Thermodynamic limit and twisted boundary energy of the XXZ spin chain with antiperiodic boundary condition

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Abstract

We investigate the thermodynamic limit of the inhomogeneous $T-Q$ relation of the antiferromagnetic XXZ spin chain with antiperiodic boundary condition. It is shown that the contribution of the inhomogeneous term at the ground state can be neglected when the system-size $N$ tends to infinity, which enables us to reduce the inhomogeneous Bethe ansatz equations (BAEs) to the homogeneous ones. Then the quantum numbers at the ground states are obtained, by which the system with arbitrary size can be studied. We also calculate the twisted boundary energy of the system.

Keywords: XXZ Spin chain; Bethe ansatz; T-Q relation

1 Introduction

The XXZ spin chain with the antiperiodic boundary condition (or the twist boundary condition) is a very interesting quantum system\cite{1,2,3,4}. By using the Jordan-Wigner transformation, the model can describe a p-wave Josephson junction embedded in a spinless Luttinger liquid\cite{5,6,7}. Although there exists a twisted bound at the boundary which breaks the usual $U(1)$-symmetry of the bulk system (or the closed chain case)\cite{8}, it can be proved that the system is still integrable. By using the off-diagonal Bethe ansatz (ODBA) method\cite{9,10,11}, the exact solution of the model was obtained\cite{9}, which is described by an inhomogeneous $T-Q$ relation (c.f. the ordinary homogeneous $T-Q$ one\cite{12,13}). Such an inhomogeneous $T-Q$ relation has played a universal role to describe the eigenvalue of the transfer matrix for quantum integrable systems\cite{8}. However, due to the fact that Bethe roots should satisfy the inhomogeneous Bethe ansatz equations (BAEs), it is hard to study the thermodynamic properties\cite{14} of the corresponding systems\cite{15,16,17}.

Based on an intelligent trick, the thermodynamic limit of the spin-$\frac{1}{2}$ XXZ chain with the generic off-diagonal boundary terms in the gapless region (i.e., the isotropic parameter $\eta$ in\cite{21} below being an imaginary number) was succeeded in obtaining\cite{18}. The most important observation in the paper is that the contribution of the inhomogeneous term at the ground state, in the gapless region, can be neglected when the system-size $N$ tends to infinity. Such a fact has been confirmed recently by the studies of other integrable models\cite{19,20,21,22} whose eigenvalue of the transfer matrix is given in terms of the inhomogeneous $T-Q$ relation.

In this paper, we propose a method to study the thermodynamic limit of the XXZ spin chain with the twist boundary condition at the antiferromagnetic region (i.e., $\eta$ being a real number). We first study the
contribution of the inhomogeneous term with finite system-size \( N \). We find that the contribution of the inhomogeneous term in the associated \( T-Q \) relation to the ground state energy can be neglected when the system-size \( N \) tends to infinity. Because we consider the massive region of the system, the ground state energy with even \( N \) and that with odd \( N \) are different. The value of energy difference is proportional to the energy of one bond. We also check our results by using the density matrix renormalization group (DMRG) method, which leads to that the numerical results and the analytic one are consistent with each other very well. As a consequence, the twist boundary energy is then calculated.

The paper is organized as follows. In the next section, the model and the associated ODBA solutions are introduced. In section 3, we study the finite-size effects of contribution of the inhomogeneous term in the \( T-Q \) relation at the ground state energy. The thermodynamic limit of the XXZ spin chain with antiperiodic and with periodic boundary conditions are discussed in section 4 and section 5, respectively. The twisted boundary energy is given in Section 6. Section 7 is the concluding remarks and discussions.

2 The model and its ODBA solution

The spin-\( \frac{1}{2} \) XXZ quantum chain is described by the Hamiltonian

\[
H = \sum_{j=1}^{N} \left[ \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \cosh \eta \sigma_j^z \sigma_{j+1}^z \right],
\]

where the anti-periodic boundary condition reads \( \sigma_{N+1}^a = \sigma_1^a \sigma_2^a \sigma_3^a \) (\( \alpha = x, y, z \)), and \( \sigma_0^a \) is the Pauli matrix. For such a topological boundary condition, the spin on the \( N \)th site couples with that on the first site after rotating by an angle \( \pi \) along the \( x \)-direction (a kink on the \( (N, 1) \) bond) and the system forms a torus in the spin space. This kink could be smoothly shifted to the \( (j, j+1) \) bond without changing the energy spectrum. That is to say that the Hamiltonian is unchanged with the transformation

\[
U_j^x = \prod_{l=1}^{j} \sigma_l^x, \quad H = [U_j^x]^{-1} HU_j^x.
\]

Due to the fact \([H, U_j^x] = 0\), the model possesses a global \( Z_2 \) invariance. Note that the braiding occurs in the quantum space rather than in the real space. Therefore, the model describes a quantum Möbius strip.

