Available online at www.sciencedirect.com
ScienceDirect
Nuclear Physics B 886 (2014) 185–201
www.elsevier.com/locate/nuclphysb

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

Junpeng Cao [a,b], Shuai Cui [a], Wen-Li Yang [c,d,*], Kangjie Shi [c], Yupeng Wang [a,b,**]

[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*

Received 16 April 2014; received in revised form 28 May 2014; accepted 30 June 2014

Available online 3 July 2014

Editor: Hubert Saleur

Abstract

The spin-$\frac{1}{2}$ XYZ model with both periodic and anti-periodic boundary conditions is studied via the off-diagonal Bethe ansatz method. The exact spectra of the Hamiltonians and the Bethe ansatz equations are derived by constructing the inhomogeneous $T-Q$ relations, which allow us to treat both the even N (the number of lattice sites) and odd N cases simultaneously in a unified approach.

1. Introduction

The spin-$\frac{1}{2}$ XYZ model is a typical model in statistical physics, one-dimensional magnetism and quantum communication. The first exact solution of the model with periodic boundary

* Corresponding author at: Institute of Modern Physics, Northwest University, Xian 710069, China.
** Corresponding author at: Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China.
E-mail addresses: wlyang@nwu.edu.cn (W.-L. Yang), yupeng@iphy.ac.cn (Y. Wang).

http://dx.doi.org/10.1016/j.nuclphysb.2014.06.026
0550-3213/

condition was derived by Baxter [1–4] based on its intrinsic relationship with the classical two-dimensional eight-vertex model. In his famous series works, the fundamental equation (the Yang–Baxter equation [5–7]) was emphasized and the $T-Q$ method was proposed. Subsequently, Takhtadzhan and Faddeev [8] resolved the model by the algebraic Bethe ansatz method [9,10]. In both Baxter's and Takhtadzhan and Faddeev's approaches, local gauge transformation played a very important role in obtaining a proper local vacuum state (or reference state) with which the general Bethe states can be constructed. However, a proper reference state is so far only available for even N (the number of lattice sites) but not for odd N. This constitutes the main obstacle for applying the conventional Bethe ansatz methods to the latter case. In fact, the lack of a reference state is a common feature of the integrable models without $U(1)$ symmetry and has been a very important and difficult issue in the field of quantum integrable models.

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

$$H = \frac{1}{2}\sum_{n=1}^{N}\big(J_x\sigma_n^x\sigma_{n+1}^x + J_y\sigma_n^y\sigma_{n+1}^y + J_z\sigma_n^z\sigma_{n+1}^z\big). \tag{1.1}$$

The coupling constants are parameterized as

$$J_x = e^{i\pi\eta}\frac{\sigma(\eta+\frac{\tau}{2})}{\sigma(\frac{\tau}{2})}, \qquad J_y = e^{i\pi\eta}\frac{\sigma(\eta+\frac{1+\tau}{2})}{\sigma(\frac{1+\tau}{2})}, \qquad J_z = \frac{\sigma(\eta+\frac{1}{2})}{\sigma(\frac{1}{2})}, \tag{1.2}$$

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

$$\sigma_{N+1}^x = \sigma_1^x, \qquad \sigma_{N+1}^y = \sigma_1^y, \qquad \sigma_{N+1}^z = \sigma_1^z, \tag{1.3}$$

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

$$\sigma_{N+1}^x = \sigma_1^x, \qquad \sigma_{N+1}^y = -\sigma_1^y, \qquad \sigma_{N+1}^z = -\sigma_1^z, \tag{1.4}$$

is integrable.

The paper is organized as follows. Section 2 serves as an introduction of our notations and some basic ingredients. After briefly reviewing the inhomogeneous XYZ spin chain with periodic boundary condition, we derive the operator product identities of the transfer matrix at some special points of the spectral parameter. In Section 3, the inhomogeneous $T-Q$ relation for the eigenvalues of the transfer matrix and the corresponding Bethe ansatz equations (BAEs) 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 antiperiodic boundary condition. In Section 5, we summarize our results. Some useful identities about the elliptic functions are listed in Appendix A. The trigonometric limit is given in Appendix B.

2. Transfer matrix

Let us fix a generic complex number η and a generic complex number τ such that $\mathrm{Im}(\tau) > 0$. For convenience, we introduce the following elliptic functions

$$\theta\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}(u,\tau) = \sum_{m=-\infty}^{\infty} \exp\big\{i\pi\big[(m+a_1)^2\tau + 2(m+a_1)(u+a_2)\big]\big\}, \tag{2.1}$$

$$\sigma(u)=\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u,\tau),\qquad \zeta(u)=\frac{\partial}{\partial u}\{\ln\sigma(u)\}. \tag{2.2}$$

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

$$R(u)=\begin{pmatrix}\alpha(u)&&&\delta(u)\\ &\beta(u)&\gamma(u)&\\ &\gamma(u)&\beta(u)&\\ \delta(u)&&&\alpha(u)\end{pmatrix}, \tag{2.3}$$

with the non-zero entries [7]

$$\alpha(u)=\frac{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)},$$
$$\beta(u)=\frac{\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)},$$
$$\gamma(u)=\frac{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)},$$
$$\delta(u)=\frac{\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)}. \tag{2.4}$$

Here u is the spectral parameter and η is the crossing parameter. In addition to satisfying the quantum Yang–Baxter equation (QYBE),

$$\begin{aligned}&R_{12}(u_1-u_2)R_{13}(u_1-u_3)R_{23}(u_2-u_3)\\&\quad=R_{23}(u_2-u_3)R_{13}(u_1-u_3)R_{12}(u_1-u_2),\end{aligned} \tag{2.5}$$

the R-matrix also possesses the following properties

$$\text{Initial condition:}\quad R_{12}(0)=P_{12}, \tag{2.6}$$

$$\text{Unitarity relation:}\quad R_{12}(u)R_{21}(-u)=-\xi(u)\,\mathrm{id},\quad \xi(u)=\frac{\sigma(u-\eta)\sigma(u+\eta)}{\sigma(\eta)\sigma(\eta)}, \tag{2.7}$$

$$\text{Crossing relation:}\quad R_{12}(u)=V_1R_{12}^{t_2}(-u-\eta)V_1,\quad V=-i\sigma^y, \tag{2.8}$$

$$\text{PT-symmetry:}\quad R_{12}(u)=R_{21}(u)=R_{12}^{t_1t_2}(u), \tag{2.9}$$

$$Z_2\text{-symmetry:}\quad d\sigma_1^i\sigma_2^iR_{1,2}(u)=R_{1,2}(u)\sigma_1^i\sigma_2^i,\quad \text{for } i=x,y,z, \tag{2.10}$$

$$\text{Antisymmetry:}\quad R_{12}(-\eta)=-(1-P_{12})=-2P_{12}^{(-)}. \tag{2.11}$$

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 $A\in\mathrm{End}(\mathbb{C}^2)$, 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

$$T_0(u) = R_{0N}(u-\theta_N)\ldots R_{01}(u-\theta_1), \tag{2.12}$$

where $\{\theta_j|j=1,\cdots,N\}$ are generic free complex parameters which are usually called inhomogeneous parameters. The transfer matrix $t(u)$ of the inhomogeneous XYZ chain with periodic boundary condition (1.3) is given by [7]

$$t(u) = tr_0\{T_0(u)\}, \tag{2.13}$$

where tr_0 denotes the trace over the "auxiliary space" 0. The Hamiltonian (1.1) with the periodic boundary condition is given by

$$H = \frac{\sigma(\eta)}{\sigma'(0)}\left\{\frac{\partial \ln t(u)}{\partial u}\bigg|_{u=0,\theta_j=0} - \frac{1}{2}N\zeta(\eta)\right\}, \tag{2.14}$$

where $\sigma'(0) = \frac{\partial}{\partial u}\sigma(u)|_{u=0}$ and the function $\zeta(u)$ is given by (2.2). It is remarked that the identities (A.1)–(A.5) (see Appendix A) are very useful to give the expressions (1.2). The QYBE (2.5) leads to that the transfer matrices with different spectral parameters are mutually commutative [10], i.e., $[t(u), t(v)] = 0$, which guarantees the integrability of the model by treating $t(u)$ as the generating functional of the conserved quantities.

