu_j + l_1\eta) + i\phi}\sigma^n(\mu_j + \frac{\eta}{2})\sigma^N(\mu_j + \eta)}{\sigma^n(\eta)} = -Q_2(\mu_j)Q_2(\mu_j + \eta), \tag{3.17}
\]
\[
\frac{c e^{-2i\pi l_1\nu_j - i\phi}\sigma^n(\nu_j + \frac{\eta}{2})\sigma^N(\nu_j)}{\sigma^n(\eta)} = -Q_1(\nu_j)Q_1(\nu_j - \eta). \tag{3.18}
\]

The resulting selection rule becomes

\[
\Lambda(0) = e^{i\phi} \prod_{j=1}^{M} \frac{\sigma(\mu_j + \eta)}{\sigma(\nu_j)} = e^{2i\pi k}, \quad k = 1, \ldots, N. \tag{3.19}
\]

The eigenvalue of the Hamiltonian (1.1) with the periodic boundary condition is given by:

\[
E = \frac{\sigma(\eta)}{\sigma(0)} \left\{ \sum_{j=1}^{M} \left[ \zeta(\nu_j) - \zeta(\mu_j + \eta) \right] + \frac{1}{2} N\zeta(\eta) + 2i\pi l_1 \right\}, \tag{3.20}
\]

where the function $\zeta(u)$ is defined by (2.2) and the parameters satisfy the corresponding BAEs (3.15)-(3.18) and the selection rule (3.19).

### 3.1 For a generic $\eta$

In this subsection we consider the case that $\eta$ is a generic complex number. When the number $N$ of the lattice size is an even number, it follows from the equations (3.17) and (3.18) that either $\mu_j = \nu_k$ or $\mu_j = \nu_k - \eta$ leads to the parameter $c$ vanishing. Hence this induces an one-to-one correspondence between $\{\mu_j\}$ and $\{\nu_k\}$, i.e., either $\mu_j = \nu_k$ or $\mu_j = \nu_k - \eta$, in the case of $c = 0$. Combining with the equation (3.15) and the fact that $\eta$ is a generic number we can conclude that in order to $c = 0$, the parameters have to satisfy the relations:

\[
l_1 = 0, \quad N = 2M, \quad \{\mu_j\} \equiv \{\lambda_j\}. \tag{3.21}
\]

The resulting T-Q relation (3.14) is thus reduced to the conventional one

\[
\Lambda(u) = e^{i\phi} \frac{\sigma^N(u + \eta)Q(u - \eta)}{\sigma^N(\eta)Q(u)} + e^{-i\phi} \frac{\sigma^N(u)Q(u + \eta)}{\sigma^N(\eta)Q(u)}, \tag{3.22}
\]
\[
Q(u) = \prod_{l=1}^{M} \frac{\sigma(u - \lambda_l)}{\sigma(\eta)}. \tag{3.23}
\]
Then we can obtain the resulting BAEs and the resulting selection rule. Namely, the $M + 1$ parameters $\phi$ and $\{\lambda_j\}$ satisfy the following BAEs

$$
\frac{\sigma^N(\lambda_j + \eta)}{\sigma^N(\lambda_j)} = -e^{-2i\phi} \frac{Q(\lambda_j + \eta)}{Q(\lambda_j - \eta)}, \quad j = 1, \ldots, M,
$$

(3.23)

$$
e^{i\phi} \prod_{j=1}^{M} \frac{\sigma(\lambda_j + \eta)}{\sigma(\lambda_j)} = e^{\frac{2i\pi k}{N}}, \quad k = 1, \ldots, N.
$$

(3.24)

Some remarks are in order. The BAEs (3.23) are just those obtained in Refs. [7, 8], while the relation (3.24) gives rise to that the parameter $\phi$ takes a discrete value labeled by $k = 1, \ldots, N$. On the other hand, $c \neq 0$ and $\mu_j \neq \nu_k$, $\nu_k - \eta$ for arbitrary $j, k$ may not lead to new solutions but different parametrizations as discussed by Baxter[17] that $M = N/2$ already gives a complete set of solutions for even $N$. We note a similar phenomenon also appears in the XXZ spin chain with unparallel boundary fields [18, 19, 20], where the number $M$ in the BAEs is also fixed. The numerical simulation [21, 22] indicates that the BAEs with a fixed $M$ indeed give the complete solutions of the model.

