Exact surface energy and helical spinons in the XXZ spin chain with arbitrary non-diagonal boundary fields

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An analytic method is proposed to compute the surface energy and elementary excitations of the XXZ spin chain with generic non-diagonal boundary fields. For the gapped case, in some boundary parameter regimes the contributions of the two boundary fields to the surface energy are non-additive. Such a correlation effect between the two boundaries also depends on the parity of the site number N even in the thermodynamic limit N → ∞. For the gapless case, contributions of the two boundary fields to the surface energy are additive due to the absence of long-range correlation in the bulk. Although the U(1) symmetry of the system is broken, exact spinon-like excitations, which obviously do not carry spin-

Quantum integrable systems with generic non-diagonal boundary fields have attracted a lot of attentions since their important applications in high energy physics [1], open string/gauge theory [2–4], condense matter physics [5] and non-equilibrium statistical physics [6, 7]. However, how to compute the physical quantities of such kind of systems has puzzled people for quite a long time. In the past several decades, many efforts have been made to approach this tough problem [8–18] but only under some special conditions the physical quantities can be calculated. Formally, the exact spectra of quantum integrable models without U(1) symmetry can be expressed in terms of inhomogeneous T–Q relations [14, 15]. Even though, to study their physical properties based on the inhomogeneous Bethe ansatz equations is still quite hard because of the complicated patterns of Bethe roots in the complex plane.

In this Letter, we propose a novel analytic method to study the surface energy and elementary excitations of the XXZ spin chain with arbitrary non-diagonal boundary fields. Our central idea lies in that instead of the Bethe roots, we use the zero roots of the transfer matrix to parameterize the spectrum. Starting from a transfer matrix including proper site-dependent inhomogeneity (described by a density σ(θ) in the thermodynamic limit), the density of the zero roots of the homogeneous transfer matrix, which is crucial to compute the physical quantities, can be obtained via analytic continuation.

The model Hamiltonian we shall consider reads

\[ H = \sum_{j=1}^{N-1} \left\{ \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \cosh \eta \sigma_j^z \sigma_{j+1}^z \right\} + \tilde{h}_- \cdot \sigma_1 + \tilde{h}_+ \cdot \sigma_N, \quad (1) \]

where \( \sigma_j^\alpha (\alpha = x, y, z) \) are the Pauli matrices on site \( j \), \( \eta \) is the anisotropic parameter and \( \tilde{h}_\pm = (h_\pm^x, h_\pm^y, h_\pm^z) \) are the boundary fields

\[ h_\pm^x = \mp \frac{\sinh \eta \cos \alpha_\pm \sinh \beta_\pm}{\sinh \alpha_\pm \cosh \beta_\pm}, \]

\[ h_\pm^y = \frac{\sinh \eta \cos \theta_\pm}{\sinh \alpha_\pm \cosh \beta_\pm}, \quad h_\pm^z = \frac{\sinh \eta \sin \theta_\pm}{\sinh \alpha_\pm \cosh \beta_\pm}, \quad (2) \]

characterized by the boundary parameters \( \alpha_\pm, \beta_\pm \) and \( \theta_\pm \). The Hamiltonian (1) is generated by the transfer matrix \( t(u) \) as

\[ H = \sinh \eta \frac{\partial \log t(u)}{\partial u} \bigg|_{u=0,(\theta_j=0)} - c_0, \quad (3) \]

where \( \{ \theta_j \} = 1, \cdots, N \) are the inhomogeneity parameters, \( c_0 = N \cosh \eta + \tanh \eta \sinh \eta, t(u) \) is defined as [19]

\[ t(u) = tr_0\{ K_{11}^+(u) R_{0N}(u - \theta_N) \cdots R_{01}(u - \theta_1) \times K_{00}^-(u) R_{1N}(u + \theta_1) \cdots R_{N0}(u + \theta_N) \}. \quad (4) \]

Here \( K_{00}^- (u) \) is the boundary reflection matrix on one end of the spin chain

\[ K_{00}^- (u) = \begin{pmatrix} K_{11}^-(u) & K_{12}^-(u) \\ K_{21}^-(u) & K_{22}^-(u) \end{pmatrix}, \]

