Thermodynamic limit of the spin- $\frac{1}{2}$ XYZ spin chain with the antiperiodic boundary condition

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ABSTRACT: Based on its off-diagonal Bethe ansatz solution, we study the thermodynamic limit of the spin- $\frac{1}{2}$ XYZ spin chain with the antiperiodic boundary condition. The key point of our method is that there exist some degenerate points of the crossing parameter $\eta_{m,l}$, at which the associated inhomogeneous $T - Q$ relation becomes a homogeneous one. This makes extrapolating the formulae deriving from the homogeneous one to an arbitrary η with $O(N^{-2})$ corrections for a large N possible. The ground state energy and elementary excitations of the system are obtained. By taking the trigonometric limit, we also give the results of antiperiodic XXZ spin chain within the gapless region in the thermodynamic limit, which does not have any degenerate points.

KEYWORDS: Bethe Ansatz, Lattice Integrable Models

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1 Introduction

The spin- $\frac{1}{2}$ XYZ chain is a typical quantum integrable model and has many applications in statistical mechanics, quantum magnetism, string theory and mathematical physics [1–3]. The periodic XYZ spin chain (or equivalent to the eight vertex model) with even number of sites was solved by Baxter [4–7]. By using the generalized algebraic Bethe ansatz [8], Takhtajan and Faddeev recovered the Baxter’s solution, where a suitable vacuum state is required. However, the proper vacuum state can be constructed only for the even number of sites case. After that, many interesting works have been done based on the exact solutions, please see [9] and references therein. In 2013, a more general method named off-diagonal Bethe ansatz (ODBA) was proposed [10] and the exact solution of the XYZ spin

chain with arbitrary number of sites is obtained [11, 12], where the eigenvalue of transfer matrix is given by an inhomogeneous $T - Q$ relation. Besides the periodic boundary condition, the XYZ model with antiperiodic and integrable open ones have been studied extensively [13–16].

So far many attempts have been done to solve the resulting BAEs from inhomogeneous $T - Q$ relations [17–22], the corresponding distribution of Bethe roots for ground-state or elementary excitation states is still an interesting open problem [12]. Here we propose a way to study the thermodynamic limit of the spin- $\frac{1}{2}$ XYZ chain with an antiperiodic boundary condition, which was successfully applied to the XXZ spin chain with open boundary conditions [18]. The main idea is that there exist some degenerate points of the crossing parameter (such as (3.1) below), at which the associated inhomogeneous $T - Q$ relation is reduced to the conventional/homogeneous one. This allows us to use the standard method to study the thermodynamic limit [23–27]. In the thermodynamic limit, the degenerate points become dense in the whole complex plain. Thus the exact results at degenerate points could approach to the actual values of physical quantities.

However, for some quantum integrable models such as the XXZ spin chain with antiperiodic boundary condition [28–32], there is no the degenerate point and the inhomogeneous BAEs can not be reduced to the traditional product ones. It is well-known that the antiperiodic XXZ spin chain is an important model and many interesting phenomena such as edge states, zero modes, boundary bound states and topological excitations are induced by the twisted boundaries [19, 20, 33]. Thus the study of the antiperiodic XXZ spin chain is another motivation of this work. The difficulty of lacking degenerate points can be overcome if we consider a more general model such as the XYZ case (the antiperiodic XXZ chain is its trigonometric limit) which has some degenerate points allowing us to investigate its thermodynamic limit.

In this paper, we study the thermodynamic limit of the antiperiodic XYZ spin chain. We obtain the distribution of Bethe roots, string structures, ground state energy and typical elementary excitations. We also check these results by the numerical calculations and the finite size scaling analysis. Particularly, we obtain the exact results of the antiperiodic XXZ spin chain in the thermodynamic limit. In order to see the boundary effects clearly, we also give the results of the XYZ spin chain with the periodic boundary condition as the comparisons.

The paper is organized as follows. In the next section, the model Hamiltonian and exact solutions are introduced. In section 3, we study the thermodynamic limit of the antiperiodic XYZ model at degenerate points. In section 4, we generalize these results to the system with general interactions. As an important component, the results of the antiperiodic XXZ model are given in section 5. Section 6 is the concluding remarks and discussions. Some supporting materials are given in appendices A–C.

2 Antiperiodic XYZ model and its exact solutions

Let us fix a generic complex number η and a generic imaginary number τ such that $\text{Im}(\tau) > 0$, which related to the coupling constants. The most anisotropic spin- $\frac{1}{2}$ XYZ chain is

described by the Hamiltonian

$$H = \frac{1}{2} \sum_{j=1}^N \left[J_x(\eta, \tau) \sigma_j^x \sigma_{j+1}^x + J_y(\eta, \tau) \sigma_j^y \sigma_{j+1}^y + J_z(\eta, \tau) \sigma_j^z \sigma_{j+1}^z \right], \quad (2.1)$$

where $J_x(\eta, \tau)$, $J_y(\eta, \tau)$ and $J_z(\eta, \tau)$ are the anisotropic coupling constants

$$J_x(\eta, \tau) = \frac{\theta_{01}(\eta)}{\theta_{01}(0)}, \quad J_y(\eta, \tau) = \frac{\theta_{00}(\eta)}{\theta_{00}(0)}, \quad J_z(\eta, \tau) = \frac{\theta_{10}(\eta)}{\theta_{10}(0)}, \quad (2.2)$$

$\theta_{00}(u)$, $\theta_{01}(u)$ and $\theta_{10}(u)$ are the elliptic theta functions defined in appendix A, η and τ are two model parameters, and σ_j^α ($\alpha = x, y, z$) are the Pauli matrices. Here we consider the Hamiltonian with the antiperiodic boundary condition

$$\sigma_{N+1}^x = \sigma_1^x \sigma_1^x \sigma_1^x = \sigma_1^x, \quad \sigma_{N+1}^y = \sigma_1^x \sigma_1^y \sigma_1^x = -\sigma_1^y, \quad \sigma_{N+1}^z = \sigma_1^x \sigma_1^z \sigma_1^x = -\sigma_1^z. \quad (2.3)$$

It is well-known that the XYZ chain with the antiperiodic boundary condition given by (2.1) and (2.3) is integrable, which is guaranteed by the eight-vertex R -matrix $R(u) \in \text{End}(\mathbb{C}^2 \otimes \mathbb{C}^2)$ given by [1]

$$R(u) = \begin{pmatrix} \alpha(u) & & \delta(u) \\ & \beta(u) & \gamma(u) \\ & \gamma(u) & \beta(u) \\ \delta(u) & & \alpha(u) \end{pmatrix}, \quad (2.4)$$

with the non-zero entries

$$\begin{aligned} \alpha(u) &= \frac{\theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(u, 2\tau) \theta \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(u + \eta, 2\tau)}{\theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(0, 2\tau) \theta \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(\eta, 2\tau)}, & \beta(u) &= \frac{\theta \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(u, 2\tau) \theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(u + \eta, 2\tau)}{\theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(0, 2\tau) \theta \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(\eta, 2\tau)}, \\ \gamma(u) &= \frac{\theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(u, 2\tau) \theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(u + \eta, 2\tau)}{\theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(0, 2\tau) \theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(\eta, 2\tau)}, & \delta(u) &= \frac{\theta \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(u, 2\tau) \theta \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(u + \eta, 2\tau)}{\theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(0, 2\tau) \theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(\eta, 2\tau)}, \end{aligned} \quad (2.5)$$

where the associated elliptic functions are defined in appendix A. In addition to satisfying the quantum Yang-Baxter equation (QYBE),

$$R_{12}(u_1 - u_2) R_{13}(u_1 - u_3) R_{23}(u_2 - u_3) = R_{23}(u_2 - u_3) R_{13}(u_1 - u_3) R_{12}(u_1 - u_2), \quad (2.6)$$

the R -matrix also possesses the Z_2 -symmetry

$$\sigma_1^i \sigma_2^i R_{12}(u) = R_{12}(u) \sigma_1^i \sigma_2^i, \quad \text{for } i = x, y, z. \quad (2.7)$$

Throughout this paper we adopt the standard notations: for any matrix $A \in \text{End}(\mathbb{C}^2)$, A_j is an embedding operator in the tensor space $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \cdots$, which acts as A on the

j -th space and as identity on the other factor spaces; $R_{ij}(u)$ is an embedding operator of R -matrix in the tensor space, which acts as identity on the factor spaces except for the i -th and j -th ones. Let us introduce the monodromy matrix

$$T_0(u) = R_{0N}(u) \dots R_{01}(u). \quad (2.8)$$

The transfer matrix $t(u)$ of the XYZ chain with the antiperiodic boundary condition (2.3) is given by

$$t(u) = \text{tr}_0 \{ \sigma_0^x T_0(u) \}, \quad (2.9)$$

where tr_0 denotes the trace over the “auxiliary space” 0. The Hamiltonian (2.1) with the antiperiodic boundary condition (2.3) can be given in terms of the transfer matrix (2.9)

$$H = \frac{\sigma(\eta)}{\sigma'(0)} \left\{ \frac{\partial \ln t(u)}{\partial u} \Big|_{u=0} - \frac{1}{2} N \zeta(\eta) \right\}, \quad (2.10)$$

where $\sigma(u) = \theta_{11}(u, \tau)$, $\sigma'(0) = \frac{\partial}{\partial u} \sigma(u) \Big|_{u=0}$ and the function $\zeta(u) = \frac{\partial}{\partial u} \ln \sigma(u)$. The QYBE (2.6) and the Z_2 -symmetry (2.7) lead to that the transfer matrices with different spectral parameters are mutually commutative [1, 2], i.e., $[t(u), t(v)] = 0$, which guarantees the integrability of the model by treating $t(u)$ as the generating functional of the conserved quantities.

The eigenvalue of the transfer matrix $t(u)$, denoted by $\Lambda(u)$, is given by an inhomogeneous $T - Q$ relation [11]

$$\begin{aligned} \Lambda(u) = & e^{\{i\pi(2l_1+1)u+i\phi\}} \frac{\sigma^N(u+\eta)}{\sigma^N(\eta)} \frac{Q_1(u-\eta)}{Q_2(u)} - \frac{e^{-i\pi(2l_1+1)(u+\eta)-i\phi} \sigma^N(u)}{\sigma^N(\eta)} \frac{Q_2(u+\eta)}{Q_1(u)} \\ & + \frac{c e^{i\pi u} \sigma^{L_1}(u+\frac{\eta}{2}) \sigma^N(u+\eta) \sigma^N(u)}{Q_1(u) Q_2(u) \sigma^N(\eta) \sigma^N(\eta)}, \end{aligned} \quad (2.11)$$

where l_1 is a certain integer and L_1 is a non-negative integer such that $N + L_1 = 2M$, the Q -functions $Q_1(u)$, $Q_2(u)$ are some elliptic polynomials of degree M

$$Q_1(u) = \prod_{j=1}^M \frac{\sigma(u - \mu_j)}{\sigma(\eta)}, \quad Q_2(u) = \prod_{j=1}^M \frac{\sigma(u - \nu_j)}{\sigma(\eta)}. \quad (2.12)$$

The $2M + 2$ parameters $\{\mu_j\}$, $\{\nu_j\}$, c and ϕ should satisfy the associated BAEs

$$\begin{aligned} \left(\frac{N}{2} - M \right) \eta - \sum_{j=1}^M (\mu_j - \nu_j) &= \left(l_1 + \frac{1}{2} \right) \tau + m_1, \quad l_1, m_1 \in \mathbf{Z}, \\ M\eta + \sum_{j=1}^M (\mu_j + \nu_j) &= \frac{1}{2} \tau + m_2, \quad m_2 \in \mathbf{Z}, \\ c e^{[2i\pi(l_1+1)\mu_j + 2i\pi(l_1+\frac{1}{2})\eta + i\phi]} \sigma^{L_1} \left(\mu_j + \frac{\eta}{2} \right) \sigma^N(\mu_j + \eta) &= \prod_{l=1}^M \sigma(\mu_j - \nu_l) \sigma(\mu_j - \nu_l + \eta), \end{aligned}$$

$$\begin{aligned}
 ce^{-2i\pi l_1 \nu_j - i\phi} \sigma^{L_1} \left(\nu_j + \frac{\eta}{2} \right) \sigma^N(\nu_j) &= - \prod_{l=1}^M \sigma(\nu_j - \mu_l) \sigma(\nu_j - \mu_l - \eta), \\
 e^{i\phi} \prod_{j=1}^M \frac{\sigma(\mu_j + \eta)}{\sigma(\nu_j)} &= e^{\frac{i\pi k_1}{N}}, \quad k_1 = 1, \dots, 2N, \quad (2.13)
 \end{aligned}$$

The eigenvalues of Hamiltonian (2.1) with the antiperiodic boundary condition (2.3) is then given in terms of the Bethe roots¹ as [11, 12]

$$E(\eta, \tau) = \frac{\sigma(\eta)}{\sigma'(0)} \left\{ \sum_{j=1}^M \left[\frac{\sigma'(\nu_j)}{\sigma(\nu_j)} - \frac{\sigma'(\mu_j + \eta)}{\sigma(\mu_j + \eta)} \right] + \frac{N}{2} \frac{\sigma'(\eta)}{\sigma(\eta)} + i\pi(2l_1 + 1) \right\}, \quad (2.14)$$

where $\sigma'(u) = \frac{\partial}{\partial u} \sigma(u)$.

