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Off-diagonal Bethe ansatz solution of the XXX spin chain with arbitrary boundary conditions

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Abstract

Employing the off-diagonal Bethe ansatz method proposed recently by the present authors, we exactly diagonalize the XXX spin chain with arbitrary boundary fields. By constructing a functional relation between the eigenvalues of the transfer matrix and the quantum determinant, the associated $T-Q$ relation and the Bethe ansatz equations are derived.

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

1. Introduction

Our understanding of quantum phase transitions and critical phenomena has been greatly enhanced by the study of exactly solvable models (or quantum integrable systems) [1]. Such exact results have provided valuable insight into the important universality classes of quantum physical systems ranging from modern condensed matter physics [2] to string and super-symmetric Yang–Mills theories [3]. Since Yang and Baxter's pioneering works [4,5,1], the quantum Yang–Baxter equation (QYBE), which defines the underlying algebraic structure, has become a cornerstone for constructing and solving the integrable models. There are several well-known methods for deriving the Bethe ansatz (BA) solution of integrable models: the coordinate BA [6,1,7–9], the

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T–Q approach [1,10], the algebraic BA [11–13], the analytic BA [14], the functional BA [15] and others [16–29].

Generally speaking, there are two classes of integrable models. One possesses $U(1)$ symmetry and the other does not. Three well-known examples without $U(1)$ symmetry are the XYZ spin chain [5,12], the XXZ spin chain with antiperiodic boundary condition [30,31,25–27,29] and the ones with unparallel boundary fields [18–21,24–29]. It has been proven that most of the conventional Bethe ansatz methods can successfully diagonalize the integrable models with $U(1)$ symmetry. However, for those without $U(1)$ symmetry, only some very special cases such as the XYZ spin chain with even site number [5,12] and the XXZ spin chain with constrained unparallel boundary fields [19,20,32,33] can be dealt with due to the existence of a proper "local vacuum state" in these special cases. The main obstacle applying the algebraic Bethe ansatz and Baxter's method to general integrable models without $U(1)$ symmetry lies in the absence of such a "local vacuum". A promising method for approaching such kind of problems is Sklyanin's separation of variables method [15] which has been recently applied to some integrable models [26–29]. However, before the very recent work [34], a systematic method was still absent to derive the Bethe ansatz equations for integrable models without $U(1)$ symmetry, which are crucial for studying the physical properties in the thermodynamic limit.

As for integrable models without $U(1)$ symmetry, some off-diagonal elements of monodromy matrix enter into expression of the transfer matrix. This breaks down the usual $U(1)$ symmetry. Very recently, we have proposed a method [34] for dealing with the integrable models without $U(1)$ symmetry. The central idea of the method is to construct the functional relations between eigenvalues $\Lambda(\lambda)$ of the transfer matrix (the trace of the monodromy matrix) and its quantum determinant $\Delta_q(\lambda)$, i.e., $\Lambda(\theta_j)\Lambda(\theta_j-\eta)\sim\Delta_q(\theta_j)$ (see below (4.17)) based on the zero points of the product of off-diagonal elements of monodromy matrix $B(u)B(u-\eta)=0$. Since the trace and the determinant are two basic quantities of a matrix which are independent of the representation basis, this method could overcome the obstacle of absence of a reference state which is crucial in the conventional Bethe ansatz methods.

Our primary motivation for this work comes from the long standing problem of solving the open spin-$\frac{1}{2}$ XXX spin chain with unparallel boundary fields, defined by the Hamiltonian [35,36]

$$H=\sum_{j=1}^{N-1}\vec{\sigma}_j\vec{\sigma}_{j+1}+h_N\sigma_N^z+h_1^x\sigma_1^x+h_1^z\sigma_1^z. \tag{1.1}$$

N is the site number of the system and σ_j^α $(\alpha=x,y,z)$ is the Pauli matrix on the site j along the α direction. The parameters h_N, h_1^x and h_1^z are related to boundary fields. Solving this problem for generic values of these three parameters is a crucial step in formulating the thermodynamics of the spin chain, due to the fact that this problem has important applications in condensed matter physics and statistical mechanics. In this paper, we shall use the method developed in [34] to solve the eigenvalue problem of the above Hamiltonian with generic h_N, h_1^x and h_1^z.

The paper is organized as follows. Section 2 serves as an introduction of our notation and some basic ingredients. We briefly describe the inhomogeneous open XXX chain with non-diagonal boundary terms. In Section 3, we derive the exchange relations among the matrix entries of the monodromy matrix algebras (or the Yang–Baxter algebras). In Section 4 after obtaining some properties of the eigenvalue as a function of spectrum parameter u, we derive the very relation between the eigenvalue and the quantum determinant of the double-row monodromy matrix. This allows us to construct a generalized T–Q relation type solution of eigenvalue. In Section 5, we consider the homogeneous limit of the results of the previous section and give the energy spectrum of the Hamiltonian of the open spin-$\frac{1}{2}$ XXX spin chain with unparallel boundary fields. In Section 6, we summarize our results and give some discussions. Some detailed technical proof is given in Appendix A.

2. Transfer matrix

Throughout, $\mathbf{V}$ denotes a two-dimensional linear space. The well-known rational six-vertex model R-matrix $R(u) \in \mathrm{End}(\mathbf{V} \otimes \mathbf{V})$ is given by

$$R(u) = \begin{pmatrix} u+1 & & & \\ & u & 1 & \\ & 1 & u & \\ & & & u+1 \end{pmatrix}. \tag{2.1}$$

Here u is the spectral parameter. Without losing the generality we have set the so-called bulk anisotropy parameter (or crossing parameter) $\eta = 1$. The R-matrix satisfies the quantum Yang–Baxter equation (QYBE)

$$\begin{aligned} &R_{12}(u_1 - u_2)R_{13}(u_1 - u_3)R_{23}(u_2 - u_3) \\ &\quad = R_{23}(u_2 - u_3)R_{13}(u_1 - u_3)R_{12}(u_1 - u_2), \end{aligned} \tag{2.2}$$

and the properties,

$$\text{Initial condition:} \quad R_{12}(0) = P_{12}, \tag{2.3}$$

$$\text{Unitarity relation:} \quad R_{12}(u)R_{21}(-u) = -\xi(u)\mathrm{id}, \quad \xi(u) = (u+1)(u-1), \tag{2.4}$$

$$\text{Crossing relation:} \quad R_{12}(u) = V_1 R_{12}^{t_2}(-u-1)V_1, \quad V = -i\sigma^y, \tag{2.5}$$

$$\text{PT-symmetry:} \quad R_{12}(u) = R_{21}(u) = R_{12}^{t_1 t_2}(u), \tag{2.6}$$

$$\text{Antisymmetry:} \quad R_{12}(-1) = -(1-P) = -2P^{(-)}. \tag{2.7}$$

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. Here and below we adopt the standard notations: for any matrix $A \in \mathrm{End}(\mathbf{V})$, A_j is an embedding operator in the tensor space $\mathbf{V} \otimes \mathbf{V} \otimes \cdots$, 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.