The integrability of the model (2.1) is associated with the well-known six-vertex \( R \)-matrix

\[
R_{0,j}(u) = \frac{1}{2} \left[ \frac{\sinh(u + \eta)}{\sinh \eta} (1 + \sigma_j^x \sigma_0^z) + \frac{\sinh u}{\sinh \eta} (1 - \sigma_j^z \sigma_0^z) \right] + \frac{1}{2} (\sigma_j^x \sigma_0^x + \sigma_j^y \sigma_0^y),
\]

where \( u \) is the spectral parameter and \( \eta \) is the crossing parameter (or isotropic parameter). The \( R \)-matrix satisfies the Yang-Baxter equation

\[
R_{12}(u-v)R_{13}(u)R_{23}(v) = R_{23}(v)R_{13}(u)R_{12}(u-v),
\]

and possesses the properties:

Initial condition: \( R_{12}(0) = P_{1,2} \),

Unitarity: \( R_{12}(u)R_{21}(-u) = -\frac{\sinh(u + \eta) \sinh(u - \eta)}{\sinh^2 \eta} \times \text{id} \),

Crossing relation: \( R_{12}(u) = -\sigma^y_1 R_{1,2} t_{1,2} \sigma^y_1 \),

\( Z_2 \)-symmetry: \( \sigma^a_1 \sigma^a_2 R_{1,2}(u) = R_{1,2}(u) \sigma^a_1 \sigma^a_2 \), \quad \text{for } \alpha = x, y, z,

where \( P_{1,2} \) is the permutation operator, and \( t_i \) denotes the transposition in the \( i \)th space. Here and below we adopt the standard notations: for any matrix \( A \in \text{End}(C^2) \), \( A_i \) is an embedding operator in the tensor space.
space $C^2 \otimes C^2 \otimes \cdots$, which acts as $A$ on the $i$-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.

The associated monodromy matrix is given as

$$T_0(u) = \sigma_0^\circ R_{0,N}(u - \theta_N) \cdots R_{0,1}(u - \theta_1) = \begin{pmatrix} C(u) & D(u) \\ A(u) & B(u) \end{pmatrix}. \quad (2.9)$$

Because of the $Z_2$-symmetry (2.8), the following relation holds

$$R_{0,\bar{0}}(u - v)T_0(u)T_0(v) = T_0(v)T_0(u)R_{0,\bar{0}}(u - v), \quad (2.10)$$

which directly gives rise to the fact that

$$[t(u), t(v)] = 0, \quad (2.11)$$

where the transfer matrix $t(u)$ is defined as

$$t(u) = tr_0 T_0(u) = B(u) + C(u). \quad (2.12)$$

The first order derivative of the logarithm of the transfer matrix gives the Hamiltonian (2.1)

$$H = 2 \sinh \eta \frac{\partial \ln t(u)}{\partial u} \big|_{u=0, \theta_j=0} - N \cosh \eta.$$  

(2.13)

This ensures the integrability of the model.

By means of the off-diagonal Bethe ansatz method, the eigenvalues $\Lambda(u)$ of the transfer matrix $t(u)$ is given by the inhomogeneous $T - Q$ relation [8]

$$\Lambda(u) = e^u a(u) Q(u - \eta) - e^{-u - \eta} d(u) \frac{Q(u + \eta)}{Q(u)} - c(u) a(u) d(u) \frac{1}{Q(u)}, \quad (2.14)$$

where $Q(u)$ is a trigonometric polynomial of the type

$$Q(u) = \prod_{j=1}^N \frac{\sinh(u - \lambda_j)}{\sinh \eta}, \quad (2.15)$$

and

$$d(u) = a(u - \eta) = \prod_{j=1}^N \frac{\sinh(u - \theta_j)}{\sinh \eta}, \quad (2.16)$$

$$c(u) = e^{u - N \eta + \sum_{j=1}^N (\theta_j - \lambda_j)} - e^{-u - \eta - \sum_{j=1}^N (\theta_j - \lambda_j)}. \quad (2.17)$$

The $N$ parameters $\{\lambda_j\}$ in Eq. (2.15) should satisfy the associated BAEs

$$e^{\lambda_j} a(\lambda_j) Q(\lambda_j - \eta) - e^{-\lambda_j - \eta} d(\lambda_j) Q(\lambda_j + \eta) - c(\lambda_j) a(\lambda_j) d(\lambda_j) = 0, \quad j = 1, \cdots , N. \quad (2.18)$$