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

\[ K_{12}^- (u) = e^{-i\theta_-} \sinh (2u), \quad K_{21}^- (u) = e^{i\theta_-} \sinh (2u), \]
\[ K_{2n}(u) = 2 \sinh \alpha_\cdot \cosh \beta_\cdot \cosh u \]
\[-2 \cosh \alpha_\cdot \sinh \beta_\cdot \sinh u, \]
and \( K_0^+(u) \) is the dual boundary matrix on the other end.

\[ K^+ = K^-(u - \eta) \big|_{(\alpha_-,\beta_+,\theta_+) \to -(\alpha_+,\beta_-,\theta_-)}. \]

The six-vertex \( R \)-matrix
\[ R_{0,j}(u) = \frac{\sinh(u + \eta) + \sinh u}{2 \sinh \eta} + \frac{1}{2} \left( \frac{\sigma_j^\tau \sigma_0^\tau + \sigma_j^\tau \sigma_0^\tau}{\sinh(u + \eta) - \sinh u} \right), \]
satisfies the Yang-Baxter equation (YBE) [20, 21] and the reflection equation (RE) or the dual one [19, 22–24]. The YBE and REs lead to that the transfer matrices with different spectral parameters commute mutually, i.e., \( t(u), t(v) = 0 \), which ensures the integrability of the model (1).

Given an arbitrary eigenvalue \( \Lambda(u) \) of the transfer matrix \( t(u) \), we have the identities [25]

\[ \Lambda(\theta_j)\Lambda(-\theta_j - \eta) = a(\theta_j)a(-\theta_j), \quad j = 1, \cdots, N, \]
\[ \Lambda(0) = a(0), \quad \Lambda(\frac{i\pi}{2}) = a(\frac{i\pi}{2}), \]
with

\[ a(u) = -\frac{\sinh(2u + 2\eta)}{\sinh(2u + \eta)} \sinh(u - \alpha_\cdot) \cosh(u - \beta_\cdot) \]
\[ \times \sinh(u - \alpha_+) \cosh(u - \beta_+) \]
\[ \times \prod_{l=1}^{N} \frac{\sinh(u - \eta) \sinh(u + \eta)}{\sinh^2 \eta}. \]

From the definition of \( t(u) \) in (4), we deduce that \( \Lambda(u) \) is a degree \( 2N + 4 \) trigonometric polynomial of \( u \). It also possesses the properties \( \Lambda(u) = \Lambda(-u - \eta) \) and \( \Lambda(u + i\pi) = \Lambda(u) \). Thus we can parameterize the eigenvalue \( \Lambda(u) \) by its roots \( \{ z_j \} \) as

\[ \Lambda(u) = \Lambda_0 \prod_{j=1}^{N+2} \sinh(u - z_j + \frac{\eta}{2}) \sinh(u + z_j + \frac{\eta}{2}). \]

\[ \Lambda_0 = -8 \cos(\theta_- - \theta_+) \sinh^{-2N} \eta \]
is determined by the asymptotic behavior of \( t(u) \) when \( u \to \infty \). In such a sense, Eqs.(8-10) determine the roots \( \{ z_j | j = 1, \cdots, N + 2 \} \) completely for a given set of inhomogeneity parameters. In the homogeneous limit \( \theta_j = 0 \), Eq.(8) is replaced by [14]

\[ [\Lambda(u)\Lambda(u - \eta)]|_{u=0}^{(n)} = [a(u)a(-u)]|_{u=0}^{(n)}, \]

where the superscript \( n \) indicates the \( n \)-th order derivative and \( n = 0, 1, \cdots, N - 1 \). From (3) and (11), the eigenvalues of the Hamiltonian (1) can be expressed as

\[ E = \sinh \eta \sum_{j=1}^{N+2} \left[ \coth(z_j + \frac{\eta}{2}) - \coth(z_j - \frac{\eta}{2}) \right] - c_0. \]
\( \beta_+ \rightarrow \beta_-, \beta_- \rightarrow \beta_+ \). Therefore, we consider only the case of \( \alpha_+ + \beta_+ > 0 \) and \( |\beta_+| \geq |\beta_-| \). It is sufficient to quantify the boundary contributions by tuning \( \beta_- \) in four regimes: (I) \( \beta_+ > \beta_- > \eta/2 \), (II) \( \eta/2 \geq \beta_- \geq 0 \), (III) \( 0 > \beta_- > -\eta/2 \) and (IV) \( -\eta/2 \geq \beta_- > -\beta_- \).

