Twisted boundary energy and low energy excitation of the XXZ spin torus at the ferromagnetic region

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Abstract

We investigate the thermodynamic limit of the one-dimensional ferromagnetic XXZ model with twisted (or antiperiodic) boundary conditions. It is shown that the distribution of the Bethe roots of the inhomogeneous Bethe ansatz equations (BAEs) for the ground state as well as for the low-lying excited states satisfy the string hypothesis, although the inhomogeneous BAEs are not in the standard product form which has made the study of the corresponding thermodynamic limit nontrivial. We also obtain the twisted boundary energy induced by the nontrivial twisted boundary conditions in the thermodynamic limit.

1. Introduction

The XXZ spin-½ torus model is the XXZ spin chain with twisted (or antiperiodic) boundary condition [1–4], and it is tightly related to the recent study on the boundary states of matter. In the works [1, 2], Baxter’s ‘pair propagation through a vertex’ was used and BA-like equations were derived and solved for the gapped antiferromagnetic regime. Based on the BA solutions, the interfacial tension are also obtained [2]. In the critical regime, some very interesting results about the low-lying excitations are calculated and conformal field theory signatures are derived by Niekamp, Wirth and Frahm [3]. By means of the separation of variables, the BA-like equations and form factors are obtained [4]. The integrability of this model is associated with the six-vertex R-matrix [5–8]. Due to the twisted boundary condition, the U(1)-symmetry is broken, making it very different from the periodic XXZ chain. For an example, the lack of an obvious reference state prevents us from applying the conventional Bethe ansatz methods [9–15] to solve the model.

The off-diagonal Bethe ansatz (ODBA) method is a newly developed analytic theory to compute exact solutions of quantum integrable models, especially for those with nontrivial integrable boundaries [16–19]. Exact solution of such a system is characterized by an inhomogeneous T–Q relations where the Bethe roots should satisfy the inhomogeneous Bethe ansatz equations (BAEs). Then, a natural question is what is the distribution of the Bethe roots of the inhomogeneous BAEs in the complex plane. It is very important because it is the start point to study the thermodynamic properties of the system. However, due to the existence of the inhomogeneous term, it is hard to use the usual thermodynamic Bethe Ansatz method [15]. Some interesting approaches are proposed [20, 21]. For examples, because the inhomogeneous BAEs can reduce to the conventional ones when the model parameters taking some special values, then one can use the results at the degenerate points to get the actual values [20]. Another method is that one can study the contribution of the inhomogeneous term, then the thermodynamic limit can be obtained by using the finite-size scaling behavior
In this paper, we directly investigate the Bethe roots from the inhomogeneous BAEs with an approximation for finite system-size that converges to the correct thermodynamic limit. We use the XXZ spin-1/2 torus as the example. From the numerical analysis, we obtain the structure of the Bethe roots for the ground state as well as for the low-lying excited states in the thermodynamic limit. Based on them, the physical quantities such as the twisted boundary energy and the gap are studied.

The paper is organized as follows. Section 2 serves as an introduction of the model and its exact solution. In section 3, we discuss the distribution of Bethe roots of the ground state. Base on them, we calculate the twisted boundary energy. In section 4, the nearly degenerate states are studied. In section 5, we discuss the elementary excitation and the energy gap. In section 6, the limiting behavior is considered, which is used to check our results. Concluding remarks are given in section 7.

2. Spin-1/2 XXZ torus

The spin-1/2 XXZ torus is characterized by the Hamiltonian

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

(2.1)

where \( N \) is the number of sites, \( \eta \) is the crossing parameter (or anisotropic parameter) and the boundary condition is the twisted one, namely,

\[ \sigma_{N+1}^\alpha = \sigma_1^\alpha, \quad \text{for } \alpha = x, y, z. \]  

(2.2)

Note that the twisted boundary condition (2.2) breaks the bulk \( U(1) \)-symmetry (see the spin-1/2 XXZ chain with the periodic boundary condition: \( \sigma_{N+1}^\alpha = \sigma_1^\alpha \)).

