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The open XXZ chain with boundary impurities

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Abstract. We propose an integrable open XXZ chain coupled to the boundary impurities with arbitrary exchange constants. The Bethe ansatz equation and eigenvalues are obtained by using the quantum inverse scattering method. The ground-state properties are discussed by solving the Bethe equation in some special cases. In addition, we present an approach for constructing the reflecting matrix K which produces the boundary term coupled to impurities.

1. Introduction

Since the Heisenberg model was exactly solved by Bethe [1] in 1931, there has been considerable progress in the investigation of quantum integrable systems. In the last decade, quantum integrable models have again attracted much attention because of the growing interest in strongly correlated systems. The Heisenberg chain is one of the most important integrable models which has been studied extensively. In the early decades, most of the work concentrated on the case with periodic or twisted boundary conditions because they are usually compatible with the Yang–Baxter equation [2].

In addition, the quantum impurity problem, which has been extensively investigated with renormalizing group techniques [3] and conformal field theory [4], is also very interesting in itself. Andrei and Johannesson [5] first considered an impurity spin S embedded in an integrable spin- $\frac{1}{2}XXX$ chain with periodic boundary conditions. Subsequently, Schlottmann *et al* [6] generalized it to the arbitrary spin chain. The standard approach to dealing with the impurity integrable problem is the quantum inverse scattering method [7]. In general, the Hamiltonian of an integrable spin chain can be represented as the logarithmic derivative of a homogeneous transfer matrix, which is constructed from the direct products of some local vertex matrices, at a special point of the spectrum parameter. Similarly, the Hamiltonian of the impurity integrable spin chain can be constructed from the corresponding inhomogeneous transfer matrix. Different from the homogeneous one, the inhomogeneous transfer matrix includes some inhomogeneous local vertex matrices. The key point is to find some inhomogeneous vertex matrices, which satisfy the same Yang–Baxter relation of the homogeneous matrices, corresponding to impurity spins.

The pioneering work on the open boundary spin chain was carried out by Gaudin [8] using the Bethe ansatz method. Lately, this work has been generalized to the Schrödinger model by Woynarovich [9], the Hubbard model by Schulz [10] and the spin chain by Alcaraz

et al [11]. Recently, investigations of the boundary bound states (see, e.g., [12–17]) have also attracted much attention.

A general approach to constructing open integrable quantum spin chains with independent boundary conditions on each end was proposed by Sklyanin [18] on the basis of the previous work of Cherednik [19]. This problem was then extensively studied and developed by many authors [20, 21]. Central to their approach is the introduction of a K matrix which fulfils the reflecting equation. Physically, the K matrix can be interpreted as the amplitude of a particle scattering at the boundaries or as boundary S matrices in a two-dimensional integrable quantum field. It is well known that not all the boundary K matrices comply with the integrability and only the solution of the reflecting equation is compatible with a given R matrix. In general, a family of conserved quantities can always be constructed corresponding to those given K and R matrices; therefore, the Hamiltonian of the open integrable chain is derived.

We note that Sklyanin and many other authors used a constant number K matrix to construct their model, where the K matrix induces the boundary fields. Recently, Wang and coworkers first introduced the operator K matrix to study the Kondo problem in one-dimensional strongly correlated electron systems [22]. In a previous paper [23], the problem of an open spin- $\frac{1}{2}$ Heisenberg chain coupled to two spin S impurities sited at the ends has been studied. In this paper, we continue to study the XXZ chain coupled to impurity spins with different coupling constants on the boundary. The Hamiltonian we will consider reads

$$H = \sum_{n=1}^{N-1} J(\sigma_n^1 \sigma_{n+1}^1 + \sigma_n^2 \sigma_{n+1}^2 + \cosh \eta \sigma_n^3 \sigma_{n+1}^3) + J_i [\cosh c (\sigma_1^1 \sigma_L^1 + \sigma_1^2 \sigma_L^2) + \cosh \eta \sigma_1^3 \sigma_L^3] \\ + J_i [\cosh c (\sigma_N^1 \sigma_R^1 + \sigma_N^2 \sigma_R^2) + \cosh \eta \sigma_N^3 \sigma_R^3] \quad (1)$$

where σ_n^i ($i = 1, 2, 3$) are the Pauli matrices in the n th quantum vector space, and J , J_i , η and c are constants with the relation

$$J_i = \frac{J \sinh^2 \eta}{(\sinh^2 \eta - \sinh^2 c)}. \quad (2)$$

Here η parametrizes the bulk anisotropy and an additional free parameter c is inducted to indicate the boundary XXZ -like exchange coupling. J and J_i are the coupling constants which describe the coupling in bulk or between the bulk and the impurities, respectively. From the relation of J and J_i , it can be seen that J_i may have the same or opposite sign to J depending on the values of c and η . This means that the boundary coupling can possess the same type coupling (antiferromagnetic or ferromagnetic) or the opposite type comparing with bulk coupling. Based on the quantum inverse scattering method, the Bethe ansatz equation and the eigenvalue of the Hamiltonian will be obtained.