Although many attempts have been done to solve the resulting BAEs from inhomogeneous $T - Q$ relations [17–22], the corresponding distributions of Bethe roots for ground-state or elementary excitation states is still an interesting open problem. This motivates us in this paper to look for another way, instead of solving the BAEs (2.13) for a large N , to study the thermodynamic limit of the spin- $\frac{1}{2}$ XYZ chain with the antiperiodic boundary condition.

3 Thermodynamic limit at the degenerate points

It was shown [11, 12] that if the crossing parameter η takes the discrete values

$$\eta_{m_1, l_1} = \frac{2l_1 + 1}{N - 2M} \tau + \frac{2m_1}{N - 2M}, \quad l_1, m_1 \in \mathbf{Z}, \quad (3.1)$$

there exists a solution with $c = 0$ of eq. (2.13), and the resulting $T - Q$ relation reduces to the conventional/homogeneous one

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

where $Q(u)$ is an elliptic polynomial with a degree of M

$$Q(u) = \prod_{j=1}^M \frac{\sigma(u - \lambda_j)}{\sigma(\eta)}. \quad (3.2)$$

Without losing the generality,² we take $M = N$, $l_1 = -1$, $m_1 = -m$ as an example to demonstrate our method. In this particular case, eq. (3.1) becomes

$$\eta_{-m, -1} = \frac{\tau}{N} + \frac{2m}{N} \equiv \eta_m, \quad m \in \mathbf{Z}. \quad (3.3)$$

¹It is remarked that for any choice of l_1 , m_1 , m_2 and L_1 the solutions to (2.13) may give rise to the complete set of the eigenvalues of the transfer matrix $t(u)$, which is a conjecture based on the numerical evidence [11, 12].

²It is straightforward to generalize our method in this paper to study the most general case (3.1).

It is clear that the degenerate point η_m (3.3) contains an imaginary part $\frac{\tau}{N}$. For a finite τ , the imaginary part of η_m will tend to zero in the thermodynamic limit $N \rightarrow \infty$. Further, we require³ $0 < \frac{2m}{N} \leq \frac{1}{2}$ in this paper. At the degenerate point of η_m , the BAEs (2.13) reduce to

$$e^{\pi x_j + 2i\phi} \frac{\sigma^N[\frac{i}{2}(x_j - \eta_m i)]}{\sigma^N[\frac{i}{2}(x_j + \eta_m i)]} = - \prod_{k \neq j}^N \frac{\sigma[\frac{i}{2}(x_j - x_k - 2\eta_m i)]}{\sigma[\frac{i}{2}(x_j - x_k + 2\eta_m i)]}, \quad j = 1, \dots, N, \quad (3.4)$$

$$e^{i\phi} \prod_{j=1}^N \frac{\sigma[\frac{i}{2}(x_j - \eta_m i)]}{\sigma[\frac{i}{2}(x_j + \eta_m i)]} = e^{\frac{i\pi k_1}{N}}, \quad k_1 = 1, \dots, 2N, \quad (3.5)$$

where $\{x_j\}$ are the Bethe roots related to the parameters in (3.2) by $\lambda_j = \frac{i}{2}x_j - \frac{\eta_m}{2}$. The BAEs (3.4) and (3.5) can give the complete set of solutions of the Hamiltonian [11, 34]. The eigenvalue of the Hamiltonian (2.1) with a fixed η_m given by (3.3) is expressed in terms of the Bethe roots as

$$E(\eta_m) = \frac{\sigma(\eta_m)}{\sigma'(0)} \left\{ \sum_{j=1}^N \left[\frac{\sigma'[\frac{i}{2}(x_j + \eta_m i)]}{\sigma[\frac{i}{2}(x_j + \eta_m i)]} - \frac{\sigma'[\frac{i}{2}(x_j - \eta_m i)]}{\sigma[\frac{i}{2}(x_j - \eta_m i)]} \right] + \frac{N}{2} \frac{\sigma'(\eta_m)}{\sigma(\eta_m)} - i\pi \right\}. \quad (3.6)$$

3.1 String hypothesis

Takahashi proposed that the general solutions of Bethe ansatz equations are [9, 27, 35]

$$x_\alpha^{j,k} = x_\alpha^j + (n_j + 1 - 2k)\eta i + \frac{1 - v_j}{2}i + O(e^{-\delta N}), \quad 1 \leq k \leq n_j, \quad (3.7)$$

where x_α^j is the position of the j -string on the real axis, k means the k th Bethe roots in j -string, n_j is the length of j -string, $O(e^{-\delta N})$ means the finite size correction, and $v_j = \pm 1$ denotes the parity of j -string. The center of j -string is the real axis if $v_j = 1$, while the center of j -string is the line with fixed imaginary part i in the complex plane if $v_j = -1$. Eq. (3.7) is the famous string hypothesis.

Similarly as the string hypothesis (3.7), we assume that there might exist the string solutions of the type (3.7) for the Bethe ansatz equations (3.4)–(3.5) with a large N . In our case, the length n_j and parity v_j of j -string are uniquely determined by the crossing parameter η . Focusing on the degenerate points η_m , the string structures are uniquely determined by the $\frac{2m}{N}$. In order to show the string structures more clearly, we expand the $\frac{2m}{N}$ into a simple continued fraction (SCF) with length l as that of [9]

$$\frac{2m}{N} = \frac{c_2}{c_1} = \cfrac{1}{a_1 + \cfrac{1}{\cdots + \cfrac{1}{a_l}}}, \quad a_l \geq 2. \quad (3.8)$$

³For the case of $0 < \eta \leq \frac{1}{2}$, we can obtain the distributions of the Bethe roots for the ground state and hole excitation in the following parts of the paper. The generalization to the case of $\frac{1}{2} < \eta \leq 1$ is straightforward although the corresponding distributions are slightly different. Hence without losing the generality we restrict ourselves in the region $0 < \eta \leq \frac{1}{2}$ in this paper.

j	1	2	3	4	5	6	7	8	9	10	11	12	13	14
n_j	1	2	3	4	5	6	1	8	15	7	29	51	22	73
v_j	+	+	+	+	+	+	−	+	−	+	−	+	+	−
q_j	$\frac{63}{10}$	$\frac{53}{10}$	$\frac{43}{10}$	$\frac{33}{10}$	$\frac{23}{10}$	$\frac{13}{10}$	−1	$-\frac{7}{10}$	$-\frac{4}{10}$	$\frac{3}{10}$	$\frac{2}{10}$	$\frac{1}{10}$	$-\frac{1}{10}$	0
z_s	$z_0 = 0$						$z_1 = 7$			$z_2 = 10$			$z_3 = 13$	

Table 1. Length n_j and parity v_j of strings for a given $\frac{2m}{N} = \frac{10}{73} = [7, 3, 3]$. From eq. (3.9), we have $a_1 = 7$, $a_2 = 3$ and $a_3 = 3$. The values of n_j and v_j for all the strings are determined by eqs. (3.10)–(3.11). We also list the values of q_j [please see eq. (3.17) below] for late use.

Here c_1 and c_2 are co-prime numbers, and $a_1 \geq 2$ because of $0 < \frac{2m}{N} \leq \frac{1}{2}$. For convenience, we rewrite the above SCF (3.8) as a compact form

$$\frac{2m}{N} = \frac{c_2}{c_1} = [a_1, a_2, \dots, a_l], \quad a_l \geq 2. \quad (3.9)$$

Define the integers z_s and quantities y_s as

$$\begin{aligned} z_0 &= 0, & z_k &= \sum_{j=1}^k a_j, & k &= 1, 2, \dots, l, \\ y_{-1} &= 0, & y_0 &= 1, & y_k &= a_k y_{k-1} + y_{k-2}. \end{aligned} \quad (3.10)$$

Then the length n_j and parity v_j of string solutions should satisfy [9, 27]:

$$\begin{aligned} n_j &= y_{s-1} + (j - z_s)y_s, & s &= 0, 1, \dots, l, & z_s &\leq j < z_{s+1}, & j &= 1, 2, \dots, z_l, \\ n_{z_l+1} &= y_l, \\ v_j &= (-1)^{\lfloor (n_j-1)\frac{2m}{N} \rfloor}, & j &\neq z_1, \\ v_{z_1} &= -1. \end{aligned} \quad (3.11)$$

Here $\lfloor x \rfloor$ denotes the maximum integer less than or equal to x (the Gauss symbol). From the eqs. (3.8) and (3.10), we have $y_l = c_1$ which corresponds to the length of the $(z_l + 1)$ -string. From eq. (3.11), we see that the number of string types is $z_l + 1$. We note that the $(z_l + 1)$ -string with length $n_{z_l+1} = y_l$ should be considered in the present case, because the corresponding energy is not zero.

In order to shown the string structure clearly, we give an example $\frac{2m}{N} = \frac{10}{73} = [7, 3, 3]$ in table 1. From it, the length n_j and parity v_j of strings can be found. Taking the data in table 1 into eq. (3.7), we can visualize the shape of the strings in the complex plane. The results with $N = 73$, $\tau = i$ and $\eta_m = \frac{i}{73} + \frac{10}{73}$ are shown in figure 1. From it we see that the string solutions are not parallel to the imaginary axis any more, this is because that the parameters η_m (3.3) has an imaginary part with order N^{-1} .