One introduces the "row-to-row" (or one-row) monodromy matrices $T(u)$ and $\hat{T}(u)$, which are a 2×2 matrix with elements being operators acting on $\mathbf{V}^{\otimes N}$,

$$T_0(u) = R_{0N}(u - \theta_N)R_{0N-1}(u - \theta_{N-1}) \cdots R_{01}(u - \theta_1), \tag{2.8}$$

$$\hat{T}_0(u) = R_{01}(u + \theta_1)R_{02}(u + \theta_2) \cdots R_{0N}(u + \theta_N). \tag{2.9}$$

Here $\{\theta_j \mid j = 1, \ldots, N\}$ are arbitrary free complex parameters which are usually called inhomogeneous parameters.

Integrable open chain can be constructed as follows [35]. Let us introduce a pair of K-matrices $K^-(u)$ and $K^+(u)$. The former satisfies the reflection equation (RE)

$$\begin{aligned} &R_{12}(u_1 - u_2)K_1^-(u_1)R_{21}(u_1 + u_2)K_2^-(u_2) \\ &\quad = K_2^-(u_2)R_{12}(u_1 + u_2)K_1^-(u_1)R_{21}(u_1 - u_2), \end{aligned} \tag{2.10}$$

and the latter satisfies the dual RE

$$\begin{aligned} &R_{12}(u_2-u_1)K_1^+(u_1)R_{21}(-u_1-u_2-2)K_2^+(u_2) \\ &\quad = K_2^+(u_2)R_{12}(-u_1-u_2-2)K_1^+(u_1)R_{21}(u_2-u_1). \end{aligned} \tag{2.11}$$

For open spin chains, other than the standard "row-to-row" monodromy matrix $T(u)$ (2.8), one needs to consider the double-row monodromy matrix $\mathbb{T}(u)$

$$\mathbb{T}(u) = T(u)K^-(u)\hat{T}(u). \tag{2.12}$$

Then the double-row transfer matrix of the XXX chain with open boundary (or the open XXX chain) is given by

$$\tau(u) = tr\big(K^+(u)\mathbb{T}(u)\big). \tag{2.13}$$

The QYBE (2.2) and (dual) REs (2.10) and (2.11) lead to the fact that the transfer matrices with different spectral parameters commute with each other [35]: $[\tau(u), \tau(v)] = 0$. Then $\tau(u)$ serves as the generating functional of the conserved quantities of the corresponding system, which ensures the integrability of the open XXX chain.

In this paper in order to study the system described by the Hamiltonian (1.1), we consider the K-matrix $K^-(u)$ which is a diagonal solution to the RE (2.10) associated with the six-vertex model R-matrix [36,37]

$$K^-(u) = \begin{pmatrix} p+u & 0 \\ 0 & p-u \end{pmatrix}. \tag{2.14}$$

At the same time, we introduce the corresponding *dual* K-matrix $K^+(u)$ which is a generic solution to the dual reflection equation (2.11)

$$K^+(u) = \begin{pmatrix} q+u+1 & \xi(u+1) \\ \xi(u+1) & q-u-1 \end{pmatrix}. \tag{2.15}$$

The first order derivative of logarithm of the transfer matrix $\tau(u)$ (2.13) with the K-matrices $K^\pm$ given by (2.14) and (2.15) yields the Hamiltonian (1.1)

$$\begin{aligned} H &= \frac{\partial \ln\tau(\lambda)}{\partial\lambda}\bigg|_{\lambda=0,\theta_j=0} - (N-1) \\ &= 2\sum_{j=1}^{N-1} P_{j,j+1} + \frac{K_N^{-\prime}(0)}{K_N^-(0)} + 2\frac{K_1^{+\prime}(0)}{K_1^+(0)} \\ &= \sum_{j=1}^{N-1} \vec{\sigma}_j\vec{\sigma}_{j+1} + \frac{1}{p}\sigma_N^z + \frac{1}{q}\big(\sigma_1^z + \xi\sigma_1^x\big). \end{aligned} \tag{2.16}$$

Therefore, $h_N = 1/p$, $h_1^x = \xi/q$ and $h_1^z = 1/q$.

3. Exchange relations of the monodromy matrices

The Yang–Baxter algebra is a corner stone of the QISM and it has been successfully explored in order to construct integrable systems and to get their exact solutions.

From the quantum Yang–Baxter equation (2.2), one may derive the following "RLL" relations among the one-row monodromy matrices $T(u)$ and $\hat{T}(u)$

$$R_{12}(u-v)T_1(u)T_2(v)=T_2(v)T_1(u)R_{12}(u-v), \tag{3.1}$$

$$R_{12}(v-u)\hat{T}_2(v)\hat{T}_1(u)=\hat{T}_1(u)\hat{T}_2(v)R_{12}(v-u), \tag{3.2}$$

$$\hat{T}_2(v)R_{12}(u+v)T_1(u)=T_1(u)R_{12}(u+v)\hat{T}(v). \tag{3.3}$$

The crossing relation of the R-matrix (2.5) allows us to derive the following relation between $T(u)$ and $\hat{T}(u)$

$$\hat{T}_0(u)=(-1)^{N-1}V_0T^{t_0}(-u-1)V_0. \tag{3.4}$$

Let us decompose the monodromy matrices $T(u)$ and $\hat{T}(u)$ in terms of its components

$$T(u)=\begin{pmatrix}\alpha(u) & \beta(u)\\ \gamma(u) & \delta(u)\end{pmatrix}, \qquad \hat{T}(u)=(-1)^{N-1}\begin{pmatrix}\delta(-u-1) & -\beta(-u-1)\\ -\gamma(-u-1) & \alpha(-u-1)\end{pmatrix}. \tag{3.5}$$