The Fourier spectrum \( k \) takes integer values and \( \hat{b}_n(k) = -2\text{sign}(k)\pi e^{-\eta|nk|} \). In the homogeneous limit, we take \( \sigma(\bar{\theta}) = \delta(\bar{\theta}) \). The ground state energy of the Hamiltonian (1) can thus be expressed as

\[
E_{g1} = \frac{Ni\sinh \eta}{2\pi} \sum_{k = -\infty}^{\infty} [\bar{\alpha}_1(k) - \bar{\alpha}_3(k)]\bar{\rho}(k) - c_0, \tag{16}
\]

where the \( \bar{\alpha}_n(k) = 2\pi i e^{-\eta|nk|} \) is the Fourier transformation of \( a_n(x) = \cot(x - \frac{\eta}{2}) - \cot(x + \frac{\eta}{2}) \). We note that the boundary parameters \( \theta_\pm \) do not appear in (14), implying that they contribute nothing to the surface energy in the leading order. Direct calculation gives the surface energy \( E_{b1} \) in regime (I) as

\[
E_{b1} = e_b(\alpha_+, \beta_+) + e_b(\alpha_-, \beta_-) + e_{b0},
\]

\[
e_b(\alpha, \beta) = -2\sinh \eta \sum_{k = 1}^{\infty} \tanh(k\eta)|(-1)^k e^{-2k\eta} + e^{-2k|\alpha|} + (-1)^k e^{-2k|\beta|} - \tanh \eta \sinh \eta, \tag{17}
\]

where \( e_b(\alpha, \beta) \) indicates the contribution of one boundary field and \( e_{b0} \) is the surface energy induced by the free open boundary [11].

In regime (II), besides the bulk conjugate pairs around the \( \pm \eta i \) lines, there exist two boundary conjugate pairs \( \frac{\pi}{2} \pm (\beta_- + \frac{\pi}{2})i \) and \( \frac{\pi}{2} \pm (\beta_+ + \frac{\pi}{2})i \) fixed by (9) as shown in Fig.2(b). Taking the boundary roots into account, with a similar procedure used in regime (I) we find that the bare contribution of the boundary conjugate pairs to the energy is exactly cancelled by that of the back flow of the continuous root density, as happened in the diagonal boundary case [11]. The surface energy \( E_{b2} \) takes exactly the same form of (17). Taking \( \alpha_- \rightarrow \infty \) and \( \beta_- \rightarrow 0 \), \( \bar{h}_- = 0 \), \( e_b(\infty, 0) = 0 \). Therefore, the contributions of the two boundary fields and the free open boundary to the surface energy are additive in regimes (I) and (II).

In regime (III), there also exist two boundary conjugate pairs. However, the absolute value of the imaginary part of the inner conjugate pair is \( \beta_- + \frac{\pi}{4} < \frac{\pi}{2} \). In this case, the inner boundary conjugate pair indeed contributes a nonzero value to energy and the surface energy reads

\[
E_{b3} = 4\sinh \eta \sum_{k = 1}^{\infty} (-1)^k e^{-kn} \tanh(k\eta) \cosh(2k\beta_- + kn)

+ e_{b1} + \sinh \eta[\tanh(\beta_- + \eta) - \tanh(\beta_-)]. \tag{18}
\]

The contributions of the two boundaries to the surface energy are no longer additive and a correlation effect between the two boundary fields appears.

In regime (IV), only one boundary conjugate pair exist as shown in Fig.2(c). However, due to the symmetry of

\[
\begin{align*}
\hat{\rho}(k) &= [2N\hat{b}_2\hat{\sigma}(k) + [1 + (-1)^k](\bar{b}_2 - \bar{b}_1) + \hat{b}_{2\alpha_+} \\
&+ \hat{b}_{2\alpha_-} + (-1)^k(\hat{b}_{2\alpha_+} + \hat{b}_{2\alpha_-})]/[N(\bar{b}_1 + \bar{b}_3)], \tag{15}
\end{align*}
\]
The boundary conjugate pair contributes nothing to the surface energy but the two real roots do contribute a nonzero value to energy and the surface energy reads

\[ E_{b4} = E_{b1} + E_h, \]
\[ E_h = 2 \sinh \eta \left[ \sum_{k=1}^{\infty} \frac{(-1)^{k+1} \tanh(k\eta)}{e^{k\eta}} + \tanh \frac{\eta}{2} \right]. \]  

In this regime, the correlation effect of the two boundary does not rely on the magnitudes of the boundary fields but on the sign of \( \beta_+ \beta_- \).

