Non-regular eigenstate of the XXX model as some limit of the Bethe state

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Abstract

For the one-dimensional XXX model under the periodic boundary conditions, we discuss two types of eigenvectors, regular eigenvectors which have finite-valued rapidities satisfying the Bethe ansatz equations, and non-regular eigenvectors which are descendants of some regular eigenvectors under the action of the SU(2) spin-lowering operator. It was pointed out by many authors that the non-regular eigenvectors should correspond to the Bethe ansatz wavefunctions which have multiple infinite rapidities. However, it has not been explicitly shown whether such a delicate limiting procedure should be possible. In this paper, we discuss it explicitly in the level of wavefunctions: we prove that any non-regular eigenvector of the XXX model is derived from the Bethe ansatz wavefunctions through some limit of infinite rapidities. We formulate the regularization also in terms of the algebraic Bethe ansatz method. As an application of infinite rapidity, we discuss the period of the spectral flow under the twisted periodic boundary conditions.

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I. INTRODUCTION

The one-dimensional Heisenberg model (XXX model) under the periodic boundary conditions is one of the fundamental models of integrable quantum spin systems. Under the spin $SU(2)$ symmetry any eigenvector of the Hamiltonian is given by a highest-weight vector or a descendant of some highest-weight vector. It has been shown by the algebraic Bethe ansatz method that any regular Bethe ansatz eigenstate of the XXX model gives a highest weight vector. Let us consider the XXX Hamiltonian under the periodic boundary conditions

$$H = -\frac{J}{4} \sum_{\ell=1}^{L} \vec{\sigma}_{\ell} \cdot \vec{\sigma}_{\ell+1}, \quad \text{where} \quad \vec{\sigma}_{L+1} = \vec{\sigma}_1. \quad (1.1)$$

Here the symbol $\vec{\sigma}_\ell = (\sigma^x_\ell, \sigma^y_\ell, \sigma^z_\ell)$ denotes the spin angular-momentum operator with $S = 1/2$ acting on the $\ell$-th site of the ring. Let us denote by the symbol $\vec{S}_{\text{tot}}$ the total spin-operator: $\vec{S}_{\text{tot}} = \sum_{\ell=1}^{L} \vec{\sigma}_\ell/2$. Then, it is easy to show that the Hamiltonian is invariant under the action of the $SU(2)$: $[H, \vec{S}_{\text{tot}}] = 0$.

Let us introduce some notation of the coordinate Bethe ansatz. We denote by $x_1, x_2, \ldots, x_M$ the coordinates of the $M$ down-spins set in increasing order: $1 \leq x_1 < x_2 < \cdots < x_M \leq L$. Then, we define the Bethe ansatz wavefunction with $M$ parameters $k_1, k_2, \ldots, k_M$ by the following:

$$f_M^{(B)}(x_1, \ldots, x_M; k_1, \ldots, k_M) = \sum_{P \in S_M} A_M(P) \exp \left( i \sum_{j=1}^{M} k_{Pj} x_j \right), \quad (1.2)$$

where the sum is over all the permutations of $M$ letters of the set $\{1, 2, \ldots, M\}$, and the symbol $Pj$ denotes the action of permutation $P$ on letter $j$. Here the symbol $S_M$ denotes the permutation group of $M$ letters. We define the amplitudes $A_M(P)$’s of the Bethe ansatz wavefunction by

$$A_M(P) = C \epsilon(P) \prod_{1 \leq j < \ell \leq M} \frac{\exp[i(k_{Pj} + k_{P\ell})] + 1 - 2 \exp(ik_{Pj})}{\exp[i(k_j + k_\ell)] + 1 - 2 \exp(ik_j)}, \quad \text{for} \quad P \in S_M. \quad (1.3)$$

Here the symbol $\epsilon(P)$ denotes the sign of permutation $P$, and $C$ is a constant. Let the symbol $|0\rangle$ denote the vacuum state where all spins are up ($M = 0$). Then, we construct the following vector from the Bethe ansatz wavefunction

2
$$||M|| = \sum_{1 \leq x_1 < x_2 < \cdots < x_M \leq L} f_M^{(B)}(x_1, \ldots, x_M; k_1, \ldots, k_M) \sigma_{x_1}^- \sigma_{x_2}^- \cdots \sigma_{x_M}^- |0\rangle.$$  
(1.4)

Here, the summation is over all the possible values of $x_j$'s given in increasing order. We call the vector $||M||$ with the amplitudes defined by eq. $|1.3\rangle$, a **formal Bethe vector** (or **formal Bethe state**). We recall that there is no constraint on the $M$ parameters $k_1, k_2, \ldots, k_M$. When they are generic, the formal Bethe state $|1.4\rangle$ is not an eigenvector of the XXX Hamiltonian.