The eigenvalue of the Hamiltonian (2.1) is then expressed in terms of the associated Bethe roots as

$$E = 2 \sinh \eta \frac{\partial \ln \Lambda(u)}{\partial u} \big|_{u=0, \theta_j=0} - N \cosh \eta \quad = \quad -2 \sinh \eta \sum_{j=1}^N \left[ \coth(\lambda_j + \eta) - \coth(\lambda_j) \right] + N \cosh \eta + 2 \sinh \eta,$$

(2.19)
where the Bethe roots \{\lambda_j\} should satisfy the inhomogeneous Bethe ansatz equations (BAEs) (2.18), namely,

\[
\begin{align*}
&\sum_{k=1}^{N} \frac{\sinh(\lambda_j - \lambda_k - \eta)}{\sinh(\lambda_j)} - \sum_{k=1}^{N} \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j + \eta)} \\
&\quad - \left[ e^{\lambda_j - N\eta - \sum_{k=1}^{N} \lambda_k} - e^{-\lambda_j - \eta + \sum_{k=1}^{N} \lambda_k} \right] = 0.
\end{align*}
\]

(2.20)

The numerical simulation implies that the inhomogeneous BAEs (2.20) indeed give the correct and complete spectrum of the model [8].

3 Finite-size effects

In this paper, we consider the massive region with a real \(\eta\). In order to study the contribution of the inhomogeneous term [the last term in Eq. (2.14)] to the ground state energy, we first introduce a homogeneous \(T-Q\) relation as

\[
\Lambda_{\text{hom}}(u) = e^{u} a(u) \frac{Q_1(u - \eta)}{Q_1(u)} - e^{-u - \eta} d(u) \frac{Q_1(u + \eta)}{Q_1(u)},
\]

(3.1)

where

\[
Q_1(u) = \prod_{i=1}^{M} \sinh(u - \lambda_i).
\]

(3.2)

It should be remarked that the number of Bethe roots in Eq. (3.1) \(N\) is reduced to \(M\) (\(M \leq N\)). The singular analyzing of the \(T-Q\) relation (3.1) gives rise to homogeneous BAEs

\[
e^{2\lambda_j + \eta} \frac{\sinh^{N}(\lambda_j + \eta)}{\sinh^{N}(\lambda_j)} = \prod_{k=1}^{M} \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)}.
\]

(3.3)

Putting \(\lambda_j = \frac{\eta}{2}(ix_j - 1)\), we obtain

\[
e^{i\eta x_j} \frac{\sin^{N}\frac{\eta}{2}(x_j - i)}{\sin^{N}\frac{\eta}{2}(x_j + i)} = \prod_{k=1}^{M} \frac{\sin^{\frac{\eta}{2}}(x_j - x_k - 2i)}{\sin^{\frac{\eta}{2}}(x_j - x_k + 2i)}.
\]

(3.4)

Taking the logarithm of Eq. (3.4), we have

\[
\eta x_j + N\theta_1(x_j) = 2\pi I_j + \sum_{k=1}^{M} \theta_2(x_j - x_k),
\]

(3.5)

where

\[
\theta_m(x) = 2 \arctan \frac{\tan \frac{\eta x}{2}}{\tanh \frac{\eta m}{2}} + 2\pi \left[ \frac{\eta x + \pi}{2\pi} \right].
\]

(3.6)

Here the notation \([ \ ]\) represents the Gauss Mark, and the quantum number \{\(I_j\)\} are certain integers (half odd integers) for \(N - M\) even (\(N - M\) odd). Corresponding to Eq. (2.19), we define

\[
E_{\text{hom}} = 2 \sinh \eta \frac{\partial \ln \Lambda_{\text{hom}}(u)}{\partial u} \bigg|_{u=0} - N \cosh \eta
\]

\[
= -4 \sinh \eta \sum_{j=1}^{M} \frac{\sinh \eta}{\cosh \eta - \cos(\eta x_j)} + N \cosh \eta + 2 \sinh \eta.
\]

(3.7)

Now, we define the contribution of the inhomogeneous term to the ground state energy as

\[
E^{\eta}_{\text{inh}} = E^{\eta}_{\text{hom}} - E^{\eta},
\]

(3.8)
where $E^g$ is the ground state energy of the Hamiltonian (2.1) obtained from Eq. (2.19) and $E^g_{hom}$ is the minimal energy calculated by Eqs. (3.7) and (3.5).