One may find the commutation relations among $\alpha(u)$, $\beta(u)$, $\gamma(u)$ and $\delta(u)$. Here we give the relevant ones for our purpose,

$$\beta(\lambda)\beta(\mu)=\beta(\mu)\beta(\lambda), \tag{3.6}$$

$$\beta(\lambda)\gamma(\mu)=\gamma(\mu)\beta(\lambda)+\frac{1}{\lambda-\mu}\big[\delta(\mu)\alpha(\lambda)-\delta(\lambda)\alpha(\mu)\big], \tag{3.7}$$

$$\alpha(\lambda)\beta(\mu)=\frac{\lambda-\mu-1}{\lambda-\mu}\beta(\mu)\alpha(\lambda)+\frac{1}{\lambda-\mu}\beta(\lambda)\alpha(\mu), \tag{3.8}$$

$$\delta(\lambda)\beta(\mu)=\frac{\lambda-\mu+1}{\lambda-\mu}\beta(\mu)\delta(\lambda)-\frac{1}{\lambda-\mu}\beta(\lambda)\delta(\mu). \tag{3.9}$$

Let us decompose the double-row monodromy matrix $\mathbb{T}(u)$ in terms of its components which can be expressed in terms of the components of $T(u)$

$$\begin{aligned}\mathbb{T}(\lambda)&=\begin{pmatrix}A(\lambda) & B(\lambda)\\ C(\lambda) & D(\lambda)\end{pmatrix}\\ &=\begin{pmatrix}\alpha(\lambda) & \beta\lambda\\ \gamma(\lambda) & \delta(\lambda)\end{pmatrix}\begin{pmatrix}p+\lambda & 0\\ 0 & p-\lambda\end{pmatrix}\begin{pmatrix}\delta(-\lambda-1) & -\beta(-\lambda-1)\\ -\gamma(-\lambda-1) & \alpha(-\lambda-1)\end{pmatrix}.\end{aligned}$$

Namely,

$$\begin{aligned}A(\lambda)&=(p+\lambda)\alpha(\lambda)\delta(-\lambda-1)-(p-\lambda)\beta(\lambda)\gamma(-\lambda-1),\\ B(\lambda)&=-(p+\lambda)\alpha(\lambda)\beta(-\lambda-1)+(p-\lambda)\beta(\lambda)\alpha(-\lambda-1),\\ C(\lambda)&=(p+\lambda)\gamma(\lambda)\delta(-\lambda-1)-(p-\lambda)\delta(\lambda)\gamma(-\lambda-1),\\ D(\lambda)&=-(p+\lambda)\gamma(\lambda)\beta(-\lambda-1)+(p-\lambda)\delta(\lambda)\alpha(-\lambda-1).\end{aligned} \tag{3.10}$$

Moreover, the RE (2.10) and the "RLL" relations (3.1)–(3.3) enable us to derive exchange relation of the double-row monodromy matrix $\mathbb{T}(u)$

$$\begin{aligned}&R_{12}(u_1-u_2)\mathbb{T}_1(u_1)R_{21}(u_1+u_2)\mathbb{T}_2(u_2)\\ &\quad=\mathbb{T}_2(u_2)R_{12}(u_1+u_2)\mathbb{T}_1(u_1)R_{21}(u_1-u_2),\end{aligned} \tag{3.11}$$

which allows one to obtain the commutation relations among $A(u)$, $B(u)$, $C(u)$ and $D(u)$. Here we give the relevant ones given by [35] for our purpose,

$$C(\lambda)B(\mu) = B(\mu)C(\lambda) + \frac{\lambda+\mu}{(\lambda+\mu+1)(\lambda-\mu)(2\lambda+1)}A(\mu)\bar{D}(\lambda)$$
$$+ \frac{(\lambda-\mu+1)(2\lambda)}{(\lambda+\mu+1)(\lambda-\mu)(2\lambda+1)}A(\mu)A(\lambda) - \frac{2\lambda[A(\lambda)\bar{D}(\mu)+A(\lambda)A(\mu)]}{(\lambda-\mu)(2\lambda+1)(2\mu+1)}$$
$$- \frac{[\bar{D}(\lambda)\bar{D}(\mu)+\bar{D}(\lambda)A(\mu)]}{(\lambda+\mu+1)(2\lambda+1)(2\mu+1)}, \tag{3.12}$$

$$A(\lambda)B(\mu) = \frac{(\lambda+\mu)(\lambda-\mu-1)}{(\lambda-\mu)(\lambda+\mu+1)}B(\mu)A(\lambda) - \frac{1}{(\lambda+\mu+1)(2\mu+1)}B(\lambda)\bar{D}(\mu)$$
$$+ \frac{2\mu}{(\lambda-\mu)(2\mu+1)}B(\lambda)A(\mu), \tag{3.13}$$

$$\bar{D}(\lambda)B(\mu) = \frac{(\lambda-\mu+1)(\lambda+\mu+2)}{(\lambda-\mu)(\lambda+\mu+1)}B(\mu)\bar{D}(\lambda) - \frac{2(\lambda+1)}{(\lambda-\mu)(2\mu+1)}B(\lambda)\bar{D}(\mu)$$
$$+ \frac{4(\lambda+1)\mu}{(2\mu+1)(\lambda+\mu+1)}B(\lambda)A(\mu). \tag{3.14}$$

Here we have introduced the operator $\bar{D}(\lambda) = (2\lambda+1)D(\lambda) - A(\lambda)$. At this stage, we have provided most of the ingredients required to obtain a fundamental functional relation the eigenvalue of the transfer matrix (2.13) with K-matrices given by (2.14) and (2.15).