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

\[ R(u, v) = \frac{1}{2} \begin{pmatrix} \sinh(u + \eta) & \sinh(u \eta) \\ \sinh(1 + \eta) & \sinh(1 - \eta) \end{pmatrix} + \frac{1}{2} (\sigma_0^x + \sigma_0^y), \]  

(2.3)

where \( u \) is the spectral parameter. From the \( R \)-matrix, we can define the monodromy matrix as

\[ T_{0}(u) = \sigma_0^x R_{0,N}(u - \theta_N) \cdots R_{0,1}(u - \theta_1) = \begin{pmatrix} C(u) & D(u) \\ A(u) & B(u) \end{pmatrix}. \]  

(2.4)

The \( R \)-matrix and the monodromy matrix satisfy the RTT relation

\[ R_{0,0}(u - v) T_{0}(u) T_{0}(v) = T_{0}(v) T_{0}(u) R_{0,0}(u - v). \]  

(2.5)

The transfer matrix of the system is defined as

\[ t(u) = t_0 T_{0}(u) = B(u) + C(u). \]  

(2.6)

From the RTT relation, one can prove that

\[ [t(u), t(v)] = 0, \]  

(2.7)

thus the system is integrable. The transfer matrix can generate all the conserved quantities and the Hamiltonian (2.1) is chosen as the first order derivative of the logarithm of the transfer matrix

\[ H = -2 \sinh \eta \left. \frac{\partial \ln t(u)}{\partial u} \right|_{u=0, \theta=0} + N \cosh \eta. \]  

(2.8)

The Hamiltonian (2.1) can be exactly solved by using the ODBA method [16, 17]. The energy is then expressed in terms of the Bethe roots

\[ E = 2 i \sinh \eta \sum_{j=1}^{N} \left[ \cot \left( u_j + \frac{\eta i}{2} \right) - \cot \left( u_j - \frac{\eta i}{2} \right) \right] + N \cosh \eta - 2 \sinh \eta, \]  

(2.9)

where the Bethe roots \( \{ u_j \} \) should satisfy the inhomogeneous BAEs

\[ e^{iu_j} \prod_{l=1}^{N} \frac{\sin(u_j - u_l + \frac{\eta i}{2})}{\sin(u_j - \frac{\eta i}{2})} = e^{-iu_j} \prod_{l=1}^{N} \frac{\sin(u_j - u_l - \frac{\eta i}{2})}{\sin(u_j - \frac{\eta i}{2})} + 2i e^{-2N\eta} \sin \left( u_j - \sum_{l=1}^{N} u_l \right), \]  

(2.10)

We note that the period of Bethe roots is \( \pi \), thus we fix the real part of Bethe roots in the interval \([-\frac{\pi}{2}, \frac{\pi}{2})\).
constant and the value is \( i \). Here, we consider the case that the real part of Bethe roots is nearly \( -\pi/2 \), and the difference between the imaginary part of two Bethe roots is nearly \( \eta \). Thus the Bethe roots form a single string \([15]\). In order to see this point clearly, we draw them in figure 1. From it we see that the string is located at the boundary of the period \( (-\pi/2) \). The difference among the imaginary part of Bethe roots is equal to \( \eta i \).

### 3. Bethe roots for the ground state

Here, we consider the case that \( \eta \) is real and solve the inhomogeneous BAEs (2.10) numerically. The values of Bethe roots for the ground states for finite system-size are listed in tables 1 and 2. From the data, we find that the real part of Bethe roots is nearly \( -\pi/2 \), and the difference between the imaginary part of two Bethe roots is nearly constant and the value is \( \eta i \). Thus the Bethe roots form a single string \([15]\). In order to see this point clearly, we draw them in figure 1. From it we see that the string is located at the boundary of the period \( (-\pi/2) \).

