Surface energy and elementary excitations of the XXZ spin chain with arbitrary boundary fields

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Abstract
The thermodynamic properties of the XXZ spin chain with integrable open boundary conditions at the gaped region (i.e. the anisotropic parameter $\eta$ being a real number) are investigated. It is shown that the contribution of the inhomogeneous term in the $T-Q$ relation of the ground state and elementary excited state can be neglected when the size of the system $N$ tends to infinity. The surface energy and elementary excitations induced by the unparallel boundary magnetic fields are obtained.

Keywords: thermodynamic Bethe ansatz, $T-Q$ relation, surface energy, elementary excitation

(Some figures may appear in colour only in the online journal)
1. Introduction

Since Yang and Baxter’s pioneering works [1, 2], the exactly solvable quantum systems have attracted a great deal of interest because they can provide us solid benchmarks for understanding the many-body effects. Especially the exact solutions are very important in nano-scale systems where alternative approaches involving mean field approximations or perturbations have failed. At present, the integrable models have many applications in statistical physics, low-dimensional condensed matter physics [3], and even some mathematical areas such as quantum groups and quantum algebras.

The coordinate Bethe ansatz [4] and the algebraic Bethe ansatz [5, 6] are the standard methods to obtain the exact solutions of models with \( U(1) \) symmetry. However, when the \( U(1) \) symmetry is broken, these methods cannot be directly applied to due to lacking the reference states. Then the off-diagonal Bethe ansatz (ODBA) was proposed to study the models with or without \( U(1) \) symmetry [7–11]. For further information, we refer the reader to the [12].

In this paper, we consider the open spin-\( \frac{1}{2} \) XXZ quantum spin chain with nondiagonal boundary terms, which is given by the Hamiltonian

\[
H = \sum_{j=1}^{N-1} \left[ \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \cosh \eta \sigma_j^z \sigma_{j+1}^z \right] + \vec{h}_1 \cdot \vec{\sigma}_1 + \vec{h}_N \cdot \vec{\sigma}_N,
\]

where \( \sigma_j^\alpha (\alpha = x, y, z) \) are the Pauli matrices at site \( j \) and \( \{ \vec{h}_i = (h_i^x, h_i^y, h_i^z) | i = 1, N \} \) are two boundary magnetic fields, \( \eta \) is the so-called anisotropic parameter. This is a prototypical integrable quantum spin chain with boundary fields. It can be related to many other models such as the sine-Gordon field theory [13]. Moreover, this model has applications in various branches of physics, including condensed matter and statistical mechanics.

The Bethe ansatz solution of model (1.1) with diagonal boundary fields (\( \{ \vec{h}_i = 0, i = 1, N \} \)), which means that the two boundary magnetic fields are parallel and along the \( z \)-direction, where the corresponding reflection matrices only have diagonal elements, has been known [4, 6]. If the boundary reflection have the off-diagonal elements, the eigenvalue and the eigenstates has been obtained by the off-diagonal Bethe ansatz [8, 10, 14–16]. The eigenvalues of the system for arbitrary boundary fields is given by an inhomogeneous \( T - Q \) relation, giving rise to the fact that the study of the thermodynamic limit becomes more involved in. However, if the anisotropic parameter \( \eta \) is an arbitrary imaginary number, there exist a series of infinite special points at which the inhomogeneous \( T - Q \) relation reduces to the homogeneous one and thus the associated Bethe ansatz equations become the standard ones [11]. In the thermodynamic limit, these points become dense on the imaginary line which allows ones to study the thermodynamics properties such as the ground state and the surface energy when the anisotropic parameter \( \eta \) is an imaginary number (namely, the open XXZ chain at the gapless region) [11]. However, if \( \eta \) is an arbitrary real number, there does not exist the series points and thus the previous analysis fails.

In this paper, we study the thermodynamic limit of the model (1.1) with \( \eta \) being an arbitrary real number under the nondiagonal boundary terms. We first address the contribution of the inhomogeneous term with finite system-size. It is shown that the contribution of the inhomogeneous term in the associated \( T - Q \) relation to the ground state energy and elementary excitation can be neglected when the system-size \( N \) tends to infinity. Then based on the reduced Bethe ansatz equation, we study the surface energy [17–19] which contains the effects induced by the unparallel boundary fields. Furthermore, we obtain the elementary excitation energy.
The paper is organized as follows. In section 2, the exact solution of the model is briefly reviewed. In section 3, we give the reduced homogeneous $T-Q$ relation and calculate the surface excitations which comes from the boundary strings. In section 4, we focus on the contribution of the inhomogeneous term to the ground state energy. In section 5, we study the thermodynamic limit and surface energy of the model with $\eta$ being an arbitrary real number. In section 6, we further calculate the elementary excitation energy induced by the boundary fields. Section 7 gives some discussions.

2. The model and its ODBA solution

In order to address the boundary reflection clearly, we rewrite the Hamiltonian (1.1) as

\[
H = \sum_{j=1}^{N-1} \left[ \sigma_+^j \sigma_+^{j+1} + \sigma_-^j \sigma_-^{j+1} + \cosh \eta \sigma_+^j \sigma_-^{j+1} \right] 
\]

where $\alpha_\pm$, $\beta_\pm$ and $\theta_\pm$ are the boundary parameters which parameterize the components of boundary fields and are related to the parameters of the $\mathcal{K}$-matrices (see (2.4) and (2.5) below). The integrability of the model is associated with the $R$-matrix

\[
R_{0j}(u) = \frac{1}{2} \left[ \frac{\sinh(u + \eta)}{\sinh(\eta)} (1 + \sigma_+^j \sigma_-^0) + \frac{\sinh u}{\sinh \eta} (1 - \sigma_+^j \sigma_-^0) \right] + \frac{1}{2} (\sigma_+^j \sigma_-^0 + \sigma_-^j \sigma_+^0),
\]

where $u$ is the spectral parameter and $\eta$ is the bulk anisotropic parameter. The $R$-matrix satisfies the Yang–Baxter equation (YBE)

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

The boundary magnetic fields are described by the reflection matrix [13, 20]

\[
\mathcal{K}^-(u) = \begin{pmatrix} \mathcal{K}_{11}^-(u) & \mathcal{K}_{12}^-(u) \\ \mathcal{K}_{21}^-(u) & \mathcal{K}_{22}^-(u) \end{pmatrix},
\]

\[
\mathcal{K}_{11}^-(u) = 2 [\sinh(\alpha_-) \cosh(\beta_-) \cosh(u) + \cosh(\alpha_-) \sinh(\beta_-) \sinh(u)],
\]

\[
\mathcal{K}_{22}^-(u) = 2 [\sinh(\alpha_-) \cosh(\beta_-) \cosh(u) - \cosh(\alpha_-) \sinh(\beta_-) \sinh(u)],
\]

\[
\mathcal{K}_{12}^-(u) = e^{\theta_-} \sinh(2u), \quad \mathcal{K}_{21}^-(u) = e^{-\theta_-} \sinh(2u),
\]

and the dual reflection matrix

\[
\mathcal{K}^+(u) = \mathcal{K}^-(-u - \eta) \left| \begin{array}{cc} \alpha_- & \beta_- \\ \theta_- & \eta \end{array} \right| \left| \begin{array}{cc} \alpha_- & \beta_- \\ \theta_- & \eta \end{array} \right|^{-1} = \mathcal{K}^-(-u)\mathcal{K}^+(u),
\]