4. Functional relations and the T–Q relation

Following the method in [38,39] and using the crossing relation of the R-matrix (2.5) and the explicit expressions of the K-matrices (2.14) and (2.15), one can show that the corresponding transfer matrix $\tau(u)$ has the following properties,

$$\text{Crossing symmetry:} \quad \tau(-u-1) = \tau(u), \tag{4.1}$$

$$\text{Initial condition:} \quad \tau(0) = 2pq\prod_{j=1}^{N}(1-\theta_j)(1+\theta_j) \times \text{id}, \tag{4.2}$$

$$\text{Asymptotic behavior:} \quad \tau(u) \sim 2u^{2N+2} \times \text{id} + \cdots, \quad \text{for } u \to \pm\infty. \tag{4.3}$$

The commutativity of the transfer matrix $\tau(u)$ implies that one can find the common eigenstate of $\tau(u)$, which indeed does not depend upon u. Suppose $\langle\Psi|$ is an eigenstate of $\tau(u)$ with an eigenvalue $\Lambda(u)$, namely,

$$\langle\Psi|\tau(u) = \Lambda(u)\langle\Psi|.$$

The properties of the transfer matrix $\tau(u)$ given by (4.1)–(4.3) imply that the corresponding eigenvalue $\Lambda(u)$ satisfies the following relations:

$$\text{Crossing symmetry:} \quad \Lambda(-u-1) = \Lambda(u), \tag{4.4}$$

$$\text{Initial condition:} \quad \Lambda(0) = 2pq\prod_{j=1}^{N}(1-\theta_j)(1+\theta_j) = \Lambda(-1), \tag{4.5}$$

$$\text{Asymptotic behavior:} \quad \Lambda(u) \sim 2u^{2N+2} + \cdots, \quad \text{for } u \to \pm\infty. \tag{4.6}$$

The analyticity of the R-matrix and K-matrices and independence on u of the eigenstate lead to that the eigenvalue $\Lambda(u)$ further obeys the property

$$\text{Analyticity:} \quad \Lambda(u), \text{ as a function of } u, \text{ is a polynomial of degree } 2N+2. \tag{4.7}$$

Therefore the values of $\Lambda(u)$ at generic $2N+3$ points suffice to determine the function uniquely. However, we have already obtained the corresponding values of $\Lambda(u)$ at points $u = 0, -1, \infty$. For this purpose, we shall find the associated equations to determine the values of $\Lambda(u)$ at the other $2N$ points, for example at $u = \theta_j, -\theta_j - 1$.

Let us define the state $|0\rangle = \otimes|\uparrow\rangle_j$ which now has nothing to do with the eigenstate of the transfer matrix $\tau(u)$ as it does in the conventional algebraic Bethe ansatz [13]. On the other hand, the components of the double-row monodromy matrix $\mathbb{T}(u)$ act on the states, giving rise to:

$$C(u)|0\rangle = 0, \tag{4.8}$$

$$A(u)|0\rangle = (p+u)\prod_{j=1}^{N}(u-\theta_j+1)(u+\theta_j+1) = a(u)|0\rangle, \tag{4.9}$$

$$\bar{D}(u)|0\rangle = 2u(p-u-1)\prod_{j=1}^{N}(u-\theta_j)(u+\theta_j) = d(u)|0\rangle. \tag{4.10}$$

From the explicit expression (2.15) of the K-matrix $K^+(u)$, one can express the transfer matrix in terms of the components of the monodromy matrix $\mathbb{T}(u)$,

$$\begin{aligned}\tau(u) &= (q+u+1)A(u) + \xi(u+1)\big[C(u)+B(u)\big] + (q-u-1)D(u)\\ &= \frac{2(u+q)(u+1)}{2u+1}A(u) + \xi(u+1)\big[B(u)+C(u)\big] + \frac{q-u-1}{2u+1}\bar{D}(u).\end{aligned} \tag{4.11}$$

Now let us compute the action of $\tau(\theta_j)\tau(\theta_j-1)$ on the state $|0\rangle$. Keeping in mind the fact that the function $a(u)$ (or $d(u)$) vanishes at $u = \theta_j - 1$ (or $u = \theta_j$), namely,

$$a(\theta_j - 1) = 0 = d(\theta_j), \quad j = 1, \ldots, N, \tag{4.12}$$

and using the relations (4.8)–(4.10), we have

$$\begin{aligned}\tau(\theta_j)\tau(\theta_j-1)|0\rangle &= \frac{2(\theta_j+q)(\theta_j+1)(q-\theta_j)}{(2\theta_j+1)(2\theta_j-1)}a(\theta_j)d(\theta_j-1)|0\rangle\\ &\quad + \xi^2\theta_j(\theta_j+1)C(\theta_j)B(\theta_j-1)|0\rangle\\ &\quad + \frac{\xi(q-\theta_j)(\theta_j+1)}{2\theta_j-1}d(\theta_j-1)B(\theta_j)|0\rangle\\ &\quad + \frac{2\xi\theta_j(\theta_j+q)(\theta_j+1)}{2\theta_j+1}A(\theta_j)B(\theta_j-1)|0\rangle\\ &\quad + \frac{\xi\theta_j(q-\theta_j-1)}{2\theta_j+1}\bar{D}(\theta_j)B(\theta_j-1)|0\rangle\\ &\quad + \xi^2\theta_j(\theta_j+1)B(\theta_j)B(\theta_j-1)|0\rangle\\ &= \frac{2(\theta_j+1)(q^2-(1+\xi^2)\theta_j^2)}{(2\theta_j-1)(2\theta_j+1)}a(\theta_j)d(\theta_j-1)|0\rangle\\ &\quad + \xi^2\theta_j(\theta_j+1)B(\theta_j)B(\theta_j-1)|0\rangle.\end{aligned} \tag{4.13}$$

In the derivation of the second equality of the above equation, we have used the exchange relation (3.12)–(3.14) and (4.12). One can compute the last terms of (4.13) by expanding the operator

$B(u)$ in terms of the components of one-row monodromy matrix $T(u)$ via (3.10). Direct calculation shows that

$$B(\theta_j)B(\theta_j-1)=0. \tag{4.14}$$

The proof of the above very relation is relegated to Appendix A. Finally, we obtain

$$\tau(\theta_j)\tau(\theta_j-1)|0\rangle=\frac{2(\theta_j+1)(q^2-(1+\xi^2)\theta_j^2)}{(2\theta_j-1)(2\theta_j+1)}a(\theta_j)d(\theta_j-1)|0\rangle. \tag{4.15}$$