2. The model

It is well known that an integrable problem is often related to the following Yang–Baxter equation:

$$R_{12}(\lambda - \mu) R_{13}(\lambda) R_{23}(\mu) = R_{23}(\mu) R_{13}(\lambda) R_{12}(\lambda - \mu). \quad (3)$$

As usual, R_{12} , R_{13} and R_{23} are matrices acting in $V^n \otimes V^n \otimes V^n$, for example, $R_{12}(\lambda) = R_{12}(\lambda) \otimes I_3$, $R_{23}(\mu) = I_1 \otimes R_{23}(\mu)$. It can be shown that the R -matrix of the XXZ model

given by

$$R(\lambda) = \frac{1}{\sinh \eta} \begin{pmatrix} \sinh(\lambda + \eta) & & & \\ & \sinh \lambda & \sinh \eta & \\ & \sinh \eta & \sinh \lambda & \\ & & & \sinh(\lambda + \eta) \end{pmatrix} \quad (4)$$

possesses P and T invariance

$$P_{12}R_{12}(\lambda)P_{12} \equiv R_{21}(\lambda) = R_{12}(\lambda) \quad R_{12}^{t_1} = R_{12}^{t_2} \quad (5)$$

where P_{12} is the permutation matrix and t_i denotes the transposition in the i th space. It also has the properties of unitarity and crossing unitarity

$$R_{12}(\lambda)R_{12}(-\lambda) = \rho(\lambda) \quad R_{12}^{t_1}(\lambda)R_{12}^{t_1}(-\lambda - 2\eta) = \tilde{\rho}(\lambda) \quad (6)$$

where

$$\rho(\lambda) = \frac{1}{\sinh^2 \eta} \sinh(\lambda + \eta) \sinh(\eta - \lambda) \quad \text{and} \quad \tilde{\rho}(\lambda) = \rho(\lambda + \eta)$$

are scalar functions of λ . Let us define the monodromy matrix

$$T(\lambda) = L_N(\lambda)L_{N-1}(\lambda) \dots L_n(\lambda) \dots L_1(\lambda)$$

with $L_n(\lambda) = R_{an}(\lambda)$, where the subindex a indicates the auxiliary space and $n = 1, \dots, N$ labels a quantum vector space at site number n ; thus we have

$$T_a(\lambda) = R_{aN}(\lambda)R_{a,N-1}(\lambda) \dots R_{a1}(\lambda). \quad (7)$$

It can be inferred from the Yang–Baxter equation (3) that the monodromy matrix fulfils the relation

$$R_{12}(\lambda - \mu)T_1(\lambda)T_2(\mu) = T_2(\mu)T_1(\lambda)R_{12}(\lambda - \mu). \quad (8)$$

In order to construct an integrable open chain with boundary impurities, it is necessary to introduce the reflection matrices $K_-(\mu)$ and $K_+(\mu)$. The reflection matrix fulfils the following reflecting equations [18]

$$\begin{aligned} R_{12}(\lambda - \mu) \overset{1}{K}_-(\lambda)R_{12}(\lambda + \mu) \overset{2}{K}_-(\mu) &= \overset{2}{K}_-(\mu)R_{12}(\lambda + \mu) \overset{1}{K}_-(\lambda)R_{12}(\lambda - \mu) \\ R_{12}(-\lambda + \mu) \overset{1}{K}_+(\lambda)R_{12}(-\lambda - \mu - 2\eta) \overset{2}{K}_+(\mu) & \\ &= \overset{2}{K}_+(\mu)R_{12}(-\lambda - \mu - 2\eta) \overset{1}{K}_+(\lambda)R_{12}(-\lambda + \mu) \end{aligned} \quad (9)$$

with $\overset{1,2}{K}_\pm$ and R_{12} acting on the space $V_{1,2}$ and $V_1 \otimes V_2$, respectively. It is obvious that $\overset{1}{K}_-(\lambda) = I$ and $\overset{1}{K}_+(\lambda) = I$, where I means the identity matrix, are the simplest reflection matrices which satisfy the reflecting equations. Following Sklyanin [18], the transfer matrix $t(\lambda)$ given by

$$t(\lambda) = \text{Tr} K_+(\lambda)T(\lambda)K_-(\lambda)T^{-1}(-\lambda) \quad (10)$$

forms a one-parameter commutative family

$$[t(\lambda), t(\mu)] = 0$$

where the monodromy matrix $T(\lambda)$ is given by (7). By virtue of the unitary property of the R -matrix for the XXZ model, $R_{12}(\lambda)$ has the same algebraic structure with $R_{12}^{-1}(-\lambda)$. Construct $\hat{T}(\lambda)$ which has the same algebra structure with $T^{-1}(-\lambda)$ by defining

$$\hat{T}(\lambda) = R_{a1}(\lambda)R_{a2}(\lambda) \dots R_{aN}(\lambda). \quad (11)$$

Thus the transfer matrix $t(\lambda)$ can also be constructed by

$$t(\lambda) = \text{Tr} K_+(\lambda) T(\lambda) K_-(\lambda) \hat{T}(\lambda). \quad (12)$$

It can be proved that if τ obeys the Yang relation

$$R_{12}(\lambda - \mu) \tau_1(\lambda) \tau_2(\mu) = \tau_2(\mu) \tau_1(\lambda) R_{12}(\lambda - \mu)$$

then

$$K_-(\lambda) = \tau(\lambda) \tau^{-1}(-\lambda) \quad (13)$$

also obeys the reflecting equation. In order to prove this, we will use the following relations.

From the Yang relation, one concludes that

$$\tau_2^{-1}(-\mu) R_{12}(\lambda + \mu) \tau_1(\lambda) = \tau_1(\lambda) R_{12}(\lambda + \mu) \tau_2^{-1}(-\mu) \quad (14)$$

or

$$\tau_1^{-1}(-\lambda) R_{12}(\lambda + \mu) \tau_2(\mu) = \tau_2(\mu) R_{12}(\lambda + \mu) \tau_1^{-1}(-\lambda). \quad (15)$$