The former satisfies the reflection equation (RE)

\[
R_{12}(u_1 - u_2)\mathcal{K}_1^-(u_1)R_{23}(u_1 + u_2)\mathcal{K}_2^-(u_2) = \mathcal{K}_2^-(u_2)R_{12}(u_1 + u_2)\mathcal{K}_1^-(u_1)R_{23}(u_1 - u_2),
\]

and the latter satisfies the dual RE.
\[
R_{12}(u_2 - u_1)K_1^+ (u_1)R_{21}(-u_1 - u_2 - 2\eta)K_2^+ (u_2) = K_2^+ (u_2)R_{12}(-u_1 - u_2 - 2\eta)K_1^+ (u_1)R_{21}(u_2 - u_1). \tag{2.7}
\]

In order to show the integrability of the system, we first introduce the ‘row-to-row’ monodromy matrices \( T_0(u) \) and \( \hat{T}_0(u) \)
\[
T_0(u) = R_{0N}(u - \theta_N)R_{0N-1}(u - \theta_{N-1}) \cdots R_{01}(u - \theta_1), \tag{2.8}
\]
\[
\hat{T}_0(u) = R_{10}(u + \theta_1)R_{20}(u + \theta_2) \cdots R_{N0}(u + \theta_N), \tag{2.9}
\]
where \( V_0 \) is the auxiliary space, \( V_1 \otimes V_2 \otimes \cdots \otimes V_N \) is the physical or quantum space, \( N \) is the number of sites and \( \{ \theta_j, j = 1, \cdots , N \} \) are the inhomogeneous parameters. The one-row monodromy matrices are the \( 2 \times 2 \) matrices in the auxiliary space \( 0 \) and their elements act on the quantum space \( \mathbb{V} \otimes \mathbb{N} \). The transfer matrix of the system reads
\[
t(u) = \text{tr}_0 \{ K_2^+ (u)T_0(u)K_1^+ (u)\hat{T}_0(u) \}. \tag{2.10}
\]
Using the YBE (2.3), RE (2.6) and dual RE (2.7), one can prove that the transfer matrices with different spectral parameters commute with each other, namely, \( [t(u), t(v)] = 0 \). Therefore, \( t(u) \) serves as the generating function of all the conserved quantities of the system. The model Hamiltonian (2.1) is constructed by taking the derivative of the logarithm of the transfer matrix
\[
H = \sinh \eta \frac{\partial \ln t(u)}{\partial u} \big|_{u=0, \theta=0} - N \cosh(\eta) - \tanh \eta \sinh \eta. \tag{2.11}
\]
By using the off-diagonal Bethe ansatz method, the eigenvalue \( \Lambda(u) \) of the transfer matrix \( t(u) \) can be given by the inhomogeneous \( T-Q \) relation [8],
\[
\Lambda(u) = a(u) \frac{Q(u - \eta)}{Q(u)} + d(u) \frac{Q(u + \eta)}{Q(u)} + 2c \frac{\sinh(2u) \sinh(2u + 2\eta)}{Q(u)} \Lambda(u) \bar{\Lambda}(-u - \eta), \tag{2.12}
\]
where
\[
c = \cosh \left[ [(N + 1)\eta + \alpha_- + \beta_- + \alpha_+ + \beta_+] - \cosh(\theta_- - \theta_+) \right],
\]
\[
\bar{\Lambda}(u) = \prod_{j=1}^{N} \frac{\sinh(u - \theta_j + \eta) \sinh(u + \theta_j + \eta)}{\sinh^2 \eta},
\]
\[
Q(u) = \prod_{j=1}^{N} \frac{\sinh(u - u_j) \sinh(u + u_j + \eta)}{\sinh^2 \eta},
\]
\[
a(u) = d(-u - \eta) = -\frac{\sinh(2u + 2\eta)}{\sinh(2u + \eta)} \sinh(u - \alpha_-) \sinh(u - \alpha_+) \times \cosh(u - \beta_-) \cosh(u - \beta_+) \bar{\Lambda}(u).
\]\( \tag{2.13} \)
The \( N \) Bethe roots \( \{ u_j \}_{j=1}^{N} \) should satisfy the Bethe ansatz equations (BAEs)
\[
a(u_j)Q(u_j - \eta) + d(u_j)Q(u_j + \eta) + 2c \sinh(2u_j) \sinh(2u_j + 2\eta) \Lambda(u_j) \bar{\Lambda}(-u_j - \eta) = 0. \tag{2.14}
\]
The eigenvalue of the Hamiltonian (2.1) in terms of the Bethe roots is
\[ E = - \sinh \eta [\coth \alpha_- + \tanh \beta_- + \coth \alpha_+ + \tanh \beta_+] \]
\[ + 2 \sum_{j=1}^{N} \frac{\sinh^2 \eta}{\sinh u_j \sinh(u_j + \eta)} + (N - 1) \cosh \eta. \]  

(2.15)

3. Reduced \( T - Q \) relation and surface excitations

In order to study the contribution of the inhomogeneous term in (2.12), we first consider the following reduced \( T - Q \) relation

\[ \Lambda_{\text{hom}}(u) = a(u) \frac{Q(u - \eta)}{Q(u)} + d(u) \frac{Q(u + \eta)}{Q(u)}. \]  

(3.1)

We note that the non-diagonal boundary parameters are included in the above reduced \( T - Q \) relation. For convenience, we put \( u_j = i \frac{\lambda_j}{2} - \frac{\eta}{2} \) with \( \eta > 0, \lambda_j \in (-\pi, \pi] \). From the singularity analysis of \( \Lambda_{\text{hom}}(u) \), we obtain the reduced BAEs

\[ \frac{\sin(\frac{\lambda_j}{2} - i\eta_j^0)}{\sin(\frac{\lambda_j}{2} + i\eta_j^0)} 2^N \sin(\lambda_j - \eta_j) \sin(\frac{\lambda_j}{2} + i\eta_j^0 + i\alpha_+)} \sin(\lambda_j + \eta_j) \sin(\frac{\lambda_j}{2} - i\eta_j - i\alpha_+) \].
\[ \times \frac{\sin(\frac{\lambda_j}{2} + i\eta_j + i\alpha_-)}{\sin(\frac{\lambda_j}{2} - i\eta_j - i\alpha_-)} \cos(\frac{\lambda_j}{2} + i\eta_j^0 + i\beta_+) \cos(\frac{\lambda_j}{2} + i\eta_j + i\beta_-) \cos(\frac{\lambda_j}{2} - i\eta_j^0 - i\beta_+) \].
\[ = \prod_{j=1}^{M} \frac{\sin(\frac{\lambda_j - \lambda_j^0}{2} - i\eta_j)}{\sin(\frac{\lambda_j - \lambda_j^0}{2} + i\eta_j)} \sin(\frac{\lambda_j + \lambda_j^0}{2} + i\eta_j), \quad j = 1, \ldots, M. \]  