Multiplying the eigenstate $\langle\Psi|$ from the left on the both sides of the above equation, we have

$$\langle\Psi|\tau(\theta_j)\tau(\theta_j-1)|0\rangle=\frac{2(\theta_j+1)(q^2-(1+\xi^2)\theta_j^2)}{(2\theta_j-1)(2\theta_j+1)}a(\theta_j)d(\theta_j-1)\langle\Psi|0\rangle, \tag{4.16}$$

which leads to the following equations[1]

$$\begin{aligned}\Lambda(\theta_j)\Lambda(\theta_j-1)&=\frac{2(\theta_j+1)(q^2-(1+\xi^2)\theta_j^2)}{(2\theta_j-1)(2\theta_j+1)}a(\theta_j)d(\theta_j-1)\\&=\frac{\Delta_q(\theta_j)}{(1-2\theta_j)(1+2\theta_j)},\quad j=1,\ldots,N.\end{aligned} \tag{4.17}$$

The expression of the quantum determinant $\Delta_q(u)$ is given by [41,42]

$$\Delta_q(u)=\mathrm{Det}\{T(u)\}\,\mathrm{Det}\{\hat{T}(u)\}\,\mathrm{Det}\{K^-(u)\}\,\mathrm{Det}\{K^+(u)\}, \tag{4.18}$$

and the corresponding determinants can be directly calculated

$$\mathrm{Det}\{T(u)\}\mathrm{id}=tr_{12}\big(P_{12}^{(-)}T_1(u-1)T_2(u)P_{12}^{(-)}\big)=\prod_{j=1}^{N}(u-\theta_j+1)(u-\theta_j-1)\mathrm{id},$$

$$\mathrm{Det}\{\hat{T}(u)\}\mathrm{id}=tr_{12}\big(P_{12}^{(-)}\hat{T}_1(u-1)\hat{T}_2(u)P_{12}^{(-)}\big)=\prod_{j=1}^{N}(u+\theta_j+1)(u+\theta_j-1)\mathrm{id},$$

$$\mathrm{Det}\{K^-(u)\}=tr_{12}\big(P_{12}^{(-)}K_1^-(u-1)R_{12}(2u-1)K_2^-(u)\big)=2(u-1)\big(p^2-u^2\big),$$

$$\begin{aligned}\mathrm{Det}\{K^+(u)\}&=tr_{12}\big(P_{12}^{(-)}K_2^+(u)R_{12}(-2u-1)K_1^+(u-1)\big)\\&=2(u+1)\big(\big(1+\xi^2\big)u^2-q^2\big).\end{aligned}$$

Eqs. (4.17) play an important role in our method, which gives rise to the functional relations between eigenvalues $\Lambda(u)$ of the transfer matrix (the trace of the monodromy matrix algebra) and its quantum determinant $\Delta_q(u)$, i.e., $\Lambda(\theta_j)\Lambda(\theta_j-1)\sim\Delta_q(\theta_j)$ when the spectrum u is taken at some particular points $\{\theta_j\}$ which are the zero points of $B(u)B(u-1)|0\rangle=0$. Since the trace and the determinant are two basic quantities of a matrix which are independent of the representation basis, this method can overcome the obstacle of absence of a reference state which is crucial in the conventional Bethe ansatz methods. Moreover, Eqs. (4.4)–(4.7) and (4.17) enable one to determine the functions $\Lambda(u)$. In the following part of the section, we shall express the solutions of these equations in terms of a generalized T–Q relation formulism.

[1] Here we assume that the scalar product $\langle\Psi|0\rangle$ is nonzero. The relations (4.14) and (4.17) were also obtained previously by the Sklyanin's separation of variables method for the boundary parameters with some constraint [40].

Let us introduce some functions $\bar{a}^{(\pm)}(u)$ and $\bar{d}^{(\pm)}(u)$

$$\bar{a}^{(\pm)}(u)=\frac{2u+2}{2u+1}(u\pm p)\big(\sqrt{1+\xi^2}u\pm q\big)\prod_{j=1}^{N}(u+\theta_j+1)(u-\theta_j+1), \tag{4.19}$$

$$\begin{aligned}\bar{d}^{(\pm)}(u)&=\frac{2u}{2u+1}(u\mp p+1)\big(\sqrt{1+\xi^2}(u+1)\mp q\big)\prod_{j=1}^{N}(u+\theta_j)(u-\theta_j)\\&=\bar{a}^{(\pm)}(-u-1).\end{aligned} \tag{4.20}$$

We can construct the solutions of (4.4)–(4.7) by the following ansatz

$$\begin{aligned}\Lambda^{(\pm)}(u)={}&\bar{a}^{(\pm)}(u)\frac{Q^{(\pm)}(u-1)Q_1^{(\pm)}(u-1)}{Q^{(\pm)}(u)Q_2^{(\pm)}(u)}+\bar{d}^{(\pm)}(u)\frac{Q^{(\pm)}(u+1)Q_2^{(\pm)}(u+1)}{Q^{(\pm)}(u)Q_1^{(\pm)}(u)}\\&+2\big(1-\sqrt{1+\xi^2}\big)u(u+1)\frac{\prod_{j=1}^{N}(u+\theta_j)(u-\theta_j)(u+\theta_j+1)(u-\theta_j+1)}{Q^{(\pm)}(u)Q_1^{(\pm)}(u)Q_2^{(\pm)}(u)}.\end{aligned} \tag{4.21}$$

The functions $Q^{(\pm)}(u)$, $Q_1^{(\pm)}(u)$ and $Q_2^{(\pm)}(u)$ are parameterized by N Bethe roots $\{\lambda_j^{(\pm)} \mid j=1,\ldots,N-2M\}$, $\{\mu_j^{(\pm)} \mid j=1,\ldots,M\}$ and $\{\nu_j^{(\pm)} \mid j=1,\ldots,M\}$ with $M=0,\ldots,[\frac{N}{2}]$ as follows,

$$Q^{(\pm)}(u)=\prod_{j=1}^{N-2M}\big(u-\lambda_j^{(\pm)}\big)\big(u+\lambda_j^{(\pm)}+1\big), \tag{4.22}$$

$$Q_1^{(\pm)}(u)=\prod_{j=1}^{M}\big(u-\mu_j^{(\pm)}\big)\big(u+\nu_j^{(\pm)}+1\big), \tag{4.23}$$

$$Q_2^{(\pm)}(u)=\prod_{j=1}^{M}\big(u-\nu_j^{(\pm)}\big)\big(u+\mu_j^{(\pm)}+1\big). \tag{4.24}$$