Because we consider the massive region, the thermodynamic limit of the system with even $N$ and that with odd $N$ are different. We first study the contribution of inhomogeneous term $E^g_{inh}$ with even $N$. In this case, $M = \frac{N}{2}$, and all the Bethe roots in Eq. (3.5) are real and are determined completely by the quantum number

$$I_j = -\frac{M}{2} + 1, -\frac{M}{2} + 2, \ldots, \frac{M}{2}. \quad (3.9)$$

Substituting the values of Bethe roots into Eq. (3.7), we obtain the value of $E^g_{hom}$. From Eq. (3.8), the contribution of the inhomogeneous term can be calculated and the results are shown in Fig. 1. From the fitting, we find that $E^g_{inh}$ and $N$ satisfy the power law

$$\frac{1}{\cosh \eta} E^g_{inh}(N) = a_1 N^{b_1}. \quad (3.10)$$

Due to the fact that $b_1 < 0$, the value of $E^g_{inh}$ tends to zero when the system-size $N$ tends to infinity, which means that the contribution of the inhomogeneous term at the ground state can be neglected in the thermodynamic limit.

For the odd $N$, we consider the case $M = \frac{N+1}{2}$ in which all the Bethe roots are real. The $E^g_{hom}$ can be calculated by Eq. (3.7) where the Bethe roots in Eq. (3.5) are completely determined by the quantum number

$$I_j = -\frac{M-1}{2}, -\frac{M-1}{2} + 1, \ldots, \frac{M-1}{2}. \quad (3.11)$$

The contributions of the inhomogeneous term are shown in Fig. 2. From the fitting, we find that $E^g_{inh}$ and $N$ satisfy the exponential law

$$\frac{1}{\cosh \eta} E^g_{inh}(N) = a_2 e^{b_2 N}. \quad (3.12)$$

Again, due to the fact that $b_2 < 0$, the value of $E^g_{inh}$ tends to zero when $N \to \infty$. Therefore, the contribution of the inhomogeneous term at the ground state can be neglected in the thermodynamic limit.

Through above finite-size scaling analysis, we conclude that the contribution of the inhomogeneous term at the ground state energy can be neglected when $N \to \infty$. The similar results have also been obtained [22]. Therefore, the reduced BAEs (3.4) and the Eq. (3.7) can be use to calculate the ground state energy of the system (2.1) in the thermodynamic limit.

From Figs. 1 and 2, we also find that $E^g_{inh} > 0$ for the even $N$ case and $E^g_{inh} < 0$ for the odd $N$ case. Which means that $E_{hom}$ is larger than the actual value for the even $N$ case while $E_{hom}$ is smaller than the actual value for the odd $N$ case.
Figure 2: The contribution of the inhomogeneous term to the ground state energy \( \frac{1}{\cosh \eta} E_{\text{inh}}^g \) versus the odd system-size \( N \). The data can be fitted as \( \frac{1}{\cosh \eta} E_{\text{inh}}^g (N) = a_2 e^{b_2 N} \). Here (a) \( \eta = 2, a_2 = -0.2042 \) and \( b_2 = -0.3658 \); (b) \( \eta = 3, a_2 = -0.1828 \) and \( b_2 = -0.8585 \). Due to the fact \( b_2 < 0 \), when the \( N \) tends to infinity, the contribution of the inhomogeneous term tends to zero.

4 The thermodynamic limit

Now, we consider the thermodynamic limit of the system. For convenience, we define the counting function

\[
Z_t(x) = \frac{1}{2π} \left[ \frac{\eta x}{N} + \theta_1(x) - \frac{1}{N} \sum_{k=1}^{M} \theta_2(x - x_k) \right].
\] (4.1)

In the thermodynamic limit, \( N \to \infty \), \( M \to \infty \) and \( N/M \) takes the finite value. Taking the derivative of Eq. (4.1) with respect to \( x \), we obtain

\[
\frac{dZ_t(x)}{dx} = \frac{\eta}{2\pi N} + a_1(x) - \int_{-Q}^{Q} a_2(x - y) \rho(y) dy
\equiv \rho(x) + \rho^h(x),
\] (4.2)

and

\[
a_m(x) = \frac{1}{2\pi} \frac{\partial \theta_m(x)}{\partial x} = \frac{\eta}{2\pi} \frac{\sinh(m\eta)}{\cosh(m\eta) - \cos(\eta x)},
\] (4.3)

where \( Q \) is chosen as \( \pi/\eta \), \( \rho(x) \) and \( \rho^h(x) \) are the densities of particles and holes, respectively. For the arbitrary periodic function \( f(x), x \in [-Q, Q] \), we introduce the Fourier transformation

\[
\hat{f}(k) = \int_{-Q}^{Q} f(x) e^{-ikx} dx,
\] (4.4)

\[
f(x) = \frac{1}{2Q} \sum_{k=-\infty}^{\infty} \hat{f}(k) e^{ikx}, \quad k = \cdots, -2, -1, 0, 1, 2, \cdots.
\] (4.5)