3.2 Distribution of Bethe roots

Substituting eq. (3.7) into (3.4) and omitting the exponentially small corrections, and then taking the product of the BAEs (3.5) for n_j components of a j -string, we obtain following

Figure 1. Strings on the complex plane for $N = 73$, $\tau = i$ and $\frac{2m}{N} = \frac{10}{73}$. The strings are arranged from left to right in the order of string length determined by eq. (3.11). The centers of strings with parity $v_j = 1$ are on the real axis, while the centers of strings with parity $v_j = -1$ are on the blue dashed line which is given by shifting the real axis up by one. All the strings are not parallel to the vertical axis, because the degenerate crossing parameters η_m contain an imaginary part with order N^{-1} .

equation for the position x_α^j of j -string

$$e^{\varphi_j(x_\alpha^j)} g^N(x_\alpha^j; n_j, v_j) = (-1)^{n_j+1} \prod_{r=1}^{z_l+1} \prod_{\beta=1}^{M_r} \prod_{k=1}^{\min(n_r, n_j)-1} g(x_\alpha^j - x_\beta^r; n_r + n_j, v_r v_j) \quad (3.12)$$

$$\times g(x_\alpha^j - x_\beta^r; |n_r - n_j|, v_r v_j) g^2(x_\alpha^j - x_\beta^r; |n_r - n_j| + 2k, v_r v_j),$$

where M_r is the number of r -strings and

$$\varphi_j(x) = \pi n_j \left(x + \frac{1-v_j}{2} i \right) + 2n_j \phi i, \quad g(x; n, v) = \frac{\sigma[\frac{i}{2}(x - n\eta_m i + \frac{1-v}{2} i)]}{\sigma[\frac{i}{2}(x + n\eta_m i + \frac{1-v}{2} i)]}. \quad (3.13)$$

Taking the logarithm of eq. (3.12), we have

$$\frac{1}{i} \varphi_j(x_\alpha^j) + N \vartheta_j(x_\alpha^j) = 2\pi I_\alpha^j + \sum_{r=1}^{z_l+1} \sum_{\beta=1}^{M_r} \Theta_{jr}(x_\alpha^j - x_\beta^r), \quad (3.14)$$

where I_α^j is an integer (or half-odd integer) for $n_j + M_j + 1 - N \frac{1+v_j}{2}$ even (or odd) and

$$\vartheta_j(x) = \vartheta(x; n_j, v_j) = -i \ln[(-v_j)g(x; n_j, v_j)], \quad (3.15)$$

$$\Theta_{jr}(x) = \vartheta(x; n_r + n_j, v_j v_r) + \vartheta(x; |n_r - n_j|, v_j v_r) + 2 \sum_{k=1}^{\min(n_r, n_j)-1} \vartheta(x; |n_r - n_j| + 2k, v_j v_r). \quad (3.16)$$

The $\vartheta_j(x)$ is the elliptic function with double quasi-periodicities $2i$ and $2\frac{\tau}{i}$. It is sufficient to consider their values in one periodicity. In order to shift the variables into the region of $[-i, i]$, we define

$$q_j \equiv (-1)^s (p_s - (j - z_s)p_{s+1}), \quad s = 0, 1, \dots, l, \quad j = 1, 2, \dots, z_l, \quad z_s \leq j < z_{s+1},$$

$$q_{z_l+1} = (-1)^{l+1} p_{l+1}, \quad (3.17)$$

where the series $\{p_s\}$ are

$$\begin{aligned} p_0 &= \frac{N}{2m}, \quad p_1 = 1, \quad p_n = p_{n-2} - p_{n-1}a_{n-1}, \\ a_{n-1} &= \left\lfloor \frac{p_{n-2}}{p_{n-1}} \right\rfloor, \quad n = 2, 3, \dots, l+1. \end{aligned} \quad (3.18)$$

We note that the series $\{p_s\}$ are completely determined by the SCF expansion of $\frac{2m}{N}$ (3.8). Thus $p_{l+1} = 0$. From eq. (3.17), we know $|q_r| \leq |q_j|$ if $r > j$, and $-1 \leq q_j \leq \frac{N}{2m} - 1$ for $j = 1, 2, \dots, z_l + 1$. These results can be seen clearly from table 1. In appendix B, we prove that q_j can also be parameterized as

$$\begin{aligned} q_j &= \omega_j \frac{N}{2m} - n_j, \\ \omega_{z_1} &= 0, \quad \omega_j = \left\lfloor (n_j - 1) \frac{2m}{N} \right\rfloor + 1, \quad j \neq z_1. \end{aligned} \quad (3.19)$$

We see that the quantity q_j and integer ω_j are only determined by the length n_j of j -string. By using q_j and integer ω_j in (3.19), we express $\vartheta_j(x)$ as

$$\vartheta_j(x) = \frac{1}{i} \ln \frac{\theta_{10}[\frac{i}{2}(x + (q_j \frac{2m}{N}i + \frac{n_j}{N} \frac{\tau}{i}))]}{\theta_{10}[\frac{i}{2}(x - (q_j \frac{2m}{N}i + \frac{n_j}{N} \frac{\tau}{i}))]}, \quad (3.20)$$

where $\theta_{10}(x)$ is the elliptic theta function defined in appendix A. Then we conclude that the function $\vartheta_j(x)$ is a monotonically increasing function of x for $q_j > 0$ and a monotonically decreasing function of x for $q_j < 0$.

Substituting eq. (3.7) into the selection rule (3.5) and taking the logarithm, we have

$$\sum_{j=1}^{z_l+1} \left\{ \sum_{\alpha=1}^{M_j} \frac{1}{2\pi} \vartheta_j(x_{\alpha}^j) \right\} = I + \frac{k_1}{2N} - \frac{\phi}{2\pi}, \quad k_1 = 1, \dots, 2N, \quad (3.21)$$

where I is an integer (of half-odd integer) for $\sum_{j=1}^{z_l+1} M_j(1 + v_j)/2$ even (or odd). From above equation, we see that the value of ϕ and the distributions of Bethe roots quantifying by function $\vartheta_j(x)$ are not independent. For each given states, the distributions of strings are determined, thus the value of ϕ is determined.

Define the counting function $Z_j(x)$ as

$$Z_j(x) = \frac{\varphi_j(x)}{2\pi N i} + \frac{1}{2\pi} \vartheta_j(x) - \frac{1}{N} \sum_{r=1}^{z_l+1} \sum_{\beta=1}^{M_r} \frac{1}{2\pi} \Theta_{jr}(x - x_{\beta}^r). \quad (3.22)$$

It is clear that $Z_j(x_{\alpha}^j) = \frac{I_{\alpha}^j}{N}$ corresponds to the eq. (3.14). In the thermodynamic limit $N \rightarrow \infty$, the distribution of Bethe roots tends to continuous. Thus x_{α}^j becomes a continuous variable and the counting function $Z_j(x)$ becomes a continuous function. Define

$$\frac{d}{dx} Z_j(x) = \text{sign}(q_j) [\rho_j(x) + \rho_j^h(x)], \quad (3.23)$$

where $\rho_j(x)$ is the density of states characterized by j -string, $\rho_j^h(x)$ is the density of corresponding holes, and the sign function $\text{sign}(q_j)$ is added because of the monotonicity of function $\vartheta_j(x)$.

Taking the derivative of eq. (3.22) with respect to x , we obtain the integral equations for the densities of states

$$\text{sign}(q_j)\rho_j^h(x) = a_j(x) + \frac{n_j}{2Ni} - \sum_{r=1}^{z_l+1} \int_{-Q}^Q A_{jr}(x-y)\rho_r(y)dy, \quad (3.24)$$

where Q is the integral bound and the functions $a_j(x)$, $A_{jr}(x)$ are

$$\begin{aligned} a_j(x) &= \frac{1}{2\pi} \frac{d}{dx} \vartheta_j(x) = a(x; n_j, v_j) \\ &= -\frac{1}{4\pi} \left\{ \frac{\theta'_{10}[\frac{i}{2}(x - (q_j \frac{2m}{N}i + \frac{n_j\tau}{Ni}))]}{\theta_{10}[\frac{i}{2}(x - (q_j \frac{2m}{N}i + \frac{n_j\tau}{Ni}))]} - \frac{\theta'_{10}[\frac{i}{2}(x + (q_j \frac{2m}{N}i + \frac{n_j\tau}{Ni}))]}{\theta_{10}[\frac{i}{2}(x + (q_j \frac{2m}{N}i + \frac{n_j\tau}{Ni}))]} \right\}, \end{aligned} \quad (3.25)$$

$$\begin{aligned} A_{jr}(x) &= \frac{1}{2\pi} \frac{d}{dx} \Theta_j(x) + \delta_{jr} \text{sign}(q_j) \delta(x) \\ &= a(x; n_r + n_j, v_r v_j) + a(x; |n_r - n_j|, v_r v_j) \\ &\quad + 2 \sum_{k=1} a(x; |n_r - n_j| + 2k, v_r v_j) + \delta_{jr} \text{sign}(q_j) \delta(x). \end{aligned} \quad (3.26)$$

The functions $a_j(x)$ and $A_{jr}(x)$ are elliptic functions with double-periodic $2i$ and $2\frac{\tau}{i}$. Since the j -strings are distributed in the interval $[-\frac{\tau}{i}, \frac{\tau}{i}]$ on the real axis (noting that τ is pure imaginary), we can choose $Q = \frac{\tau}{i}$.

3.3 Ground state energy

Now, we are ready to calculate the physical quantities in the thermodynamic limit. Since the real Bethe roots contribute negative energies, the Bethe roots should fill the real axis as far as possible at the ground state. In general, the maximum number of real Bethe roots is $\frac{N}{2}$, and the remaining roots will be repelled to the complex plane and form the strings satisfying the rule (3.11).

We express the real Bethe roots as 1-strings, which correspond $n_j = 1$ and $v_j = +1$ in eq. (3.11). From (3.26), we obtain the function $A_{1r}(x)$ at the ground state

$$A_{1r}(x) = a(x; n_r + 1, v_r) + a(x; n_r - 1, v_r) + \delta_{1r} \text{sign}(q_1) \delta(x). \quad (3.27)$$

Above equation can be solved by the Fourier transformation. The Fourier transformation of a periodic function $F(x)$ is defined as

$$\tilde{F}(k) = \int_{-T}^T F(x) e^{-ik\frac{\pi}{T}x} dx, \quad F(x) = \frac{1}{2T} \sum_{k=-\infty}^{\infty} \tilde{F}(k) e^{ik\frac{\pi}{T}x}, \quad k \in \mathbf{Z},$$

where $x \in [-T, T]$ and $2T$ is the periodicity. The Fourier transformation of function $A_{1r}(x)$ is

$$\tilde{A}_{1r}(k) = 2 \cosh\left(\frac{i}{\tau} k \pi \eta_m\right) \frac{\sinh[\frac{i}{\tau} k \pi (q_r \frac{2m}{N} - n_r \frac{\tau}{N})]}{\sinh(\frac{i}{\tau} k \pi)}. \quad (3.28)$$

Taking the Fourier transformation of eq. (3.24) with $j = 1$ and using eq. (3.28), we obtain the densities of states at the ground state

$$\tilde{\rho}_1(k) = \frac{1}{2 \cosh(\frac{i}{\tau} k \pi \eta_m)} - \frac{\tilde{\rho}_1^h(k)}{\tilde{A}_{11}(k)} - \frac{\tau \delta_{k0}}{N \tilde{A}_{11}(k)} - \sum_{r \neq 1}^{z_l+1} \frac{\sinh[\frac{i}{\tau} k \pi (q_r \frac{2m}{N} - n_r \frac{\tau}{N})]}{\sinh[\frac{i}{\tau} k \pi (1 - \eta_m)]} \tilde{\rho}_r(k). \quad (3.29)$$

We see that the real Bethe roots, holes and strings are coupled together, thus the distribution of real Bethe roots depends on the densities of holes and strings.