When the number $N$ of the lattice size is an odd number, it follows from (3.17) and (3.18) that the vanishing condition of $c$ also leads to the parameters $\{\mu_j\}$ and $\{\nu_j\}$ having to form pairs either $\mu_j = \nu_k$ or $\mu_j = \nu_k - \eta$. However, for a generic $\eta$ both $\mu_j = \nu_k$ or $\mu_j = \nu_k - \eta$ cannot make the equation (3.15) satisfied due to the fact that in this case $\frac{N}{2} - M = -\frac{1}{2}$. This means that the solutions of the BAEs (3.15)-(3.18) with $c = 0$ actually do not exist for an odd $N$. Therefore for the XYZ chain with odd number sites and $\eta$ being a generic complex number, the generalized T-Q relation (3.14) cannot be reduced to the conventional one like (3.22).

3.2 For some degenerate values of $\eta$

In this subsection we consider the case that $\eta$ takes some discrete series of values in which case the corresponding T-Q relation (3.14) can be reduced to the conventional one [7, 8] no matter that $N$ be even or odd.

For this purpose, let us first focus on the BAEs (3.17) and (3.18). In order to have the solution corresponding to $c = 0$, the parameters $\{\mu_j\}$ and $\{\nu_j\}$ have to satisfy the following relations

$$
\mu_j = \nu_j \equiv \lambda_j, \quad j = 1, \ldots, M_1,
$$

$$
\mu_{j+M_1} = \nu_{j+M_1} - \eta, \quad j = 1, \ldots, M - M_1.
$$
It should be remarked that (3.16) is not necessary any more since \( c = 0 \). The relation (3.15) now reads
\[
\left( \frac{N}{2} - M_1 \right) \eta = l_1 \tau + m_1, \quad l_1, m_1 \in \mathbb{Z}.
\] (3.25)

This implies that if the crossing parameter \( \eta \) takes some discrete values:
\[
\frac{2l_1}{N - 2M_1} \tau + \frac{2m_1}{N - 2M_1} \quad \text{for some non-negative integer } M_1 \text{ and some integers } l_1 \text{ and } m_1,
\]
our general T-Q relation (3.14) is indeed reduced to the conventional one \([7, 8]\) because of \( c = 0 \), namely,
\[
\Lambda(u) = e^{2i\pi l_1 u + i\phi} \frac{\sigma^N(u + \eta)}{\sigma^N(\eta)} Q(u - \eta) + e^{-\{2i\pi l_1 (u + \eta) + \phi\}} \frac{\sigma^N(u)}{\sigma^N(\eta)} \frac{Q(u + \eta)}{Q(u)},
\] (3.26)
\[
Q(u) = \prod_{l=1}^{M_1} \frac{\sigma(u - \lambda_l)}{\sigma(\eta)}.
\]
The \( M_1 + 1 \) parameters \( \phi \) and \( \{\lambda_j\} \) satisfy the associated BAEs
\[
e^{(2i\pi (2l_1 \lambda_j + l_1 \eta) + 2i\phi)} \frac{\sigma^N(\lambda_j + \eta)}{\sigma^N(\lambda_j)} = \frac{Q(\lambda_j + \eta)}{Q(\lambda_j - \eta)}, \quad j = 1, \ldots, M_1,
\] (3.27)
\[
e^{i\phi} \prod_{j=1}^{M_1} \frac{\sigma(\lambda_j + \eta)}{\sigma(\lambda_j)} = e^{\frac{2i\pi k}{N}}, \quad k = 1, \ldots, N.
\] (3.28)