Let us evaluate the transfer matrix of the closed chain at some special points. The initial condition of the R-matrix (2.6) implies that

$$t(\theta_j) = R_{j\,j-1}(\theta_j-\theta_{j-1})\ldots R_{j\,1}(\theta_j-\theta_1) \times R_{j\,N}(\theta_j-\theta_N)\ldots R_{j\,j+1}(\theta_j-\theta_{j+1}). \tag{2.15}$$

The crossing relation (2.8) enables one to have

$$t(\theta_j-\eta) = (-1)^N R_{j\,j+1}(-\theta_j+\theta_{j+1})\ldots R_{j\,N}(-\theta_j+\theta_N) \times R_{j\,1}(-\theta_j+\theta_1)\ldots R_{j\,j-1}(-\theta_j+\theta_{j-1}). \tag{2.16}$$

With (2.15)–(2.16) and the unitary relation (2.7) we readily obtain the following operator identities

$$t(\theta_j)t(\theta_j-\eta) = \Delta_q(\theta_j), \quad j=1,\ldots,N, \tag{2.17}$$

where the quantum determinant $\Delta(u)$ of the monodromy matrix is proportional to the identity operator

$$\Delta_q(u) = a(u)d(u-\eta)\times \mathrm{id}, \tag{2.18}$$

$$a(u) = \prod_{l=1}^{N}\frac{\sigma(u-\theta_l+\eta)}{\sigma(\eta)}, \qquad d(u) = a(u-\eta) = \prod_{l=1}^{N}\frac{\sigma(u-\theta_l)}{\sigma(\eta)}. \tag{2.19}$$

In addition, (2.7) and (2.15) give rise to the following operator identity [14–16]

$$\prod_{j=1}^{N} t(\theta_j) = \prod_{j=1}^{N} a(\theta_j)\times \mathrm{id}. \tag{2.20}$$

The Z_2-symmetry (2.10) of the R-matrix implies

$$U^i\, t(u)\, U^i = tr_0\big(U^i\, T_0(u)\, U^i\big) = tr_0\big(\sigma_0^i\, T_0(u)\, \sigma_0^i\big) = t(u), \tag{2.21}$$

$$U^i = \sigma_1^i \sigma_2^i \ldots \sigma_N^i, \quad i = x, y, z. \tag{2.22}$$

Notice that $\{U^i\}$ form an (non)abelian group when N is even (odd), i.e.

$$\big(U^i\big)^2 = \mathrm{id}, \qquad U^i\, U^j = (-1)^N U^j\, U^i, \quad \text{for } i \neq j, \text{ and } i, j = x, y, z. \tag{2.23}$$

The quasi-periodicity of the σ-function

$$\sigma(u+\tau) = -e^{-2i\pi(u+\frac{\tau}{2})}\sigma(u), \qquad \sigma(u+1) = -\sigma(u), \tag{2.24}$$

indicates that the R-matrix possesses the following quasi-periodic properties

$$R_{12}(u+1) = -\sigma_1^z R_{12}(u) \sigma_1^z,$$

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

which lead to the quasi-periodicity of the transfer matrix $t(u)$

$$t(u+\tau) = (-1)^N e^{-2\pi i\{Nu + N(\frac{\eta+\tau}{2}) - \sum_{j=1}^N \theta_j\}} t(u), \tag{2.25}$$

$$t(u+1) = (-1)^N t(u). \tag{2.26}$$

In the subsequent section we shall show that (2.17), (2.20) and (2.25)–(2.26), allow us to determine the eigenvalue $\Lambda(u)$ of the transfer matrix $t(u)$ completely.

3. Functional relations and the $T-Q$ relation

Let $|\Psi\rangle$ be an eigenstate (independent of u) of $t(u)$ with the eigenvalue $\Lambda(u)$, i.e.,

$$t(u)|\Psi\rangle = \Lambda(u)|\Psi\rangle.$$

The analyticity of the R-matrix implies that

$$\Lambda(u) \text{ is an entire function of } u. \tag{3.1}$$

The quasi-periodic properties of the transfer matrix (2.25) and (2.26) indicate that the corresponding eigenvalue $\Lambda(u)$ also possesses the following quasi-periodic properties

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

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

The analytic property (3.1) and the quasi-periodic properties (3.2)–(3.3) indicate that $\Lambda(u)$, as a function of u, is an elliptic polynomial of degree N. This implies that one needs $N+1$ conditions to fix the function. The very operator identities (2.17) and (2.20) lead to that the corresponding eigenvalue $\Lambda(u)$ satisfies the following relations (the same functional relations to (3.4) were previously derived in [17] via separation of variables method)

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

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

Therefore, Eqs. (3.1)–(3.5) will completely characterize the spectrum of the transfer matrix. Following the work [11–13], we can construct the following inhomogeneous T–Q relation for the eigenvalue $\Lambda(u)$

$$\Lambda(u) = e^{2i\pi l_1 u + i\phi} a(u) \frac{Q_1(u-\eta)Q(u-\eta)}{Q_2(u)Q(u)} + e^{-2i\pi l_1(u+\eta)-i\phi} d(u) \frac{Q_2(u+\eta)Q(u+\eta)}{Q_1(u)Q(u)} + c\,\frac{\sigma^m(u+\frac{\eta}{2})a(u)d(u)}{\sigma^m(\eta)Q_1(u)Q_2(u)Q(u)}, \tag{3.6}$$

where l_1 is a certain integer and m is a non-negative integer. The functions $Q_1(u)$, $Q_2(u)$ and $Q(u)$ are parameterized by $2M + M_1$ unequal Bethe roots $\{\mu_j | j = 1, \ldots, M\}$, $\{\nu_j | j = 1, \ldots, M\}$ and $\{\lambda_j | j = 1, \ldots, M_1\}$ as follows

$$Q_1(u) = \prod_{j=1}^{M} \frac{\sigma(u-\mu_j)}{\sigma(\eta)}, \qquad Q_2(u) = \prod_{j=1}^{M} \frac{\sigma(u-\nu_j)}{\sigma(\eta)}, \tag{3.7}$$

$$Q(u) = \prod_{j=1}^{M_1} \frac{\sigma(u-\lambda_j)}{\sigma(\eta)}. \tag{3.8}$$

These non-negative integers m, M and M_1 satisfy the following relation

$$N + m = 2M + M_1. \tag{3.9}$$

It should be remarked that the minimal number of the Bethe roots is N when $m = 0$. In the following text, we put $m = 0$. It is believed that any choice of m might give a complete set of eigenvalues $\Lambda(u)$ of the transfer matrix.