Taking the Fourier transformation of Eq. (4.2), we obtain

\[
\hat{\rho}(k) + \hat{\rho}^h(k) = \frac{1}{N} \delta_{k,0} + \hat{a}_1(k) - \hat{a}_2(k) \hat{\rho}(k),
\] (4.6)

where

\[
\hat{a}_m(k) = e^{-m|\eta|}.
\] (4.7)

Then we have

\[
\hat{\rho}(k) = \frac{1}{e^{\eta|k|} + e^{-\eta|k|}} + \frac{\delta_{k,0}}{N} \frac{\delta_{k,0}}{1 + e^{-2\eta|k|}} - \frac{\hat{\rho}^h(k)}{1 + e^{-2\eta|k|}}.
\] (4.8)
In the thermodynamic limit, the eigenvalue (3.7) can be expressed by the density of particles as

\[ E_{\text{hom}} = E = -\frac{8\pi}{\eta}N \sinh \eta \int_{-Q}^{Q} a_1(x) \rho(x) dx + N \cosh \eta + 2 \sinh \eta. \]  (4.9)

For the even \( N \) case, we have \( M = \frac{N}{2} \) at the ground state. Thus the following equation must hold

\[ \frac{M}{N} = \int_{-Q}^{Q} \rho(x) dx = \bar{\rho}(0) = \frac{1}{2}. \]  (4.10)

From Eqs. (4.8) and (4.10), we find that at the ground state, there exists one hole at \( x_0 \in [-\frac{\pi}{\eta}, \frac{\pi}{\eta}] \). The density of holes is given by

\[ \rho^h(x) = \frac{1}{N} \delta(x - x_0). \]  (4.11)

With the Fourier transformation, we have

\[ \tilde{\rho}^h(k) = \frac{1}{N} e^{-ikx_0}. \]  (4.12)

Thus the solution of (4.12) can be derived as

\[ \tilde{\rho}(k) = \frac{1}{e^{\eta k} + e^{-\eta k}} + \frac{1}{N} \frac{\delta_{k,0}}{1 + e^{2\eta k}} - \frac{1}{N} \frac{e^{-ikx_0}}{1 + e^{-2\eta k}}. \]  (4.13)

With the help of Eqs. (4.11) and (4.13), we obtain

\[ E^{\text{even}} = \left( -8 \sinh \eta \sum_{k=1}^{\infty} \frac{1}{1 + e^{2\eta k}} - 2 \sinh \eta + \cosh \eta \right) N + 4 \sinh \eta \sum_{k=-\infty}^{\infty} \frac{e^{ikx_0}}{2 \cosh(\eta k)} \]
\[ = e_0 N + e_h(x_0), \]  (4.14)

where \( e_0 \) is exactly the density of ground state energy of the XXZ spin chain with periodic boundary condition

\[ e_0 = -8 \sinh \eta \sum_{k=1}^{\infty} \frac{1}{1 + e^{2\eta k}} - 2 \sinh \eta + \cosh \eta, \]  (4.15)

and \( e_h(x_0) \) is the energy carried by one hole as

\[ e_h(x_0) = 4 \sinh \eta \sum_{k=-\infty}^{\infty} \frac{e^{ikx_0}}{2 \cosh(\eta k)}. \]  (4.16)

At the ground state, the position of hole should be put at \( x_0 = \frac{\pi}{\eta} \) to minimize the energy. Thus the ground state energy in the thermodynamic limit can be written as

\[ E^{g,\text{even}} = e_0 N + e_h\left(\frac{\pi}{\eta}\right). \]  (4.17)

For the odd \( N \) case, we consider the case that \( M = \frac{N+1}{2} \) at the ground state. Thus the following equation must hold

\[ \frac{M}{N} = \int_{-Q}^{Q} \rho(x) dx = \bar{\rho}(0) = \frac{1}{2} + \frac{1}{2N}. \]  (4.18)

Such a configuration gives that there is no hole and the ground state is completely determined by the density of particles

\[ \tilde{\rho}(k) = \frac{1}{e^{\eta k} + e^{-\eta k}} + \frac{1}{N} \frac{\delta_{k,0}}{1 + e^{-2\eta k}}. \]  (4.19)
With the help of Eqs. (4.9) and (4.19), we have

\[ E_{g,\text{odd}} = \left( -8 \sinh \eta \sum_{k=1}^{\infty} \frac{1}{1 + e^{2\eta k}} - 2 \sinh \eta + \cosh \eta \right) N \]

\[ = e_0 N. \]  

(4.20)

with \( e_0 \) defined as (4.15).