4 Results for the XYZ chain with antiperiodic boundary condition

4.1 Functional relations

Now let us consider the XYZ spin chain described by the Hamiltonian (1.1) but with an antiperiodic boundary condition (1.4), whose integrability is guaranteed by the associated transfer matrix \( t(a)(u) \) given by
\[
t^{(a)}(u) = tr_0 \{ \sigma_0^x T_0(u) \},
\] (4.1)
where the monodromy matrix is still given by (2.13). Following the method that we have used in Section 2, we can derive the following important functional relations of the transfer matrix \( t^{(a)}(u) \) which allow us to determine the eigenvalue of the transfer matrix
\[
t^{(a)}(\theta_j) t^{(a)}(\theta_j - \eta) = -a(\theta_j) d(\theta_j - \eta), \quad j = 1, \ldots, N,
\] (4.2)
\[
\prod_{j=1}^{N} t^{(a)}(\theta_j) = \prod_{j=1}^{N} a(\theta_j) \times U, \quad U = \sigma_1^x \sigma_2^x \cdots \sigma_N^x,
\] (4.3)
\[ t^{(a)}(u + 1) = (-1)^{N-1} t^{(a)}(u), \quad (4.4) \]
\[ t^{(a)}(u + \tau) = (-1)^N e^{-2\pi i \{Nu + N \frac{2\pi}{2} - \sum_{l=1}^N \theta_l\}} t^{(a)}(u). \quad (4.5) \]

It is easy to check that
\[ [t^{(a)}(u), U] = 0, \quad U^2 = \text{id}, \quad (4.6) \]

which implies that the eigenvalue of the operator \( U \) given by (4.3) takes the values \( \pm 1 \) and it can be diagonalized with the transfer matrix \( t^{(a)}(u) \) simultaneously. Let us denote the eigenvalue of the transfer matrix \( t^{(a)}(u) \) by \( \Lambda(u) \), then the above identities enable us to derive the following relations of its eigenvalue
\[ \Lambda(\theta_j)\Lambda(\theta_j - \eta) = -a(\theta_j) d(\theta_j - \eta), \quad j = 1, \ldots N, \quad (4.7) \]
\[ \prod_{j=1}^N \Lambda(\theta_j) = \pm \prod_{j=1}^N a(\theta_j), \quad (4.8) \]
\[ \Lambda(u + 1) = (-1)^{N-1} \Lambda(u), \quad (4.9) \]
\[ \Lambda(u + \tau) = (-1)^N e^{-2\pi i \{Nu + N \frac{2\pi}{2} - \sum_{l=1}^N \theta_l\}} \Lambda(u). \quad (4.10) \]

The analyticity of the R-matrix implies the following analytic property of eigenvalue \( \Lambda(u) \) of the transfer matrix \( t^{(a)}(u) \):
\[ \Lambda(u) \text{ is an entire function of } u. \quad (4.11) \]

### 4.2 T-Q relation

Similarly as that of the (inhomogeneous) XYZ spin chain with the periodic boundary condition, the relations (4.7)-(4.11) allow us to determine the eigenvalue \( \Lambda(u) \) of the transfer matrix \( t^{(a)}(u) \) for the inhomogeneous XYZ spin chain with the antiperiodic boundary condition. After taking the homogeneous limit \( \theta_j \to 0 \), we obtain the eigenvalue of the transfer matrix with the homogeneous limit. Namely the eigenvalue \( \Lambda(u) \) of the transfer matrix \( t^{(a)}(u) \) (in the homogeneous limit) is given by
\[ \Lambda(u) = e^{i\pi (2l_1 + 1)(u + \eta)} \frac{\sigma^N(u + \eta) Q_1(u - \eta)}{\sigma^N(\eta) Q_2(u)} - e^{-i\pi (2l_1 + 1)(u + \eta)} \frac{\sigma^N(u) Q_2(u + \eta)}{\sigma^N(\eta) Q_1(u)} \]
\[ + ce^{i\pi u} \frac{\sigma^N(u + \frac{\eta}{2})}{\sigma^N(\eta)} Q_1(u) Q_2(u) \frac{\sigma^N(u + \eta) \sigma^N(u)}{\sigma^N(\eta) \sigma^N(\eta)}. \quad (4.12) \]
where \( l_1 \) is a certain integer, the functions \( Q_1(u) \) and \( Q_2(u) \) are given by (3.8). The non-negative integers \( N, M \) and \( n \) satisfy the relation
\[
N + n = 2M. \tag{4.13}
\]