In order that the function (3.6) becomes the solution of (3.1)–(3.3), the $N + 2$ parameters ϕ, c, $\{\mu_j\}$, $\{\nu_j\}$ and $\{\lambda_j\}$ have to satisfy the following $N + 2$ equations

$$\left(\frac{N}{2} - M - M_1\right)\eta - \sum_{j=1}^{M}(\mu_j - \nu_j) = l_1\tau + m_1, \quad l_1, m_1 \in Z, \tag{3.10}$$

$$\frac{N}{2}\eta - \sum_{l=1}^{N}\theta_l + \sum_{j=1}^{M}(\mu_j + \nu_j) + \sum_{j=1}^{M_1}\lambda_j = m_2, \quad m_2 \in Z, \tag{3.11}$$

$$c e^{2i\pi(l_1\mu_j + l_1\eta) + i\phi} a(\mu_j) = -Q_2(\mu_j)Q_2(\mu_j + \eta)Q(\mu_j + \eta), \quad j = 1, \ldots, M, \tag{3.12}$$

$$c e^{-2i\pi l_1\nu_j - i\phi} d(\nu_j) = -Q_1(\nu_j)Q_1(\nu_j - \eta)Q(\nu_j - \eta), \quad j = 1, \ldots, M, \tag{3.13}$$

$$\frac{e^{2i\pi l_1(2\lambda_j+\eta)+2i\phi}a(\lambda_j)}{d(\lambda_j)} + \frac{Q_2(\lambda_j)Q_2(\lambda_j+\eta)Q(\lambda_j+\eta)}{Q_1(\lambda_j)Q_1(\lambda_j-\eta)Q(\lambda_j-\eta)} = \frac{-c e^{2i\pi l_1(\lambda_j+\eta)+i\phi}a(\lambda_j)}{Q_1(\lambda_j)Q_1(\lambda_j-\eta)Q(\lambda_j-\eta)}, \quad j = 1, \ldots, M_1. \tag{3.14}$$

Eqs. (3.12)–(3.14) ensure that the function (3.6) is an entire function of u, namely, the function satisfies (3.1). Eqs. (3.10) and (3.11) imply that the function (3.6) has the same quasi-periodic properties to (3.2)–(3.3). As $\sigma(0) = 0$, $\Lambda(u)$ given by (3.6) at the points $u = \theta_j$ and $u = \theta_j - \eta$ takes the values

$$\Lambda(\theta_j) = e^{2i\pi l_1\theta_j + i\phi} a(\theta_j) \frac{Q_1(\theta_j - \eta)Q(\theta_j - \eta)}{Q_2(\theta_j)Q(\theta_j)}, \quad j = 1, \ldots, N,$$

$$\Lambda(\theta_j-\eta)=e^{-2i\pi l_1\theta_j-i\phi}d(\theta_j-\eta)\frac{Q_2(\theta_j)Q(\theta_j)}{Q_1(\theta_j-\eta)Q(\theta_j-\eta)},\quad j=1,\ldots,N, \tag{3.15}$$

which directly yield

$$\Lambda(\theta_j)\Lambda(\theta_j-\eta)=a(\theta_j)d(\theta_j-\eta),\quad j=1,\ldots,N,$$

namely, $\Lambda(u)$ given by (3.6) indeed satisfies (3.1)–(3.4) and is the eigenvalue of the transfer matrix, provided that the BAEs (3.10)–(3.14) hold. Taking the homogeneous limit $\theta_j\to 0$, the $T-Q$ relation becomes

$$\begin{aligned}\Lambda(u)=&\,e^{2i\pi l_1 u+i\phi}\frac{\sigma^N(u+\eta)}{\sigma^N(\eta)}\frac{Q_1(u-\eta)Q(u-\eta)}{Q_2(u)Q(u)}\\&+\frac{e^{-2i\pi l_1(u+\eta)-i\phi}\sigma^N(u)}{\sigma^N(\eta)}\frac{Q_2(u+\eta)Q(u+\eta)}{Q_1(u)Q(u)}\\&+\frac{c\,\sigma^N(u+\eta)\sigma^N(u)}{Q_1(u)Q_2(u)Q(u)\sigma^N(\eta)\sigma^N(\eta)},\end{aligned} \tag{3.16}$$

with the corresponding BAEs

$$\left(\frac{N}{2}-M-M_1\right)\eta-\sum_{j=1}^{M}(\mu_j-\nu_j)=l_1\tau+m_1,\quad l_1,m_1\in Z, \tag{3.17}$$

$$\frac{N}{2}\eta+\sum_{j=1}^{M}(\mu_j+\nu_j)+\sum_{j=1}^{M_1}\lambda_j=m_2,\quad m_2\in Z, \tag{3.18}$$

$$\begin{aligned}&\frac{ce^{2i\pi(l_1\mu_j+l_1\eta)+i\phi}\sigma^N(\mu_j+\eta)}{\sigma^N(\eta)}\\&\quad=-Q_2(\mu_j)Q_2(\mu_j+\eta)Q(\mu_j+\eta),\quad j=1,\ldots,M,\end{aligned} \tag{3.19}$$

$$\frac{ce^{-2i\pi l_1\nu_j-i\phi}\sigma^N(\nu_j)}{\sigma^N(\eta)}=-Q_1(\nu_j)Q_1(\nu_j-\eta)Q(\nu_j-\eta),\quad j=1,\ldots,M, \tag{3.20}$$

$$\begin{aligned}&\frac{e^{2i\pi l_1(2\lambda_j+\eta)+2i\phi}\sigma^N(\lambda_j+\eta)}{\sigma^N(\lambda_j)}+\frac{Q_2(\lambda_j)Q_2(\lambda_j+\eta)Q(\lambda_j+\eta)}{Q_1(\lambda_j)Q_1(\lambda_j-\eta)Q(\lambda_j-\eta)}\\&\quad=\frac{-ce^{2i\pi l_1(\lambda_j+\eta)+i\phi}\sigma^N(\lambda_j+\eta)}{Q_1(\lambda_j)Q_1(\lambda_j-\eta)Q(\lambda_j-\eta)\sigma^N(\eta)},\quad j=1,\ldots,M_1,\end{aligned} \tag{3.21}$$

and the selection rule

$$\Lambda(0)=e^{i\phi}\left\{\prod_{j=1}^{M}\frac{\sigma(\mu_j+\eta)}{\sigma(\nu_j)}\right\}\left\{\prod_{j=1}^{M_1}\frac{\sigma(\lambda_j+\eta)}{\sigma(\lambda_j)}\right\}=e^{\frac{2i\pi k}{N}},\quad k=1,\ldots,N. \tag{3.22}$$

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

$$\begin{aligned}E=&\,\frac{\sigma(\eta)}{\sigma'(0)}\left\{\sum_{j=1}^{M}\big[\zeta(\nu_j)-\zeta(\mu_j+\eta)\big]+\sum_{j=1}^{M_1}\big[\zeta(\lambda_j)-\zeta(\lambda_j+\eta)\big]\right.\\&\left.+\frac{1}{2}N\zeta(\eta)+2i\pi l_1\right\}.\end{aligned} \tag{3.23}$$

Some remarks are in order. The integers l_1, m_1 and m_2 that appeared in the BAEs (3.17)–(3.21) are due to the quasi-periodicity of the R-matrix (2.3)–(2.4) in terms of u. Any choices of these integers may give rise to the complete set of eigenvalues $\Lambda(u)$. In addition, the numerical simulation for the open XXZ chain [18] indicates that the BAEs with a fixed M (or M_1) indeed give the complete solutions of the model (see also [19]). Similarly, in our case, different M might only give different parameterizations of the eigenvalues but not different eigenstates. To support this conjecture, numerical simulations for $N = 3, 5, 4$ with random choice of η and τ are performed. The results are listed in Tables 1, 2, 3 respectively. Moreover, (2.21) and (2.23) imply that $\Lambda(u)$ has no degeneracy for even N but indeed has a double degeneracy for odd N. As a consequence, for the even N case there exists a one-to-one correspondence between the solutions of the BAEs (3.29)–(3.30) (see below) and the eigenstates of the transfer matrix, while for the odd N case there are multiple solutions of the BAEs (3.17)–(3.22) corresponding to one $\Lambda(u)$ due to its degeneracy. This phenomenon has been checked numerically for some small N.