(3.2)

We define the reduced eigenvalues as

\[ E_{\text{hom}} = \sinh \eta \frac{\partial \ln \Lambda_{\text{hom}}(u)}{\partial u}\big|_{u=0, \theta_j=0} = N \cosh \eta - \tanh \eta \sinh \eta \]
\[ = \sum_{j=1}^{M} 4 \sinh^2 \eta \cos \lambda_j - \cosh \eta + N \cosh \eta + E_0, \]  

(3.3)

where

\[ E_0 = -\sinh \eta [\coth \alpha_- + \coth \alpha_+ + \tanh \beta_+ + \tanh \beta_-] - \cosh(\eta). \]  

(3.4)

Taking the logarithm of BAEs (3.2), we obtain

\[ 2N \phi_1(\lambda_j) + \phi_2(2\lambda_j) - \phi(2\alpha_-/\eta_{j+1})(\lambda_j) - \phi(2\alpha_+/\eta_{j+1})(\lambda_j) + \gamma_+(\lambda_j) + \gamma_-(\lambda_j) + \pi \]
\[ = 2\pi I_j + \sum_{j=1}^{M} [\phi_2(\lambda_j - \lambda_j) + \phi_2(\lambda_j + \lambda_j)], \quad j = 1, \ldots, M, \]  

(3.5)

with \( I_j \) being an integer which determine the eigenvalue and

\[ \phi_m(\lambda_j) = -i \ln \frac{\sin(\frac{\lambda_j}{2} - i\eta_j^0)}{\sin(\frac{\lambda_j}{2} + i\eta_j^0)}, \quad \gamma_{\pm}(\lambda_j) = -i \ln \frac{\cos(\lambda_j - i\eta_j + i\beta_{\pm})}{\cos(\lambda_j - i\eta_j - i\beta_{\pm})}. \]  

(3.6)
Define the counting function as $Z(\lambda_j) = \frac{1}{2\pi}$, then the BAEs (3.5) read

$$Z(\lambda) = \frac{1}{2\pi} \left\{ \phi_1(\lambda) + \frac{1}{2N} \left[ \phi_2(2\lambda) - \phi_{2\alpha_-/\eta+1}(\lambda) - \phi_{2\alpha_+/\eta+1}(\lambda) + \gamma_+(\lambda) + \gamma_-(\lambda) 
+ \pi - \sum_{l=1}^{M} (\phi_2(\lambda - \lambda_l) + \phi_2(\lambda + \lambda_l)) \right] \right\}. \quad (3.7)$$

In the thermodynamic limit $N \to \infty$, the distribution of Bethe roots tend to continuous and

$$\frac{dZ(\lambda)}{d\lambda} = \rho(\lambda) + \rho_h(\lambda), \quad (3.8)$$

where $\rho(\lambda)$ is the density of particles and $\rho_h(\lambda)$ is the density of holes. From equation (3.7), the density of the roots $\rho(\lambda)$ satisfies

$$\rho(\lambda) = \frac{dZ(\lambda)}{d\lambda} - \frac{1}{2N} \delta(\lambda) - \frac{1}{2N} \delta(\lambda - \pi) = g_1(\lambda) + \frac{1}{2N} \left[ 2q(\lambda) - g_{2\alpha_-/\eta+1}(\lambda) - g_{2\alpha_+/\eta+1}(\lambda) + h_+(\lambda) + h_-(\lambda) 
- \delta(\lambda) - \delta(\lambda - \pi) \right] - \int_{-\pi}^{\pi} g_2(\lambda - v) \rho(v) dv, \quad (3.9)$$

where

$$g_m(\lambda) = \frac{1}{2\pi} \frac{d\phi_m(\lambda)}{d\lambda} = \frac{1}{2\pi} \frac{\sinh(m\lambda)}{\cosh(m\lambda) - \cos(\lambda)},$$

$$h_{\pm}(\lambda) = \frac{1}{2\pi} \frac{d\gamma_{\pm}(\lambda)}{d\lambda} = \mp \frac{1}{2\pi} \frac{\sin(2\beta_{\pm} + \eta)}{\cosh(2\beta_{\pm} + \eta)},$$

$$q(\lambda) = g_2(2\lambda). \quad (3.10)$$

In equation (3.9), the presence of delta-functions is due to the fact that $\lambda_j = 0$ and $\lambda_j = \pi$ are the solutions of (3.5), which should be excluded, since they make the wavefunction vanish identically [21].

Now, we consider the elementary excitations of this model. We first consider the spin excitation, which means that one spin is flipped. The one spin excitation corresponds add two holes in the ground state distribution of $I_j$. Denote the positions of holes as $\lambda_h$ and $-\lambda_h$. In the thermodynamic limit $N \to \infty$, we obtain the density of state $\rho(\lambda)$ in this case is

$$\tilde{\rho}(\lambda) = g_1(\lambda) + \frac{1}{2N} \left[ 2q(\lambda) - g_{2\alpha_-/\eta+1}(\lambda) - g_{2\alpha_+/\eta+1}(\lambda) + h_+(\lambda) + h_-(\lambda) 
- \delta(\lambda) - \delta(\lambda - \pi) - \delta(\lambda - \lambda_h) - \delta(\lambda + \lambda_h) \right] - \int_{-\pi}^{\pi} g_2(\lambda - v) \tilde{\rho}(v) dv. \quad (3.11)$$

From equations (3.9) and (3.11), we obtain the difference between $\tilde{\rho}(\lambda)$ and $\rho(\lambda)$ as

$$\delta \rho(\lambda) = \tilde{\rho}(\lambda) - \rho(\lambda), \text{ which satisfies}$$

$$\delta \rho(\lambda) = \frac{1}{2N} \left[ \delta(\lambda - \lambda_h) - \delta(\lambda + \lambda_h) \right] - \int_{-\pi}^{\pi} g_2(\lambda - v) \delta \rho(v) dv. \quad (3.12)$$

By using the Fourier transformation
\[ \hat{f}(\omega) = \int_{-\pi}^{\pi} f(\lambda) e^{i\omega \lambda} d\lambda, \quad f(\lambda) = \frac{1}{2\pi} \sum_{\omega = -\infty}^{\infty} \hat{f}(\omega) e^{-i\omega \lambda}, \quad (3.13) \]

we obtain the solution of \( \delta \rho(\lambda) \) as

\[ \delta \rho(\omega) = - \frac{\cos(\lambda_0 \omega)}{N(1 + g_2^2(\omega))}, \quad (3.14) \]

where \( g_m(\omega) = e^{-m|\omega|} \). The energy of a bulk hole at the position \( \lambda_0 \) can be calculated as

\[ \delta_{ch} = 2 \sinh \eta \sum_{\omega = -\infty}^{\infty} \frac{e^{-i\omega \lambda_0}}{\cosh(\omega \eta)}, \quad (3.15) \]

which is shown in figure 1. The spin of this excitation is \( S_z = N \int_{-\pi}^{\pi} \delta \rho(\lambda) d\lambda = -1/2 \).