The parameters \( c, \phi, \{\mu_j\} \) and \( \{\nu_j\} \) satisfy the associated BAEs
\[
\frac{(N - M)\eta - \sum_{j=1}^{M} (\mu_j - \nu_j)}{\sigma^n(\eta)} = (l_1 + \frac{1}{2})\tau + m_1, \quad l_1, m_1 \in \mathbb{Z}, \tag{4.14}
\]
\[
M\eta + \sum_{j=1}^{M} (\mu_j + \nu_j) = \frac{1}{2}\tau + m_2, \quad m_2 \in \mathbb{Z}, \tag{4.15}
\]
\[
\frac{c e^{2i\pi(l_1+1)\mu_j+2i\pi(l_1+\frac{1}{2})\eta+i\phi} \sigma^n(\mu_j + \eta)}{\sigma^n(\eta)} = Q_2(\mu_j)Q_2(\mu_j + \eta), \tag{4.16}
\]
\[
\frac{c e^{-2i\pi l_1 \nu_j - i\phi} \sigma^n(\nu_j + \eta)}{\sigma^n(\eta)} = -Q_1(\nu_j)Q_1(\nu_j - \eta), \tag{4.17}
\]
and the selection rule
\[
\Lambda(0) = e^{i\phi} \prod_{j=1}^{M} \frac{\sigma(\mu_j + \eta)}{\sigma(\nu_j)} = e^{\frac{i\pi k}{N}}, \quad k = 1, \ldots, 2N. \tag{4.18}
\]

The eigenvalue of the Hamiltonian (1.1) with the anti-periodic boundary condition is then given by:
\[
E = \frac{\sigma(\eta)}{\sigma'(0)} \left\{ \sum_{j=1}^{M} [\zeta(\nu_j) - \zeta(\mu_j + \eta)] + \frac{1}{2} N \zeta(\eta) + 2i\pi(l_1 + \frac{1}{2}) \right\}, \tag{4.19}
\]
where the function \( \zeta(u) \) is defined by (2.2) and the parameters satisfy the corresponding BAEs (4.14)-(4.17) and the selection rule (4.18).

For a generic \( \eta \), in contrast with the XYZ spin chain with the periodic boundary condition, there does not exist the solution with \( c = 0 \) of the BAEs (4.14)-(4.17). However, when \( \eta \) takes some discrete values labeled by two integers \( l_1 \) and \( m \) as follows:
\[
\frac{(N - M_1)\eta - \sum_{j=1}^{M_1} (\mu_j - \nu_j)}{\sigma^n(\eta)} = (l_1 + \frac{1}{2})\tau + m, \quad l_1, m \in \mathbb{Z}, \tag{4.20}
\]
there does exist the solution with \( c = 0 \) of the BAEs (4.14)-(4.17). In this case, the T-Q relation (4.12) reduces to the conventional one
\[
\Lambda(u) = e^{2i\pi(l_1 + \frac{1}{2})u + i\phi} \sigma^N(u + \eta) Q(u - \eta) \frac{Q(u - \eta)}{\sigma^N(\eta)} Q(u) - e^{-2i\pi(l_1 + \frac{1}{2})(u + \eta) + i\phi} \sigma^N(u) Q(u + \eta) \frac{Q(u + \eta)}{\sigma^N(\eta)} Q(u), \tag{4.21}
\]
\[
Q(u) = \prod_{i=1}^{M_1} \frac{\sigma(u - \lambda_i)}{\sigma(\eta)}. \tag{4.22}
\]
The $M_1 + 1$ parameters $\phi$ and $\{\lambda_j\}$ satisfy the associated BAEs