Substituting $K_-(\lambda)$ into the reflecting equation, one gets

$$\begin{aligned} R_{12}(\lambda - \mu) \overset{1}{K}_-(\lambda) R_{12}(\lambda + \mu) \overset{2}{K}_-(\mu) & \\ &= R_{12}(\lambda - \mu) \tau_1(\lambda) \tau_1^{-1}(-\lambda) R_{12}(\lambda + \mu) \tau_2(\mu) \tau_2^{-1}(-\mu) \\ &= R_{12}(\lambda - \mu) \tau_1(\lambda) \tau_2(\mu) R_{12}(\lambda + \mu) \tau_1^{-1}(-\lambda) \tau_2^{-1}(-\mu) \\ &= \tau_2(\mu) \tau_1(\lambda) R_{12}(\lambda - \mu) R_{12}(\lambda + \mu) \tau_1^{-1}(-\lambda) \tau_2^{-1}(-\mu) \\ &= \tau_2(\mu) \tau_1(\lambda) R_{12}(\lambda + \mu) R_{12}(\lambda - \mu) \tau_1^{-1}(-\lambda) \tau_2^{-1}(-\mu) \\ &= \tau_2(\mu) \tau_2^{-1}(-\mu) R_{12}(\lambda + \mu) \tau_1(\lambda) \tau_2(-\mu) R_{12}(\lambda - \mu) \tau_1^{-1}(-\lambda) \tau_2^{-1}(-\mu) \\ &= \tau_2(\mu) \tau_2^{-1}(-\mu) R_{12}(\lambda + \mu) \tau_1(\lambda) \tau_1^{-1}(-\lambda) R_{12}(\lambda - \mu) \tau_2(-\mu) \tau_2^{-1}(-\mu) \\ &= \overset{2}{K}_-(\mu) R_{12}(\lambda + \mu) \overset{1}{K}_-(\lambda) R_{12}(\lambda - \mu). \end{aligned}$$

From (14) and (15), we find that the relations

$$\tau_2^{-1}(-\mu + c) R_{12}(\lambda + \mu) \tau_1(\lambda + c) = \tau_1(\lambda + c) R_{12}(\lambda + \mu) \tau_2^{-1}(-\mu + c) \quad (16)$$

$$\tau_1^{-1}(-\lambda + c) R_{12}(\lambda + \mu) \tau_2(\mu + c) = \tau_2(\mu + c) R_{12}(\lambda + \mu) \tau_1^{-1}(-\lambda + c) \quad (17)$$

are also satisfied, where c is a constant. By using previous relations (16) and (17), with the same procedure as the above we can prove that the matrix

$$K_-(\lambda) = \tau(\lambda + c) \tau^{-1}(-\lambda + c)$$

also satisfies the reflecting equation. Thus we can construct the reflection matrix as

$$K_-(\lambda) = L_L(\lambda + c_L) L_L^{-1}(-\lambda + c_L) = R_{aL}(\lambda + c_L) R_{aL}^{-1}(-\lambda + c_L). \quad (18)$$

Because the R -matrix of the XXZ model has P symmetry and the property of unitarity, $R_{12}(\lambda - c_L) R_{12}(-\lambda + c_L) = \rho(\lambda - c_L)$. It is convenient to multiply $K_-(\lambda)$ by a constant $\rho(\lambda - c_L)$, so thus we obtain

$$K_-(\lambda) = R_{aL}(\lambda + c_L) R_{aL}(\lambda - c_L) \quad (19)$$

where c_L is a constant decided by the left boundary. In the following we will work with this left reflection matrix.

In order to obtain our integrable Hamiltonian in the open boundary, we define the monodromy matrix as

$$U_a(\lambda) = K_+(\lambda) T'_a(\lambda) K_-(\lambda) \hat{T}'_a(\lambda). \quad (20)$$

Here we take $K_+(\lambda) = I$ and $K_-(\lambda)$ given in (18), and define $T'(\lambda)$ and $\hat{T}'(\lambda)$ as

$$T'_a(\lambda) = R_{aR}(\lambda + c_R)R_{aN}(\lambda) \dots R_{a2}(\lambda)R_{a1}(\lambda) \quad (21)$$

$$\hat{T}'_a(\lambda) = R_{a1}(\lambda)R_{a2}(\lambda) \dots R_{aN}(\lambda)R_{aR}(\lambda - c_R) \quad (22)$$

where c_R is a constant decided by the right boundary. With the same method discussed above, one can prove that $U(\lambda)$ satisfies the reflecting equation:

$$R_{12}(\lambda - \mu)U_1(\lambda)R_{12}(\lambda + \mu)U_2(\mu) = U_2(\mu)R_{12}(\lambda + \mu)U_1(\lambda)R_{12}(\lambda - \mu). \quad (23)$$

The Hamiltonian H can be constructed from the transfer matrix $X(\lambda)$, which is given by

$$X(\lambda) = \text{Tr}_a U_a(\lambda) = \text{Tr} K_+(\lambda)T'_a(\lambda)K_-(\lambda)\hat{T}'_a(\lambda). \quad (24)$$

We note that

$$K_-(\lambda)|_{\lambda=0} = R_{aL}(c_L)R_{aL}(-c_L) = \left(1 - \frac{\sinh^2 c_L}{\sinh^2 \eta}\right)I_{aL}$$

and $R_{am}(\lambda)|_{\lambda=0} = P_{am}$, where I_{aL} is the identity matrix in the space $V_a \otimes V_L$ and P_{am} represents the permutation operator in the space $V_a \otimes V_m$. Differentiating $X(\lambda)$ with respect to λ at $\lambda = 0$, one gets

$$X'(0) = x + x_{NR} + \sum_{n=1}^{N-1} x_{n,n+1} + x_{L1} \quad (25)$$

where the first term is

$$\begin{aligned} x &= \text{Tr}_a \left[\frac{\partial}{\partial \lambda} R_{aR}(\lambda + c_R)|_{\lambda=0} R_{aR}(-c_R)K_-(0) + R_{aR}(c_R) \frac{\partial}{\partial \lambda} R_{aR}(\lambda - c_R)|_{\lambda=0} K_-(0) \right] \\ &= 2 \frac{\cosh \eta}{\sinh \eta} \left(1 - \frac{\sinh^2 c_L}{\sinh^2 \eta}\right) \end{aligned}$$