Now, let us consider the Bethe ansatz equations. They correspond to the periodic boundary conditions for the Bethe ansatz wavefunction.

$$\exp(i L k_j) = (-1)^{M-1} \prod_{\ell=1, \ell \neq j}^{M} \frac{\exp[i(k_j + k_\ell)] + 1 - 2 \exp(ik_j)}{\exp[i(k_j + k_\ell)] + 1 - 2 \exp(ik_\ell)},$$
for $j = 1, \ldots, M$.  
(1.5)

If all the parameters $k_1, k_2, \ldots, k_M$ satisfy the Bethe ansatz equations, then the formal Bethe vector $||M||$ becomes an eigenvector of the XXX Hamiltonian. Furthermore, if the $k_j$'s satisfy the conditions that $k_j \neq 0 \mod 2\pi$ for $j = 1, \ldots, M$, then we call the eigenvector **regular**, and denote it by the symbol $|M\rangle$. It is called regular, since it is well defined as an eigenstate given by the Bethe ansatz wavefunction. In this sense, it is also called a regular Bethe ansatz state or a Bethe state, in short.

A regular eigenstate can lead to a series of non-highest weight eigenvectors of the $SU(2)$ symmetry. Let $|R\rangle$ denote a given regular eigenstate with $R$ down-spins. Then, it is a highest weight vector of the $SU(2)$ symmetry with $S_{tot} = L/2 - R$ and $S_{z_{tot}} = L/2 - R$. Here we assume that the number $R$ should satisfy the condition: $0 \leq R \leq L/2$, for regular eigenvectors. From the eigenvector $|R\rangle$, we can derive a sequence of non-highest weight eigenvectors: $(S_{tot}^-)^K |R\rangle$ for $K = 1, \ldots, L - 2R$. We call the series of descendant eigenstates **non-regular**. We denote them by

$$|R, K\rangle = \frac{1}{K!} (S_{tot}^-)^K |R\rangle \quad \text{for} \quad K = 1, \ldots, L - 2R.$$  
(1.6)

It is remarked that the eigenvectors $|R, K\rangle$'s are fundamental in the completeness of the spectrum of the XXX model, although they are called non-regular in this paper.
The main question of this paper is how non-regular eigenvectors of the XXX model are related to the Bethe ansatz wavefunctions. In fact, it has already been observed by Gaudin [1] that the non-regular eigenvectors are associated with the Bethe ansatz wavefunction with several parameters $k_j$’s being equal to zero. Furthermore, it was shown by Takhtajan and Faddeev [3] that the creation operator $B(v)$ is equivalent to the spin-lowering operator $S_{\text{tot}}$ by sending the rapidity $v$ to infinity (see also Refs. [8–11]). We note that the limit of sending the parameter $k_j$ to zero corresponds to the limit of the infinite rapidity. Here, for a given parameter $k$, the rapidity $v$ has been defined by the relation: $\exp(ik) = (v + i)/(v - i)$; rapidity $v$ is finite if and only if $k \neq 0 \, (\text{mod} \, 2\pi)$. In spite of the observations, however, it has not been clearly shown yet whether one can construct the non-regular eigenvector $|R, K\rangle$ from the Bethe ansatz wavefunctions for the case of general $K$. In the case of multiple infinite rapidities, the limit of the wavefunction depends not only on its normalization but also on how we control the differences among the infinite rapidities. Thus, under a naive limiting procedure, the amplitudes of the formal Bethe state become indefinite; it can vanish or diverge depending on the limiting procedure. (For example, see also [12].) Furthermore, if a set of parameters $k_j$’s contains multiple zeros, then it is not clear whether the Bethe ansatz wavefunction should vanish or not. In fact, for any given regular eigenvector, we can show that if two momenta (or two rapidities) have the same value, then the norm of the eigenvector is given by zero. This fact is called the “Pauli principle” of the Bethe ansatz wavefunction. Thus, the question has been nontrivial. In this paper, we make it clear. We show that there exists a certain limiting procedure through which any non-regular eigenvector of the XXX model is derived from the formal Bethe state.