These N parameters are different from each other and satisfy the following Bethe ansatz equations

$$\begin{aligned}&-\frac{\bar{a}^{(\pm)}(\lambda_j^{(\pm)})}{\bar{d}^{(\pm)}(\lambda_j^{(\pm)})}-\frac{Q^{(\pm)}(\lambda_j^{(\pm)}+1)Q_2^{(\pm)}(\lambda_j^{(\pm)})Q_2^{(\pm)}(\lambda_j^{(\pm)}+1)}{Q^{(\pm)}(\lambda_j^{(\pm)}-1)Q_1^{(\pm)}(\lambda_j^{(\pm)})Q_1^{(\pm)}(\lambda_j^{(\pm)}-1)}\\&=\frac{(1-\sqrt{1+\xi^2})(\lambda_j^{(\pm)}+1)(2\lambda_j^{(\pm)}+1)\prod_{l=1}(\lambda_j^{(\pm)}+\theta_l+1)(\lambda_j^{(\pm)}-\theta_l+1)}{(\lambda_j^{(\pm)}\mp p+1)(\sqrt{1+\xi^2}(\lambda_j^{(\pm)}+1)\mp q)Q^{(\pm)}(\lambda_j^{(\pm)}-1)Q_1^{(\pm)}(\lambda_j^{(\pm)})Q_1^{(\pm)}(\lambda_j^{(\pm)}-1)},\\&j=1,\ldots,N-2M,\end{aligned} \tag{4.25}$$

$$\begin{aligned}&\frac{(1-\sqrt{1+\xi^2})(\mu_j^{(\pm)}+1)(2\mu_j^{(\pm)}+1)\prod_{l=1}(\mu_j^{(\pm)}+\theta_l+1)(\mu_j^{(\pm)}-\theta_l+1)}{(\mu_j^{(\pm)}\mp p+1)(\sqrt{1+\xi^2}(\mu_j^{(\pm)}+1)\mp q)Q^{(\pm)}(\mu_j^{(\pm)}+1)Q_2^{(\pm)}(\mu_j^{(\pm)})Q_2^{(\pm)}(\mu_j^{(\pm)}+1)}\\&=-1,\quad j=1,\ldots,M,\end{aligned} \tag{4.26}$$

$$\frac{(1-\sqrt{1+\xi^2})\nu_j^{(\pm)}(2\nu_j^{(\pm)}+1)\prod_{l=1}(\nu_j^{(\pm)}+\theta_l)(\nu_j^{(\pm)}-\theta_l)}{(\nu_j^{(\pm)}\pm p)(\sqrt{1+\xi^2}\nu_j^{(\pm)}\pm q)Q^{(\pm)}(\nu_j^{(\pm)}-1)Q_1^{(\pm)}(\nu_j^{(\pm)})Q_1^{(\pm)}(\nu_j^{(\pm)}-1)}=-1,$$
$$j=1,\ldots,M. \tag{4.27}$$

Some remarks are in order. The completeness [43,10] of the two sets of eigenvalues in the XXZ spin chain with constrained unparallel boundary fields case suggests that in our case, the eigenvalues $\Lambda^{(-)}(u)$ and $\Lambda^{(+)}(u)$ *together* constitute the complete set of eigenvalues of the transfer matrix $t(u)$ of the open XXX spin chain. The last term of our generalized T–Q relation (4.21) (cf. the conventional type [1]) is crucial, which has encoded the contribution from the off-diagonal element of the K-matrix and vanishes when two boundary fields are parallel. Taking the limit: $\xi\to 0$, the set of parameter $\{\mu_j\}$ coincides with that of $\{\nu_j\}$, the corresponding T–Q relation (4.21) becomes the usual type

$$\Lambda^{(\pm)}(u)=\bar{a}^{(\pm)}(u)\frac{\bar{Q}^{(\pm)}(u-1)}{\bar{Q}^{(\pm)}(u)}+\bar{d}^{(\pm)}(u)\frac{\bar{Q}^{(\pm)}(u+1)}{\bar{Q}^{(\pm)}(u)}, \tag{4.28}$$

where $\bar{Q}^{(\pm)}(u)=Q^{(\pm)}(u)Q_1^{(\pm)}(u)$. Then the resulting solutions are reduced to those in [35].

5. Homogeneous limit

The results of the previous sections focus on the inhomogeneous spin-$\frac{1}{2}$ XXX open chain. In this section we consider the homogeneous limit, i.e. $\{\theta_j\}\longrightarrow 0$, of the above results. The corresponding eigenvalue $\Lambda(u)$ of the transfer matrix of the homogeneous model satisfies the following relations:

$$\text{Crossing symmetry:}\quad \Lambda(-u-1)=\Lambda(u), \tag{5.1}$$
$$\text{Initial condition:}\quad \Lambda(0)=2pq=\Lambda(-1), \tag{5.2}$$
$$\text{Asymptotic behavior:}\quad \Lambda(u)\sim 2u^{2N+2}+\cdots,\quad \text{for } u\to\pm\infty, \tag{5.3}$$
$$\text{Analyticity:}\quad \Lambda(u),\ \text{as a function of } u,\ \text{is a polynomial of degree } 2N+2. \tag{5.4}$$

The corresponding relations (4.17) now read

$$\frac{\partial^l}{\partial u^l}\big\{\Lambda(u)\Lambda(u-1)\big\}\big|_{u=0}=\frac{\partial^l}{\partial u^l}\left\{\frac{\bar{\Delta}_q(u)}{(1+2u)(1-2u)}\right\}\bigg|_{u=0},\quad l=0,1,\ldots,2N-1. \tag{5.5}$$

Here the quantum determinant $\bar{\Delta}_q(u)$ becomes

$$\bar{\Delta}_q(u)=4\big(u^2-1\big)\big(p^2-u^2\big)\big((1+\xi^2)^2u^2-q^2\big)(u+1)^{2N}(u-1)^{2N}. \tag{5.6}$$