Next, we consider the new solutions of BAEs (3.2), that is the boundary strings. The analysis is close to that of [22]. The fundamental boundary 1-string is the root located at \( \lambda_0 = 2i(\alpha_\pm + \frac{\eta}{2}) \) for \( \alpha_\pm > -\frac{\eta}{2} \) and at \( \lambda_0 = \pi + 2i(\beta_\pm + \frac{\eta}{2}) \) for \( \beta_\pm > -\frac{\eta}{2} \). One can check that these strings are the solutions of BAEs (3.2).

Substituting the string solution \( \lambda_0 = 2i(\alpha_\pm + \frac{\eta}{2}) \) into BAEs (3.2) and taking the thermodynamic limit, we obtain the density of states \( \tilde{\rho}_\alpha(\lambda) \)

\[ \tilde{\rho}_\alpha(\lambda) = g_1(\lambda) + \frac{1}{2N} \left[ 2g(\lambda) - g_{2\alpha-1/\eta+1}(\lambda) - g_{2\alpha-1/\eta+1}(\lambda) + h_+(\lambda) + h_-(\lambda) \right. \]
\[ \left. - \delta(\lambda) - \delta(\lambda - \pi) - g_2(\lambda - 2i(\alpha_\pm + \frac{1}{2} \eta)) - g_2(\lambda + 2i(\alpha_\pm + \frac{1}{2} \eta)) \right] \]
\[- \int_{-\pi}^{\pi} g_2(\lambda - v) \tilde{\rho}_\alpha(v) dv. \quad (3.16) \]

Denote the difference between \( \tilde{\rho}_\alpha(\lambda) \) and \( \rho(\lambda) \) as \( \delta \rho_\alpha(\lambda) = \tilde{\rho}_\alpha(\lambda) - \rho(\lambda) \). From equations (3.9) and (3.16), we find \( \delta \rho_\alpha(\lambda) \) should satisfy

\[ \delta \rho_\alpha(\lambda) = \frac{1}{2N} \left[ - g_2(\lambda - 2i(\alpha_\pm + \frac{1}{2} \eta)) - g_2(\lambda + 2i(\alpha_\pm + \frac{1}{2} \eta)) \right] \]
\[- \int_{-\pi}^{\pi} g_2(\lambda - v) \delta \rho_\alpha(v) dv. \quad (3.17) \]

The solution of equation (3.17) is

\[ \delta \rho_\alpha(\omega) = \begin{cases} 
\frac{1}{2N(1 + g_2(\omega))} \left[ g_{\pm \alpha + 1/2\eta}(\omega) + g_{\pm \alpha + 1/2\eta}(\omega) \right], & -\frac{\eta}{2} < \alpha_\pm < \frac{\eta}{2}, \\
\frac{1}{2N(1 + g_2(\omega))} \left[ 2e^{-2|\omega|} \cosh(2\omega \alpha + \omega \eta) - 2 \cosh(2\omega \alpha - \omega \eta) \right], & \alpha_\pm > \frac{\eta}{2}.
\end{cases} \]

Thus, the energy carried by the boundary string is

\[ \delta_{\alpha} = \begin{cases} 
\frac{4 \sinh \eta}{\cosh(2\alpha_\pm + \eta) - \cosh \eta}, & -\frac{\eta}{2} < \alpha_\pm < \frac{\eta}{2}, \\
+2 \sinh \eta \sum_{\omega = -\infty}^{\infty} \frac{e^{-2|\omega|} \cosh(2\alpha_\pm + \omega \eta)}{\cosh(\omega \eta)}, & -\frac{\eta}{2} < \alpha_\pm < \frac{\eta}{2}, \\
0, & \alpha_\pm > \frac{\eta}{2},
\end{cases} \quad (3.18) \]

which is shown in figure 2. The corresponding spinor carries the spin \( S_z = -1/2 \).
Substituting the string solution $\lambda_0 = \pi + 2i(\beta \pm \eta/2)$ into BAEs (3.2) and taking the thermodynamic limit, we obtain the density of states $\bar{\rho}_\beta(\lambda)$.

**Figure 1.** The energy carried by one bulk hole, where $\eta = 2.0$ and $-\pi < \lambda < \pi$. We find $3.8655 < \delta_{eh} < 11.7183$.

**Figure 2.** The energy $\delta_{e\alpha}$ carried by the boundary string located at $\lambda_0 = 2i(\alpha \pm \eta/2)$, where $\eta = 2.0$. We find that the absolute value of the energy $\delta_{e\alpha}$ is bigger than the maximum $11.7183$ of the energy $\delta_{eh}$, $|\delta_{e\alpha}| > \delta_{eh}^{\max} = 11.7183$ if $-\frac{\pi}{2} < \alpha < \frac{\pi}{2}$.
\[
\tilde{\rho}_\beta(\lambda) = g_1(\lambda) + \frac{1}{2N} \left[ 2g_1(\lambda) - g_{2n-\eta+1}(\lambda) - g_{2n+\eta+1}(\lambda) + h_+(\lambda) + h_-(\lambda) - \delta(\lambda) - \delta(\pi - \lambda) - g_2(\lambda - \pi - 2i(\beta_\pm + \frac{1}{2}\eta)) - g_2(\lambda + \pi + 2i(\beta_\pm + \frac{1}{2}\eta)) \right] - \int_{-\pi}^{\pi} g_2(\lambda - v)\tilde{\rho}_\beta(v)dv.
\]

(3.19)

Denote the difference between \(\tilde{\rho}_\beta(\lambda)\) and \(\rho(\lambda)\) as \(\delta\rho_\beta(\lambda) = \tilde{\rho}_\beta(\lambda) - \rho(\lambda)\). From equations (3.9) and (3.19), we find such solution an

\[
\delta\rho_\beta(\lambda) = \frac{1}{2N} \left[ - g_2(\lambda - \pi - 2i(\beta_\pm + \frac{1}{2}\eta)) - g_2(\lambda + \pi + 2i(\beta_\pm + \frac{1}{2}\eta)) \right] - \int_{-\pi}^{\pi} g_2(\lambda - v)\delta\rho_\beta(v)dv.
\]

(3.20)

Thus, the energy carried by the boundary string is

\[
\delta\varepsilon_\beta = \begin{cases} 
\frac{4\sinh^2\eta}{\cosh(2\beta_\pm + \eta) + \cosh\eta} 
+ 2\sinh\eta \sum_{\omega=-\infty}^{\infty} \frac{(-1)^{\omega}e^{-2i\omega\eta}}{\cosh(\eta)}
, & -\frac{\eta}{2} < \beta_\pm < \frac{\eta}{2}, \\
0, & \beta_\pm > \frac{\eta}{2},
\end{cases}
\]

(3.21)

which is shown in figure 3. The corresponding spinor carries the spin \(S_z = -1/2\).