Let us explain our derivation of non-regular eigenvectors from the formal Bethe states, briefly. We consider a given regular Bethe ansatz eigenstate $|R\rangle$ with $R$ down-spins. It has $R$ rapidities $v_1, v_2, \ldots, v_R$, satisfying the Bethe ansatz equations for $R$ down-spins. For a given positive integer $K$, we consider the non-regular eigenstate $|R, K\rangle$. We recall that it has been defined in eq. (1.6) and is derived from $|R\rangle$. Then, we introduce an additional set of the rapidities $v_{R+1}, \ldots, v_{R+K}$ as follows.
Here we call the parameter \( \Lambda \) the “center” of the additional \( K \) rapidities \( v_{R+1}, \ldots, v_{R+K} \). We assume that the \( \delta_j \) ’s are arbitrary non-zero parameters, which can be sent to infinity.

Let us now consider a formal Bethe vector \(| |R + K\rangle\) with \( R + K \) down-spins that has \( R \) rapidities of the given regular eigenstate \(| R\rangle \) (i.e., \( v_1, \ldots, v_R \)) together with the additional \( K \) rapidities given by eq. (1.7) (i.e., \( v_{R+1}(\Lambda), \ldots, v_{R+K}(\Lambda) \)). We denote it by \(| |R, K; \Lambda\rangle\).

Then, we can show that the vector \(| |R, K; \Lambda\rangle\) becomes the non-regular eigenstate \(| R, K\rangle\) by sending \( \Lambda \) to infinity:

\[
\lim_{\Lambda \to \infty} | |R, K; \Lambda\rangle = C | R, K\rangle
\]  

(1.8)

Here \( C \) denotes a constant. Thus, the non-regular eigenstate is derived from the Bethe ansatz wavefunction.

We discuss only regular eigenvectors of the XXX model and their descendants which we call non-regular eigenvectors. We do not consider other types of solutions in this paper. In fact, it was shown that the so-called string hypothesis predicts the correct number of appropriate solutions to the Bethe ansatz equations of the XXX model under the periodic boundary conditions [1,13,14]. Although the hypothesis fails to count the particular type of solutions, all the known numerical or analytical researches have shown that the total number of solutions to the Bethe ansatz equations is given correctly [1,15,16,11]. Thus, it is conjectured that all the regular eigenvectors and their descendants give the complete set of eigenvectors of the XXX model. In fact, it is proven that the number of solutions of the Bethe ansatz equations is given correctly for the XXX model under the twisted boundary conditions with the \textit{generic} twisting parameter [17]. It seems that the theorem does not cover the case of the periodic boundary conditions, since it corresponds to a non-generic point of the twisting parameter. However, the result of the paper might also shed some light on the mathematical understanding of the string hypothesis and the number counting arguments in general, as we shall discuss in sections 5 and 6.
The contents of the paper consists of the following. In section 2 we give a formula describing the action of powers of the spin-lowering operator. Then, through some examples, we explicitly discuss the derivation of non-regular eigenvectors from formal Bethe states. It is shown that infinite rapidities do not always satisfy the Bethe ansatz equations, although the limit of the Bethe ansatz wavefunction satisfies the periodic boundary conditions. In section 3, we give an explicit proof for the construction of non-regular eigenstates from the formal Bethe states. We show in section 4 that the formal Bethe state can be defined naturally in the algebraic Bethe ansatz. In fact, the formal Bethe state $|M\rangle$ is equivalent to the vector generated by the $B$ operators on the vacuum: $B(v_1)\cdots B(v_M)|0\rangle$ with the $M$ rapidities $v_1, \ldots, v_M$ being generic. In section 5, we show how the concept of formal Bethe states is useful in the analysis of the spectral flow of the XXX model under the twisted boundary conditions. In fact, we can derive the $4\pi$-period of the spectral flow under the twisted boundary conditions, almost rigorously. In section 6, we give some discussions. In order to make the paper self-consistent, some Appendices are provided. The formula for the action of spin-lowering operator is proven in Appendix A. An example of the formal Bethe state with three infinite rapidities is discussed in Appendix B. Some fundamental properties of the symmetric group are given in Appendix C, which are important in sec. 3. The “Pauli principle” of the Bethe ansatz wavefunction is explicitly proven in Appendix D. Finally, we formulate rigorously the coordinate Bethe ansatz method introduced by Bethe in Appendix E.