From the above calculation, we find that the ground state energy of the XXZ spin torus with even \( N \) and that with odd \( N \) are different. This is consistent with the fact that we consider the antiferromagnetic coupling and the massive region of the model (2.1), i.e., \( \Delta = \cosh \eta \geq 1 \) with real \( \eta \). The values of \( e_0 \) and \( e_h(\pi/\eta) \) have the same order. In the thermodynamic limit, the most contributions come from \( e_0 N \) and the \( e_h(\pi/\eta) \) can be neglected. Thus the thermodynamic quantities calculated by the density of ground state energy \( e_0 \) do no depend on the even or odd of \( N \). However, in this paper, we focus on the effects induced by the boundary degree of freedom, thus the contribution of \( e_h(\pi/\eta) \) can not be neglected. If \( \eta \to 0 \), then \( e_h(\pi/\eta) \to 0 \).

5 The thermodynamic limit of the periodic XXZ spin chain

In order to study the effects induced by the twisted boundary, now we should study the thermodynamic limit of the XXZ spin chain with periodic boundary condition. The model Hamiltonian reads

\[ H_p = \sum_{j=1}^{N} \left[ \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \cosh \eta \sigma_j^z \sigma_{j+1}^z \right], \]  

(5.1)

with the constraint \( \sigma_{N+1}^N = \sigma_1^1 \). We consider the same case that \( \eta \) is real, thus the eigenvalues of the Hamiltonian (5.1) is

\[ E_p = -4 \cdot \sinh \eta \sum_{j=1}^{M} \frac{\sinh \eta}{\cosh \eta - \cos(\eta x_j)} + N \cosh \eta, \]

(5.2)

where the \( M \) Bethe roots \( \{x_j\} \) are determined by the BAEs [14]

\[ \frac{\sin^N \frac{\pi}{2}(x_j - i)}{\sin^N \frac{\pi}{2}(x_j + i)} = -\prod_{k=1}^{M} \frac{\sin \frac{\pi}{2}(x_j - x_k - 2i)}{\sin \frac{\pi}{2}(x_j - x_k + 2i)}. \]

(5.3)

Taking the logarithm of Eq. (5.3), we have

\[ N \theta_1(x_j) = 2\pi I_j + \sum_{k=1}^{M} \theta_2(x_j - x_k), \]

(5.4)

where \( \{I_j\} \) are certain integers (half odd integers) for \( N - M \) odd (\( N - M \) even). For convenience, we define the counting function

\[ Z_p(x) = \frac{1}{2\pi} \left[ \theta_1(x) - \frac{1}{N} \sum_{k=1}^{M} \theta_2(x - x_k) \right]. \]

(5.5)

Obviously, \( Z_p(x_j) = \frac{I_j}{N} \) corresponds to the Eq. (5.4) and it will turn to be a continuous function in the thermodynamic limit. When \( N \to \infty \) and \( M \to \infty \), the distribution of Bethe roots are continuous, i.e., \( Z_p(x_j) = Z_p(x) \). Taking the derivative of Eq. (5.5) with respect to \( x \), we obtain

\[ \frac{dZ_p(x)}{dx} = a_1(x) - \int_{-Q}^{Q} a_2(x - y)\rho(y)dy \]

\[ = \rho(x) + \rho^N(x), \]

(5.6)
where $\rho(x)$ and $\rho^h(x)$ are the densities of the particles and holes, respectively. Taking the Fourier transformation of Eq. (5.6), we obtain

$$\tilde{\rho}(k) + \tilde{\rho}^h(k) = a_1(k) - a_2(k)\tilde{\rho}(k).$$

(5.7)

Thus the density of particles can be expressed as

$$\tilde{\rho}(k) = \frac{1}{e^{\eta|k|} + e^{-\eta|k|}} - \frac{\tilde{\rho}^h(k)}{1 + e^{-2\eta|k|}}.$$ 

(5.8)

In the thermodynamic limit, the energy (5.2) of the periodic XXZ spin chain is

$$E_p = -\frac{8\pi}{\eta} N \sinh \eta \int_{-Q}^{Q} a_1(x)\rho(x)dx + N \cosh \eta.$$ 

(5.9)

For the even $N$, all the Bethe roots are real at the ground state and fill the region $(-\frac{\pi}{\eta}, \frac{\pi}{\eta})$. Meanwhile, the number of Bethe roots $M = \frac{N}{2}$. Thus the following equation must hold

$$M = \int_{-Q}^{Q} \rho(x)dx = \tilde{\rho}(0) = \frac{1}{2},$$ 

(5.10)

which means the magnetization at the ground state is $0$. From Eqs. (5.8) and (5.10), we find that such a configuration is described by $\rho^h(x) = 0$ and the density of particles is

$$\tilde{\rho}(k) = \frac{1}{2 \cosh(\eta k)}.$$ 

(5.11)

With the help of Eqs. (5.9) and (5.11), we have

$$E_{p,even} = \left( -8 \sinh \eta \sum_{k=1}^{\infty} \frac{1}{1 + e^{2\eta k}} - 2\sinh \eta + \cosh \eta \right) N = e_0 N,$$ 

(5.12)

where $e_0$ is the density of ground state energy of the system defined by Eq. (4.15).