Combining the results (3.15), (3.18) and (3.21), we find that the excitation energy caused by the boundary parameter \(\alpha_\pm\) (3.18) is bigger than the maximum of energy of one bulk hole \(\delta\varepsilon_\eta\) (3.15) if \(-\frac{\eta}{2} < \alpha_\pm < \frac{\eta}{2}\), while the excitation energy caused by the boundary parameter \(\beta_\pm\) (3.21) is smaller than the minimum of energy of one bulk hole \(\delta\varepsilon_\eta\) (3.15) if \(-\frac{\eta}{2} < \beta_\pm < \frac{\eta}{2}\). In addition, we conclude that

\[
\delta\varepsilon_\alpha < \delta\varepsilon_\beta < 0 < \delta\varepsilon_\eta; \quad -\delta\varepsilon_\alpha > \delta\varepsilon_\eta > -\delta\varepsilon_\beta, \quad \text{if} \quad -\frac{\eta}{2} < \alpha_\pm < 0, \quad -\frac{\eta}{2} < \beta_\pm < 0,
\]

\[
\delta\varepsilon_\alpha > \delta\varepsilon_\eta > \delta\varepsilon_\beta > 0, \quad \text{if} \quad 0 < \alpha_\pm < \frac{\eta}{2}, \quad 0 < \beta_\pm < \frac{\eta}{2}.
\]

(3.22)

Another conclusion is that the energy of the boundary bound state in the regime of \(-\frac{\eta}{2} < \alpha_\pm < 0\) is bigger than the top of the energy band. Therefore it is stable, in spite of its huge energy.

Besides the fundamental boundary 1-string, there exists an infinite set of ‘long’ boundary strings, consisting of roots \(\lambda_0 - 2ik\eta, \lambda_0 - 2i(k - 1)\eta, \ldots, \lambda_0 + 2in\eta\) with \(n, k \geq 0\). We call such solution an \((n, k)\) boundary string, where \((0, 0)\) string is the fundamental boundary string. By using the same arguments in [23], we can prove that the \((n, k)\) string is a solution of BAEs when its ‘centre of mass’ has positive imaginary part and the lowest root \(\lambda_0 - 2ik\eta\) lies below the real axis. However, a direct calculation shows that the energy of the \((n, k)\) strings vanishes with \(k \geq 1\). For the \((n, 0)\) strings with \(n \geq 1\), they have the same energy as that of the boundary bound state given by (3.18) and (3.21), so they represent charged boundary excitations.
4. Finite size correction

Now, we consider the contribution of the inhomogeneous term in the $T - Q$ relation (2.12) to the ground state energy of the system. For this purpose, we define

$$E_{inh} \equiv E_{hom} - E_{true},$$

(4.1)

where $E_{true}$ is the ground state energy of the Hamiltonian (2.1) which can be obtained by using the density matrix renormalization group (DMRG) [24, 25], while $E_{hom}$ is the minimal energy which can be obtained from (3.3), where Bethe roots should satisfy the BAEs (3.5).

Without losing generality, we choose $\theta_{\pm} = 0$, $\alpha_{\pm} = \eta$ and $N$ is even. The number of Bethe roots constructed in (3.3) is related to the total magnetization $m = N^2 - N \int_{-\pi}^{\pi} \rho(\lambda) d\lambda = \frac{N^2}{2} - M$.

In this framework, the ground state should have an integer charge [22], which means the total magnetization should be an integer. We analyze the structure of the Bethe roots at the ground state based on equation (3.22). For the $(0,0)$ string and one bulk hole shown in section 3, the charges of boundary excitations and of the bulk excitations turned out to be half-integer. Then we conclude that the number of excitations should be even if the total magnetization corresponds to the real Bethe roots is an integer, and the number of excitations should be odd if the total magnetization corresponds to the real Bethe roots is a half-integer. In addition, the energy must be the minimum for all the cases that satisfy the condition with integer charges.

For example, we consider the special boundary parameters $(\alpha_{+} > 0, \alpha_{-} > 0, \beta_{+} > \frac{2}{\eta}, \beta_{-} < -\frac{2}{\eta})$ in table 1. Based on the equation (3.9), the total magnetization is given by $m = \frac{N^2}{2} - N \int_{-\pi}^{\pi} \rho(\lambda) d\lambda = \frac{1}{2}$ if the state only have real roots. In addition, from equation (3.22) we know that the energy comes from the boundary string $\lambda_0 = 2i(\alpha_{\pm} + \frac{2}{\eta})$ is bigger than that of one bulk hole. So there must exist one bulk hole. Then we obtain that the structure of the Bethe roots at the ground state is $\frac{N}{2} - 1$ real roots plus one bulk hole.
Table 1. The Bethe roots at the ground state which have no boundary strings.

| No. | Regimes of boundary parameters | Bethe roots |
|-----|--------------------------------|-------------|
| 1.1 | $\alpha_+ > 0, \alpha_- > 0, \beta_+ > \frac{\pi}{2}, \beta_- < -\frac{\pi}{2}$ | $\frac{N}{2} - 1$ real roots |
| 1.2 | $\alpha_+ > 0, \alpha_- < -\frac{\pi}{2}, \beta_+ > \frac{\pi}{2}, \beta_- < \frac{\pi}{2}$ | + one bulk hole |
| 1.3 | $\alpha_+ > 0, \alpha_- > 0, -\frac{\pi}{2} < \beta_+ < 0, -\beta_- < \beta_+ < \frac{\pi}{2}$ | $\frac{N}{2} - 1$ real roots |
| 1.4 | $\alpha_+ > 0, \alpha_- > 0, -\frac{\pi}{2} < \beta_+ < 0, \beta_- > \frac{\pi}{2}$ | $\frac{N}{2}$ real roots |
| 1.5 | $\alpha_+ > 0, \alpha_- > 0, 0 < \beta_+ < \frac{\pi}{2}, 0 < \beta_- < \frac{\pi}{2}$ | $\frac{N}{2} - 1$ real roots |
| 1.6 | $\alpha_+ > 0, \alpha_- > 0, 0 < \beta_+ < \frac{\pi}{2}, \beta_- > \frac{\pi}{2}$ | $\frac{N}{2}$ real roots |
| 1.7 | $\alpha_+ > 0, \alpha_- > 0, \beta_+ > \frac{\pi}{2}, \beta_- < -\frac{\pi}{2}$ | + one bulk hole |
| 1.8 | $\alpha_+ > 0, \alpha_- > 0, \beta_+ < -\frac{\pi}{2}, \beta_- > -\frac{\pi}{2}$ | $\frac{N}{2}$ real roots |
| 1.9 | $\alpha_+ > 0, \alpha_- < -\frac{\pi}{2}, -\beta_- < \beta_+ < 0, \beta_- < -\beta_+$ | $\frac{N}{2}$ real roots |
| 1.10 | $\alpha_+ > 0, \alpha_- < -\frac{\pi}{2}, 0 < \beta_+ < \frac{\pi}{2}, \beta_- < -\beta_+$ | $\frac{N}{2}$ real roots |
| 1.11 | $\alpha_+ > 0, \alpha_- < -\frac{\pi}{2}, \beta_+ > \frac{\pi}{2}, \beta_- < -\beta_+$ | $\frac{N}{2}$ real roots |
| 1.12 | $\alpha_+ > 0, \alpha_- < -\frac{\pi}{2}, \beta_+ < \frac{\pi}{2}, \beta_- < -\beta_+$ | $\frac{N}{2}$ real roots |