the second term is

$$\begin{aligned} x_{NR} &= 2 \text{Tr}_a \left[R_{aR}(c_R) \frac{\partial}{\partial \lambda} R_{aN}(\lambda)|_{\lambda=0} P_{aN} R_{aR}(-c_R)K_-(0) \right] \\ &= \frac{2}{\sinh \eta} \left(1 - \frac{\sinh^2 c_L}{\sinh^2 \eta}\right) \left[\cosh c_R (\sigma_N^1 \sigma_R^1 + \sigma_N^2 \sigma_R^2) \right. \\ &\quad \left. + \cosh \eta (\sigma_N^3 \sigma_R^3 + 1) - \cosh \eta \frac{\sinh^2 c_R}{\sinh^2 \eta} \right] \end{aligned}$$

the third term is

$$\begin{aligned} x_{n,n+1} &= 2 \text{Tr}_a \left[R_{aR}(c_R)R_{aR}(-c_R) \frac{\partial}{\partial \lambda} R_{n,n+1}(\lambda)|_{\lambda=0} P_{n,n+1} K_-(0) \right] \\ &= \frac{2}{\sinh \eta} \prod_{R,L} \left(1 - \frac{\sinh^2 c_{R,L}}{\sinh^2 \eta}\right) [\sigma_n^1 \sigma_{n+1}^1 + \sigma_n^2 \sigma_{n+1}^2 + \cosh \eta (\sigma_n^3 \sigma_{n+1}^3 + 1)] \end{aligned}$$

and the last term is

$$\begin{aligned} x_{L1} &= \left[\frac{\partial}{\partial \lambda} R_{1L}(\lambda + c_L)|_{\lambda=0} R_{1L}(-c_L) + R_{1L}(c_L) \frac{\partial}{\partial \lambda} R_{1L}(\lambda - c_L)|_{\lambda=0} \right] \text{Tr}_a R_{aR}(c_R)R_{aR}(-c_R) \\ &= \frac{2}{\sinh \eta} \left(1 - \frac{\sinh^2 c_R}{\sinh^2 \eta}\right) [\cosh c_L (\sigma_1^1 \sigma_L^1 + \sigma_1^2 \sigma_L^2) + \cosh \eta (\sigma_1^3 \sigma_L^3 + 1)]. \end{aligned}$$

Thus the Hamiltonian H can be obtained:

$$\begin{aligned}
 H &= \frac{J}{2} \sinh \eta \frac{\sinh^4 \eta}{\prod_{R,L} (\sinh^2 \eta - \sinh^2 c_{R,L})} X'(0) - C \\
 &= \sum_{n=1}^{N-1} J (\sigma_n^1 \sigma_{n+1}^1 + \sigma_n^2 \sigma_{n+1}^2 + \cosh \eta \sigma_n^3 \sigma_{n+1}^3) \\
 &\quad + J_L [\cosh c_L (\sigma_1^1 \sigma_L^1 + \sigma_1^2 \sigma_L^2) + \cosh \eta \sigma_1^3 \sigma_L^3] \\
 &\quad + J_R [\cosh c_R (\sigma_N^1 \sigma_R^1 + \sigma_N^2 \sigma_R^2) + \cosh \eta \sigma_N^3 \sigma_R^3] \tag{26}
 \end{aligned}$$

where

$$J_{L,R} = \frac{J \sinh^2 \eta}{(\sinh^2 \eta - \sinh^2 c_{L,R})}$$

and the constant C is given by

$$C = (NJ + J_L + J_R) \cosh \eta.$$

Although $c_{L,R}$ can take arbitrary values, for simplicity we only consider the case $c_L = c_R = c$ ($J_L = J_R = J_i$) which corresponds to the Hamiltonian (1). The general case can be studied easily by following the same procedure.

3. The algebraic Bethe ansatz

In the following, we will use the algebraic Bethe ansatz developed by Sklyanin to solve the spectrum of $X(\lambda)$. For simplicity of calculation, it is convenient to shift λ to $\lambda - (\eta/2)$. We define

$$U_a(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}.$$

From the reflecting equation (22), some useful commutation relations between $A(\lambda)$, $D(\lambda)$ and $B(\lambda)$ can be obtained:

$$\begin{aligned}
 A(\lambda)B(\mu) &= \frac{\sinh(\lambda - \mu - \eta) \sinh(\lambda + \mu - \eta)}{\sinh(\lambda - \mu) \sinh(\lambda + \mu)} B(\mu)A(\lambda) \\
 &\quad + \frac{\sinh \eta \sinh(\lambda + \mu - \eta)}{\sinh(\lambda - \mu) \sinh(\lambda + \mu)} B(\lambda)A(\mu) - \frac{\sinh \eta}{\sinh(\lambda + \mu)} B(\lambda)D(\mu) \tag{27}
 \end{aligned}$$

$$\begin{aligned}
 D(\lambda)B(\mu) &= \frac{-2 \sinh^2 \eta \cosh \eta}{\sinh(\lambda - \mu) \sinh(\lambda + \mu)} B(\mu)A(\lambda) \\
 &\quad + \frac{\sinh(\lambda - \mu + \eta) \sinh(\lambda + \mu + \eta)}{\sinh(\lambda - \mu) \sinh(\lambda + \mu)} B(\mu)D(\lambda) \\
 &\quad + \frac{\sinh \eta \sinh(\lambda - \mu + 2\eta)}{\sinh(\lambda - \mu) \sinh(\lambda + \mu)} B(\lambda)A(\mu) - \frac{\sinh \eta \sinh(\lambda + \mu + \eta)}{\sinh(\lambda - \mu) \sinh(\lambda + \mu)} B(\lambda)D(\mu). \tag{28}
 \end{aligned}$$

It is very convenient to use the notation

$$\tilde{D}(\lambda) = D(\lambda) \sinh 2\lambda - A(\lambda) \sinh \eta. \tag{29}$$