3.1. For a generic η

Let us consider the $c = 0$ solutions of (3.17)–(3.21). In this case, the corresponding inhomogeneous T–Q relation (3.16) is reduced to Baxter's homogeneous form [7]. Obviously, (3.18) is not necessary since $c = 0$.

It follows from (3.19) and (3.20) that for $c = 0$, the parameters $\{\mu_j\}$ and $\{\nu_j\}$ have to form the pairs with either $\mu_j = \nu_k$ or $\mu_j = \nu_k - \eta$. Suppose

$$\begin{aligned} &\mu_j = \nu_j \overset{\text{Redef}}{=} \lambda_{M_1+j}, \quad j = 1, \ldots, \bar{m}, \text{ and } 0 \le \bar{m} \le M, \\ &\mu_{\bar{m}+k} = \nu_{k+\bar{m}} - \eta, \quad k = 1, \ldots, M - \bar{m}. \end{aligned} \tag{3.24}$$

Combining (3.24) with (3.17), we have

$$\left(\frac{N}{2} - \bar{m} - M_1\right)\eta = l_1\tau + m_1. \tag{3.25}$$

- **Even N case**. Suppose $N = 2\bar{M}$. Because τ and η are generic complex numbers, the only solution to (3.25) is

$$l_1 = m_1 = 0, \qquad N = 2\bar{M} = 2(M_1 + \bar{m}). \tag{3.26}$$

The resulting T–Q relation (3.16) is reduced to Baxter's one

$$\Lambda(u) = e^{i\phi}\frac{\sigma^N(u+\eta)}{\sigma^N(\eta)}\frac{Q(u-\eta)}{Q(u)} + e^{-i\phi}\frac{\sigma^N(u)}{\sigma^N(\eta)}\frac{Q(u+\eta)}{Q(u)}, \tag{3.27}$$

$$Q(u) = \prod_{l=1}^{M_1}\frac{\sigma(u-\lambda_l)}{\sigma(\eta)}\prod_{k=1}^{\bar{m}}\frac{\sigma(u-\nu_k)}{\sigma(\eta)} = \prod_{l=1}^{\bar{M}}\frac{\sigma(u-\lambda_l)}{\sigma(\eta)}. \tag{3.28}$$

The resulting BAEs and the selection rule thus read

$$\frac{\sigma^N(\lambda_j+\eta)}{\sigma^N(\lambda_j)} = -e^{-2i\phi}\frac{Q(\lambda_j+\eta)}{Q(\lambda_j-\eta)}, \quad j = 1, \ldots, \bar{M}, \tag{3.29}$$

$$e^{i\phi}\prod_{j=1}^{\bar{M}}\frac{\sigma(\lambda_j+\eta)}{\sigma(\lambda_j)} = e^{\frac{2i\pi k}{N}}, \quad k = 1, \ldots, N. \tag{3.30}$$

Table 1
Numerical solutions of the BAEs (3.17)–(3.22) for $N = 3$, $M = 1$, $\eta = 0.20$, $\tau = i$, $l_1 = m_1 = m_2 = 0$. The eigenvalues E_n calculated from (3.23) are exactly the same to those from the exact diagonalization of the Hamiltonian. n denotes the number of the energy levels.

μ_1	ν_1	λ_1	c	ϕ	k	E_n	n
$0.35000 + 0.02632i$	$0.45000 + 0.02632i$	$-1.10000 - 0.05263i$	$-0.08948 + 0.00000i$	$-0.08501 - 0.00000i$	1	−1.40865	1
$0.35000 - 0.02632i$	$0.45000 - 0.02632i$	$-1.10000 + 0.05263i$	$-0.08948 + 0.00000i$	$0.08501 - 0.00000i$	2	−1.40865	1
$-0.15000 + 0.08693i$	$-0.05000 + 0.08693i$	$-0.10000 - 0.17387i$	$3.04065 + 0.00000i$	$4.10893 - 0.00000i$	2	−1.40865	1
$-0.15000 - 0.08693i$	$-0.05000 - 0.08693i$	$-0.10000 + 0.17387i$	$3.04065 - 0.00000i$	$-4.10893 - 0.00000i$	1	−1.40865	1
$-0.65000 - 0.27875i$	$-0.55000 - 0.27875i$	$0.90000 + 0.55749i$	$-0.28951 - 0.00000i$	$0.35925 - 0.00000i$	0	1.18468	2
$-0.28066 + 0.31196i$	$-0.18066 + 0.31196i$	$0.16133 - 0.62392i$	$-0.61188 + 0.36729i$	$-0.27657 + 0.04967i$	0	1.18468	2
$0.15828 + 0.12139i$	$0.25828 + 0.12139i$	$-0.71655 - 0.24279i$	$-0.09303 - 0.16695i$	$-0.29190 + 0.31832i$	0	1.63263	3
$-0.42198 + 0.50000i$	$-0.32198 + 0.50000i$	$0.44397 - 1.00000i$	$3.33371 - 7.57925i$	$-0.94248 - 0.14392i$	0	1.63263	3

Table 2
Numerical solutions of the BAEs (3.17)–(3.22) for $N = 5$, $\eta = 0.20$, $M = 1$, $\tau = i$, $l_1 = m_1 = m_2 = 0$. The eigenvalues E_n calculated from (3.23) are exactly the same to those from the exact diagonalization of the Hamiltonian. n denotes the number of the energy levels.