Actually Eqs, (5.1)–(5.5) enable one to determine the functions $\Lambda(u)$. We shall express the solutions of these equations in terms of a generalized T–Q relation formulism. For this purpose, let us introduce the following functions $H^{(\pm)}(u)$ and $\Lambda^{(\pm)}(u)$

$$H^{(\pm)}(u)=\frac{2u+2}{2u+1}(u\pm p)\big(\sqrt{1+\xi^2}u\pm q\big)(u+1)^{2N}, \tag{5.7}$$

$$\Lambda^{(\pm)}(u)=H^{(\pm)}(u)\frac{Q^{(\pm)}(u-1)Q_1^{(\pm)}(u-1)}{Q^{(\pm)}(u)Q_2^{(\pm)}(u)}+H^{(\pm)}(-u-1)\frac{Q^{(\pm)}(u+1)Q_2^{(\pm)}(u+1)}{Q^{(\pm)}(u)Q_1^{(\pm)}(u)}$$
$$+\frac{2(1-\sqrt{1+\xi^2})u^{2N+1}(u+1)^{2N+1}}{Q^{(\pm)}(u)Q_1^{(\pm)}(u)Q_2^{(\pm)}(u)}, \tag{5.8}$$

where the functions $Q^{(\pm)}(u)$, $Q_1^{(\pm)}(u)$ and $Q_2^{(\pm)}(u)$ are also given by (4.22)–(4.24). Then the functions $\Lambda^{(\pm)}(u)$ become the solutions of Eqs. (5.1)–(5.5) provided that the parameters $\{\lambda_j^{(\pm)}\}$, $\{\mu_j^{(\pm)}\}$ and $\{\nu_j^{(\pm)}\}$ satisfy the following Bethe ansatz equations respectively

$$-\frac{H^{(\pm)}(\lambda_j^{(\pm)})}{H^{(\pm)}(-\lambda_j^{(\pm)}-1)}-\frac{Q^{(\pm)}(\lambda_j^{(\pm)}+1)Q_2^{(\pm)}(\lambda_j^{(\pm)})Q_2^{(\pm)}(\lambda_j^{(\pm)}+1)}{Q^{(\pm)}(\lambda_j^{(\pm)}-1)Q_1^{(\pm)}(\lambda_j^{(\pm)})Q_1^{(\pm)}(\lambda_j^{(\pm)}-1)}$$
$$=\frac{(1-\sqrt{1+\xi^2})(\lambda_j^{(\pm)}+1)(2\lambda_j^{(\pm)}+1)(\lambda_j^{(\pm)}+1)^{2N}}{(\lambda_j^{(\pm)}\mp p+1)(\sqrt{1+\xi^2}(\lambda_j^{(\pm)}+1)\mp q)Q^{(\pm)}(\lambda_j^{(\pm)}-1)Q_1^{(\pm)}(\lambda_j^{(\pm)})Q_1^{(\pm)}(\lambda_j^{(\pm)}-1)},$$
$$j=1,\ldots,N-2M, \tag{5.9}$$

$$\frac{(1-\sqrt{1+\xi^2})(\mu_j^{(\pm)}+1)(2\mu_j^{(\pm)}+1)(\mu_j^{(\pm)}+1)^{2N}}{(\mu_j^{(\pm)}\mp p+1)(\sqrt{1+\xi^2}(\mu_j^{(\pm)}+1)\mp q)Q^{(\pm)}(\mu_j^{(\pm)}+1)Q_2^{(\pm)}(\mu_j^{(\pm)})Q_2^{(\pm)}(\mu_j^{(\pm)}+1)}$$
$$=-1,\quad j=1,\ldots,M, \tag{5.10}$$

$$\frac{(1-\sqrt{1+\xi^2})\nu_j^{(\pm)}(2\nu_j^{(\pm)}+1)\nu_j^{(\pm)2N}}{(\nu_j^{(\pm)}\pm p)(\sqrt{1+\xi^2}\nu_j^{(\pm)}\pm q)Q^{(\pm)}(\nu_j^{(\pm)}-1)Q_1^{(\pm)}(\nu_j^{(\pm)})Q_1^{(\pm)}(\nu_j^{(\pm)}-1)}=-1,$$
$$j=1,\ldots,M. \tag{5.11}$$

With the help of the relation (2.16) between the Hamiltonian (1.1) and the transfer matrix $\tau(u)$, the energy value E of the Hamiltonian is given as

$$E^{(\pm)}=2\sum_{j=1}^{N-2M}\frac{1}{\lambda_j^{(\pm)}(\lambda_j^{(\pm)}+1)}+2\sum_{j=1}^{M}\left(\frac{1}{\nu_j^{(\pm)}}-\frac{1}{\mu_j^{(\pm)}+1}\right)+\text{const.}, \tag{5.12}$$

where the parameters $\{\lambda_j^{(\pm)}\}$ and $\{\mu_j^{(\pm)}\}$ need to satisfy the associated Bethe ansatz equations (5.9)–(5.11) respectively. It would be believed that the eigenvalues $E^{(-)}(u)$ and $E^{(+)}(u)$ *together* constitute the complete set of energy spectrum of the Hamiltonian (1.1).

6. Discussions

In this paper, the open spin-$\frac{1}{2}$ XXX spin chain with unparallel boundary fields defined by the Hamiltonian (1.1) is exactly diagonalized by the off-diagonal Bethe ansatz method proposed in [34]. There are two sets of eigenvalues $E^{(\pm)}$ given by (5.12), which are expressed in terms of the roots of the associated Bethe ansatz equations (5.9)–(5.11).