The commutation relations are then simplified to

$$A(\lambda)B(\mu) = \frac{\sinh(\lambda - \mu - \eta) \sinh(\lambda + \mu - \eta)}{\sinh(\lambda - \mu) \sinh(\lambda + \mu)} B(\mu)A(\lambda) + \frac{\sinh \eta \sinh(2\mu - \eta)}{\sinh(\lambda - \mu) \sinh 2\mu} B(\lambda)A(\mu) - \frac{\sinh \eta}{\sinh(\lambda + \mu) \sinh 2\mu} B(\lambda)\tilde{D}(\mu) \quad (30)$$

$$\begin{aligned} \tilde{D}(\lambda)B(\mu) &= \frac{\sinh(\lambda - \mu + \eta) \sinh(\lambda + \mu + \eta)}{\sinh(\lambda - \mu) \sinh(\lambda + \mu)} B(\mu)\tilde{D}(\lambda) \\ &\quad - \frac{\sinh \eta \sinh(2\lambda + \eta)}{\sinh(\lambda - \mu) \sinh 2\mu} B(\lambda)\tilde{D}(\mu) \\ &\quad + \frac{\sinh \eta \sinh(2\lambda + \eta) \sinh(2\mu - \eta)}{\sinh 2\mu \sinh(\lambda + \mu)} B(\lambda)A(\mu). \end{aligned} \quad (31)$$

The trace of $U_a(\lambda)$ can be expressed as

$$X(\lambda) = \text{Tr}_a U_a(\lambda) = \frac{\sinh 2\lambda + \sinh \eta}{\sinh 2\lambda} A(\lambda) + \frac{1}{\sinh 2\lambda} \tilde{D}(\lambda). \quad (32)$$

Define the pseudovacuum state $|0\rangle$ as the state which has all N bulk spins and two boundary impurity spins up:

$$|0\rangle = |\uparrow\uparrow \cdots \uparrow\rangle = \prod_k \otimes |\uparrow\rangle_k$$

where $|\uparrow\rangle_k = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_k$, $k = L, 1, \dots, N, R$. Obviously,

$$\sigma_j^+ |0\rangle = 0.$$

Writing the R -matrix as a 2×2 matrix in the auxiliary space, it follows that

$$L_j(\lambda) = R_{aj}(\lambda) = \begin{pmatrix} \omega_0 + \omega_3 \sigma_j^3 & \sigma_j^- \\ \sigma_j^+ & \omega_0 - \omega_3 \sigma_j^3 \end{pmatrix} \quad (33)$$

where

$$\omega_0 = \frac{1}{\sinh \eta} \sinh \lambda \cosh \frac{1}{2} \eta \quad \text{and} \quad \omega_3 = \frac{1}{\sinh \eta} \cosh \lambda \sinh \frac{1}{2} \eta.$$

It should be noted that the R -matrix is different from (3) only with the λ shifted to $\lambda - (\eta/2)$. From the definition of $U_a(\lambda)$, it is easy to see

$$C(\lambda)|0\rangle = 0.$$

After some algebraic calculations, we also get

$$A(\lambda)|0\rangle = a(\lambda)|0\rangle \quad D(\lambda)|0\rangle = d(\lambda)|0\rangle.$$

$a(\lambda)$ and $d(\lambda)$ are given by

$$\begin{aligned} a(\lambda) &= \frac{1}{\sinh^{2(N+2)} \eta} \mathbf{a}_{L^+} \mathbf{a}_{L^-} \mathbf{a}_{R^+} \mathbf{a}_{R^-} \mathbf{a}^{2N} \\ &= \frac{1}{\sinh^{2(N+2)} \eta} \sinh^2 \left(\lambda + c + \frac{1}{2} \eta \right) \sinh^2 \left(\lambda - c + \frac{1}{2} \eta \right) \sinh^{2N} \left(\lambda + \frac{1}{2} \eta \right) \end{aligned} \quad (34)$$

$$\begin{aligned}
d(\lambda) &= \frac{1}{\sinh^{2(N+2)} \eta} \left[\mathbf{a}_{L^+} \mathbf{a}_{L^-} \mathbf{a}^{2N} + \mathbf{a}_{L^+} \mathbf{a}_{L^-} \mathbf{d}_{R^+} \mathbf{d}_{R^-} \sum_{k=1}^N \mathbf{a}^{2(N-k)} \mathbf{d}^{2(k-1)} \right. \\
&\quad \left. + \mathbf{d}_{L^+} \mathbf{d}_{L^-} \mathbf{d}_{R^+} \mathbf{d}_{R^-} \mathbf{d}^{2N} \right] \\
&= \frac{1}{\sinh^{2(N+2)} \eta} \left[\mathbf{a}_{L^+} \mathbf{a}_{L^-} \left(\mathbf{a}^{2N} + \mathbf{d}_{R^+} \mathbf{d}_{R^-} \frac{\mathbf{a}^{2N} - \mathbf{d}^{2N}}{\mathbf{a}^2 - \mathbf{d}^2} \right) + \mathbf{d}_{L^+} \mathbf{d}_{L^-} \mathbf{d}_{R^+} \mathbf{d}_{R^-} \mathbf{d}^{2N} \right]
\end{aligned} \tag{35}$$

where

$$\begin{aligned}
\mathbf{a} &= \sinh \left(\lambda + \frac{1}{2} \eta \right) & \mathbf{d} &= \sinh \left(\lambda - \frac{1}{2} \eta \right) & \mathbf{a}_{L^+} &= \mathbf{a}_{R^+} = \sinh \left(\lambda + c + \frac{1}{2} \eta \right) \\
\mathbf{a}_{L^-} &= \mathbf{a}_{R^-} = \sinh \left(\lambda - c + \frac{1}{2} \eta \right) & \mathbf{d}_{L^+} &= \mathbf{d}_{R^+} = \sinh \left(\lambda + c - \frac{1}{2} \eta \right) \\
\mathbf{d}_{L^-} &= \mathbf{d}_{R^-} = \sinh \left(\lambda - c - \frac{1}{2} \eta \right).
\end{aligned}$$