μ_1	ν_1	λ_1	λ_2	λ_3	c	ϕ	k	E_n	n
−0.55827 − 0.02265i	−0.25827 − 0.02265i	−0.10018 + 0.08190i	−0.10011 − 0.01038i	0.51684 − 0.02622i	−0.08617 − 0.00699i	0.10696 − 0.03689i	1	−3.51343	1
−0.55827 + 0.02265i	−0.25827 + 0.02265i	−0.10018 − 0.08190i	−0.10011 + 0.01038i	0.51684 + 0.02622i	−0.08617 + 0.00699i	−0.10696 − 0.03689i	4	−3.51343	1
−0.35211 + 0.07575i	−0.05211 + 0.07575i	−2.07865 + 0.00704i	0.90992 − 0.07849i	1.07296 − 0.08006i	−0.26973 + 6.70848i	1.26914 + 1.97113i	1	−3.51343	1
−0.35211 − 0.07575i	−0.05211 − 0.07575i	−2.07865 − 0.00704i	0.90992 + 0.07849i	1.07296 + 0.08006i	−0.26973 − 6.70848i	−1.26914 + 1.97113i	4	−3.51343	1
−1.42021 − 0.00000i	−1.12021 − 0.00000i	−0.06738 + 0.09747i	2.17518 + 0.00000i	−0.06738 − 0.09747i	−3.95699 + 0.00000i	0.00000 + 1.74063i	0	−1.42192	2
0.44197 − 0.00000i	0.74197 − 0.00000i	−4.09984 + 0.09712i	−1.09984 − 0.09712i	3.51573 − 0.00000i	−0.09625 − 0.00000i	−0.00000 − 0.02711i	0	−1.42192	2
−0.37881 − 0.02198i	−0.07881 − 0.02198i	−0.08454 + 0.09207i	−0.02749 − 0.11816i	0.06967 + 0.07005i	10.06245 − 5.20522i	−2.60644 + 2.33291i	2	−1.25055	3
−0.37881 + 0.02198i	−0.07881 + 0.02198i	−0.08454 − 0.09207i	−0.02749 + 0.11816i	0.06967 − 0.07005i	10.06245 + 5.20522i	2.60644 + 2.33291i	3	−1.25055	3
0.25000 − 0.04330i	0.55000 − 0.04330i	−0.77352 − 0.43943i	−0.42648 + 0.56057i	−0.10000 − 0.03454i	−0.60291 + 1.15659i	0.09819 − 0.00000i	2	−1.25055	3
0.25000 + 0.04330i	0.55000 + 0.04330i	−0.77352 + 0.43943i	0.57352 − 0.56057i	−1.10000 + 0.03454i	−0.60291 − 1.15659i	−0.09819 − 0.00000i	3	−1.25055	3
−0.45598 − 0.05509i	−0.15598 − 0.05509i	−0.87080 − 0.05853i	1.09356 + 0.20136i	−0.11080 − 0.03264i	−1.36773 + 1.60135i	0.51434 + 1.26882i	2	−0.86239	4
−0.45598 + 0.05509i	−0.15598 + 0.05509i	−0.87080 + 0.05853i	1.09356 − 0.20136i	−0.11080 + 0.03264i	−1.36773 − 1.60135i	−0.51434 + 1.26882i	3	−0.86239	4
0.25000 + 0.00965i	0.55000 + 0.00965i	−2.10000 − 0.03122i	0.40000 − 0.16249i	0.40000 + 0.17440i	−0.08524 − 0.00000i	−0.03396 − 0.00000i	2	−0.86239	4
0.25000 − 0.00965i	0.55000 − 0.00965i	−2.10000 + 0.03122i	0.40000 + 0.16249i	0.40000 − 0.17440i	−0.08524 + 0.00000i	0.03396 − 0.00000i	3	−0.86239	4
−0.75000 + 0.11275i	−0.45000 + 0.11275i	−1.90029 − 0.08059i	−0.29971 − 0.08059i	2.90000 − 0.06432i	0.23171 − 0.00000i	−0.58316 + 0.00000i	2	0.70428	5
−0.75000 − 0.11275i	−0.45000 − 0.11275i	−1.90029 + 0.08059i	−0.29971 + 0.08059i	2.90000 + 0.06432i	0.23171 + 0.00000i	0.58316 + 0.00000i	3	0.70428	5
−1.55828 + 0.03094i	−1.25828 + 0.03094i	−0.20115 − 0.04899i	1.51859 + 0.03613i	0.99912 − 0.04902i	−0.07119 + 0.01370i	−0.16566 − 0.04516i	2	0.70428	5
−1.55828 − 0.03094i	−1.25828 − 0.03094i	−0.20115 + 0.04899i	1.51859 − 0.03613i	0.99912 + 0.04902i	−0.07119 − 0.01370i	0.16566 − 0.04516i	3	0.70428	5
0.05720 + 0.13634i	0.35720 + 0.13634i	−2.06490 − 0.15055i	1.37567 + 0.08642i	−0.22517 − 0.20856i	−0.23061 + 0.32198i	−0.81379 − 0.24504i	1	1.02350	6
0.05720 − 0.13634i	0.35720 − 0.13634i	−2.06490 + 0.15055i	1.37567 − 0.08642i	−0.22517 + 0.20856i	−0.23061 − 0.32198i	0.81379 − 0.24504i	4	1.02350	6
0.25000 − 0.11861i	0.55000 − 0.11861i	−1.10000 − 0.14588i	−0.42425 + 0.69155i	0.22425 − 0.30845i	−0.38487 + 0.76419i	0.23725 − 0.00000i	1	1.02350	6
0.25000 + 0.11861i	0.55000 + 0.11861i	−1.10000 + 0.14588i	−0.42425 − 0.69155i	0.22425 + 0.30845i	−0.38487 − 0.76419i	−0.23725 − 0.00000i	4	1.02350	6
0.90991 − 0.30523i	1.20991 − 0.30523i	−3.10036 − 0.12527i	0.11226 + 0.64836i	0.36829 + 0.08736i	0.51259 + 0.05215i	7.25665 + 0.11304i	1	1.08128	7
0.90991 + 0.30523i	1.20991 + 0.30523i	−3.10036 + 0.12527i	0.11226 − 0.64836i	0.36829 − 0.08736i	0.51259 − 0.05215i	−7.25665 + 0.11304i	4	1.08128	7
0.25000 + 0.30649i	0.55000 + 0.30649i	−1.10000 − 0.12487i	−0.60000 − 0.55900i	0.40000 + 0.07089i	0.25098 − 0.00000i	5.34851 + 0.00000i	1	1.08128	7
0.25000 − 0.30649i	0.55000 − 0.30649i	−1.10000 + 0.12487i	−0.60000 + 0.55900i	0.40000 − 0.07089i	0.25098 − 0.00000i	−5.34851 − 0.00000i	4	1.08128	7
0.04768 − 0.36108i	0.34768 − 0.36108i	−0.70037 + 0.60978i	0.07267 − 0.43720i	−0.26765 + 0.54957i	−0.45482 + 0.61880i	0.94953 + 0.00473i	0	2.00622	8
−0.75000 + 0.35671i	−0.45000 + 0.35671i	−1.46212 − 0.58320i	−0.10000 − 0.54702i	2.26212 + 0.41680i	−0.43735 − 0.51456i	−0.93370 − 0.00000i	0	2.00622	8
0.25000 + 0.31675i	0.55000 + 0.31675i	−1.60000 + 0.08844i	−0.10000 − 0.43539i	0.40000 − 0.28655i	0.42608 − 0.00000i	−1.21388 + 0.00000i	0	2.35931	9
−1.08828 − 0.00000i	−0.78828 − 0.00000i	0.11378 − 0.00000i	0.13139 + 0.44094i	1.13139 − 0.44094i	−1.85262 + 0.00000i	−0.00000 + 0.50365i	0	2.35931	9
0.39331 − 0.09117i	0.69331 − 0.09117i	0.46344 − 0.00267i	0.48984 − 0.16274i	−2.53991 + 0.34774i	−0.01886 − 0.06929i	0.30512 − 0.18507i	0	2.69100	10
−1.36802 + 0.13801i	−1.06802 + 0.13801i	−0.26550 + 0.14338i	1.63970 − 0.35821i	0.56183 − 0.06119i	−0.14181 + 0.59662i	−0.50305 − 0.73047i	0	2.69100	10

Table 3
Numerical solutions of the BAEs (3.29)–(3.30) for $N = 4$, $\eta = 0.4$, $\tau = i$. The eigenvalues E_n are exactly the same to those from the exact diagonalization. n denotes the number of the energy levels.