$$e^{2i\pi((2l_1+1)\lambda_j+(l_1+\frac{1}{2})\eta)+2i\phi} \frac{\sigma^N(\lambda_j + \eta)}{\sigma^N(\lambda_j)} = \frac{Q(\lambda_j + \eta)}{Q(\lambda_j - \eta)}, \quad j = 1, \ldots, M_1, \quad (4.23)$$

$$e^{i\phi} \prod_{j=1}^{M_1} \frac{\sigma(\lambda_j + \eta)}{\sigma(\lambda_j)} = e^{i\pi k}, \quad k = 1, \ldots, 2N. \quad (4.24)$$

5 Conclusions

The spin-$\frac{1}{2}$ XYZ model described by the Hamiltonian (1.1) with the periodic boundary condition (1.3) and the anti-periodic boundary condition (1.4) are studied via the off-diagonal Bethe ansatz method [11, 12, 13]. The eigenvalues of the transfer matrix of the model are given in terms of an extended T-Q ansatz (3.14) and (4.12) which allow us to treat both even $N$ and odd $N$ cases in an unified framework. For a generic crossing parameter $\eta$, our solution can be reduced to Baxter’s solution only for the periodic chain with an even $N$, while for all the other cases (odd $N$ and antiperiodic boundary condition) an extra term (the third term in (3.14) or (4.12)) has to be added in the T-Q relation. However, if the crossing parameter $\eta$ take some degenerate values ((3.25) for the periodic boundary condition and (4.20) for the antiperiodic boundary condition), the corresponding T-Q relation indeed can be reduced to the conventional one. It should be emphasized that these degenerate points become dense in the whole complex $\eta$-plane in the thermodynamic limit ($N \to \infty$). This enables one to obtain the thermodynamic properties (up to the order of $O(N^{-2})$) of the XYZ model for generic values of $\eta$ via the conventional thermodynamic Bethe ansatz methods [10, 23]. This method has been proven to be very successful in the study of the surface energy of the XXZ spin chain with arbitrary boundary fields [24].

Acknowledgments

The financial supports from the National Natural Science Foundation of China (Grant Nos. 11174335, 11031005, 11375141, 11374334), the National Program for Basic Research of MOST (973 project under grant No. 2011CB921700) and the State Education Ministry of China (Grant No. 2011610110017) and BCMIS are gratefully acknowledged. Two of the authors (W.-L Yang and K. Shi) would like to thank IoP/CAS for the hospitality and they enjoyed during their visit there.
Appendix A: Identities of the elliptic functions

In this appendix, we list some identities of the elliptic functions which have been used in the derivations of the paper. Besides the identity (2.3), the elliptic functions defined by (2.1)-(2.2) satisfy the following identities:

\[ \sigma(2u) = \frac{2\sigma(u)\sigma(u + \frac{1}{2})\sigma(u + \frac{\tau}{2})\sigma(u - \frac{1}{2} - \frac{\tau}{2})}{\sigma(\frac{\tau}{2})\sigma(\frac{\tau}{2})\sigma(-\frac{1}{2} - \frac{\tau}{2})}, \]  
(A.1)

\[ \frac{\sigma(u)}{\sigma(\frac{\tau}{2})} = \frac{\theta \left[ \begin{array}{c} 0 \\ \frac{1}{2} \end{array} \right] (u, 2\tau) \theta \left[ \begin{array}{c} \frac{1}{2} \\ \frac{1}{2} \end{array} \right] (u, 2\tau)}{\theta \left[ \begin{array}{c} 0 \\ \frac{1}{2} \end{array} \right] (\frac{\tau}{2}, 2\tau) \theta \left[ \begin{array}{c} \frac{1}{2} \\ \frac{1}{2} \end{array} \right] (\frac{\tau}{2}, 2\tau)}, \]  
(A.2)