For the special boundary parameters $(\alpha_+ > 0, \alpha_- > 0, 0 < \beta_+ < \frac{\pi}{2}, \beta_- < -\frac{\pi}{2})$ in table 2, the total magnetization will be $m = \frac{N}{2} - N \int_{-\pi}^{\pi} \rho(\lambda) d\lambda = 1$ if the state only have real roots. In addition, from equation (3.22) we know that the energy comes from the boundary string $\lambda_0 = \pi + 2i(\beta_+ + \frac{\pi}{2})$ is bigger than that of one bulk hole, while the energy comes from the boundary string $\lambda_0 = 2i(\alpha_+ + \frac{\pi}{2})$ is bigger than that of one bulk hole. So there must exist one boundary string. Then we obtain that the structure of the Bethe roots at the ground state is $\frac{N}{2} - 1$ real roots plus the boundary string $\lambda_0 = \pi + 2i(\beta_+ + \frac{\pi}{2})$.

For the special boundary parameters $(\alpha_+ > 0, \alpha_- > 0, -\frac{\pi}{2} < \beta_+ < 0, \beta_- < -\beta_+)$ in table 3, the total magnetization will be $m = \frac{N}{2} - N \int_{-\pi}^{\pi} \rho(\lambda) d\lambda = 1$ if the state only have real roots. In addition, from equation (3.22) we know that the sum of the energy comes from the boundary strings $\lambda_0 = \pi + 2i(\beta_+ + \frac{\pi}{2})$ and $\lambda_0 = \pi + 2i(\beta_- + \frac{\pi}{2})$ is the minimum which satisfies the condition with integer charges. So there must exist two boundary strings. Then we obtain that the structure of the Bethe roots at the ground state is $\frac{N}{2} - 2$ real roots plus the boundary strings $\lambda_0 = \pi + 2i(\beta_+ + \frac{\pi}{2})$ and $\lambda_0 = \pi + 2i(\beta_- + \frac{\pi}{2})$.

Now we can determine the structures of Bethe roots at the ground state for all the cases in tables 1–3. Let us consider them separately.

I. The ground state has no boundary strings.

We first consider the case that there is no boundary strings at the ground state. The corresponding regimes of the boundary parameters are given by table 1. We calculate the energy $E_{inh}$ in these regimes. We find that $E_{inh}$ satisfies the finite-size behavior, $E_{inh}(N) = q_1e^{\beta N}$, where $q_1 < 0$. Which means if $N \to \infty$, then $E_{inh} \to 0$. Thus $E_{inh}$ equals to the true ground state energy in the thermodynamic limit. Without losing generality, figure 4 gives the detailed results in the regimes 6 and 8 as the examples.

II. The ground state has one $(0, 0)$ string.

Next, we consider the case that there is one boundary strings at the ground state. The corresponding regimes of the boundary parameters are given by table 2 and the finite-size behavior of $E_{inh}$ is shown in figure 5. Again, we see that the inhomogeneous term in (2.12) can be neglected in the thermodynamic limit.
III. The ground state has two (0, 0) strings.

Last, we consider the case that there are two boundary strings at the ground state. The corresponding regimes of the boundary parameters are given by table 3 and the finite-size behavior of $E_{\text{inh}}$ is shown in figure 6. Again, we see that the inhomogeneous term in the $T - Q$ relation (2.12) can be neglected in the thermodynamic limit.

5. Surface energy

Now we consider the surface energy induced by the boundary magnetic fields. For the condition that shown in table 1, in which all the Bethe roots are real at the ground state. Taking the Fourier transformation of equation (3.9), we obtain

Table 2. The Bethe roots of the ground state which have one (0,0) string.

| No. | Regimes of boundary parameters | Bethe Roots |
|-----|--------------------------------|-------------|
| 2.1 | $\alpha_+ > 0, \alpha_- > 0, 0 < \beta_+ < \frac{\pi}{2}, \beta_- < -\frac{\pi}{2}$ | $\frac{\pi}{2} - 1$ real roots |
| 2.2 | $\alpha_+ > 0, \alpha_- > 0, -\frac{\pi}{2} < \beta_+ < 0, \beta_- < -\frac{\pi}{2}$ | $\pi + 2i(\beta_+ + \frac{\pi}{2})$ |
| 2.3 | $\alpha_+ > 0, \alpha_- < -\frac{\pi}{2}, \beta_+ < 0, \beta_- > \frac{\pi}{2}$ | $\pi + 2i(\beta_- + \frac{\pi}{2})$ |
| 2.4 | $\alpha_+ > 0, \alpha_- < -\frac{\pi}{2}, 0 < \beta_+ < \frac{\pi}{2}, \beta_- > \frac{\pi}{2}$ | $\pi + 2i(\beta_- + \frac{\pi}{2})$ |
| 2.5 | $\alpha_+ > 0, \alpha_- < -\frac{\pi}{2}, -\frac{\pi}{2} < \beta_+ < 0, 0 < \beta_- < \frac{\pi}{2}$ | $\pi + 2i(\beta_- + \frac{\pi}{2})$ |

Table 3. The Bethe roots of the ground state which have two (0,0) strings.