λ_1	λ_2	ϕ	k	E_n	n
$0.80000 + 0.11349i$	$0.80000 + 0.88651i$	2.51327	2	−3.21353	1
$0.80000 + 0.00000i$	$0.80000 + 0.50000i$	1.25664	1	−2.34227	2
$0.80000 + 0.00000i$	$0.30000 + 0.50000i$	1.25664	1	−1.71217	3
$0.30000 + 0.00000i$	$0.80000 + 0.00000i$	0	0	−0.61387	4
$0.30000 + 0.70000i$	$0.80000 + 0.80000i$	3.76991	3	0.00000	5
$0.30000 + 0.30000i$	$0.80000 + 0.20000i$	1.25664	1	0.00000	5
$0.30000 + 0.86676i$	$0.80000 + 0.13324i$	2.51327	2	0.00000	5
$0.30000 + 0.13324i$	$0.80000 + 0.86676i$	2.51327	2	0.00000	5
$0.62340 + 0.25000i$	$0.97660 + 0.25000i$	1.25664	1	0.00000	5
$0.62340 + 0.75000i$	$0.97660 + 0.75000i$	3.76991	3	0.00000	5
0.6	1.0	0	0	0.00000	5
$0.03367 + 0.50000i$	$0.56633 + 0.50000i$	2.51327	2	0.58230	6
$0.30000 + 0.50000i$	$0.80000 + 0.50000i$	2.51327	2	0.61387	7
$0.30000 + 0.00000i$	$0.80000 + 0.50000i$	1.25664	1	1.71217	8
$0.30000 + 0.00000i$	$0.30000 + 0.50000i$	1.25664	1	2.34227	9
$0.30000 + 0.16022i$	$0.30000 + 0.83978i$	2.51327	2	2.63122	10

Some remarks are in order. The BAEs (3.29) are just those obtained in Refs. [7,8], while the relation (3.30) gives rise to that the parameter ϕ takes a discrete value labeled by $k = 1, \ldots, N$. On the other hand, $c \neq 0$ and $\mu_j \neq \nu_k$ for arbitrary j, k may not lead to new solutions but different parameterizations as discussed by Baxter [20] that $\bar{M} = N/2$ already gives a complete set of solutions for even N. To show this clearly, the numerical solutions for $N = 4$ and random choice of η and τ are listed in Table 3.

- **Odd** N **case**. Since τ and η are generic complex numbers, (3.25) cannot be satisfied for any odd N. This means that the $c = 0$ solution of the BAEs (3.17)–(3.21) does not exist for an odd N and generic τ and η.

3.2. *For some degenerate values of* η

For some degenerate values of η, the $c = 0$ solutions indeed exist no matter N is even or odd. In this case, (3.18) is not necessary, and the parameters η and τ are no longer independent but have to obey the relation (3.25). This implies that if the crossing parameter η takes some discrete values

$$\eta = \frac{2l_1}{N - 2\bar{M}}\tau + \frac{2m_1}{N - 2\bar{M}}, \tag{3.31}$$

for any non-negative integer $\bar{M} = M_1 + \bar{m}$ and any integers l_1 and m_1, our generalized T–Q relation (3.16) is reduced to the conventional one [7,8]

$$\Lambda(u) = e^{2i\pi l_1 u + i\phi}\frac{\sigma^N(u+\eta)}{\sigma^N(\eta)}\frac{Q(u-\eta)}{Q(u)} + e^{-2i\pi l_1(u+\eta) - i\phi}\frac{\sigma^N(u)}{\sigma^N(\eta)}\frac{Q(u+\eta)}{Q(u)}, \tag{3.32}$$

where the Q-function is given by (3.28). The $\bar{M} + 1$ parameters ϕ and $\{\lambda_j\}$ satisfy the associated BAEs

$$e^{\{2i\pi(2l_1\lambda_j + l_1\eta) + 2i\phi\}}\frac{\sigma^N(\lambda_j + \eta)}{\sigma^N(\lambda_j)} = -\frac{Q(\lambda_j + \eta)}{Q(\lambda_j - \eta)}, \quad j = 1, \ldots, \bar{M}, \tag{3.33}$$

$$e^{i\phi}\prod_{j=1}^{\bar{M}}\frac{\sigma(\lambda_j+\eta)}{\sigma(\lambda_j)}=e^{\frac{2i\pi k}{N}},\quad k=1,\dots,N. \tag{3.34}$$

4. Results for the XYZ chain with anti-periodic boundary condition

4.1. Functional relations

Now let us turn to the XYZ spin chain described by the Hamiltonian (1.1) but with the anti-periodic boundary condition (1.4). Its integrability is associated with the mutually commutative transfer matrix $t^{(a)}(u)$ given by

$$t^{(a)}(u)=tr_0\{\sigma_0^x\,T_0(u)\}. \tag{4.1}$$

Following the method introduced in Section 2, we can derive the following functional relations

$$t^{(a)}(\theta_j)t^{(a)}(\theta_j-\eta)=-a(\theta_j)\,d(\theta_j-\eta),\quad j=1,\dots N, \tag{4.2}$$

$$\prod_{j=1}^{N}t^{(a)}(\theta_j)=\left\{\prod_{j=1}^{N}a(\theta_j)\right\}\times U^x, \tag{4.3}$$

$$t^{(a)}(u+1)=(-1)^{N-1}t^{(a)}(u), \tag{4.4}$$

$$t^{(a)}(u+\tau)=(-1)^N e^{-2i\pi\{Nu+N\frac{\eta+\tau}{2}-\sum_{l=1}^{N}\theta_l\}}\,t^{(a)}(u), \tag{4.5}$$

where the operator U^x is given by (2.22). It is easy to check that

$$\left[t^{(a)}(u),\,U^x\right]=0,\quad \left(U^x\right)^2=\mathrm{id},$$

which implies that the eigenvalue of the operator U^x takes the values ±1 and can be diagonalized with the transfer matrix $t^{(a)}(u)$ simultaneously. Let us denote the eigenvalue of the transfer matrix $t^{(a)}(u)$ as $\Lambda(u)$. (4.2)–(4.5) enable us to derive the following functional relations

$$\Lambda(\theta_j)\Lambda(\theta_j-\eta)=-a(\theta_j)\,d(\theta_j-\eta),\quad j=1,\dots,N, \tag{4.6}$$

$$\prod_{j=1}^{N}\Lambda(\theta_j)=\pm\prod_{j=1}^{N}a(\theta_j), \tag{4.7}$$

$$\Lambda(u+1)=(-1)^{N-1}\Lambda(u), \tag{4.8}$$

$$\Lambda(u+\tau)=(-1)^N e^{-2i\pi\{Nu+N\frac{\eta+\tau}{2}-\sum_{l=1}^{N}\theta_l\}}\Lambda(u). \tag{4.9}$$

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

$$\Lambda(u)\ \text{is an entire function of}\ u. \tag{4.10}$$

4.2. T–Q relation

As for the periodic case, (4.6)–(4.10) allow us to determine the eigenvalues of the transfer matrix $t^{(a)}(u)$. After taking the homogeneous limit $\theta_j\to0$, we obtain the following inhomogeneous T–Q relation

$$\Lambda(u)=e^{\{i\pi(2l_1+1)u+i\phi\}}\frac{\sigma^N(u+\eta)}{\sigma^N(\eta)}\,\frac{Q_1(u-\eta)Q(u-\eta)}{Q_2(u)Q(u)}$$

$$
\begin{aligned}
&- \frac{e^{-i\pi(2l_1+1)(u+\eta)-i\phi}\sigma^N(u)}{\sigma^N(\eta)} \frac{Q_2(u+\eta)Q(u+\eta)}{Q_1(u)Q(u)} \\
&+ \frac{ce^{i\pi u}\sigma^N(u+\eta)\sigma^N(u)}{Q_1(u)Q_2(u)Q(u)\sigma^N(\eta)\sigma^N(\eta)},
\end{aligned} \tag{4.11}
$$