From eqs. (3.6) and (3.25), the energy of r -string is

$$\begin{aligned} \varepsilon_r(\eta_m) &= \frac{\sigma(\eta_m)}{\sigma'(0)} \left\{ \frac{\theta'_{10}[\frac{i}{2}(x - (q_r \frac{2m}{N} i + \frac{n_r \tau}{N i}))]}{\theta_{10}[\frac{i}{2}(x - (q_r \frac{2m}{N} i + \frac{n_r \tau}{N i}))]} - \frac{\theta'_{10}[\frac{i}{2}(x + (q_r \frac{2m}{N} i + \frac{n_r \tau}{N i}))]}{\theta_{10}[\frac{i}{2}(x + (q_r \frac{2m}{N} i + \frac{n_r \tau}{N i}))]} \right\} \\ &= -4\pi \frac{\sigma(\eta_m)}{\sigma'(0)} a_r(x). \end{aligned} \quad (3.30)$$

From eqs. (3.6), (3.29) and (3.30), the ground state energy reads

$$\begin{aligned} E_g(\eta_m) &= -4\pi N \frac{\sigma(\eta_m)}{\sigma'(0)} \left\{ \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} a_1(x) \rho_1(x) dx + \sum_{r \neq 1}^{z_l+1} \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} a_r(x) \rho_r(x) dx \right\} \\ &\quad - i\pi \frac{\sigma(\eta_m)}{\sigma'(0)} + \frac{N}{2} \frac{\sigma'(\eta_m)}{\sigma'(0)} \\ &= -\frac{2i\pi N}{\tau} \frac{\sigma(\eta_m)}{\sigma'(0)} \sum_{k=-\infty}^{\infty} \left\{ \frac{\tilde{a}_1(k)}{2 \cosh(\frac{i}{\tau} k \pi \eta_m)} - \frac{\tilde{\rho}_1^h(k)}{2 \cosh(\frac{i}{\tau} k \pi \eta_m)} \right\} + \frac{N}{2} \frac{\sigma'(\eta_m)}{\sigma'(0)} \\ &= e_0(\eta_m) N + \epsilon_h(\eta_m), \end{aligned} \quad (3.31)$$

where $e_0(\eta_m)$ is the density of ground state energy at degenerate point η_m and $\epsilon_h(\eta_m)$ is the energy carried by the holes in the real axis

$$e_0(\eta_m) = -\frac{i\pi}{\tau} \frac{\sigma(\eta_m)}{\sigma'(0)} \sum_{k=-\infty}^{\infty} \frac{\sinh[\frac{i}{\tau} k \pi (1 - \eta_m)]}{\sinh(\frac{i}{\tau} k \pi) \cosh(\frac{i}{\tau} k \pi \eta_m)} + \frac{1}{2} \frac{\sigma'(\eta_m)}{\sigma'(0)}, \quad (3.32)$$

$$\epsilon_h(\eta_m) = \frac{i\pi N}{\tau} \frac{\sigma(\eta_m)}{\sigma'(0)} \sum_{k=-\infty}^{\infty} \frac{\tilde{\rho}_1^h(k)}{\cosh(\frac{i}{\tau} k \pi \eta_m)}. \quad (3.33)$$

From eq. (3.31), we find that the ground state energy is only related to the real Bethe roots and corresponding holes. Although the strings could affect the densities of sates, their contribution to the energies is zero. This is because of the rearrangement of Fermi sea. From eqs. (3.32) and (3.33), we know that the ground state energy density is negative while the energy of hole is positive. Thus at the ground state, the number of holes should be as less as possible to minimize the energy. Due to the constraints of the BAEs, the density of holes should satisfy (3.29).

As we mentioned before, the strings can affect the distribution of holes. Now, let us analyze the string solutions satisfying the rule (3.11). Suppose at the ground state, there are M_r r -strings ($r \geq 2$). From eq. (3.17), we know $-1 \leq q_r \leq \frac{N}{2m} - 1$ for $r = 2, \dots, z_l + 1$. Because we have shifted all the variables into one periodicity to compute the values of

elliptic functions, these strings should also be moved to the same periodicity. In order to minimize the energy, we require

$$-1 < \sum_{r \neq 1}^{z_l+1} M_r q_r < \frac{N}{2m} - 1. \quad (3.34)$$

Based on eq. (3.34), it is straightforward that

$$\left\lfloor \left(\sum_{r \neq 1}^{z_l+1} M_r n_r - 1 \right) \frac{2m}{N} \right\rfloor + 1 = \sum_{r \neq 1}^{z_l+1} M_r \omega_r, \quad (3.35)$$

where $\sum_{r \neq 1}^{z_l+1} M_r n_r$ is the total number of string solutions. Substituting eq. (3.35) into (3.19), we arrive at

$$\sum_{r \neq 1}^{z_l+1} M_r q_r = \left(\left\lfloor \left(\sum_{r \neq 1}^{z_l+1} M_r n_r - 1 \right) \frac{2m}{N} \right\rfloor + 1 \right) \frac{N}{2m} - \sum_{r \neq 1}^{z_l+1} M_r n_r. \quad (3.36)$$

It is clear that the contribution of strings depends on the parity of system-size N . Thus the number of holes and the ground state energy depend on the parity of N , and we should consider them separately.

If N is odd. At the ground state, there are $M_1 = \frac{N-1}{2}$ real Bethe roots and $\frac{N+1}{2}$ string solutions

$$\sum_{r \neq 1}^{z_l+1} M_r n_r = \frac{N+1}{2}. \quad (3.37)$$

Substituting (3.37) into (3.36), we have

$$\sum_{r \neq 1}^{z_l+1} M_r q_r = \left(\left\lfloor \left(\frac{N+1}{2} - 1 \right) \frac{2m}{N} \right\rfloor + 1 \right) \frac{N}{2m} - \frac{N+1}{2} = -\frac{1}{2}. \quad (3.38)$$

Because the number of real Bethe roots is $M_1 = \frac{N-1}{2}$, we have

$$\frac{M_1}{N} = \frac{1}{2} - \frac{1}{2N} = \int_{-\frac{\pi}{i}}^{\frac{\pi}{i}} \rho_1(x) dx = \tilde{\rho}_1(0). \quad (3.39)$$

From the density of states (3.29), we obtain the values of $\tilde{\rho}_1(0)$ as

$$\tilde{\rho}_1(0) = \frac{1}{2} - \frac{\tilde{\rho}_1^h(0)}{2(1 - \eta_m)} + \frac{\eta_m}{2N(1 - \eta_m)}. \quad (3.40)$$

Substituting (3.40) into (3.39), we obtain

$$\tilde{\rho}_1^h(0) = \int_{-\frac{\pi}{i}}^{\frac{\pi}{i}} \rho_1^h(x) dx = \frac{1}{N}. \quad (3.41)$$

Comparing this relation with the definition of counting function, we know that such a configuration gives that there is only one hole in the real axis at the ground state. The density of holes $\rho_1^h(x)$ can be expressed by the δ -function as

$$\rho_1^h(x) = \frac{1}{N} \delta(x - x^h), \quad \tilde{\rho}_1^h(k) = \frac{1}{N} e^{\frac{k\pi}{\tau} x^h}, \quad (3.42)$$

where x^h is the position of hole. Substituting (3.42) into (3.33), we obtain the energy carried by one hole

$$\epsilon_h(x^h, \eta_m) = \frac{i\pi}{\tau} \frac{\sigma(\eta_m)}{\sigma'(0)} \sum_{k=-\infty}^{\infty} \frac{e^{k\pi x^h/\tau}}{\cosh(\frac{i}{\tau} k\pi \eta_m)}. \quad (3.43)$$

In the thermodynamic limit, the position x^h of hole can take continuous values in the interval $[-\frac{\tau}{i}, \frac{\tau}{i}]$. It should be noted that the function $\epsilon_h(x^h, \eta_m)$ takes the minimum value at $x^h = \frac{\tau}{i}$, which corresponding to the ground state. Thus the ground state energy reads

$$E_g^{\text{odd}}(\eta_m) = e_0(\eta_m)N + \epsilon_h(\frac{\tau}{i}, \eta_m). \quad (3.44)$$

If the system size N is even, there are $M_1 = \frac{N}{2}$ real Bethe roots and $\frac{N}{2}$ string solutions at the ground state

$$\sum_{r \neq 1}^{z_l+1} M_r n_r = \frac{N}{2}. \quad (3.45)$$

Substituting (3.45) into (3.36), we have

$$\sum_{r \neq 1}^{z_l+1} M_r q_r = \left(\left\lfloor \left(\frac{N}{2} - 1 \right) \frac{2m}{N} \right\rfloor + 1 \right) \frac{N}{2m} - \frac{N}{2} = 0. \quad (3.46)$$

From the eqs. (3.29), (3.45) and (3.46), we have

$$\frac{M_1}{N} = \frac{1}{2} = \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} \bar{\rho}_1(x) dx = \tilde{\rho}_1(0) = \frac{1}{2} - \frac{\tilde{\rho}_1^h(0)}{2(1 - \eta_m)}, \quad (3.47)$$

where $\bar{\rho}_1(x)$ is the density of real Bethe roots and $\tilde{\rho}_1(k)$ is the density of corresponding holes. Such a configuration gives that there is no hole at the ground state, i.e., $\tilde{\rho}_1^h(x) = 0$. Then the ground state energy is

$$E_g^{\text{even}}(\eta_m) = e_0(\eta_m)N. \quad (3.48)$$

3.4 Elementary excitations

Now, we consider a typical elementary excitations that is the hole excitation. The hole excitations of present model also have the parity. We first consider the odd N case. Obviously, the simplest excitation is putting one hole in the real axis, where the position of hole deviates from τ/i . The corresponding excited energy is quantified by

$$\Delta E^{\text{odd}}(x^h, \eta_m) = E_e^{\text{odd}}(\eta_m) - E_g^{\text{odd}}(\eta_m) = \epsilon_h(x^h, \eta_m) - \epsilon_h\left(\frac{\tau}{i}, \eta_m\right), \quad (3.49)$$

where $E_e^{\text{odd}}(\eta_m)$ is the energy at the excited state. In the thermodynamic limit, the hole can move smoothly in the real axis which means x^h can tend to τ/i infinitely. Then we conclude that the excitation spectrum is continuous

$$\Delta E^{\text{odd}}(\eta_m) = \lim_{x^h \rightarrow \tau/i} \Delta E^{\text{odd}}(x^h, \eta_m) \rightarrow 0. \quad (3.50)$$

The simplest hole excitation for even N case is that a real Bethe root is replaced by a z_1 -string in the configuration of Bethe roots at the ground state. The length of z_1 -string is $n_{z_1} = 1$ and the corresponding parity is $v_{z_1} = -1$, which is shown as the ninth column in table 1 and the red dot in figure 1. The energy carried by z_1 -string is positive. In this kind of excited state, there are $M_1 = (\frac{N}{2} - 1)$ real Bethe roots and $(\frac{N}{2} + 1)$ string solutions. The real Bethe roots satisfies

$$\frac{M_1}{N} = \frac{1}{2} - \frac{1}{N} = \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} \rho'_1(x) dx = \tilde{\rho}'_1(0), \quad (3.51)$$

and the string solutions satisfy

$$\sum_{r \neq 1}^{z_l+1} M_r n_r = \frac{N}{2} + 1, \quad (3.52)$$

$$\sum_{r \neq 1}^{z_l+1} M_r q_r = \left(\left\lfloor \left(\frac{N}{2} - 1 \right) \frac{2m}{N} \right\rfloor + 1 \right) \frac{N}{2m} - \frac{N}{2} + q_{z_1} = -1. \quad (3.53)$$

Due to the constraints (3.52) and (3.53), the density of states (3.29) with $k = 0$ reads

$$\tilde{\rho}'_1(0) = \frac{1}{2} - \frac{\tilde{\rho}_1^h(0)}{2(1 - \eta_m)} + \frac{\eta_m}{N(1 - \eta_m)}. \quad (3.54)$$

Substituting (3.54) into (3.51), we obtain

$$\tilde{\rho}_1^h(0) = \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} \rho_1^h(x) dx = \frac{2}{N}, \quad (3.55)$$

which indicates that there exist two holes in the real axis. The density of holes can be expressed as

$$\rho_1^h(x) = \frac{1}{N} [\delta(x - x_1^h) + \delta(x - x_2^h)], \quad (3.56)$$

where x_1^h and x_2^h are the positions of holes. The energy of hole excitation is defined as

$$\Delta E^{\text{even}}(x_1^h, x_2^h, \eta_m) = E_e^{\text{even}}(\eta_m) - E_g^{\text{even}}(\eta_m) = \epsilon_h(x_1^h, \eta_m) + \epsilon_h(x_2^h, \eta_m), \quad (3.57)$$

where $E_e^{\text{even}}(\eta_m)$ is the energy at excited state. The values of $\Delta E^{\text{even}}(x_1^h, x_2^h, \eta_m)$ can be minimized by putting two holes at the point of τ/i in the thermodynamic limit. Then we have

$$\Delta E^{\text{even}}(\eta_m) = \lim_{x_1^h, x_2^h \rightarrow \tau/i} \Delta E^{\text{even}}(x_1^h, x_2^h, \eta_m) = 2\epsilon_h\left(\frac{\tau}{i}, \eta_m\right), \quad (3.58)$$

which means that the hole excitation has a gap.