For the odd $N$, the ground state of the system (5.1) is described by $\frac{N-1}{2}$ real Bethe roots in the region $(-\frac{\pi}{\eta}, \frac{\pi}{\eta})$ and one hole at $x_0 \in [-\frac{\pi}{\eta}, \frac{\pi}{\eta}]$. Thus the following equation must hold

$$M = \int_{-Q}^{Q} \rho(x)dx = \tilde{\rho}(0) = \frac{1}{2} - \frac{1}{2N}.$$ 

(5.13)

In this case, the density of holes is given by Eq. (4.11).

Then from Eq. (5.8), we obtain the density of particles as

$$\tilde{\rho}(k) = \frac{1}{2 \cosh(\eta k)} - \frac{e^{-i\eta x_0}}{1 + e^{-2\eta|k|}}.$$ 

(5.14)

With the help of Eqs. (5.9) and (5.14), we have

$$E_{p,odd} = \left( -8 \sinh \eta \sum_{k=1}^{\infty} \frac{1}{1 + e^{2\eta k}} - 2\sinh \eta + \cosh \eta \right) N + 4 \sinh \eta \sum_{k=-\infty}^{\infty} \frac{e^{i\eta x_0}}{2 \cosh(\eta k)} = e_0 N + e_h(x_0),$$ 

(5.15)

where $e_h(x_0)$ is the energy carried by one hole defined by Eq. (4.16). At the ground state, $x_0 = \frac{\pi}{\eta}$ to minimize the energy. Thus the ground state energy in the thermodynamic limit can be expressed by

$$E_{p,odd} = e_0 N + e_h\left(\frac{\pi}{\eta}\right).$$ 

(5.16)
Again, we find that the ground state energy of the periodic XXZ spin chain with even \( N \) and that with odd \( N \) are different. In the thermodynamic limit, comparing with \( e_0N \), the \( e_0(\pi/\eta) \) is a small quantity and can be neglected. The thermodynamic behavior of the system with even \( N \) and those with odd \( N \) obtained by the density of ground state energy \( e_0 \) are the same.

Comparing the relations (5.12) and (4.17), (5.16) and (4.20), we find that the parity of \( N \) of the XXZ spin torus and the parity of \( N \) of the periodic XXZ spin chain are reversed. That is to say, the ground state energy of the periodic XXZ spin chain with even \( N \) equals to that of the antiperiodic XXZ spin chain with odd \( N \). While the ground state energy of the periodic XXZ spin chain with odd \( N \) equals to that of the antiperiodic XXZ spin chain with even \( N \). This is because of the existence of the twisted bond.

6 The twisted boundary energy

![Graphs](image)

**Figure 3:** The twisted boundary energies \( E_b \) versus the system size \( N \). The data in (a) and (b) can be fitted as \( \frac{1}{\cosh \eta} E_{b,even}^{even} = a_3 b_3 N + c_3 \), where (a) \( \eta = 2 \), \( a_3 = 1.028 \), \( b_3 = -0.3787 \) and \( c_3 = 1.027 \); (b) \( \eta = 3 \), \( a_3 = 1.461 \), \( b_3 = -0.8706 \) and \( c_4 = 1.614 \). Due to the fact \( b_3 < 0 \), when the system size \( N \) tends to infinity, \( c_3 \) is the corresponding twisted boundary energy. The data in (c) and (d) can be fitted as \( \frac{1}{\cosh \eta} E_{b,odd}^{odd} = a_4 b_4 N + c_4 \), where (c) \( \eta = 2 \), \( a_4 = -8.696 \), \( b_4 = -1.945 \) and \( c_4 = -1.027 \); (d) \( \eta = 3 \), \( a_4 = -2.342 \), \( b_4 = -1.988 \) and \( c_4 = -1.614 \). Due to the \( b_4 < 0 \), when the system size \( N \) tends to infinity, \( |c_4| \) is the corresponding twisted boundary energy.