We should mention that for the odd \( N \) case, there exists another \( N \)-string which locates at the imaginary axis. These two kinds of strings give the same ground state energy thus the corresponding Bethe states are degenerate.
Based on above facts, we conclude that all the Bethe roots may form the string solution for the ground state

\[
u_j = -\frac{\pi}{2} + \left(\frac{N + 1}{2} - j\right)\eta\bar{\eta} + o(N), \quad j = 1, \cdots, N, \tag{3.1}\]

where \(o(N)\) stands for a small correction which is related with \(N\), and \(i\) is the imaginary unit. Substituting the string hypothesis (3.1) into the energy expression (2.9) and neglecting the small correction, we obtain the ground state energy

\[
E_0 = -N \cosh \eta - 2 \sinh \eta + 4 \sinh \eta \tanh \left(\frac{N\eta}{2}\right). \tag{3.2}
\]

In order to check the validity of string hypothesis (3.1), we calculate the ground state energy of the system by exactly diagonalizing the Hamiltonian (2.1) up to \(N = 19\) and compare the results with those obtained by the equation (3.2). The data is listed in table 3. We see that the analytical and numerical results agree with each other very well. For the larger system-size, we also check the validity of (3.1) and (3.2) by the density matrix renormalization group (DMRG) method. The result is shown in figure 2. Then, we can conclude that the Bethe roots for the ground state form the string solution in the thermodynamic limit and equation (3.2) gives the energy of the system.

Now, we calculate the twisted boundary energy. It is well-known that the ground state energy of the XXZ spin chain with periodic boundary condition is [15]
We define the twisted boundary energy as
\[ E_i^b = -N \cosh \eta. \] (3.3)

Substituting equations (3.2) and (3.3) into (3.4), we obtain
\[ E_i = -2 \sinh \eta + 4 \sinh \eta \tanh \left( \frac{N\eta}{2} \right). \] (3.5)

In the thermodynamic limit, the twisted boundary energy arrives at
\[ E_i = 2 \sinh \eta. \] (3.6)

4. Nearly degenerate states

From the numerical calculation, we also find that the XXZ spin torus model has some nearly degenerate states with the ground state, which have following properties:

1. They are almost degenerate states with exponentially small gaps for the finite system-size. As shown in figure 3, the energy difference between the ground state and nearly degenerate states satisfies the law \( \Delta E \propto e^{-\beta N}, \beta \approx \eta \), which means that the difference will exponentially tends to zero with the increasing \( N \). Thus in the thermodynamic limit, the nearly degenerate states are degenerate to the ground state.

2. The number of the nearly degenerate states is \( 2N - 2 \). In the case of \( \eta \to +\infty \), the model degenerates to a Ising-like model. The system possesses \( Z_2 \) symmetry and the boundary conditions at different site number are equivalent. It is easy to find that the degeneracy of the ground state is \( 2N \), which is consistent with the numerical results. When the crossing parameter \( \eta \) tends to infinity, the main contribution in Hamiltonian (2.1) to the energy comes from the \( \sigma_i^x \sigma_{i+1}^x \) terms, and the degeneracy of the ground state is \( 2N \). When the \( \eta \) is finite, the rest parts of Hamiltonian make contributions and the ground state splits into several separate energies, corresponding to the ground state, where the total momentum is zero, and the nearly degenerate states, where the total momentum is finite. The degeneracy of the ground state is 2 and we have \( 2N - 2 \) nearly degenerate states.

The physical picture of the nearly degenerate states is as follows. There are two domains with oppositely pointing spins. One domain wall sits between sites \( N \) and 1. The other domain wall could be anywhere. If \( \eta \) tends to infinite, the second domain may be empty. This in total gives \( 2N \) configurations, which is consist with the case of Ising limit. For the large but finite \( \eta \), the states are probably plain waves in the second, free domain wall\(^8\).

3. As shown in figure 4, the Bethe roots for the nearly degenerate states also form a \( N \)-string structure, but the position is moved and the deviation \( \phi \) is larger than that for the ground state.

\( \quad \)

\( ^8 \) We thank the anonymous referee for pointing it out for us.
A general $N$-string is

$$u_j = x + \left( \frac{N + 1}{2} - j \right) \eta i + o(N), \quad j = 1, \ldots, N,$$

(4.1)

where the string position $x$ is real, $x \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ and $o(N)$ stands for a small correction which is related with $N$. Substituting the string hypothesis (4.1) into the energy expression (2.9) and neglecting the small correction, we obtain

$$E_{N \text{ string}} = -N \cosh \eta - 2 \sinh \eta + 4 \sinh \eta \frac{\tanh \left( \frac{N \eta}{2} \right)}{\sin^2 x + \tanh \left( \frac{N \eta}{2} \right) \cos^2 x}.$$  

(4.2)

If $N$ is large, we have $\tanh \left( \frac{N \eta}{2} \right) \to 1$, then $\sin^2 x + \tanh \left( \frac{N \eta}{2} \right) \cos^2 x \to \sin^2 x + \cos^2 x = 1$ for arbitrary $x$.