II. FORMAL BETHE STATES AND NON-REGULAR EIGENSTATES

A. Non-regular eigenstates

Let us discuss the action of spin-lowering operator on arbitrary vectors with $M$ down-spins, explicitly. For an illustration we consider the case of $M = 1$. Let $|1\rangle$ denote a vector with one down-spin
\[ |1\rangle = \sum_{x_1=1}^{L} g(x_1) \sigma_{x_1}^- |0\rangle, \quad (2.1) \]

where \( g(x) \) is any given arbitrary function. Applying to it the spin-lowering operator \( S_{\text{tot}}^- = \sum_{j=1}^{L} \sigma_j^- \), we have

\[
S_{\text{tot}}^- \, |1\rangle = \sum_{x_2=1}^{L} \sum_{x_1=1}^{L} g(x_1) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle \\
= \left( \sum_{1 \leq x_1 < x_2 \leq L} + \sum_{1 \leq x_2 < x_1 \leq L} \right) g(x_1) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle \\
= \sum_{1 \leq x_1 < x_2 \leq L} (g(x_1) + g(x_2)) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle \\
= \sum_{1 \leq x_1 < x_2 \leq L} \left( \sum_{1 \leq j \leq 2} g(x_j) \right) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle \quad (2.2)
\]

Here we note that \((\sigma_x^-)^2 |0\rangle = 0\).

We can generalize the expression (2.2). Let us denote by the symbol \(|M\rangle\) a vector with \(M\) down-spins

\[
|M\rangle = \sum_{1 \leq x_1 < x_2 < \ldots < x_M \leq L} g(x_1, x_2, \ldots, x_M) \sigma_{x_1}^- \sigma_{x_2}^- \cdots \sigma_{x_M}^- |0\rangle, \quad (2.3)
\]

where \(g(x_1, x_2, \ldots, x_M)\) is an arbitrary function of \(x_j\)'s. Then, it is clear that any vector with \(M\) down-spins can be considered as a vector \(|M\rangle\) with some function \(g(x_1, x_2, \ldots, x_M)\).

Now, we introduce the following formula

\[
\frac{1}{K!} (S_{\text{tot}}^-)^K |M\rangle = \sum_{1 \leq x_1 < \ldots < x_{M+K} \leq L} \left( \sum_{1 \leq j_1 < \ldots < j_{M+K} \leq M+K} g(x_{j_1}, \ldots, x_{j_M}) \right) \sigma_{x_1}^- \cdots \sigma_{x_{M+K}}^- |0\rangle. \quad (2.4)
\]

We note that the expression (2.2) corresponds to the case \(M = K = 1\). An explicit proof of the formula (2.4) will be given in Appendix A. In sec. 2.C, we shall consider the special case of \(K = 2\) and \(M = 1\), which is given in the following

\[
\frac{1}{2} (S_{\text{tot}}^-)^2 |1\rangle = \sum_{1 \leq x_1 < x_2 < x_3 \leq L} \sum_{1 \leq j \leq 3} g(x_j) \sigma_{x_1}^- \sigma_{x_2}^- \sigma_{x_3}^- |0\rangle \\
= \sum_{1 \leq x_1 < x_2 < x_3 \leq L} (g(x_1) + g(x_2) + g(x_3)) \sigma_{x_1}^- \sigma_{x_2}^- \sigma_{x_3}^- |0\rangle. \quad (2.5)
\]
Here we note that \( M + K = 1 + 2 = 3 \).

Let us consider a regular eigenstate \(|R\rangle\) with \( R \) down-spins, and the non-regular eigenstate \(|R, K\rangle\) given by eq. (1.6). We recall that \(|R\rangle\) is a highest weight vector of the \( SU(2) \) with \( S = L/2 - R \) and \( S_z = L/2 - R \). By applying the formula (2.4) to the definition (1.6) of the non-regular eigenvector, then it is explicitly expressed in terms of the Bethe ansatz wavefunctions

\[
|R, K\rangle = \sum_{1 \leq x_1 < \cdots < x_{R+K} \leq L} \left( \sum_{1 \leq j_1 < \cdots < j_{R+K} \leq L} f_R^{(B)}(x_{j_1}, \ldots, x_{j_R}) \right) \sigma_{x_1}^{-} \cdots \sigma_{x_{R+K}}^{-} |0\rangle.
\]  

Here we recall that the function \( f_R^{(B)}(x_1, \ldots, x_R; k_1, \ldots, k_M) \) is the Bethe ansatz wavefunction defined in eq. (1.2), where the \( k_j \)'s satisfy the Bethe ansatz equations.