where l_1 is a certain integer, the Q-functions $Q_1(u)$, $Q_2(u)$ and $Q(u)$ are given by (3.7)–(3.8). The $N+2$ parameters c, ϕ, $\{\mu_j | j = 1, \ldots, M\}$, $\{\nu_j | j = 1, \ldots, M\}$ and $\{\lambda_j | j = 1, \ldots, M_1\}$ satisfy the associated BAEs

$$
\left(\frac{N}{2} - M - M_1\right)\eta - \sum_{j=1}^{M}(\mu_j - \nu_j) = \left(l_1 + \frac{1}{2}\right)\tau + m_1, \quad l_1, m_1 \in Z, \tag{4.12}
$$

$$
\frac{N}{2}\eta + \sum_{j=1}^{M}(\mu_j + \nu_j) + \sum_{j=1}^{M_1}\lambda_j = \frac{1}{2}\tau + m_2, \quad m_2 \in Z, \tag{4.13}
$$

$$
\begin{aligned}
&\frac{ce^{\{2i\pi(l_1+1)\mu_j + 2i\pi(l_1+\frac{1}{2})\eta + i\phi\}}\sigma^N(\mu_j+\eta)}{\sigma^N(\eta)} \\
&\quad = Q_2(\mu_j)Q_2(\mu_j+\eta)Q(\mu_j+\eta), \quad j = 1, \ldots, M,
\end{aligned} \tag{4.14}
$$

$$
\begin{aligned}
&\frac{ce^{\{-2i\pi l_1\nu_j - i\phi\}}\sigma^N(\nu_j)}{\sigma^N(\eta)} \\
&\quad = -Q_1(\nu_j)Q_1(\nu_j-\eta)Q(\nu_j-\eta), \quad j = 1, \ldots, M,
\end{aligned} \tag{4.15}
$$

$$
\begin{aligned}
&e^{i\pi(2l_1+1)(2\lambda_j+\eta)+2i\phi}\frac{\sigma^N(\lambda_j+\eta)}{\sigma^N(\lambda_j)} - \frac{Q_2(\lambda_j)Q_2(\lambda_j+\eta)Q(\lambda_j+\eta)}{Q_1(\lambda_j)Q_1(\lambda_j-\eta)Q(\lambda_j-\eta)} \\
&\quad = \frac{-ce^{2i\pi(l_1+1)\lambda_j + i\pi(2l_1+1)\eta + i\phi}\sigma^N(\lambda_j+\eta)}{Q_1(\lambda_j)Q_1(\lambda_j-\eta)Q(\lambda_j-\eta)\sigma^N(\eta)}, \quad j = 1, \ldots, M_1,
\end{aligned} \tag{4.16}
$$

and the selection rule

$$
\Lambda(0) = e^{i\phi}\left\{\prod_{j=1}^{M}\frac{\sigma(\mu_j+\eta)}{\sigma(\nu_j)}\right\}\left\{\prod_{j=1}^{M_1}\frac{\sigma(\lambda_j+\eta)}{\sigma(\lambda_j)}\right\} = e^{\frac{i\pi k}{N}}, \quad k = 1, \ldots, 2N. \tag{4.17}
$$

The eigenvalue of the Hamiltonian (1.1) with the anti-periodic boundary condition is then given by

$$
\begin{aligned}
E = \frac{\sigma(\eta)}{\sigma'(0)}\Bigg\{&\sum_{j=1}^{M}\left[\zeta(\nu_j) - \zeta(\mu_j+\eta)\right] + \sum_{j=1}^{M_1}\left[\zeta(\lambda_j) - \zeta(\lambda_j+\eta)\right] \\
&+ \frac{1}{2}N\zeta(\eta) + 2i\pi\left(l_1 + \frac{1}{2}\right)\Bigg\}.
\end{aligned} \tag{4.18}
$$

For a generic η, in contrast to the periodic case, there does not exist the $c = 0$ solution of the BAEs (4.12)–(4.16) no matter N is even or odd. However, when η takes some discrete values labeled by a non-negative integer $\bar{M}$ and two integers l_1 and m_1

$$
\eta = \frac{2l_1+1}{N-2\bar{M}}\tau + \frac{2m_1}{N-2\bar{M}}, \quad l_1, m_1 \in Z, \tag{4.19}
$$

the $c = 0$ solutions of the BAEs (4.12)–(4.16) do exist. In this case, the T–Q relation (4.11) is reduced to the conventional one

$$\Lambda(u) = e^{2i\pi(l_1+\frac{1}{2})u+i\phi}\frac{\sigma^N(u+\eta)}{\sigma^N(\eta)}\frac{Q(u-\eta)}{Q(u)} - e^{-2i\pi(l_1+\frac{1}{2})(u+\eta)-i\phi}\frac{\sigma^N(u)}{\sigma^N(\eta)}\frac{Q(u+\eta)}{Q(u)}, \tag{4.20}$$

with the associated BAEs and selection rule

$$e^{\{2i\pi((2l_1+1)\lambda_j+(l_1+\frac{1}{2})\eta)+2i\phi\}}\frac{\sigma^N(\lambda_j+\eta)}{\sigma^N(\lambda_j)} = \frac{Q(\lambda_j+\eta)}{Q(\lambda_j-\eta)}, \quad j = 1, \ldots, \bar{M}, \tag{4.21}$$

$$e^{i\phi}\prod_{j=1}^{\bar{M}}\frac{\sigma(\lambda_j+\eta)}{\sigma(\lambda_j)} = e^{\frac{i\pi k}{N}}, \quad k = 1, \ldots, 2N. \tag{4.22}$$

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 [11–13]. The eigenvalues of the transfer matrices are given in terms of the inhomogeneous T–Q relations (3.16) and (4.11) which allow us to treat both even N and odd N cases in a unified framework. For a generic crossing parameter η, our solution can be reduced to Baxter's solution only for the periodic chain and even N, while for all the other cases (the periodic chain with odd N and the anti-periodic chain), an extra inhomogeneous term (the third term in (3.16) or (4.11)) has to be included in the T–Q relations. However, if the crossing parameter η takes some degenerate values ((3.31) for the periodic case and (4.19) for the antiperiodic case), the corresponding T–Q relation can be reduced to the conventional one. It should be emphasized that these degenerate points become dense in the whole complex η-plane in the thermodynamic limit ($N \to \infty$). This enables one to obtain the thermodynamic properties (up to the order of $O(N^{-2})$) [21] for generic values of η via the conventional thermodynamic Bethe ansatz methods [10,22].

Acknowledgements

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), the State Education Ministry of China (Grant No. 20116101110017) and BCMIIS 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

The following identities for the elliptic functions defined by (2.1)–(2.2) are quite useful in the derivations

$$\sigma(u+x)\sigma(u-x)\sigma(v+y)\sigma(v-y) - \sigma(u+y)\sigma(u-y)\sigma(v+x)\sigma(v-x) = \sigma(u+v)\sigma(u-v)\sigma(x+y)\sigma(x-y), \tag{A.1}$$

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

$$\frac{\sigma(u)}{\sigma(\frac{\tau}{2})} = \frac{\theta\begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(u,2\tau)\,\theta\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(u,2\tau)}{\theta\begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(\frac{\tau}{2},2\tau)\,\theta\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(\frac{\tau}{2},2\tau)}, \tag{A.3}$$

$$\theta\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(2u,2\tau) = \theta\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(\tau,2\tau) \times \frac{\sigma(u)\sigma(u+\frac{1}{2})}{\sigma(\frac{\tau}{2})\sigma(\frac{1}{2}+\frac{\tau}{2})}, \tag{A.4}$$

$$\theta\begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(2u,2\tau) = \theta\begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(0,2\tau) \times \frac{\sigma(u-\frac{\tau}{2})\sigma(u+\frac{1}{2}+\frac{\tau}{2})}{\sigma(-\frac{\tau}{2})\sigma(\frac{1}{2}+\frac{\tau}{2})}. \tag{A.5}$$

Appendix B. Trigonometric limit

The results of the XXZ spin chain can be recovered by taking the limit $\tau \to +i\infty$ of the XYZ model. Here we take the periodic case as an example. Its generalization to the anti-periodic case is straightforward.