The twisted boundary energy is a physical quantity to measure the effects induced by twisted boundary at the ground state, which is defined as

\[
E_b = |E^g - E^p_p|, \tag{6.1}
\]

which is a function of the crossing parameter \( \eta \). The symbol of absolute value in Eq. (6.1) is used because that \( E^g > E^p_p \) for even \( N \) while \( E^g < E^p_p \) for odd \( N \). From Eqs. (5.12) and (4.17), we find that \( E_{g,even}^g - E_{p,even}^p \)
equals to the twisted boundary energy for even $N$

$$E_{\text{even}}^b(\eta) = E^{g,\text{even}}(\eta) - E^{g,\text{even}}_p(\eta) = E_b(\eta) = 4 \sinh \eta \sum_{k=1}^{\infty} \frac{\cos(k\pi)}{\cosh(\eta k)} + 2 \sinh \eta. \quad (6.2)$$

While from Eqs. (5.16) and (4.20), we find that $E^{g,\text{odd}} - E^{g,\text{odd}}_p$ equals to the minus of twisted boundary energy for odd $N$

$$E_{\text{odd}}^b(\eta) = E^{g,\text{odd}}(\eta) - E^{g,\text{odd}}_p(\eta) = -E_b(\eta). \quad (6.3)$$

Therefore, the twisted boundary energy $E_{\text{even}}^b$ with even $N$ equals to the minus of twisted boundary energy $E_{\text{odd}}^b$ with odd $N$

$$E_{\text{odd}}(\eta) = -E_{\text{even}}(\eta). \quad (6.4)$$

The twisted boundary energies with $\eta = 2$ and $\eta = 3$ are derived as

$$\frac{1}{\cosh 2} E_{\text{even}}^b(2) = -\frac{1}{\cosh 2} E_{\text{odd}}^b(2) = 1.02746,$$

$$\frac{1}{\cosh 3} E_{\text{even}}^b(3) = -\frac{1}{\cosh 3} E_{\text{odd}}^b(3) = 1.61356. \quad (6.5)$$

Now, we check the above results by the DMRG method. The twisted boundary energies for different system-size $N$ obtained by DMRG are shown in Fig. 3. For the even $N$ case, the data in Fig. 3(a) and Fig. 3(b) can be fitted as

$$\frac{1}{\cosh \eta} E_{\text{even}}^b(\eta) = a_3 e^{b_3 N} + c_3. \quad (6.6)$$

Due to the fact $b_3 < 0$, when the system size $N$ tends to infinity, $c_3$ should be the twisted boundary energy, $c_3 = E_b$. The DMRG results are

$$c_3 = 1.027, \quad \text{for} \quad \eta = 2,$$

$$c_3 = 1.614, \quad \text{for} \quad \eta = 3, \quad (6.7)$$

which are highly consistent with the analytical results (6.5).

For the odd $N$ case, the data in Fig. 3(c) and Fig. 3(d) can be fitted as

$$\frac{1}{\cosh \eta} E_{\text{odd}}^b(\eta) = a_4 N^{b_4} + c_4. \quad (6.8)$$

Due to the fact $b_4 < 0$, when the system size $N$ tends to infinity, $|c_4|$ should be the twisted boundary energy, $|c_4| = E_b$. The DMRG results are

$$c_4 = -1.027, \quad \text{for} \quad \eta = 2,$$

$$c_4 = -1.614, \quad \text{for} \quad \eta = 3, \quad (6.9)$$

which are also highly consistent with the analytical results (6.5).

Now, we consider the degenerate case. When $\eta = 0$, the XXZ spin torus degenerates into the isotropic XXX spin chain with the anti-periodic boundary conditions. From Eq. (4.16), we have

$$\lim_{\eta \to 0} e_h(\frac{\pi}{\eta}) = 0. \quad (6.10)$$

Thus the parity of $N$ vanishes and the ground state energy reads

$$E_{\text{XXX}}^g = \lim_{\eta \to 0} \frac{e_0(\eta) N}{\cosh \eta} = (1 - 4 \ln 2) N. \quad (6.11)$$

The ground state energy of the periodic XXX spin chain is

$$E_{\text{p,XXX}}^g = (1 - 4 \ln 2) N. \quad (6.12)$$

Therefore, the twisted boundary energy of the XXX spin torus is zero.
7 Conclusions

In this paper, we have studied the thermodynamic limits of the spin-$\frac{1}{2}$ XXZ chain both with the antiperiodic and the periodic boundary conditions. We find that due to the twisted bond, the ground state energy of the antiperiodic XXZ spin chain with even $N$ equals to that of the periodic XXZ spin chain with odd $N$. While the ground state energy of the antiperiodic XXZ spin chain with odd $N$ equals to that of the periodic XXZ spin chain with even $N$. We also find that the contribution of the inhomogeneous term in the $T - Q$ relation of the antiperiodic XXZ spin chain at the ground state can be neglected when the system-size $N$ tends to the infinity. By using the reduced BAEs, we study the twisted boundary energy and show that the twisted boundary energy $E_{\text{even}}^b$ of the system with even $N$ differs from the one $E_{\text{odd}}^b$ with odd $N$ by a minus sign. We check these results by the DMRG, which leads to that the analytical results and the numerical ones agree with each other very well.

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