4 Thermodynamic limit with arbitrary couplings

4.1 Main ideas

In this section, we generalize above results from degenerate points η_m to the arbitrary real η in the interval $0 < \text{Re}(\eta) \leq \frac{1}{2}$. The main idea is as follows. In principle, a physical quantity $E(\eta)$ which is a function of model parameter η can be expressed as

$$E(\eta) = N f_0(\eta) + f_1(\eta) + \frac{1}{N} f_2(\eta) + O(N^{-2}), \quad (4.1)$$

where $f_n(\eta)$ ($n = 0, 1, 2$) are some unknown functions and $O(N^{-2})$ means the corrections up to the order of N^{-2} . We do not know the explicit forms of $E(\eta)$ and $f_n(\eta)$ for the general η . What we know is the value of $E(\eta)$ at the point of η_m

$$E(\eta_m) = N e_0(\eta_m) + e_1(\eta_m) + \frac{1}{N} e_2(\eta_m) + O(N^{-2}), \quad (4.2)$$

where the functions $e_n(\eta_m)$ ($n = 0, 1, 2$) have been determined. With the changing of m , there are a series of degenerate points $\{\eta_m\}$. Substituting the $\eta = \eta_m, \eta_{m+1}$ into (4.1) and comparing with (4.2), we obtain

$$f_n(\eta_m) = e_n(\eta_m), \quad f_n(\eta_{m+1}) = e_n(\eta_{m+1}). \quad (4.3)$$

From eq. (3.1), the difference between two degenerate points η_m and η_{m+1} is proportional to N^{-1} , which means that the $\eta_{m+1} - \eta_m$ is a small quantity with the order of N^{-1} .

Now, we consider a generic η where $\eta_m \leq \eta \leq \eta_{m+1}$. Suppose both $f_n(\eta)$ and $e_n(\eta)$ are the smooth functions of η . We take the Taylor expansions of functions $f_n(\eta)$ and $e_n(\eta)$ at the point of η_m

$$f_n(\eta) = f_n(\eta_m) + f'_n(\eta_m)(\eta - \eta_m) + O(N^{-2}), \quad (4.4)$$

$$e_n(\eta) = e_n(\eta_m) + e'_n(\eta_m)(\eta - \eta_m) + O(N^{-2}). \quad (4.5)$$

Substituting $\eta = \eta_{m+1}$ into eqs. (4.4)–(4.5), we have

$$f_n(\eta_{m+1}) = f_n(\eta_m) + f'_n(\eta_m)(\eta_{m+1} - \eta_m) + O(N^{-2}), \quad (4.6)$$

$$e_n(\eta_{m+1}) = e_n(\eta_m) + e'_n(\eta_m)(\eta_{m+1} - \eta_m) + O(N^{-2}). \quad (4.7)$$

Eq. (4.6) minus (4.7) gives

$$f'_n(\eta_m) = e'_n(\eta_m) + O(N^{-1}). \quad (4.8)$$

Substituting (4.8) into (4.4), we have

$$f_n(\eta) = e_n(\eta_m) + e'_n(\eta_m)(\eta - \eta_m) + O(N^{-2}) = e_n(\eta) + O(N^{-2}), \quad (4.9)$$

which means that the functions $f_n(\eta)$ can be obtained from the determined ones $e_n(\eta)$ up to the order of N^{-2} . In the thermodynamic limit, the correction $O(N^{-2})$ can be neglected and the physical quantity $E(\eta)$ can be obtained from $E(\eta_m)$ with great accuracy.

Some remarks are in order. Because the degenerate point η_m contains an imaginary part τ/N , the above extrapolations are valid for the line τ/N in the complex plain with varying the value of m . That is to say, we obtain the physical quantities along this line. In the thermodynamic limit, we have $\tau/N \rightarrow 0$ thus can study the physics with real model parameter η , i.e., $0 < \eta \leq \frac{1}{2}$ due to $0 < \frac{2m}{N} \leq \frac{1}{2}$. However, our method also allows us to study the thermodynamic limit of the XYZ model with η taking others values beyond a real one. If l_1 tends to infinite while l_1/N is finite in the thermodynamic limit, the degenerate points are $\eta_{m,l_1} = -\frac{2l_1+1}{N}\tau + \frac{2m}{N}$, where we have put $M = N$ and $m_1 = -m$ in eq. (3.1). Because τ is pure imaginary, the η_{m,l_1} is complex. We note that the above method can also be applied directly and one can obtain the corresponding results for the generic complex η with a finite imaginary part. If η is pure imaginary, we can put $M = N$ and $m_1 = 0$ in eq. (3.1). Then with the changing of l_1 , there exist sufficient degenerate points in the thermodynamic limit. Based on them, we can obtain the associated results similarly.

4.2 Ground state energy

Using above technique, we obtain the ground state energy of Hamiltonian (2.1) with odd N and generic η as

$$E_g^{\text{odd}}(\eta) = e_0(\eta)N + \epsilon_h\left(\frac{\tau}{i}, \eta\right), \quad (4.10)$$

where the density $e_0(\eta)$ and function $\epsilon_h(x, \eta)$ are given by (3.32) and (3.43) provided that η_m is replaced by η , respectively.

Next, we check the result (4.10) by numerical calculations. In the verifications, we randomly chose the values of model parameters τ and η . Meanwhile, we require that $\eta \neq \eta_m$, because we have proved analytically that eq. (4.10) is correct if $\eta = \eta_m$. In order to quantify the validity of eq. (4.10), we define

$$\delta^{\text{odd}} = \frac{E_g^{\text{odd}}(\eta)}{\bar{E}_g^{\text{odd}}(\eta)} - 1, \quad (4.11)$$

where $\bar{E}_g^{\text{odd}}(\eta)$ is the ground state energy of Hamiltonian (2.1) obtained by the exact diagonalization and $E_g^{\text{odd}}(\eta)$ is the ground state energy obtained by eq. (4.10).

In table 2, we list the results with $\tau = 0.5i$ and $\eta = 0.4$. We see that the value of δ^{odd} has the order of 10^{-9} when the system size $N = 25$, which indicates that eq. (4.10) can describe the ground state energy with satisfied accuracy even for the system with small size.

In figure 2, the finite size effect of δ^{odd} with $\tau = 0.5i$ and $\eta = \sqrt{2}/4$ is given. From the fitting, we find that δ^{odd} satisfies the exponential law

$$\delta^{\text{odd}} = \alpha_1 \exp(\beta_1 N), \quad (4.12)$$

where α_1 and β_1 are the fitting factors. Due to the fact $\beta_1 < 0$, the δ^{odd} tends to zero when the system size $N \rightarrow \infty$, which indicates that eq. (4.10) gives the correct ground state energy of antiperiodic XYZ spin chain in the thermodynamic limit.

N	$\bar{E}_g^{\text{odd}}$	E_g^{odd}	$\delta^{\text{odd}} (\times 10^{-3})$
5	-4.24631809	-4.25772417	2.68611098
7	-6.58795792	-6.59092288	0.45005755
9	-8.92330609	-8.92412158	0.09138932
11	-11.25708902	-11.25732029	0.02054430
13	-13.59045214	-13.59051899	0.00491948
15	-15.92369811	-15.92371770	0.00122998
17	-18.25691061	-18.25691640	0.00031735
19	-20.59011338	-20.59011511	0.00008386
21	-22.92331330	-22.92331381	0.00002258
23	-25.25651236	-25.25651252	0.00000617
25	-27.58971118	-27.58971122	0.00000171

Table 2. Numerical results for the odd N . Here $\bar{E}_g^{\text{odd}}$ is the ground state energy of Hamiltonian (2.1) obtained by the exact diagonalization with the help of the sparse matrix method, E_g^{odd} is the ground state energy obtained by eq. (4.10), δ^{odd} characterizes the difference, $\tau = 0.5i$ and $\eta = 0.4$.

Figure 2. The deviation δ^{odd} versus the system-size N . The data can be fitted as $\delta^{\text{odd}} = \alpha_1 \exp(\beta_1 N)$. Here $\tau = 0.5i$, $\eta = \frac{\sqrt{2}}{4}$, $\alpha_1 = 0.05447$ and $\beta_1 = -0.5632$. Due to the fact $\beta_1 < 0$, the δ^{odd} tends to zero when $N \rightarrow \infty$.

The ground state energy of model (2.1) with even N and generic η is

$$E_g^{\text{even}}(\eta) = e_0(\eta)N. \quad (4.13)$$

In order to check the validity of eq. (4.13), we define

$$\delta^{\text{even}} = \frac{E_g^{\text{even}}(\eta)}{\bar{E}_g^{\text{even}}(\eta)} - 1, \quad (4.14)$$

where $\bar{E}_g^{\text{even}}(\eta)$ is the ground state energy obtained by the exact diagonalization and $E_g^{\text{even}}(\eta)$ is the ground state energy obtained by eq. (4.13).

In table 3, we list the numerical results with $\tau = 0.5i$ and $\eta = 0.4$. The data show that the value of δ^{even} has the order of 10^{-15} when the system size $N = 24$, which indicates

N	$\bar{E}_g^{\text{even}}$	E_g^{even}	$\delta^{\text{even}} (\times 10^{-4})$
4	-4.66414993812	-4.66639740988	4.81860959229
6	-6.99945302886	-6.99959611482	0.20442450017
8	-9.33278427176	-9.33279481977	0.01130210061
10	-11.66599268867	-11.66599352471	0.00071664895
12	-13.99919216041	-13.99919222965	0.00004945726
14	-16.33239092868	-16.33239093459	0.00000361594
16	-18.66558963902	-18.66558963953	0.00000027571
18	-20.99878834443	-20.99878834447	0.00000002169
20	-23.33198704941	-23.33198704941	0.00000000174
22	-25.66518575436	-25.66518575436	0.00000000015
24	-27.99838445930	-27.99838445930	0.00000000002

Table 3. Numerical results for the even N . Here $\bar{E}_g^{\text{even}}$ is the ground state energy obtained by the exact diagonalization, E_g^{even} is the ground state energy obtained by eq. (4.13), δ^{even} characterizes the difference, $\tau = 0.5i$ and $\eta = 0.4$.

Figure 3. The deviation δ^{even} versus the system-size N . The data can be fitted as $\delta^{\text{even}} = \alpha_2 \exp(\beta_2 N)$. Here $\tau = 0.5i$, $\eta = \frac{\sqrt{2}}{4}$, $\alpha_2 = 0.06319$ and $\beta_2 = -1.079$. Due to the fact $\beta_2 < 0$, the δ^{even} tends to zero when $N \rightarrow \infty$.

that eq. (4.13) can quantify the ground state energy with satisfied accuracy even for the system with small size.