The definition of the elliptic functions (2.1)–(2.2) implies

$$\sigma\left(u+\frac{\tau}{2}\right) = e^{-i\pi(u+\frac{1}{2}+\frac{\tau}{4})}\,\theta\begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(u,\tau), \tag{B.1}$$

and the following asymptotic behaviors

$$\lim_{\tau\to+i\infty} \sigma(u) = -2e^{\frac{i\pi\tau}{4}}\sin\pi u + \ldots, \tag{B.2}$$

$$\lim_{\tau\to+i\infty} \theta\begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(u,\tau) = 1 + \ldots. \tag{B.3}$$

The above asymptotic behaviors lead to the well-known XXZ R-matrix

$$\lim_{\tau\to+i\infty} R(u) = \frac{1}{\sin\pi\eta}\begin{pmatrix} \sin\pi(u+\eta) & & & \\ & \sin\pi u & \sin\pi\eta & \\ & \sin\pi\eta & \sin\pi u & \\ & & & \sin\pi(u+\eta) \end{pmatrix}. \tag{B.4}$$

The resulting R-matrix gives rise to the associated asymptotic behaviors of the resulting transfer matrix, which are the counterparts of the quasi-periodic properties (2.25) and (2.26),

$$t(u+1) = (-1)^N t(u), \tag{B.5}$$

$$t(u) \overset{u\to-i\infty}{=} \frac{e^{i\pi(Nu-\sum_{l=1}^N\theta_l+\frac{N}{2}\eta)}}{(2\sin\pi\eta)^N}\left(e^{\frac{i\pi\eta}{2}\sum_{l=1}^N\sigma_l^z} + e^{\frac{-i\pi\eta}{2}\sum_{l=1}^N\sigma_l^z}\right) + \ldots, \tag{B.6}$$

$$t(u) \overset{u\to+i\infty}{=} (-1)^N\frac{e^{i\pi(-Nu+\sum_{l=1}^N\theta_l-\frac{N}{2}\eta)}}{(2\sin\pi\eta)^N}\left(e^{\frac{i\pi\eta}{2}\sum_{l=1}^N\sigma_l^z} + e^{\frac{-i\pi\eta}{2}\sum_{l=1}^N\sigma_l^z}\right) + \ldots. \tag{B.7}$$

Since the total spin operator $S^z = \frac{1}{2}\sum_{l=1}^N\sigma_l^z$ commutes with the transfer matrix in the trigonometric limit, one can decompose the whole Hilbert space into subspaces according to the eigenvalues of S^z

$$\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \cdots \mathbb{C}^2 = \bigoplus_{i=0}^{N} \mathcal{H}^{(i)}, \qquad S^z \mathcal{H}^{(i)} = \left(\frac{N}{2} - i\right) \mathcal{H}^{(i)}. \tag{B.8}$$

The eigenvalue $\Lambda(u)$ in the subspace $\mathcal{H}^{(M)}$ has the following asymptotic behaviors

$$\Lambda(u+1) = (-1)^N \Lambda(u), \tag{B.9}$$

$$\Lambda(u) \overset{u\to -i\infty}{=} \frac{e^{i\pi(Nu - \sum_{l=1}^{N}\theta_l)}}{(2\sin\pi\eta)^N} \left(e^{i\pi(N-M)\eta} + e^{i\pi M\eta}\right) + \ldots, \tag{B.10}$$

$$\Lambda(u) \overset{u\to +i\infty}{=} (-1)^N \frac{e^{i\pi(-Nu + \sum_{l=1}^{N}\theta_l)}}{(2\sin\pi\eta)^N} \left(e^{i\pi(-N+M)\eta} + e^{-i\pi M\eta}\right) + \ldots. \tag{B.11}$$

The limits of the identities (3.4) become

$$\Lambda(\theta_j)\Lambda(\theta_j - \eta) = \bar{a}(\theta_j)\bar{d}(\theta_j - \eta), \quad j = 1, \ldots, N,$$
$$\bar{a}(u) = \prod_{l=1}^{N} \frac{\sin\pi(u - \theta_l + \eta)}{\sin\pi\eta}, \qquad \bar{d}(u) = \bar{a}(u - \eta) = \prod_{l=1}^{N} \frac{\sin\pi(u - \theta_l)}{\sin\pi\eta}. \tag{B.12}$$

The solutions of (3.1), (B.9)–(B.12) in the subspace $\mathcal{H}^{(M)}$ (naturally $c = 0$) can be given by the usual T–Q relation

$$\Lambda(u) = \bar{a}(u)\frac{\bar{Q}(u-\eta)}{\bar{Q}(u)} + \bar{d}(u)\frac{\bar{Q}(u+\eta)}{\bar{Q}(u)}, \tag{B.13}$$

$$\bar{Q}(u) = \prod_{l=1}^{M} \frac{\sin\pi(u - \lambda_l)}{\sin\pi\eta}, \quad M = 0, 1, \ldots, N, \tag{B.14}$$

where the Bethe roots $\{\lambda_l\}$ satisfy the conventional Bethe ansatz equations [10].

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, Academic Press, London, 1982.
[8] L.A. Takhtadzhan, L.D. Faddeev, Rush. Math. Surv. 34 (1979) 11.
[9] E.K. Sklyanin, L.D. Faddeev, Sov. Phys. Dokl. 23 (1978) 902.
[10] V.E. Korepin, N.M. Boliubov, A.G. Izergin, Quantum Inverse Scattering Method and Correlation Functions, Cambridge University Press, Cambridge, 1993.
[11] J. Cao, W.-L. Yang, K.-J. Shi, Y. Wang, Phys. Rev. Lett. 111 (2013) 137201.
[12] J. Cao, W.-L. Yang, K.-J. Shi, Y. Wang, Nucl. Phys. B 875 (2013) 152.
[13] J. Cao, W.-L. Yang, K.-J. Shi, Y. Wang, Nucl. Phys. B 877 (2013) 152.
[14] N. Kitanine, J.M. Maillet, V. Terras, Nucl. Phys. B 554 (1999) 647.
[15] J.M. Maillet, V. Terras, Nucl. Phys. B 575 (2000) 627.
[16] F. Göhmann, V.E. Korepin, J. Phys. A 33 (2000) 1199.
[17] G. Niccoli, J. Phys. A 46 (2013) 075003.
[18] R.-I. Nepomechie, F. Ravanini, J. Phys. A 36 (2003) 11391;
R.-I. Nepomechie, F. Ravanini, J. Phys. A 37 (2004) 1945.
[19] J. Cao, H.-Q. Lin, K. Shi, Y. Wang, Nucl. Phys. B 663 (2003) 487.

[20] R.J. Baxter, J. Stat. Phys. 116 (2004) 43.
[21] Y.-Y. Li, J. Cao, W.-L. Yang, K. Shi, Y. Wang, Nucl. Phys. B 844 (2014) 17.
[22] M. Takahashi, Thermodynamics of One-Dimensional Solvable Models, Cambridge University Press, Cambridge, 1999.