\[ \theta \left[ \begin{array}{c} \frac{1}{1} \\ \frac{1}{2} \end{array} \right] (2u, 2\tau) = \theta \left[ \begin{array}{c} \frac{1}{1} \\ \frac{1}{2} \end{array} \right] (\tau, 2\tau) \times \frac{\sigma(u)\sigma(u + \frac{1}{2})}{\sigma(\frac{\tau}{2})\sigma(\frac{1}{2} + \frac{\tau}{2})}, \]  
(A.3)

\[ \theta \left[ \begin{array}{c} 0 \\ \frac{1}{2} \end{array} \right] (2u, 2\tau) = \theta \left[ \begin{array}{c} 0 \\ \frac{1}{2} \end{array} \right] (0, 2\tau) \times \frac{\sigma(u - \frac{\tau}{2})\sigma(u + \frac{1}{2} + \frac{\tau}{2})}{\sigma(-\frac{\tau}{2})\sigma(\frac{1}{2} + \frac{\tau}{2})}. \]  
(A.4)

References

[1] R. J. Baxter, *Phys. Rev. Lett.* **26** (1971), 832.

[2] R. J. Baxter, *Phys. Rev. Lett.* **26** (1971), 834.

[3] R. J. Baxter, *Ann. Phys. (N.Y.)* **70** (1972), 193.

[4] R. J. Baxter, *Ann. Phys. (N.Y.)* **70** (1972), 323.

[5] C. -N. Yang, *Phys. Rev. Lett.* **19**(1967), 1312.

[6] C. -N. Yang, *Phys. Rev.* **168** (1968), 1920.

[7] R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (1982) (London: Academic Press).

[8] L. A. Takhtadzhan and L. D. Faddeev, *Rush. Math. Surveys* **34** (1979), 11.

[9] E. K. Sklyanin and L. D. Faddeev, *Sov. Phys. Dokl.* **23** (1978), 902.
[10] V. E. Korepin, N. M. Boliubov and A. G. Izergin, *Quantum Inverse Scattering Method and Correlation Functions* (1993), (Cambridge: Cambridge University Press).

[11] J. Cao, W.-L. Yang, K.-J. Shi and Y. Wang, *Phys. Rev. Lett.* **111** (2013), 137201.

[12] J. Cao, W.-L. Yang, K.-J. Shi and Y. Wang, *Nucl. Phys.* **B 875** (2013), 152.

[13] J. Cao, W.-L. Yang, K.-J. Shi and Y. Wang, *Nucl. Phys.* **B 877** (2013), 152.

[14] G. Niccoli, 2013 *J. Phys. A: Math. Theor.* **46** (2013), 075003.

[15] N. Kitanine, J. M. Maillet and V. Terras, *Nucl. Phys.* **B 554** (1999), 647.

[16] J. M. Maillet and V. Terras *Nucl. Phys.* **B 575** (2000), 627.

[17] R. J. Baxter, *J. Stat. Phys.* **116** (2004), 43.

[18] J. Cao J, H.-H. Lin, K.-J. Shi and Y. Wang, *Nucl. Phys.* **B 663** (2003), 487.

[19] W.-L. Yang and R. Sasaki, *J. Math. Phys.* **45** (2004), 4301; *Nucl. Phys.* **B 679** (2004), 495.

[20] W.-L. Yang and Y.-Z. Zhang, *Nucl. Phys.* **B 744** (2006), 312.

[21] R.-I. Nepomechie and F. Ravanini, *J. Phys. A: Math. Gen.* **36** (2003), 11391.

[22] R.-I. Nepomechie and F. Ravanini, *J. Phys. A: Math. Gen.* **37** (2004), 1945.

[23] M. Takahashi, *Thermodynamics of One-Dimensional Solvable Models* (1999) (Cambridge: Cambridge University Press).

[24] Y.-Y. Li, J.-P. Cao, W.-L. Yang, K.-J. Shi and Y.-P. Wang, Thermodynamic limit of the off-diagonal Bethe ansatz solvable models, [arXiv:1401.3045](https://arxiv.org/abs/1401.3045).