| No. | Regimes of boundary parameters | Bethe Roots |
|-----|--------------------------------|-------------|
| 3.1 | $\alpha_+ > 0, \alpha_- > 0, -\frac{\pi}{2} < \beta_+ < 0, 0 < \beta_- < -\beta_+$ | $\frac{\pi}{2} - 2$ real roots |
| 3.2 | $\alpha_+ > 0, \alpha_- > 0, -\frac{\pi}{2} < \beta_+ < 0, -\frac{\pi}{2} < \beta_- < 0$ | $\pi + 2i(\beta_+ + \frac{\pi}{2})$ |
| 3.3 | $\alpha_+ > 0, -\frac{\pi}{2} < \alpha_- < 0, 0 < \beta_+ < \frac{\pi}{2}, \beta_- > \frac{\pi}{2}$ | $\frac{\pi}{2} - 2$ real roots |
| 3.4 | $\alpha_+ > 0, -\frac{\pi}{2} < \alpha_- < 0, -\frac{\pi}{2} < \beta_+ < 0, \beta_- > \frac{\pi}{2}$ | $\pi + 2i(\beta_+ + \frac{\pi}{2})$ |
| 3.5 | $\alpha_+ > 0, -\frac{\pi}{2} < \alpha_- < 0, -\frac{\pi}{2} < \beta_+ < 0, 0 < \beta_- < \frac{\pi}{2}$ | $\pi + 2i(\beta_+ + \frac{\pi}{2})$ |
| 3.6 | $\alpha_+ > 0, -\frac{\pi}{2} < \alpha_- < 0, 0 < \beta_+ < \frac{\pi}{2}, 0 < \beta_- < \frac{\pi}{2}$ | $\frac{\pi}{2} - 2$ real roots |
| 3.7 | $\alpha_+ > 0, -\frac{\pi}{2} < \alpha_- < 0, -\frac{\pi}{2} < \beta_+ < 0, -\frac{\pi}{2} < \beta_- < 0$ | $\pi + 2i(\min(\beta_+), \frac{\pi}{2})$ |

+ one bulk hole + $2i(\alpha_- + \frac{\pi}{2})$
\[ \hat{\rho}(\omega) = \hat{\rho}_0(\omega) + \hat{\rho}_\beta^0(\omega) + \hat{\rho}_\beta^+ (\omega) + \hat{\rho}_\beta^- (\omega) + \hat{\rho}_\alpha^+ (\omega) + \hat{\rho}_\alpha^- (\omega), \]  

where

Figure 4. The contribution of the inhomogeneous term to the ground state energy $E_{\text{inh}}$ versus the even system-size $N$. The data can be fitted as $E_{\text{inh}}(N) = p_1 e^{q_1 N}$. Here (a) $p_1 = 0.9139$ and $q_1 = -0.7841$; (b) $p_1 = 0.3916$ and $q_1 = -0.8501$.

Figure 5. The contribution of the inhomogeneous term to the ground state energy $E_{\text{inh}}$ versus the even system-size $N$. The data can be fitted as $E_{\text{inh}}(N) = p_1 e^{q_1 N}$. Here (a) $p_1 = -3.8560$ and $q_1 = -0.5838$; (b) $p_1 = -1.3750$ and $q_1 = -0.6165$. 

\[ p_1 = 0.9139, \quad q_1 = -0.7841 \]

\[ p_1 = 0.3916, \quad q_1 = -0.8501 \]
\[ \rho_b^0(\omega) = \frac{2\tilde{g}(\omega) - 1 - (-1)^w}{2N(1 + \tilde{g}_2(\omega))}, \quad \tilde{q}(\omega) = \frac{e^{-\eta|\omega|}}{2} (1 + (-1)^w), \]

\[ \tilde{\rho}_{\alpha,\pm}(\omega) = \begin{cases} -\frac{\tilde{g}(\omega)}{2N(1 + \tilde{g}_2(\omega))}, & \alpha_\pm > -\frac{\eta}{2}, \\ \frac{\tilde{g}(\omega)}{2N(1 + \tilde{g}_2(\omega))}, & \alpha_\pm < -\frac{\eta}{2}, \end{cases} \]

\[ \tilde{\rho}_{\beta,\pm}(\omega) = \begin{cases} -\frac{\tilde{g}(\omega)}{2N(1 + \tilde{g}_2(\omega))}, & \beta_\pm < -\frac{\eta}{2}, \\ \frac{\tilde{g}(\omega)}{2N(1 + \tilde{g}_2(\omega))}, & \beta_\pm > -\frac{\eta}{2}, \end{cases} \]

\[ \tilde{h}_b(\omega) = (-1)^w e^{-2|\beta|\omega - |\eta|}, \quad \tilde{\rho}_0(\omega) = \frac{1}{2 \cosh(\eta \omega)}. \tag{5.2} \]

The ground energy can be expressed as

\[ E = -8\pi N \sinh(\eta) \int_{-\pi}^{\pi} g_1(\lambda) \rho(\lambda) d\lambda + N \cosh(\eta) + E_0 \]

\[ = N e_g + e_b, \tag{5.3} \]

where

\[ e_b = e_b^0 + e_{\alpha_+} + e_{\alpha_-} + e_{\beta_+} + e_{\beta_-}, \]

\[ e_g = -2 \sinh(\eta) \sum_{\omega = -\infty}^{\infty} \frac{e^{-\eta|\omega|}}{\cosh(\eta \omega)} + \cosh(\eta), \]

\[ e_b^0 = -\cosh(\eta) - \sum_{\omega = -\infty}^{\infty} \frac{2\tilde{g}(\omega) - 1 - (-1)^w \sinh(\eta)}{\cosh(\eta \omega)}, \]

\[ e_{\alpha_\pm} = \begin{cases} -\sinh(\eta) \coth(\alpha_\pm) - \sinh(\eta) \sum_{\omega = -\infty}^{\infty} \frac{\tilde{g}(\omega)}{\cosh(\eta \omega)}, & \alpha_\pm > -\frac{\eta}{2}, \\ \sinh(\eta) \coth(\alpha_\pm) - \sinh(\eta) \sum_{\omega = -\infty}^{\infty} \frac{\tilde{g}(\omega)}{\cosh(\eta \omega)}, & \alpha_\pm < -\frac{\eta}{2}, \end{cases} \]

\[ e_{\beta_\pm} = \begin{cases} -\sinh(\eta) \tanh(\beta_\pm) - \sinh(\eta) \sum_{\omega = -\infty}^{\infty} \frac{\tilde{h}_b(\omega)}{\cosh(\eta \omega)}, & \beta_\pm < -\frac{\eta}{2}, \\ \sinh(\eta) \tanh(\beta_\pm) + \sinh(\eta) \sum_{\omega = -\infty}^{\infty} \frac{\tilde{h}_b(\omega)}{\cosh(\eta \omega)}, & \beta_\pm > -\frac{\eta}{2}. \end{cases} \tag{5.4} \]

Here \( e_g \) equals to the ground state energy density of the periodic chain and \( e_b \) is the surface energy induced by the open boundary and the boundary fields.

It’s easy to show that for the other conditions, which includes the one boundary \((0, 0)\) string and two boundary \((0, 0)\) strings. The ground state energy can be expressed by two parts. One of them comes from the real roots \((5.3)\) and the other comes from the bulk holes \((3.15)\) or the boundary bound strings \((3.18)-(3.21)\).\(^8\)

For simplicity, here we only give two examples.