**B. Amplitudes of formal Bethe states**

Let us recall the relation between rapidity \( v_j \) and parameter \( k_j \)

\[
\exp(ik_j) = \frac{v_j + i}{v_j - i} \quad \text{for} \quad j = 1, \ldots, M.
\]  

In terms of rapidities, the Bethe ansatz equations are given by

\[
\left( \frac{v_j + i}{v_j - i} \right)^L = \prod_{\ell=1,\ell\neq j}^{M} \left( \frac{v_j - v_\ell + 2i}{v_j - v_\ell - 2i} \right), \quad \text{for} \quad j = 1, \ldots, M.
\]  

The amplitudes \( A_M(P) \)'s defined in eq. (1.3) are given by the following

\[
A_M(P) [v_1, \cdots, v_M] = \epsilon(P) \prod_{1 \leq j < k \leq M} \frac{v_{pj} - v_{pk} + 2i}{v_j - v_k + 2i}
\]  

Here, the dependence of the amplitude \( A_M(P) \) on rapidities \( v_1, \ldots, v_M \) is expressed in the bracket \([\cdots]\), explicitly. Here we note that the expression (1.3) of the amplitude \( A_M(P) \) is proven in Appendix E.

Let us now introduce a useful formula for expressing the amplitudes of the Bethe ansatz wavefunction. We denote by the symbol \( H(x) \) the Heaviside step function defined by \( H(x) = 1 \) for \( x > 0 \), and \( H(x) = 0 \) otherwise. Then, we can show that the amplitudes \( A_M(P) \)'s given in eq. (2.3) are expressed by the following
We shall prove the expression (2.10) in sec. 3.

For an illustration, we consider the amplitudes $A_M(P)$’s for the case $M = 3$. Let us express $A_M(P)$ by $A_{P_1P_2...P_M}$. Then, they are given as follows

\[
A_{123} = 1, \quad A_{132} = \frac{v_2 - v_3 - 2i}{v_2 - v_3 + 2i}, \quad A_{213} = \frac{v_1 - v_2 - 2i}{v_1 - v_2 + 2i},
\]
\[
A_{231} = \left(\frac{v_1 - v_2 - 2i}{v_1 - v_2 + 2i}\right) \left(\frac{v_1 - v_3 - 2i}{v_1 - v_3 + 2i}\right),
\]
\[
A_{312} = \left(\frac{v_1 - v_3 - 2i}{v_1 - v_3 + 2i}\right) \left(\frac{v_2 - v_3 - 2i}{v_2 - v_3 + 2i}\right),
\]
\[
A_{321} = \left(\frac{v_1 - v_2 - 2i}{v_1 - v_2 + 2i}\right) \left(\frac{v_1 - v_3 - 2i}{v_1 - v_3 + 2i}\right) \left(\frac{v_2 - v_3 - 2i}{v_2 - v_3 + 2i}\right).
\]

(2.11)

C. Formal Bethe states with additional infinite rapidities

Let us discuss some examples of the Bethe ansatz wavefunctions with additional rapidities. We first consider the case of three down-spins with $R = 1$ and $K = 2$, i.e., the formal Bethe state $||1, 2; \Lambda\rangle$. Here, $v_2$ and $v_3$ are additional rapidities defined by eq. (1.7): $v_2 = \Lambda + \delta_1$, $v_3 = \Lambda + \delta_2$. Here we assume that $\delta_1$ and $\delta_2$ are some constants. We recall that $v_1$ is the rapidity of the state $|1\rangle$ and it satisfies the Bethe ansatz equation for $M = 1$.