By using (29) and substituting $a(\lambda)$ and $d(\lambda)$ into $\tilde{d}(\lambda)$, the relation

$$\tilde{D}(\lambda)|0\rangle = \tilde{d}(\lambda)|0\rangle$$

is given with

$$\begin{aligned}
\tilde{d}(\lambda) &= d(\lambda) \sinh 2\lambda - a(\lambda) \sinh \eta = \frac{1}{\sinh^{2N+2} \eta} (\sinh 2\lambda - \sinh \eta) \mathbf{d}_{L^+} \mathbf{d}_{L^-} \mathbf{d}_{R^+} \mathbf{d}_{R^-} \mathbf{d}^{2N} \\
&= \frac{\sinh 2\lambda - \sinh \eta}{\sinh^{2(N+2)} \eta} \sinh^2 \left(\lambda + c - \frac{1}{2} \eta \right) \\
&\quad \times \sinh^2 \left(\lambda - c - \frac{1}{2} \eta \right) \sinh^{2N} \left(\lambda - \frac{1}{2} \eta \right).
\end{aligned} \tag{36}$$

As was shown, $X(\lambda)$ and $B(\lambda)$ can be treated as the generating functional of an infinite number of conserved quantities and the creation operator of their eigenstates, respectively. Our main task is to calculate the eigenvalue of $X(\lambda)$ on their eigenstates. The eigenstate of $X(\lambda)$ with M spins down is constructed as

$$|\Omega\rangle = \prod_{j=1}^M B(\lambda_j)|0\rangle.$$

Acting with $X(\lambda)$ on the state and using the commutation relations (30) and (31), we obtain

$$X(\lambda)|\Omega\rangle = \Lambda(\lambda, \lambda_1, \dots, \lambda_M)|\Omega\rangle + \sum_{j=1}^M \Lambda_j(\lambda, \lambda_1, \dots, \lambda_M)|\lambda_1, \dots, \lambda_{j-1}, \lambda, \lambda_{j+1}, \dots, \lambda_M\rangle.$$

$\Lambda(\lambda, \lambda_1, \dots, \lambda_M)$ given by

$$\begin{aligned}
\Lambda(\lambda, \lambda_1, \dots, \lambda_M) &= \frac{1}{\sinh 2\lambda} \tilde{d}(\lambda) \prod_{j=1}^M \frac{\sinh(\lambda - \lambda_j + \eta) \sinh(\lambda + \lambda_j + \eta)}{\sinh(\lambda - \lambda_j) \sinh(\lambda + \lambda_j)} \\
&\quad + \left(1 + \frac{\sinh \eta}{\sinh 2\lambda} \right) a(\lambda) \prod_{j=1}^M \frac{\sinh(\lambda - \lambda_j - \eta) \sinh(\lambda + \lambda_j - \eta)}{\sinh(\lambda - \lambda_j) \sinh(\lambda + \lambda_j)}
\end{aligned} \tag{37}$$

is the eigenvalue if all the ‘unwanted terms’ $\Lambda_j(\lambda, \lambda_1, \dots, \lambda_M)$ vanish, that is

$$\Lambda_j(\lambda, \lambda_1, \dots, \lambda_M) = 0$$

for $j = 1, \dots, M$. This condition indicates that the spectral parameters λ_j are not independent of each other and produces the so-called Bethe ansatz equation:

$$\sinh(2\lambda_j - \eta) \frac{\cosh(\lambda_j - (\eta/2)) a(\lambda_j)}{\cosh(\lambda_j + (\eta/2)) \bar{d}(\lambda_j)} = \prod_{k=1(\neq j)}^M \frac{\sinh(\lambda_j - \lambda_k + \eta) \sinh(\lambda_j + \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta) \sinh(\lambda_j + \lambda_k - \eta)}. \quad (38)$$

Substituting (30) and (31) into it, one has

$$\begin{aligned} & \frac{\cosh^2(\lambda_j - (\eta/2)) \sinh^2(\lambda_j + c + (\eta/2)) \sinh^2(\lambda_j - c + (\eta/2))}{\cosh^2(\lambda_j + (\eta/2)) \sinh^2(\lambda_j + c - (\eta/2)) \sinh^2(\lambda_j - c - (\eta/2))} \left(\frac{\sinh(\lambda_j + (\eta/2))}{\sinh(\lambda_j - (\eta/2))} \right)^{2N} \\ &= \prod_{k=1(\neq j)}^M \frac{\sinh(\lambda_j - \lambda_k + \eta) \sinh(\lambda_j + \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta) \sinh(\lambda_j + \lambda_k - \eta)}. \end{aligned} \quad (39)$$

From equations (25) and (37), the eigenvalue of Hamiltonian (1) acting on the state $|\Omega\rangle$ is obtained:

$$\begin{aligned} E(\lambda_1, \dots, \lambda_M) &= \frac{J}{2} \sinh \eta \frac{\sinh^4 \eta}{(\sinh^2 \eta - \sinh^2 c)^2} \frac{\partial}{\partial \lambda} \Lambda(\lambda, \lambda_1, \dots, \lambda_M)|_{\lambda=\eta/2} \\ &\quad - (NJ + 2J_i) \cosh \eta \\ &= 2J \sinh \eta \sum_{j=1}^M \frac{\sinh \eta}{\cosh 2\lambda_j - \cosh \eta} + [(N - 1)J + 2J_i] \cosh \eta. \end{aligned} \quad (40)$$

4. The ground-state properties

The properties of the XXZ chain was first studied in detail by Yang and Yang [24]. In recent years, the finite-size corrections for the energy of this model have been extensively investigated by many authors [25–27]. In this section, we will discuss the ground-state properties of our model (1) in some special parameter cases.