\(^8\)The surface energy of this model with special boundary parameters \((\alpha_\pm = \alpha, \beta_\pm = \beta, \beta_\pm = -\beta)\) for a real \(\eta\) has been studied by the quantum transfer matrix method \([26]\) in \([27, 28]\).
I. For the interval that the Bethe roots of the ground state are $N^2 - 1$ real roots plus one $(0, 0)$ string, in the regime of $\alpha_+ > 0$, $\alpha_- > 0$, $0 < \beta_+ < \frac{\eta}{2} - \frac{\eta}{2}$, the ground state energy can be expressed by

$$E = N e_g + e_b + \delta e_{\beta_+},$$

(5.5)

where $e_b + \delta e_{\beta_+}$ is the surface energy induced by the open boundary and the boundary fields.

II. For the interval that the Bethe roots of the ground state are $N^2 - 2$ real roots plus two $(0, 0)$ strings, in the regime of $\alpha_+ > 0$, $\alpha_- > 0$, $-\frac{\eta}{2} < \beta_+ < 0$ and $-\frac{\eta}{2} < \beta_- < 0$, the ground state energy is

$$E = N e_g + e_b + \delta e_{\beta_+} + \delta e_{\beta_-},$$

(5.6)

where $e_b + \delta e_{\beta_+} + \delta e_{\beta_-}$ is the surface energy induced by the open boundary and the boundary fields.

6. Elementary excitation

Now, we consider the elementary excitation. First, we show that the inhomogeneous term in the $T - Q$ relation (2.12) can also be neglected in the thermodynamic limit for the excited states. For this purpose, we define

$$\Delta E = \Delta E^{\text{ED}} - \delta_e,$$

(6.1)

where $\Delta E^{\text{ED}}$ is the minimal change of energy between the ground state and the excitations of the Hamiltonian (2.1) which can be obtained by using the DMRG. Let $\delta_e$ be the minimal change of energy from the ground state obtaining from (3.3) and (3.5). From the equation (3.22), we know that the energy change $\delta_e$ are connected with the choice of boundary parameters. Let us consider them one by one.
Figure 7. $\Delta E = \Delta E_{\text{ED}} - \delta e$, where $\Delta E_{\text{ED}}$ is the minimal change of energy between the ground state and the excitations calculated by using DMRG. The figure can be fitted as $E(N) = p_2 e^{q_2 N}$. Here (a) $p_2 = 0.9875$ and $q_2 = -0.2494$; (b) $p_2 = 1.7260$ and $q_2 = -0.2733$.

Table 4. The Bethe roots at the ground state which have no boundary strings.

| Value of $\delta e$ | Regimes of boundary parameters in table 1 |
|---------------------|------------------------------------------|
| $\delta_{\text{gh}} + \delta_{\text{gh}}$ | 1.4, 1.6, 1.9, 1.10 |
| $\delta_{\text{gh}} + \delta_{\text{gh}}$ | 1.1, 1.2, 1.7, 1.8, 1.11, 1.12 |
| $\delta_{\text{gh}} + \delta_{\text{gh}}$ | 1.3, 1.5 |

Figure 8. $\Delta E = \Delta E_{\text{ED}} - \delta e$, where $\Delta E_{\text{ED}}$ is the minimal change of energy between the ground state and the excitations calculated by using DMRG. The figure can be fitted as $E(N) = p_2 e^{q_2 N}$. Here (a) $p_2 = 2.7060$ and $q_2 = -0.2732$; (b) $p_2 = 4.1750$ and $q_2 = -0.2980$. 
I. The ground state has no boundary strings.

The finite-size behaviors of $\Delta E$ in the regimes of 1.3 and 1.5 are shown in figure 7. The fitted curves give $\Delta E = p_2 e^{q_2 N}$, where $q_2 < 0$. Thus the $\Delta E$ tends to zero exponentially when the size of the system tends to infinity, and $\delta_e$ gives the minimal change of energy from the ground state in the thermodynamic limit. The energy change in the whole regimes are given by table 4.

II. The ground state contains one boundary (0,0) string.

The finite-size behaviors of $\Delta E$ in the regimes of 2.5 and 2.9 are shown in figure 8. Again, we see that the $\Delta E$ tends to zero and $\delta_e$ gives the minimal change of energy from the ground state in the thermodynamic limit. The energy change are given by table 5.

III. The ground state contains two boundary (0,0) strings.

The finite-size behaviors of $\Delta E$ in the regimes 3.1 and 3.7 are shown in figure 9 and the energy change are given by table 6.

| Table 5. The Bethe roots at the ground state which have one (0,0) string. |
|-----------------------------|-----------------------------|
| Value of $\delta$           | Regimes of boundary parameters in table 2 |
| $\delta_{\beta_\alpha} + \delta_{\beta_\theta}$ | 2.6, 2.7 |
| $\delta_{\beta_\alpha} + \delta_{\beta_\theta}$ | 2.8, 2.11, 2.12 |
| $\delta_{\beta_\alpha} - \delta_{\beta_\theta}$ | 2.5 |
| $-\delta_{\beta_\alpha} + \delta_{\beta_\theta}$ | 2.1, 2.2, 2.3, 2.4 |
| $|\delta_{\beta_\alpha} - \delta_{\beta_\theta}|$ | 2.9, 2.10 |

Figure 9. $\Delta E = \Delta E^{\text{ED}} - \delta e$, where $\Delta E^{\text{ED}}$ is the minimal change of energy between the ground state and the excitations calculated by using DMRG. The figure can be fitted as $E(N) = p_2 e^{q_2 N}$. Here (a) $p_2 = 1.7640$ and $q_2 = -0.4836$; (b) $p_2 = 7.9740$ and $q_2 = -0.5163$. 

(a) 

(b)
In this paper, we study the thermodynamic properties of one-dimensional XXZ spin chain with unparallel boundary magnetic fields at the gaped region (\(\eta\) being a real number). Firstly, we analyse the change of energy comes from the bulk hole and the boundary strings of the reduced \(T-Q\) relation. Then we give the distribution of the Bethe roots in the reduced BAES for different boundary parameters. Secondly, it is shown that the contribution of the inhomogeneous term in the \(T-Q\) relation for the ground state or for the elementary excitation states both can be neglected when the size of the system \(N\) tends to infinity. This allows us to obtain the surface energy and the elementary excitation of the model.

We should note that in the thermodynamic limit, the boundary field at one side cannot been ‘seen’ by the other side, thus the energy induced by the twist angle of two boundary fields can be neglected. However, the twist angle will affect the eigenstates of the system, which are very different from that of the parallel boundary fields case and many interesting boundary states are involved. While for the system with finite size, the twist angle has nontrivial effect on both the energy and the states.

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