We note that if \( |\beta_+| < \eta/2 \) and \( \beta_+ \beta_- < 0 \), we can always choose \( \beta_- = -\min\{|\beta_+|, |\beta_-|\} \) and \( \beta_+ = \max\{|\beta_+|, |\beta_-|\} \) in (18) to get the correct surface energy. For comparison, the density matrix renormalization group (DMRG) method [28] is performed for \( N = 212 \) and several values of \( \beta_- \). Our analytic results coincide perfectly with the numerical ones as shown in Fig 2(d). For \( \alpha_\pm \in (0, \eta/2) \), central conjugate pairs associated with the boundary fields around \( \pm i(\eta/2 + \alpha_\pm) \) exist in the ground state as shown in Fig 3(a). Exact calculation shows that these boundary roots contribute nothing to the surface energy in the thermodynamic limit, as their contributions are exactly cancelled by that of the back flow of the bulk root density. By examining the root patterns we obtain that the surface energy \( E_{b4}^{\text{odd}}(\beta_-) \) for an odd \( N \) can be given by \( E_{b4}(-\beta_-) \) for an even \( N \) as \( E_{b4}^{\text{odd}}(\beta_-) = E_{b4}(-\beta_-) - E_h \), where \( l = 1, 2, 3, 4 \) indicates the corresponding boundary parameter regime. Such a parity dependence of the surface energy is in fact due to the long range Neel order in the bulk. For an even \( N \) the two boundary spins prefer to be anti-parallel, while for an odd \( N \) the two boundary spins prefer to be parallel. Therefore, fixed boundary fields must induce different surface energies for even \( N \) and odd \( N \) in the thermodynamic limit \( N \to \infty \).

A question thus arises: Is there any spinon-like excitations in the present system? As an example to answer this question, let us consider a simple root distribution away from that of the ground state in regime (I): taking two conjugate pairs away in the ground state configuration and adding four real roots on the real axis. The four real roots are distributed symmetrically around the origin as required by the symmetry of the eigenvalue function \( \Lambda(u) \). In addition, two imaginary conjugate pairs may appear in the root configuration as shown in Fig 3(b). We denote the four real roots as \( \pm z_1 \) and \( \pm z_2 \). The excitation energy in the thermodynamic limit associated with this root pattern can be derived by following the same procedure discussed in the previous text

\[ E_e = \varepsilon(z_1) + \varepsilon(z_2), \varepsilon(z) = 2 \sinh \eta \sum_{k=-\infty}^{\infty} \frac{e^{-2kz}}{\cosh(k\eta)}. \]

It seems that the excitation energy only depends on the positions of the real roots and takes exactly the same dispersion form of spinons in the periodic chain. Even though, such kind of elementary excitations should be rather different from the traditional spinons [29] due to the broken \( U(1) \)-symmetry. In fact, these excitations must be helical in the real space to match the two unparallel boundaries. The helical structure can be visualized either by the quantity \( \langle \sigma_j \times \sigma_{j+1} \rangle \), which is nonzero in the non-diagonal boundary cases but zero in the parallel boundary cases, or by the structure of the eigenvectors constructed from a helical pseudo-vacuum state [12, 30].

FIG. 3: The distribution of \( z \)-roots for \( N = 10 \) and \( \eta = 2 \). (a) The ground state. (b) A low-lying excited state.

Usually, exact fractional excitations can be derived in most of the integrable models with \( U(1) \) symmetry. A typical kind of fractional excitations in the periodic spin chain model is spinon, which is believed carrying spin-\( \frac{1}{2} \) [29]. In the open boundary case, the unparallel boundary fields break the \( U(1) \) symmetry and the \( z \)-component of the total spin is no longer a good quantum number.
\( \Lambda^*(u) = \Lambda(-u^*) \). The roots can be classified into (i) real \( \pm z_j \); (ii) on the line \( \text{Im}\{z_j\} = -\frac{i\pi}{2} \); (iii) bulk conjugate pairs \( \text{Im}\{z_j\} \sim \pm \frac{i\pi}{n} \) (\( n \geq 2 \)) and (iv) central conjugate pairs associated with the boundaries. For convenience, let us introduce the notations \( \gamma = -i\eta \) with \( \gamma \in (0, \pi) \) and \( \alpha_{\pm} = -\alpha_{\pm} \). Without losing generality, we restrict \( -\frac{i\pi}{2} \leq \text{Im}\{z_j\} < \frac{i\pi}{2} \) for the periodicity of \( \Lambda(u) \).