In figure 3, we list the finite size effect of δ^{even} with $\tau = 0.5i$ and $\eta = \sqrt{2}/4$. The data can be fitted as

$$\delta^{\text{even}} = \alpha_2 \exp(\beta_2 N). \quad (4.15)$$

Due to the fact $\beta_2 < 0$, the δ^{even} tends to zero when the system size $N \rightarrow \infty$, which indicates that eq. (4.13) gives the correct ground state energy in the thermodynamic limit.

4.3 Elementary excitations

The energy of hole excitation with odd N and generic η is

$$\Delta E^{\text{odd}}(x^h, \eta) = \epsilon_h(x^h, \eta) - \epsilon_h\left(\frac{\tau}{i}, \eta\right). \quad (4.16)$$

Figure 4. The energy of hole excitation ΔE_e^{odd} versus the system-size N . Here $\tau = 0.5i$, $\eta = \frac{\sqrt{2}}{4}$, $\alpha_3 = 19.87$ and $\beta_3 = -1.869$. The data can be fitted as $\Delta E_e^{\text{odd}} = \alpha_3 N^{\beta_3}$. Because of $\beta_3 < 0$, the ΔE_e^{odd} tends to zero when $N \rightarrow \infty$.

In the thermodynamic limit, the position of hole x^h can take continuous values in the interval $[-\frac{\tau}{i}, \frac{\tau}{i}]$. Then we have

$$\Delta E^{\text{odd}}(\eta) = \lim_{x^h \rightarrow \tau/i} \Delta E^{\text{odd}}(x^h, \eta) \rightarrow 0, \quad (4.17)$$

which indicates that the hole excitations are continuous.

Now, we check the result (4.17) by the density matrix renormalization group (DMRG) method [36, 37]. We use the infinite chain DMRG algorithm and start with 14 sites, where the number of reserved states $m = 2^7$ and the truncation error is 10^{-8} . We note that even in the small N (less than 24) case, the DMRG results are in pretty good agreement with the direct diagonalization results, where the relative errors at ground state is 10^{-9} . The numerical results, denoted as $\Delta E_e^{\text{odd}}(\eta)$, with $\tau = 0.5i$ and $\eta = \sqrt{2}/4$ for various system size N are shown in figure 4. The data can be fitted as

$$\Delta E_e^{\text{odd}}(\eta) = \alpha_3 N^{\beta_3}. \quad (4.18)$$

Due to the fact $\beta_3 < 0$, the value $\Delta E_e^{\text{odd}}(\eta)$ tends to zero when the system size $N \rightarrow \infty$, which is consistent with the analytical result (4.17).

The energy of hole excitation with even N and generic η is

$$\Delta E^{\text{even}}(x_1^h, x_2^h, \eta) = \epsilon_h(x_1^h, \eta) + \epsilon_h(x_2^h, \eta). \quad (4.19)$$

In the thermodynamic limit, two holes x_1^h and x_2^h can be put on the point of τ/i and we have

$$\Delta E^{\text{even}}(\eta) = \lim_{x_1^h, x_2^h \rightarrow \tau/i} \Delta E^{\text{even}}(x_1^h, x_2^h, \eta) = 2\epsilon_h\left(\frac{\tau}{i}, \eta\right). \quad (4.20)$$

Now, we check the validity of eq. (4.20). Substituting $\tau = 0.5i$ and $\eta = \frac{\sqrt{2}}{4}$ into eq. (4.20) and using the definition of elliptic functions, we obtain

$$\Delta E^{\text{even}}\left(\frac{\sqrt{2}}{4}\right) = 2.54881. \quad (4.21)$$

Figure 5. The energy of hole excitation ΔE_e^{even} versus the system-size N . Here $\tau = 0.5i$, $\eta = \frac{\sqrt{2}}{4}$, $\alpha_4 = 28.46$, $\beta_4 = -1.769$ and $\varepsilon_4 = 2.548$. The data can be fitted as $\Delta E_e^{\text{even}} = \alpha_4 N^{\beta_4} + \varepsilon_4$. Due to the fact $\beta_4 < 0$, ε_4 gives the value of ΔE_e^{even} in the thermodynamic limit.

We also check the analytical result (4.21) by DMRG methods. The DMRG data, denoted as $\Delta E_e^{\text{even}}(\eta)$, with $\tau = 0.5i$ and $\eta = \frac{\sqrt{2}}{4}$ for various even system size are shown in figure 5. The data can be fitted as

$$\Delta E_e^{\text{even}}(\eta) = \alpha_4 N^{\beta_4} + \varepsilon_4. \quad (4.22)$$

Because of $\beta_4 < 0$, in the thermodynamic limit, ε_4 gives the values of energy, i.e.,

$$\varepsilon_4 = \Delta E_e^{\text{even}}(\eta). \quad (4.23)$$

Meanwhile, the numerical calculation gives $\varepsilon_4 = 2.548$, which is consistent with the analytical result (4.21).

So far, we have obtained the ground state energy and hole excitation. All these physical quantities are related to the parity of system size. From eqs. (4.10) and (4.13), we find that the ground state energy with odd N includes a term $\epsilon_h(\frac{\tau}{i}, \eta)$ induced by the hole in the real axis. The magnitude of $\epsilon_h(\frac{\tau}{i}, \eta)$ is the same as the ground state energy density $e_0(\eta)$. From eqs. (4.17) and (4.20), we find that the model with odd N has a continuous hole excitation spectrum, while the excitation for the even N case has an energy gap $2\epsilon_h(\frac{\tau}{i}, \tau)$.

5 Limit to the antiperiodic XXZ model

A very strong motivation of this paper is to study the thermodynamic limit of the antiperiodic XXZ model. Because the corresponding inhomogeneous BAEs do not have the degenerate points, the above method does not work. In this section we show that the thermodynamic limit of the antiperiodic XXZ model can be obtained from the antiperiodic XYZ model. The Hamiltonian of XXZ model reads

$$\bar{H} = \frac{1}{2} \sum_{j=1}^N \left[\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \cos(\pi\eta) \sigma_j^z \sigma_{j+1}^z \right], \quad (5.1)$$

and the antiperiodic boundary condition is given by eq. (2.3). The eigenvalue of Hamiltonian (5.1) is [10]

$$\bar{E} = -i \sin(\pi\eta) \sum_{j=1}^N [\coth(\lambda_j + i\pi\eta) - \coth(\lambda_j)] + \frac{N}{2} \cos(\pi\eta) + i \sin(\pi\eta), \quad (5.2)$$

where the N Bethe roots $\{\lambda_j\}$ satisfy the BAEs

$$e^{2\lambda_j+i\pi\eta} \frac{\sinh^N(\lambda_j+i\pi\eta)}{\sinh^N(\lambda_j)} = \prod_{k=1}^N \frac{\sinh(\lambda_j-\lambda_k+i\pi\eta)}{\sinh(\lambda_j-\lambda_k-i\pi\eta)} + c(\lambda_j) e^{\lambda_j+i\pi\eta} \prod_{k=1}^N \frac{\sinh(\lambda_j+i\pi\eta)}{\sinh(\lambda_j-\lambda_k-i\pi\eta)}, \quad j=1, \dots, N, \quad (5.3)$$

and $c(\lambda_j)$ is determined as

$$c(\lambda_j) = e^{\lambda_j-iN\pi\eta-\sum_{l=1}^N \lambda_l} - e^{-\lambda_j-i\pi\eta+\sum_{l=1}^N \lambda_l}. \quad (5.4)$$

We see that the parameter $c(\lambda_j)$ and Bethe roots $\{\lambda_j\}$ are determined together and BAEs (5.3) can not be reduced to the homogeneous ones.

It is well-known that the XXZ model can be obtained from XYZ model by taking the trigonometric limit

$$\lim_{\tau \rightarrow i\infty} J_x(\eta, \tau) \rightarrow 1, \quad \lim_{\tau \rightarrow i\infty} J_y(\eta, \tau) \rightarrow 1, \quad \lim_{\tau \rightarrow i\infty} J_z(\eta, \tau) \rightarrow \cos(\pi\eta). \quad (5.5)$$

Therefore, some physics including the exact solution, BAEs, ground state, elementary excitation and thermodynamics of XXZ model can be obtained from XYZ model by taking the same limit, provided that the limit exists.

In the following, we show that the thermodynamic limits of antiperiodic XXZ model indeed can be obtained from XYZ model. Due to the constraint $0 < \eta \leq \frac{1}{2}$, the related results are valid in the massless region $0 < \cos(\pi\eta) \leq 1$ of XXZ model. The ground state energy of antiperiodic XXZ model with odd N is obtained by taking the limit $\tau \rightarrow i\infty$ of eq. (4.10)

$$\bar{E}_g^{\text{odd}}(\eta) = \lim_{\tau \rightarrow i\infty} E_g^{\text{odd}}(\eta) = \bar{e}_0(\eta)N + \bar{\epsilon}_h(\infty, \eta). \quad (5.6)$$

Here $\bar{e}_0(\eta)$ is the ground state energy density of the antiperiodic XXZ model

$$\bar{e}_0(\eta) = \lim_{\tau \rightarrow i\infty} e_0(\eta) = -\frac{\sin(\pi\eta)}{\pi} \int_{-\infty}^{\infty} \frac{\sinh[w(1-\eta)]}{\sinh(w) \cosh(w\eta)} dw + \frac{1}{2} \cos(\pi\eta). \quad (5.7)$$

It is shown that $\bar{e}_0(\eta)$ (5.7) obtained here is the same as that of the periodic XXZ model obtained in [9]. The $\bar{\epsilon}_h(x^h, \eta)$ is the energy carried by one hole

$$\bar{\epsilon}_h(x^h, \eta) = \lim_{\tau \rightarrow i\infty} \epsilon_h(x^h, \eta) = \frac{\sin(\pi\eta)}{\eta} \frac{1}{\cosh(\frac{\pi x^h}{2\eta})}, \quad (5.8)$$

where x^h is the position of hole which is distributed in the interval $(-\infty, \infty)$. If the hole is put on the infinity, from eq. (5.8), we obtain that the minimum energy carried by hole is zero, i.e., $\bar{\epsilon}_h(\infty, \eta) = 0$.

The ground state energy with even N is obtained by taking the limit $\tau \rightarrow i\infty$ of eq. (4.13),

$$\bar{E}_g^{\text{even}}(\eta) = \lim_{\tau \rightarrow i\infty} E_g^{\text{even}}(\eta) = \bar{e}_0(\eta)N. \quad (5.9)$$

From eqs. (5.6) and (5.9), we know that the ground state energy of antiperiodic XXZ model does not depend on the parity of system size N in the thermodynamic limit. That is to say, although the distributions of Bethe roots (or the densities of states) with odd and even N are different, the ground state energy can be expressed as a unified form of

$$\bar{E}_g = \bar{e}_0(\eta)N. \quad (5.10)$$

This is because we consider the massless region and the contribution of hole is zero.

The energy of hole excitation with odd N is obtained by taking the limit $\tau \rightarrow i\infty$ of eq. (4.17). Obviously, the hole excitation is continuous

$$\Delta \bar{E}^{\text{odd}}(\eta) \rightarrow 0. \quad (5.11)$$

From eq. (4.20), we obtain the energy of hole excitation with even N

$$\Delta \bar{E}^{\text{even}}(\eta) = \lim_{\tau \rightarrow i\infty} 2\epsilon_h\left(\frac{\tau}{i}, \eta\right) \rightarrow 0. \quad (5.12)$$

Therefore, the energy gap in the XYZ model closes after taking the trigonometric limit. Comparing eqs. (5.11) and (5.12), we find that the hole excitation is gapless and the excited spectrum is continuous, which is true for both odd and even N . We note that the physical pictures of excitations with odd and even N are quite different, which have been explained in previous sections.