In the following, we mainly concentrate our discussion on the $|\cosh \eta| < 1$ and $J > 0$ case. For convenience, put $\eta = i\gamma$ (γ real) and $\Delta = \cosh \eta = \cos \gamma$. Although the parameter c can take real or imaginary values, we limit our discussion to the real c case. From (2), it can be seen this means that the boundary impurity coupling J_i has the same sign with coupling J . In this case, we will see later that there is no boundary string solution in the ground state. We define

$$\Phi\left(\lambda_j, \frac{\gamma}{2}\right) = 2 \arctan\left(\tanh \lambda_j \cot \frac{1}{2}\gamma\right). \quad (41)$$

By using $\exp(2i \arctan z) = (1 + iz)/(1 - iz)$, we have

$$e^{i\Phi(\lambda_j, \gamma/2)} = \frac{\sinh(i\gamma/2) - \lambda_j}{\sinh(i\gamma/2) + \lambda_j}. \quad (42)$$

Putting

$$e^{2i\Gamma} = \frac{\Delta - e^{i\gamma}}{\Delta e^{i\gamma} - 1} \quad (43)$$

it follows that

$$e^{i\Phi(\lambda_j, \Gamma)} = \frac{e^{ip_j} + \Delta}{e^{ip_j} \Delta + 1} = \frac{\cosh(\lambda_j + (i\gamma/2))}{\cosh(\lambda_j - (i\gamma/2))} \tag{44}$$

where $p_j = \Phi(\lambda_j, \gamma/2)$ and $\Delta = \cosh \eta = \cos \gamma = (e^{2i\Gamma} - e^{i\gamma}) / (e^{2i\Gamma} e^{i\gamma} - 1)$.

Now taking the logarithm of (39) we obtain

$$2N\Phi(\lambda_j, \gamma/2) = 2\pi I_j - 2[\Phi(\lambda_j, \Gamma) + \Phi(\lambda_j + c, \gamma/2) + \Phi(\lambda_j - c, \gamma/2)] + \sum_{k=1(\neq j)}^M \Phi(\lambda_j \pm \lambda_k, \gamma). \tag{45}$$

This equation can be written as

$$\frac{I_j}{N} = \frac{1}{\pi} \left\{ \Phi\left(\lambda_j, \frac{\gamma}{2}\right) + \frac{1}{N} [\Phi_i(\lambda_j) + \Phi_b(\lambda_j)] - \frac{1}{2N} \sum_{k=-M}^M \Phi(\lambda_j - \lambda_k, \gamma) \right\} \tag{46}$$

where

$$\Phi_i(\lambda_j) = \Phi(\lambda_j + c, \gamma/2) + \Phi(\lambda_j - c, \gamma/2) \text{ and } \Phi_b(\lambda_j) = \Phi(\lambda_j, \Gamma) + \frac{1}{2}\Phi(2\lambda_j, \gamma) + \frac{1}{2}\Phi(\lambda_j, \gamma)$$

and I_j are some integers. Here we represent $\lambda_{-j} = -\lambda_j$ and note $\Phi(0, \gamma) = 0$. We define

$$Z_N(\lambda) = \frac{1}{\pi} \left\{ \Phi\left(\lambda, \frac{\gamma}{2}\right) + \frac{1}{N} [\Phi_i(\lambda) + \Phi_b(\lambda)] - \frac{1}{2N} \sum_{k=-M}^M \Phi(\lambda - \lambda_k, \gamma) \right\}. \tag{47}$$

From this definition, the Bethe equation (46) is recovered by $Z_N(\lambda_j) = I_j/N$. For the ground state, I_j take consecutive integers symmetrically around zero. When N goes to infinity λ_j tends to a continuous distribution, thus a density of roots $\{\lambda_j\}$ can be defined as

$$\rho_N(\lambda) = \frac{dZ_N(\lambda)}{d\lambda}. \tag{48}$$

Taking the thermodynamic limit and differentiating (47) with respect to λ one gets

$$\rho_N(\lambda) = \frac{1}{\pi} \left\{ \Phi'\left(\lambda, \frac{\gamma}{2}\right) + \frac{1}{N} [\Phi'_i(\lambda) + \Phi'_b(\lambda)] \right\} - \frac{1}{2\pi} \int_{-\Lambda}^{\Lambda} d\mu \rho_N(\mu) \Phi'(\lambda - \mu, \gamma) \tag{49}$$

where Λ is the cut-off of the λ modes and is determined by the condition $\int_{-\Lambda}^{\Lambda} \rho_N(\lambda) d\lambda = (2M + 1)/N$. As discussed in many previous papers [27, 28], the eigenenergy is minimized at $\Lambda = \infty$ up to the order of $O(N^{-2})$.

We represent $\rho_N(\lambda)$ as

$$\rho_N(\lambda) = \rho_0(\lambda) + \frac{1}{N} [\rho_i(\lambda) + \rho_b(\lambda)] \tag{50}$$

with $\rho_0(\lambda)$, $\rho_i(\lambda)$ and $\rho_b(\lambda)$ given by

$$\rho_0(\lambda) = \frac{1}{\pi} \Phi'\left(\lambda, \frac{\gamma}{2}\right) - \frac{1}{2\pi} \int_{-\Lambda}^{\Lambda} d\mu \rho_0(\mu) \Phi'(\lambda - \mu, \gamma) \tag{51}$$

$$\rho_i(\lambda) = \frac{1}{\pi} \Phi'_i(\lambda) - \frac{1}{2\pi} \int_{-\Lambda}^{\Lambda} d\mu \rho_i(\mu) \Phi'(\lambda - \mu, \gamma) \tag{52}$$

$$\rho_b(\lambda) = \frac{1}{\pi} \Phi'_b(\lambda) - \frac{1}{2\pi} \int_{-\Lambda}^{\Lambda} d\mu \rho_b(\mu) \Phi'(\lambda - \mu, \gamma) \tag{53}$$

where $\rho_0(\lambda)$, $(1/N)\rho_i(\lambda)$ and $(1/N)\rho_b(\lambda)$ are the contributions of the bulk, the impurity and the open boundary to the density, respectively. Substituting