Thus the energy of $N$-string tends to the actual ground state energy, which also supports the property 1 of nearly degenerate states.

5. Elementary excitation

Now, we consider the elementary excitation of the XXZ spin torus model. As shown in figure 5, we find that the distribution of Bethe roots for the lowest excited states can be described by a $(N - 1)$-string plus an additional real root. Meanwhile, the string and the real root are nearly located at the interval boundary $-\frac{\pi}{2}$. After some more precision calculation, we conclude that the Bethe roots for the lowest excited state take the form of

$$u_1 = -\frac{\pi}{2} + o_1(N); \quad u_j = -\frac{\pi}{2} + \left( \frac{N}{2} - j + 1 \right) \eta i + o_2(N); \quad j = 2, \ldots, N,$$

(5.1)

where $o_1(N)$ and $o_2(N)$ stand for the small deviations and $i$ is the imaginary unit. The energy corresponding to this kind of excitation is

$$E_1 = -N \cosh \eta - 2 \sinh \eta + 4 \sinh \eta \tanh \left[ \frac{(N - 1) \eta}{2} \right] + 4 \sinh \eta \tanh \frac{\eta}{2}. $$

(5.2)

$^9$We regard $\frac{\pi}{2}$ as the same point with $-\frac{\pi}{2}$ due to the periodicity.
We also check the validity of equation (5.2) by the exact diagonalization and the result is shown in figure 6.
Again, we see that with the increasing $N$, the energy difference between the analytic result (5.2) and the actual values tends to zero rapidly. Thus the string solution (5.1) is correct in the thermodynamic limit.

The energy gap of the XXZ spin torus is defined as

$$E_{\text{gap}} = E_1 - E_0 = 4 \sinh \eta \tanh \frac{\eta}{2} + 4 \sinh \eta \tanh \left( \frac{(N-1)\eta}{2} \right) - 4 \sinh \eta \tanh \left( \frac{N\eta}{2} \right).$$

In the thermodynamic limit, the energy gap reads

$$E_{\text{gap}} = 4 \sinh \eta \tanh \frac{\eta}{2},$$

which is the same as that of the XXZ spin chain with periodic boundary condition.

6. Limiting behavior

In order to check above results again, now, we consider some limit case of $\eta \to +\infty$. In this case, the Ising-like spin coupling $\sigma_j^z \sigma_{j+1}^z$ in Hamiltonian (2.1) is dominated and the model degenerates into the one-dimensional Ising model with a twisted boundary condition. Evidently, the ferromagnetic state is the ground state and the corresponding ground state energy is known as

$$\frac{E_{\text{Ising}}}{\cosh \eta} = -N + 2.$$
Taking the $\eta \to +\infty$ limit of equation (3.2), we have
\[
\frac{E_{0|\eta=+\infty}}{\cosh \eta} = -N + 2,
\]
which is consistent with the result of the Ising model. The lowest excited energy of the Ising model with a twisted boundary condition is
\[
\frac{E_1^{\text{Ising}}}{\cosh \eta} = -N + 6.
\]
Taking the $\eta \to +\infty$ limit of equation (5.2), we have
\[
\frac{E_{1|\eta=+\infty}}{\cosh \eta} = -N + 6.
\]
Therefore, the results derived from the string hypothesis (3.1) and (5.1) are consistent with the already known results.

7. Conclusions

In this paper, we have studied the thermodynamic limit of the one-dimensional ferromagnetic XXZ model with the twisted (or antiperiodic) boundary condition which is described by the Hamiltonians (2.1) and (2.2). It is shown that even for the inhomogeneous BAEs (2.10), the corresponding roots for the ground state appear to form a string (3.1). This fact enables us to calculate the twisted boundary energy of the model given by (3.6). By using the similar method, we further investigate the elementary excitation and obtain the energy gap of the model which is the same as that of the periodic boundary condition case.

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