For \( \gamma \in \left[ \frac{\pi}{2}, \pi \right) \), the \( z \)-roots in the ground state for a given set of boundary parameters and \( N = 10 \) is shown in Fig.4(a). Most of the roots locate on the line \( -i\frac{\pi}{2} \) and one conjugate pair \( \pm i\left( \frac{\pi}{2} + \frac{\alpha_{\pm}}{2} \right) \) locates on the imaginary axis. The existence of this conjugate pair does not depend on the values of the boundary parameters. By tuning the value of \( \beta_- \), we find that the structure of \( z \)-roots keeps unchanged, which indicates that the ground state energy is given by an unified formula for arbitrary real boundary parameters \( \beta_{\pm} \).

By varying \( \alpha_- \), a central conjugate pair \( \pm i\left( \frac{\pi}{2} + \frac{\alpha_-}{2} \right) \) appears when \( \alpha_- \in (0, \frac{\pi}{2}) \) as shown in Fig.4(b). Direct calculation shows that the central conjugate pairs do not contribute to the surface energy. The above conclusion also holds for \( \bar{\alpha}_+ \). Besides, depending on \( \bar{\alpha}_+ \) and the parity of \( N \), two real roots may exist at the boundaries as shown in Fig.4(c).

These roots tend to \( \pm \infty \) in the thermodynamic limit and also do not contribute to the surface energy. For the case corresponding to Fig.4(a), in the thermodynamic limit the density of roots satisfies

\[
N \int_{-\infty}^{\infty} \left[ b_2(u - \theta) + b_2(u + \theta) \right] \sigma(\theta) d\theta + b_2(u) + \frac{1}{2} \left[ b_{\pm}(u + \beta_{\pm}) + b_{\pm}(u - \beta_{\pm}) \right] + b_{\pm}(u - \beta_{-}) + b_{2\alpha_{\pm}}(u) + b_{\pm}(u - \beta_{-}) = b_{\bar{z}}(u) + b_{1}(u) + N \int_{-\infty}^{\infty} b_{\bar{z}}(u - z) \rho(z) dz,
\]

where \( b_{\alpha}(x) = \cosh^2(x - \frac{\alpha}{2}) + \cosh^2(x - \frac{i\alpha}{2}) \). Taking the Fourier transformation and homogeneous limit \( \sigma(\theta) \to \delta(\theta) \), we finally obtain the surface energy

\[
E_b = -\sin \frac{\gamma}{2} \int_{-\infty}^{\infty} \frac{\tanh(k\gamma/2)}{\sinh(k\gamma/2)} \cos(\pi(\gamma - 2\gamma)) \frac{k}{2} + c - 1
\]

\[
+ \cosh \left( \frac{k(\pi - 2\gamma_{\mp} + 2\pi(\gamma_{\mp}))}{2} \right) + \cos \beta_{\pm}
\]

\[
+ \cosh \left( \frac{k(\pi - 2\gamma_{\mp} + 2\pi(\gamma_{\pm}))}{2} \right) + \cos \beta_{\pm}
\]

\[
- \cosh \frac{k\gamma}{2} - \cosh \left( \frac{k(\pi - \gamma_{\mp})}{2} \right) dk.
\]

For \( \gamma \in (0, \frac{\pi}{2}) \), most of the roots in the ground state locate on the lines \( \pm i\gamma \) and the rest roots form central conjugate pairs as shown in Fig.1(b). The surface energy is still given by Eq.(22). Comparison of the DMRG results and our analytic results is given in Fig.4(d). The present result also coincides exactly with that derived in [16]. The absence of correlation and parity effects is due to the absence of long-range order in the gapless bulk.

In conclusion, an analytic method is developed to obtain the surface energy and elementary excitations of the XXZ spin chain with generic non-diagonal boundary fields in both gapped and gapless regimes. This method provides an universal procedure to compute physical quantities of quantum integrable systems either with or without \( U(1) \) symmetry [15, 31, 32] in thermodynamic limit.

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