Let us denote the difference $\delta_1 - \delta_2$ by $\Delta$. For simplicity, we assume that $\delta_1 = -\delta_2$. Then, the additional rapidities are given by $v_2 = \Lambda + \Delta/2$ and $v_3 = \Lambda - \Delta/2$. Substituting the rapidities $v_1$, $v_2$ and $v_3$ into the amplitudes in (2.11), we have

\[
A_{123}(\Lambda) = 1, \quad A_{132}(\Lambda) = \frac{\Delta - 2i}{\Delta + 2i}, \quad A_{213}(\Lambda) = \frac{v_1 - \Lambda - \Delta/2 - 2i}{v_1 - \Lambda - \Delta/2 + 2i},
\]
\[
A_{231}(\Lambda) = \left(\frac{v_1 - \Lambda - \Delta/2 - 2i}{v_1 - \Lambda - \Delta/2 + 2i}\right) \left(\frac{v_1 - \Lambda + \Delta/2 - 2i}{v_1 - \Lambda + \Delta/2 + 2i}\right),
\]
\[
A_{312}(\Lambda) = \left(\frac{v_1 - \Lambda + \Delta/2 - 2i}{v_1 - \Lambda + \Delta/2 + 2i}\right) \left(\frac{\Delta - 2i}{\Delta + 2i}\right),
\]
\[
A_{321}(\Lambda) = \left(\frac{v_1 - \Lambda - \Delta/2 - 2i}{v_1 - \Lambda - \Delta/2 + 2i}\right) \left(\frac{v_1 - \Lambda + \Delta/2 - 2i}{v_1 - \Lambda + \Delta/2 + 2i}\right) \left(\frac{\Delta - 2i}{\Delta + 2i}\right).
\]

(2.12)
Let us denote by \( f^{(B)}_{R,K} \) the Bethe ansatz wavefunction for the formal state \( |R,K;\Lambda\rangle \). The Bethe ansatz wavefunction of \( |1,2;\Lambda\rangle \) is given by

\[
f^{(B)}_{1,2}(x_1, x_2, x_3; k_1, k_2(\Lambda), k_3(\Lambda)) = A_{123} \exp i (k_1 x_1 + k_2(\Lambda) x_2 + k_3(\Lambda) x_3) + A_{132} \exp i (k_1 x_1 + k_3(\Lambda) x_2 + k_2(\Lambda) x_3) + A_{213} \exp i (k_2(\Lambda) x_1 + k_1 x_2 + k_3(\Lambda) x_3) + A_{312} \exp i (k_3(\Lambda) x_1 + k_1 x_2 + k_2(\Lambda) x_3) + A_{231} \exp i (k_2(\Lambda) x_1 + k_3(\Lambda) x_2 + k_1 x_3) + A_{321} \exp i (k_3(\Lambda) x_1 + k_2(\Lambda) x_2 + k_1 x_3)
\]

for \( 1 \leq x_1 < x_2 < x_3 \leq L \), \( \text{(2.13)} \)

where \( k_2(\Lambda) \) and \( k_3(\Lambda) \) are given by

\[
\exp(ik_2(\Lambda)) = \left( \frac{\Lambda + \Delta/2 + i}{\Lambda + \Delta/2 - i} \right), \quad \exp(ik_3(\Lambda)) = \left( \frac{\Lambda - \Delta/2 + i}{\Lambda - \Delta/2 - i} \right).
\]

\( \text{(2.14)} \)

Sending the center \( \Lambda \) to infinity : \( \Lambda \to \infty \), we have \( k_2 = k_3 = 0 \) (mod)\( 2\pi \) and

\[
A_{123}(\infty) = A_{213}(\infty) = A_{231}(\infty) = 1
\]
\[
A_{132}(\infty) = A_{312}(\infty) = A_{321}(\infty) = \frac{\Delta - 2i}{\Delta + 2i}.
\]

\( \text{(2.15)} \)

Therefore, the limit of the Bethe ansatz wavefunction is given by

\[
\lim_{\Lambda \to \infty} f^{(B)}_{1,2}(x_1, x_2, x_3; k_1, k_2(\Lambda), k_3(\Lambda)) = C_2 \left( e^{ik_1 x_1} + e^{ik_1 x_2} + e^{ik_1 x_3} \right).
\]

\( \text{(2.16)} \)

where the constant \( C_2 \) is given by

\[
C_2 = \left( 1 + \frac{\Delta - 2i}{\Delta + 2i} \right).
\]

\( \text{(2.17)} \)

Combining the eqs. (2.16) and (2.5), we obtain the following result.