It is remarked that the process of taking limits in this paper is as follows. We first set τ to be finite, then we set N to be infinite. The resulting degenerate points (3.3) tend to real numbers which are dense in the real line. By this way, we obtain the thermodynamic limit of the XYZ model with a real η and a finite τ . The detailed results are given in sections 3 and 4. Then taking the trigonometric limit of $\tau \rightarrow i\infty$ (or $\lim_{\tau \rightarrow i\infty} \lim_{N \rightarrow \infty} \frac{\tau}{N} = 0$), we obtain the corresponding results of the XXZ model with a real η from those of the corresponding XYZ model.

6 Conclusions

We study the thermodynamic limit of the anisotropic spin- $\frac{1}{2}$ XYZ spin chain with the antiperiodic boundary condition described by the Hamiltonian (2.1) and (2.3) based on its off-diagonal Bethe ansatz solution. We overcome the difficult that it is hard to take the thermodynamic limit of the associated BAEs deriving from its inhomogeneous $T-Q$ relation. With the help of the exact results of system at degenerate points (3.3), we obtain the actual values of physical quantities such as the ground state energies and hole excitations for an arbitrary coupling η . In this paper, we consider the case that the anisotropic coupling parameter η after taking thermodynamic limit is real one and $0 < \eta \leq \frac{1}{2}$. The results with generic complex model parameters including the pure imaginary ones can be derived similarly. We also propose a method to study the thermodynamic limit of integrable model without degenerate points. As an example, the results of the antiperiodic XXZ spin chain are obtained with the help of those of the antiperiodic XYZ spin chain.

The method proposed in this paper can be generalized to study the high rank quantum integrable models such as the $su(n)$ XYZ spin chain (or the Z_n -Belavin model) with antiperiodic boundary conditions or with off-diagonal boundary reflections. In the thermodynamic limit, there are sufficient degenerate points where the inhomogeneous Bethe ansatz equations reduce to the homogeneous ones. Based on them, we can study the ground state, elementary excitations and thermodynamic quantities. Furthermore, the thermodynamic results of antiperiodic $su(n)$ XYZ model can give the corresponding results of the antiperiodic $su(n)$ XXZ model which does not have degenerate points. We also expect that this method can be applied to other quantum integrable models.

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A Some elliptic theta functions

The elliptic θ -function is defined by

$$\theta \begin{bmatrix} a \\ b \end{bmatrix} (u, \tau) = \sum_m e^{\pi i(m+a)^2 \tau + 2\pi i(m+a)(u+b)}, \quad (\text{A.1})$$

where a and b are rational numbers, and τ is a generic complex number with $\text{Im}(\tau) > 0$. For convenience, we adopt the following notations

$$\begin{aligned} \theta_{11}(u) &= \theta \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} (u, \tau), & \theta_{10}(u) &= \theta \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} (u, \tau), \\ \theta_{00}(u) &= \theta \begin{bmatrix} 0 \\ 0 \end{bmatrix} (u, \tau), & \theta_{01}(u) &= \theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix} (u, \tau). \end{aligned} \quad (\text{A.2})$$

From the definition (A.1), we know that $\theta_{11}(u)$ is an odd function of u and $\theta_{10}(u)$, $\theta_{00}(u)$, $\theta_{01}(u)$ are the even functions of u . These functions are doubly quasi-periodic and satisfy

$$\begin{aligned} \theta_{11}(u+1) &= -\theta_{11}(u), & \theta_{11}(u+\tau) &= -e^{-2i\pi(u+\frac{\tau}{2})} \theta_{11}(u), \\ \theta_{10}(u+1) &= -\theta_{10}(u), & \theta_{10}(u+\tau) &= e^{-2i\pi(u+\frac{\tau}{2})} \theta_{10}(u), \\ \theta_{00}(u+1) &= \theta_{00}(u), & \theta_{00}(u+\tau) &= e^{-2i\pi(u+\frac{\tau}{2})} \theta_{00}(u), \\ \theta_{01}(u+1) &= \theta_{01}(u), & \theta_{01}(u+\tau) &= -e^{-2i\pi(u+\frac{\tau}{2})} \theta_{01}(u). \end{aligned} \quad (\text{A.3})$$

B Proof of relation (3.19)

It is convenient to introduce a series $\{y'_{-1}, y'_0, \dots, y'_l\}$ as

$$y'_{-1} = 1, \quad y'_0 = 0, \quad y'_k = y'_{k-2} + a_k y'_{k-1}, \quad k = 1, 2, \dots, l, \quad (\text{B.1})$$

where the integers a_k are given by eq. (3.8). Combining above definition and eqs. (3.10) and (3.18), we find

$$(-1)^t p_t = y'_{t-1} p_0 - y_{t-1}, \quad t = 0, 1, \dots, l+1, \quad (\text{B.2})$$

Thus the q_j given in (3.17) reads

$$q_j = \omega_j p_0 - n_j, \quad (\text{B.3})$$

where the integer $\omega_j = y'_{s-1} + (j - z_s)y'_s$ if $z_s \leq j < z_{s+1}$, $j = 1, 2, \dots, z_l$, and $\omega_{z_l+1} = y'_l$ if $j = z_l + 1$.

From eq. (3.17), we have $0 \leq (-1)^s q_j \leq p_s$ if $z_s \leq j < z_{s+1}$, which leads to

$$0 \leq (-1)^s \left(\omega_j - \frac{n_j}{p_0} \right) \leq \frac{p_s}{p_0}. \quad (\text{B.4})$$

The value of ω_j depends on the parity of s . If s is even, ω_j can be expressed as

$$\omega_j = \left\lfloor \frac{n_j}{p_0} \right\rfloor + 1, \quad z_s \leq j < z_{s+1}, \quad (\text{B.5})$$

Based on eqs. (B.4) and (B.5), we construct the inequality

$$\left\lfloor \frac{n_j}{p_0} \right\rfloor + 1 - \frac{p_s + 1}{p_0} \leq \frac{n_j - 1}{p_0} \leq \left\lfloor \frac{n_j}{p_0} \right\rfloor + 1 - \frac{1}{p_0}. \quad (\text{B.6})$$

The relation (3.18) with even $s \geq 2$ gives

$$0 \leq 1 - \frac{p_s + 1}{p_0} < 1. \quad (\text{B.7})$$

Taking the integer part of eq. (B.6) and using eq. (B.7), we obtain

$$\left\lfloor \frac{n_j - 1}{p_0} \right\rfloor = \left\lfloor \frac{n_j}{p_0} \right\rfloor. \quad (\text{B.8})$$

If $s = 0$, due to the fact $1 \leq n_j < p_0$ if $1 \leq j < z_1$, we have

$$\left\lfloor \frac{n_j - 1}{p_0} \right\rfloor = \left\lfloor \frac{n_j}{p_0} \right\rfloor = 0, \quad 1 \leq j < z_1. \quad (\text{B.9})$$

From the above discussions, we arrive at

$$\omega_j = \left\lfloor \frac{n_j - 1}{p_0} \right\rfloor + 1. \quad (\text{B.10})$$

If s is odd, eq. (B.4) tells us that

$$\omega_j = \left\lfloor \frac{n_j}{p_0} \right\rfloor. \quad (\text{B.11})$$

Based on (B.4) and (B.11), we construct the inequality

$$\left\lfloor \frac{n_j}{p_0} \right\rfloor - \frac{1}{p_0} \leq \frac{n_j - 1}{p_0} \leq \left\lfloor \frac{n_j}{p_0} \right\rfloor + \frac{p_s - 1}{p_0}. \quad (\text{B.12})$$

The relation (3.18) with odd $s \geq 3$ gives

$$-1 < \frac{p_s - 1}{p_0} < 0. \quad (\text{B.13})$$

Taking the integer part of eq. (B.12) and using (B.13), we obtain

$$\left\lfloor \frac{n_j - 1}{p_0} \right\rfloor = \left\lfloor \frac{n_j}{p_0} \right\rfloor - 1. \quad (\text{B.14})$$

If $s = 1$ and $z_1 < j < z_2$, based on eqs. (B.4) and (B.11), we construct another inequality

$$\left\lfloor \frac{n_j}{p_0} \right\rfloor - \frac{1}{p_0} \leq \frac{n_j - 1}{p_0} < \left\lfloor \frac{n_j}{p_0} \right\rfloor + \frac{p_1 - 1}{p_0}. \quad (\text{B.15})$$

Taking the integer part of eq. (B.15) and considering

$$\frac{p_1 - 1}{p_0} = 0, \quad (\text{B.16})$$

we obtain

$$\left\lfloor \frac{n_j - 1}{p_0} \right\rfloor = \left\lfloor \frac{n_j}{p_0} \right\rfloor - 1. \quad (\text{B.17})$$

If $s = 1$ and $j = z_1$, the $\omega_{z_1} = 0$ because of $q_{z_1} = -1$. Comparing (B.11), (B.14) and (B.17), we find that ω_j can also be written as (B.10). Then we arrive at the conclusion (3.19).

C Result for the periodic XYZ model

C.1 The system

In order to study the effect induced by twisted boundaries, we consider the XYZ spin chain (2.1) with periodic boundary condition (cf. (2.3))

$$\sigma_{N+1}^\alpha = \sigma_1^\alpha, \quad \alpha = x, y, z. \quad (\text{C.1})$$

In this case, the eigenvalue of the Hamiltonian (2.1) reads

$$E_p(\eta) = \frac{\sigma(\eta)}{\sigma'(0)} \left\{ \sum_{j=1}^M \left[\frac{\sigma'(\nu_j)}{\sigma(\nu_j)} - \frac{\sigma'(\mu_j + \eta)}{\sigma(\mu_j + \eta)} \right] + \frac{N}{2} \frac{\sigma'(\eta)}{\sigma(\eta)} + 2i\pi l_1 \right\}, \quad (\text{C.2})$$

where the $2M$ Bethe roots $\{\mu_j\}$ and $\{\nu_j\}$ should satisfy the BAEs

$$\begin{aligned} \left(\frac{N}{2} - M \right) \eta - \sum_{j=1}^M (\mu_j - \nu_j) &= l_1 \tau + m_1, \quad l_1, m_1 \in \mathbf{Z}, \\ M\eta + \sum_{j=1}^M (\mu_j + \nu_j) &= m_2, \quad m_2 \in \mathbf{Z}, \\ c_p e^{[2i\pi l_1(\mu_j + \eta)\mu_j + i\phi_p]} \sigma^{\bar{L}_1} \left(\mu_j + \frac{\eta}{2} \right) \sigma^N(\mu_j + \eta) &= \prod_{l=1}^M \sigma(\mu_j - \nu_l) \sigma(\mu_j - \nu_l + \eta), \\ c_p e^{-2i\pi l_1 \nu_j - i\phi_p} \sigma^{\bar{L}_1} \left(\nu_j + \frac{\eta}{2} \right) \sigma^N(\nu_j) &= - \prod_{l=1}^M \sigma(\nu_j - \mu_l) \sigma(\nu_j - \mu_l - \eta), \\ e^{i\phi_p} \prod_{j=1}^M \frac{\sigma(\mu_j + \eta)}{\sigma(\nu_j)} &= e^{\frac{2i\pi k_1}{N}}, \quad k_1 = 1, \dots, N. \end{aligned} \quad (\text{C.3})$$