As for integrable models without $U(1)$ symmetry, some off-diagonal elements of monodromy matrix enter into expression of the transfer matrix. This breaks down the usual $U(1)$ symmetry. However the central idea of our method is to construct the functional relations such as (4.17) between eigenvalues $\Lambda(\lambda)$ of the transfer matrix (the trace of the monodromy matrix) and its quantum determinant $\Delta_q(\lambda)$ based on the zero points of the product of off-diagonal elements of monodromy matrix $B(u)B(u-\eta)=0$. In fact, with some operator product identities, we can demonstrate[2]

[2] We have directly proven such an operator identity in [44].

$$\tau(\theta_j)\tau(\theta_j-1)=\frac{\Delta_q(\theta_j)}{(1-2\theta_j)(1+2\theta_j)},\quad j=1,\dots,N, \tag{6.1}$$

which is completely independent of the representation basis and thus avoids the obstacle of absence of a reference state which is crucial in the conventional Bethe ansatz methods. Although the functional relations between eigenvalues $\Lambda(\lambda)$ and the quantum determinant $\Delta_q(\lambda)$ at some particular points can be obtained by different ways [34,29,26], the very relations would play an important role in the method. In our case, based on the relation (4.17) and some properties (4.4)–(4.7) of $\Lambda(\lambda)$ we can give a generalized T–Q relation type solution (4.21), which modifies the usual T–Q relation by adding an extra term. Such an extra term encodes the contribution of the off-diagonal element of the associated K-matrix.

The numerical results [43] strongly suggest that a fixed M might give a complete set of eigenvalues of the transfer matrix. In such a sense, different M might only give different parameterization of the eigenvalues but not different states. This allows us to simplify further the generalized T–Q relation as follows. For the case of N being even, let $M=\frac{N}{2}$ and the corresponding eigenvalue $\Lambda(u)$ can be parameterized by

$$\begin{aligned}\Lambda^{(\pm)}(u)=\bar{a}^{(\pm)}(u)\frac{Q_1^{(\pm)}(u-1)}{Q_2^{(\pm)}(u)}+\bar{d}^{(\pm)}(u)\frac{Q_2^{(\pm)}(u+1)}{Q_1^{(\pm)}(u)}\\ +2\big(1-\sqrt{1+\xi^2}\big)u(u+1)\\ \times\frac{\prod_{j=1}^N(u+\theta_j)(u-\theta_j)(u+\theta_j+1)(u-\theta_j+1)}{Q_1^{(\pm)}(u)Q_2^{(\pm)}(u)}.\end{aligned} \tag{6.2}$$

For the case of N being odd, let $M=\frac{N+1}{2}$ and the corresponding eigenvalue $\Lambda(u)$ can be parameterized by

$$\begin{aligned}\Lambda^{(\pm)}(u)=\bar{a}^{(\pm)}(u)\frac{Q_1^{(\pm)}(u-1)}{Q_2^{(\pm)}(u)}+\bar{d}^{(\pm)}(u)\frac{Q_2^{(\pm)}(u+1)}{Q_1^{(\pm)}(u)}\\ +2\big(1-\sqrt{1+\xi^2}\big)u^2(u+1)^2\\ \times\frac{\prod_{j=1}^N(u+\theta_j)(u-\theta_j)(u+\theta_j+1)(u-\theta_j+1)}{Q_1^{(\pm)}(u)Q_2^{(\pm)}(u)}.\end{aligned} \tag{6.3}$$

The above T–Q relations lead to the Bethe ansatz equations which allow one to investigate the distribution of roots of these equations and compute the physical properties in the thermodynamic limit by the usual method [13].

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Appendix A. Proof of (4.14)

In this appendix, we prove the relation (4.14). From the definition (2.8) of the one-row monodromy matrix $T(u)$ and the exchange relations (3.6)–(3.9) of its components, we have

$$\alpha(\theta_j)\beta(\theta_j-1)|0\rangle = 0 = \delta(\theta_j)\alpha(\theta_j-1)|0\rangle, \tag{A.1}$$

$$\alpha(\theta_j)\alpha(\theta_j-1)|0\rangle = 0 = \delta(\theta_j)\delta(\theta_j-1)|0\rangle, \tag{A.2}$$

$$\gamma(\theta_j)\beta(\theta_j-1)|0\rangle = -\tilde{a}(\theta_j)\tilde{d}(\theta_j-1)|0\rangle, \tag{A.3}$$

$$\delta(\theta_j)\beta(\theta_j-1)|0\rangle = -\tilde{d}(\theta_j-1)\beta(\theta_j)|0\rangle, \tag{A.4}$$

$$\alpha(\theta_j)\delta(\theta_j-1)|0\rangle = \tilde{a}(\theta_j)\tilde{d}(\theta_j-1)|0\rangle, \tag{A.5}$$

$$\beta(\theta_j)\beta(\theta_j-1)|0\rangle = 0, \tag{A.6}$$

where

$$\tilde{a}(\lambda) = \prod_{j=1}^{N}(\lambda-\theta_j+1), \qquad \tilde{d}(\lambda) = \prod_{j=1}^{N}(\lambda-\theta_j). \tag{A.7}$$

One can check the last equation (A.6) by induction. Expanding the operator $B(u)$ in terms of the components of the one-row monodromy matrix (3.10) and using the relations (A.1)–(A.6), we have

$$\begin{aligned}
&B(\theta_j)B(\theta_j-1)|0\rangle \\
&\quad= \big\{-(p+\theta_j)\alpha(\theta_j)\beta(-\theta_j-1)+(p-\theta_j)\beta(\theta_j)\alpha(-\theta_j-1)\big\} \\
&\qquad\times\big\{-(p+\theta_j-1)\alpha(\theta_j-1)\beta(-\theta_j)+(p-\theta_j+1)\beta(\theta_j-1)\alpha(-\theta_j)\big\}|0\rangle \\
&\quad= \frac{(2\theta_j+1)(\theta_j-p+1)(2p+(\theta_j-p-1)2\theta_j)}{(\theta_j+1)(2\theta_j-1)} \\
&\qquad\times\tilde{a}(-\theta_j)\tilde{a}(-\theta_j-1)\beta(\theta_j)\beta(\theta_j-1)|0\rangle \\
&\quad= 0.
\end{aligned} \tag{A.8}$$

Due to the fact that for a generic value of $\{u_j\}$ the set of vectors $\{\prod_{j=1}^{M} B(u_j)|0\rangle \mid M=0,\ldots,N\}$ spans the whole vector space $\mathbf{V}^{\otimes N}$ and the fact that the commutativity between the operators B with different spectrum, one can conclude that $B(\theta_j)B(\theta_j-1)=0$. This completes the proof of (4.14).[3]

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