$$\Phi'\left(\lambda, \frac{\gamma}{2}\right) = \frac{2 \sin \gamma}{\cosh 2\lambda - \cos \gamma} \quad \text{and} \quad \Phi'(\lambda - \mu, \gamma) = \frac{2 \sin 2\gamma}{\cosh 2(\lambda - \mu) - \cos 2\gamma}$$

into (51), in the case of $\Lambda = \infty$ the equation is exactly solved by a Fourier transform to give

$$\rho_0(\lambda) = \frac{1}{\gamma \cosh(\pi\lambda/\gamma)}. \tag{54}$$

Note that

$$\begin{aligned} \Phi'_i(\lambda) &= \frac{2 \sin \gamma}{\cosh 2(\lambda + c) - \cos \gamma} + \frac{2 \sin \gamma}{\cosh 2(\lambda - c) - \cos \gamma} \\ \Phi'_b(\lambda) &= \frac{2 \sin 2\Gamma}{\cosh 2\lambda - \cos 2\Gamma} + \frac{2 \sin 2\gamma}{\cosh 4\lambda - \cos 2\gamma} + \frac{\sin 2\gamma}{\cosh 2\lambda - \cos 2\gamma}. \end{aligned}$$

Then from (52) and (53), we obtain $\rho_i(\lambda)$ and $\rho_b(\lambda)$:

$$\rho_i(\lambda) = \frac{1}{\gamma \cosh[\pi(\lambda - c)/\gamma]} + \frac{1}{\gamma \cosh[\pi(\lambda + c)/\gamma]} \tag{55}$$

$$\begin{aligned} \rho_b(\lambda) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\xi e^{-i\lambda\xi} \\ &\times \frac{2 \sinh \frac{1}{2}\xi(\pi - 2\Gamma) + 2 \cosh \frac{1}{4}\pi\xi \sinh \frac{1}{4}\xi(\pi - 2\gamma) + \sinh \frac{1}{2}\xi(\pi - 2\gamma)}{\sinh \frac{1}{2}\pi\xi + \sinh \frac{1}{2}\xi(\pi - 2\gamma)}. \end{aligned} \tag{56}$$

In the thermodynamic limit, the ground-state energy can be expressed as

$$E_g = \frac{1}{2}N \int_{-\infty}^{\infty} d\lambda \varepsilon_0(\lambda)\rho_N(\lambda) + \text{constant} \tag{57}$$

up to the order of $O(N^{-2})$, where

$$\varepsilon_0(\lambda) = \frac{2J \sinh^2 \eta}{\cosh 2\lambda - \cosh \eta} = \frac{-2J \sin^2 \gamma}{\cosh 2\lambda - \cos \gamma}. \tag{58}$$

In the case of $c = 0$, the boundary coupling constants are equal to the bulk coupling constants, and thus the present model degenerates to the XXZ spin chain with the free boundary. It can be shown that our results coincide with those obtained by other authors [26, 27] in this limit case. Additionally, the boundary energy can be obtained by using the relation [13]

$$E_b = E_g - E_p$$

where E_p is the well known ground-state energy with periodic boundary condition. The final result is represented as

$$E_b = \int_{-\infty}^{\infty} d\lambda \frac{-J \sin^2 \gamma}{\cosh 2\lambda - \cos \gamma} [\rho_i(\lambda) + \rho_b(\lambda)] + (2J_i - J) \cos \gamma \tag{59}$$

where $\rho_i(\lambda)$ and $\rho_b(\lambda)$ are given by (55) and (56).

It should be noted that our above results for the ground-state energy are only correct when λ has no boundary string solution corresponding to the impurity terms. In our discussion for real c and imaginary η ($|\Delta| < 1$), no boundary string solution appears. However, for imaginary $c = ic'$ (c' real), the boundary string [12, 13] type solution appears.

For example, if we take $\pi/2 > c' > 0$ and $\gamma > 0$, in the case of $c' > \gamma$, it is straightforward to observe from the Bethe ansatz equation (39) that $\lambda_j = c - \frac{1}{2}\eta = i(c' - \frac{1}{2}\gamma)$ is a solution of the Bethe ansatz equation when $N \rightarrow \infty$. From (2), that is $J_i = J \sin^2 \gamma / (\sin^2 \gamma - \sin^2 c')$, it is easy to see that $\pi/2 > c' > \gamma > 0$ means the impurity coupling J_i takes the opposite sign to the bulk coupling J . To see this from the viewpoint of energy, when $2c' - \gamma < \pi/2$, the energy

$$\varepsilon_0(\lambda) = \frac{-2J \sin^2 \gamma}{\cos(2c' - \gamma) - \cos \gamma}$$

carried by the imaginary mode $\lambda = ic' - (i/2)\gamma$ is smaller than that carried by the real mode. Thus it corresponds to the boundary bound state. In other cases, for example $|\Delta| = |\cosh \eta| > 1$, we can also discuss the boundary state properties but need to be more careful. Interested readers can see the articles of Skorik *et al* [12, 13], in which a detailed discussion about the boundary bound state can be found (see also [14–17]).

In conclusion, the Hamiltonian of the XXZ chain with boundary terms coupled to impurities is derived and the ground-state properties are discussed in some limited cases. The thermodynamics of the present model can also be constructed with the standard method [29, 30] based on the string hypothesis [31]. However, how to construct the K matrix is a very interesting problem. As we know, the K matrix induces boundary terms. The constant number K matrix corresponds to the boundary term which can be interpreted as coupling with magnetic fields on the edges [32]. In this paper, the K matrix includes a boundary spin operator and produces the boundary term which is interpreted as the coupling between the bulk and the boundary spins. In the XXX chain case, the open spin chain with two arbitrary spin impurities can be constructed. The corresponding K matrix includes an arbitrary spin operator [23]. It is also interesting to investigate in depth the boundary state properties of the present model with different parameters; this work is under investigation and will be presented in the future.

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