Here c_p and ϕ_p are the constants, and the non-negative integer $\bar{L}_1$ satisfies the constraint

$$N + \bar{L}_1 = 2M. \quad (\text{C.4})$$

The BAEs (C.3) are derived from the inhomogeneous $T-Q$ relation [11]. If the system size N is even, detailed analysis of eq. (C.3) shows that either $\mu_j = \nu_l$ or $\mu_j = \nu_l - \eta$ leads to $c_p = 0$ and hence induces a one-to-one correspondence between Bethe roots $\{\mu_j\}$ and $\{\nu_l\}$, which means only one set of Bethe roots is survived. Therefore, for a generic η , if we require

$$l_1 = 0, \quad N = 2M, \quad \{\mu_j\} = \{\nu_l\}, \quad (\text{C.5})$$

then $c_p = 0$ and the BAEs reduce to the conventional ones, which are consistent with the results given in references [6–8]. That is the reason why the periodic XYZ model with even N has been studied extensively. However, if the system size N is odd, this conclusion is not true for a generic η . The correct statement is that only at following discrete points of crossing parameter η

$$\bar{\eta}_{m_1, l_1} = \frac{2l_1}{N - 2M}\tau + \frac{2m_1}{N - 2M}, \quad l_1, m_1 \in \mathbf{Z}, \quad (\text{C.6})$$

the parameter $c_p = 0$ thus the BAEs (C.3) can reduce to the conventional ones. Here we consider the case that η is real, which can be achieved by putting $l_1 = 0$. Without losing generality, we also put $M = N$ and $m_1 = -m$. Then the degenerate points (C.6) becomes

$$\bar{\eta}_m = \frac{2m}{N}, \quad m \in \mathbf{Z}, \quad (\text{C.7})$$

and the reduced BAEs are

$$\begin{aligned} e^{2i\phi_p} \frac{\sigma^N[\frac{i}{2}(x_j - \bar{\eta}_m i)]}{\sigma^N[\frac{i}{2}(x_j + \bar{\eta}_m i)]} &= \prod_{k \neq j}^N \frac{\sigma[\frac{i}{2}(x_j - x_k - 2\bar{\eta}_m i)]}{\sigma[\frac{i}{2}(x_j - x_k + 2\bar{\eta}_m i)]}, \quad j = 1, \dots, N, \\ e^{i\phi_p} \prod_{j=1}^N \frac{\sigma[\frac{i}{2}(x_j - \bar{\eta}_m i)]}{\sigma[\frac{i}{2}(x_j + \bar{\eta}_m i)]} &= e^{\frac{2i\pi k_1}{N}}, \quad k_1 = 1, \dots, N, \end{aligned} \quad (\text{C.8})$$

where $\{x_j\}$ are the Bethe roots in the degenerate cases. Accordingly, we obtain the eigenvalue of system at the degenerate points as

$$E_p(\bar{\eta}_m) = \frac{\sigma(\bar{\eta}_m)}{\sigma'(0)} \left\{ \sum_{j=1}^N \left[\frac{\sigma'[\frac{i}{2}(x_j + \bar{\eta}_m i)]}{\sigma[\frac{i}{2}(x_j + \bar{\eta}_m i)]} - \frac{\sigma'[\frac{i}{2}(x_j - \bar{\eta}_m i)]}{\sigma[\frac{i}{2}(x_j - \bar{\eta}_m i)]} \right] + \frac{N}{2} \frac{\sigma'(\bar{\eta}_m)}{\sigma(\bar{\eta}_m)} \right\}. \quad (\text{C.9})$$

Using the same idea as suggested previously, we first solve the reduced BAEs (C.8) and obtain the exact results at the degenerate points $\bar{\eta}_m$. Then we extrapolate these results to the real η case. Here, we only list the main results and neglect all the detailed treatment. Due to the fact that $\bar{\eta}_m$ is real, in the present case, the strings in the complex plane are parallel to the imaginary axis and are symmetric around the real axis or the $y = i$ line, which is shown in figure 6. We consider the same region $0 < \bar{\eta}_m \leq \frac{1}{2}$ as before.

Figure 6. Strings on the complex plane for $\bar{\eta}_m = \frac{2m}{N} = \frac{10}{73}$. The strings are arranged from left to right in the order of string length determined by eq. (3.11). The blue dashed line is given by shifting the real axis up by unit. We see the strings are symmetric distribute around the real axis or the blue dashed line.

C.2 Ground state

Repeating the similar calculation with antiperiodic case, we obtain the ground state energy of XYZ model with odd N as

$$E_{p,g}^{\text{odd}}(\eta) = e_0(\eta)N + \epsilon_h\left(\frac{\tau}{i}, \eta\right). \quad (\text{C.10})$$

Here $e_0(\eta)$ is the ground state energy density which is given by eq. (3.32) after replacing the η_m by η . $\epsilon_h(x^h, \eta)$ is the energy of hole at the point of x^h , which can be obtained by replacing η_m in eq. (3.43) with η . Obviously, the function $\epsilon_h(x^h, \eta)$ takes its minimum value if $x^h = \tau/i$.

Comparing eqs. (C.10) and (4.10), we find that the ground state energy of XYZ model with periodic boundary condition equals to that with antiperiodic one. It is reasonable because that there is only one bound is twisted in Hamiltonian (2.1). In the thermodynamic limit, it is hard that the twisted bound can affect the energy of whole system. However, the twisted bound can affect the eigenstates. The eigenstates of periodic and that of antiperiodic are totally different.

Now, we check the formula (C.10) by the exact diagonalization. Define

$$\delta_p^{\text{odd}} = \frac{E_{p,g}^{\text{odd}}(\eta)}{\bar{E}_{p,g}^{\text{odd}}(\eta)} - 1, \quad (\text{C.11})$$

where $E_{p,g}^{\text{odd}}(\eta)$ is the ground state energy obtained by eq. (C.10) and $\bar{E}_{p,g}^{\text{odd}}(\eta)$ is the ground state energy obtained by the exact diagonalization. In table 4, we list the numerical results with $\tau = 0.5i$ and $\eta = 0.4$. We find that the deviation δ_p^{odd} is about 10^{-4} if $N = 25$, which means that eq. (C.10) is still valid for the finite system size provided that N is not too small. In figure 7, the δ_p^{odd} for various N with $\tau = 0.5i$ and $\eta = \sqrt{2}/4$ are shown. The data can be fitted as power law

$$\delta_p^{\text{odd}} = \alpha_5 N^{\beta_5}. \quad (\text{C.12})$$

N	$\bar{E}_{p,g}^{\text{odd}}$	$E_{p,g}^{\text{odd}}$	$\delta_p^{\text{odd}} (\times 10^{-2})$
5	-4.0730	-4.2577	4.5353
7	-6.4903	-6.5909	1.5507
9	-8.8616	-8.9241	0.7057
11	-11.2149	-11.2573	0.3779
13	-13.5600	-13.5905	0.2253
15	-15.9007	-15.9237	0.1449
17	-18.2389	-18.2569	0.0986
19	-20.5757	-20.5901	0.0701
21	-22.9115	-22.9233	0.0516
23	-25.2467	-25.2565	0.0391
25	-27.5814	-27.5897	0.0303

Table 4. The numerical results of periodic XYZ model with $\eta = 0.4$ and $\tau = 0.5i$. Here, $\bar{E}_{p,g}^{\text{odd}}$ is the ground state energy obtained by the exact diagonalization, $E_{p,g}^{\text{odd}}$ is the ground state energy obtained by eq. (C.10), and δ_p^{odd} is the deviation.

Figure 7. The deviation δ_p^{odd} versus the system-size N . The data can be fitted as $\delta_p^{\text{odd}} = \alpha_5 N^{\beta_5}$. Here $\tau = 0.5i$, $\eta = \frac{\sqrt{2}}{4}$, $\alpha_5 = 8.225$ and $\beta_5 = -3.045$. Due to the fact $\beta_5 < 0$, the deviation $\delta_p^{\text{odd}} \rightarrow 0$ when $N \rightarrow \infty$.

Due to the fact $\beta_5 < 0$, the value δ_p^{odd} tends to zero when the system size $N \rightarrow \infty$, which indicates that eq. (C.10) can describe the ground state energy in the thermodynamic limit.

The ground state energy with even N is

$$E_{p,g}^{\text{even}}(\eta) = e_0(\eta)N. \quad (\text{C.13})$$

Comparing eqs. (C.13) and (4.13), we find that the ground state energy with periodic boundary condition and that with antiperiodic one are the same.

C.3 Elementary excitation

Repeating the similar calculation with antiperiodic case, we obtain the energy of hole excitation with odd N

$$\Delta E_p^{\text{odd}}(x^h, \eta) = \epsilon_h(x^h, \eta) - \epsilon_h\left(\frac{\tau}{i}, \eta\right). \quad (\text{C.14})$$

Figure 8. The energy of hole excitation $\Delta E_{p,e}^{\text{odd}}$ versus the system-size N . The data can be fitted as $\Delta E_{p,e}^{\text{even}} = \alpha_6 N^{\beta_6}$. Here $\tau = 0.5i$, $\eta = \frac{\sqrt{2}}{4}$, $\alpha_6 = 41.18$ and $\beta_6 = -1.899$. Due to the fact $\beta_6 < 0$, the ΔE_e^{odd} tends to zero when $N \rightarrow \infty$.

In the thermodynamic limit, the position of hole x^h can tend to τ/i infinitely, thus

$$\Delta E_p^{\text{odd}}(\eta) = \lim_{x^h \rightarrow \frac{\tau}{i}} \Delta E_p^{\text{odd}}(x^h, \eta) \rightarrow 0. \quad (\text{C.15})$$

Now, we check the analytical result (C.15) by the DMRG method. The numerical results, denoted as $\Delta E_{p,e}^{\text{odd}}$, with $\tau = 0.5i$ and $\eta = \sqrt{2}/4$ are shown in figure 8. The data are fitted as

$$\Delta E_{p,e}^{\text{odd}} = \alpha_6 N^{\beta_6}. \quad (\text{C.16})$$

Due to the fact $\beta_6 < 0$, the $\Delta E_{p,e}^{\text{odd}}$ tends to zero when the system size $N \rightarrow \infty$, which is consistent with eq. (C.15). Comparing eqs. (C.15) and (4.17), we also find that the excitation energy with periodic boundary condition is the same as that with antiperiodic one.

The hole excitation with even N has a gap

$$\Delta E_p^{\text{even}}(\eta) = 2\epsilon_h \left(\frac{\tau}{i}, \eta \right). \quad (\text{C.17})$$

Comparing eqs. (C.17) and (4.20), we find that the gap with periodic boundary condition is the same as that with antiperiodic one. Now, we check the analytic result (C.17) by the DMRG method. The numerical results, denoted as $\Delta E_{p,e}^{\text{even}}$, with $\tau = 0.5i$ and $\eta = \sqrt{2}/4$ are given in figure 9. The data can be fitted as

$$\Delta E_{p,e}^{\text{even}} = \alpha_7 N^{\beta_7} + \epsilon_7. \quad (\text{C.18})$$

Due to the fact $\beta_7 < 0$, in the thermodynamic limit, ϵ_7 gives the energy gap. The DMRG data give $\epsilon_7 = 2.548$, which is highly consistent with the analytical results (4.21). We note that although the values of fitting factors α_7 and β_7 in (C.18) are different from that of α_4 and β_4 in (4.22), the energy gap $\epsilon_7 = \epsilon_4$.

Finally, let us remark that by taking the limit $\tau \rightarrow i\infty$ of above results, one can easily obtain corresponding results for the periodic XXZ spin chain.

Figure 9. The energy of hole excitation $\Delta E_{p,e}^{\text{even}}$ versus the system-size N . The data can be fitted as $\Delta E_{p,e}^{\text{even}} = \alpha_7 N^{\beta_7} + \epsilon_7$. Here $\tau = 0.5i$, $\eta = \frac{\sqrt{2}}{4}$, $\alpha_7 = 14.71$, $\beta_7 = -1.668$ and $\epsilon_7 = 2.548$. Due to the fact $\beta_7 < 0$, in the thermodynamic limit, ϵ_7 gives the gap, i.e., $\epsilon_7 = \Delta E_p^{\text{even}}(\eta)$.

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