\[
\lim_{\Lambda \to \infty} |1,2;\Lambda\rangle = C_2 \sum_{1 \leq x_1 < x_2 < x_3 \leq L} \left( e^{ik_1 x_1} + e^{ik_1 x_2} + e^{ik_1 x_3} \right) \sigma_{x_1}^- \sigma_{x_2}^- \sigma_{x_3}^- |0\rangle
\]
\[
= C_2 \frac{1}{2} \left( S_{\text{tot}}^- \right)^2 |1\rangle
\]
\[
= C_2 |1,2\rangle
\]

\( \text{(2.18)} \)

Thus, we have shown that the limit of the formal Bethe state \( |1,2;\Lambda\rangle \) is equivalent to the non-regular eigenstate \( |1,2\rangle \). We shall prove this equivalence for the general case in sec. 3. For an illustration, we shall consider the case of \( R = 0 \) and \( K = 3 \) in Appendix B.
Let us give some remarks on eq. (2.18). We see that the limiting procedure depends on the difference \( \Delta \). If \( \Delta = -2i \), then the constant \( C_2 \) becomes infinite. If \( \Delta = 0 \), then the constant \( C_2 \) vanishes. Thus, the limit of the wavefunction with infinite rapidities \( v_2 \) and \( v_3 \) depends on how we send them into infinity.

D. The P.B.C.s for the limits of the formal Bethe states

The formal Bethe state \(|R, K; \Lambda\rangle\) satisfies the periodic boundary conditions after taking the limit: \( \Lambda \to \infty \). In fact, it is clear since the limit gives the non-regular eigenvector \(|R, K\rangle\), which satisfies the periodic boundary conditions. Here we note that the total spin operator \( \vec{S}_{\text{tot}} \) is translation invariant. However, infinite rapidities do not always satisfy the Bethe ansatz equations.

For an illustration, let us consider the formal Bethe state \(|1, 2; \Lambda\rangle\). We denote by \( f_{1,2}^{(\infty)}(x_1, x_2, x_3) \) the limit of \( f_{1,2}^{(B)}(x_1, x_2, x_3; k_1, k_2(\Lambda), k_3(\Lambda)) \) with \( \Lambda \) sent to infinity. We see that it satisfies the periodic boundary conditions: \( f_{1,2}^{(\infty)}(x_1, x_2, x_3) = f_{1,2}^{(\infty)}(x_2, x_3, x_1 + L) \) for \( 1 \leq x_1 < x_2 < x_3 \leq L \). Explicitly we have

\[
f_{1,2}^{(\infty)}(x_2, x_3, x_1 + L) = \frac{2\Delta}{\Delta + 2i} \left( e^{ik_1x_2} + e^{ik_1x_3} + e^{ik_1(x_1+L)} \right). \tag{2.19}
\]

Thus, it satisfies the periodic boundary conditions if and only if the following holds:

\[
\exp(ik_1L) = 1 \quad \tag{2.20}
\]

This is nothing but the Bethe ansatz equation for \( k_1 \), and it does hold from the assumption that \( v_1 \) is the rapidity of a regular eigenvector \(|1\rangle\).

Now let us show that the additional rapidities do not necessarily satisfy the Bethe ansatz equations, although the limiting Bethe ansatz wavefunction satisfies the periodic boundary conditions. Let us consider the Bethe ansatz equations for three rapidities \( v_1, v_2 \) and \( v_3 \)

\[
\left( \frac{v_1 + i}{v_1 - i} \right)^L = \left( \frac{v_1 - v_2 + 2i}{v_1 - v_2 - 2i} \right) \left( \frac{v_1 - v_3 + 2i}{v_1 - v_3 - 2i} \right) \\
\left( \frac{v_2 + i}{v_2 - i} \right)^L = \left( \frac{v_2 - v_1 + 2i}{v_2 - v_1 - 2i} \right) \left( \frac{v_2 - v_3 + 2i}{v_2 - v_3 - 2i} \right)
\]
Taking the limit: $\Lambda \rightarrow \infty$, the three equations are reduced into the following

\[
\left( \frac{v_1 + i}{v_1 - i} \right)^L = 1 \tag{2.22}
\]

\[
\left( \frac{\Delta + 2i}{\Delta - 2i} \right) = 1 \tag{2.23}
\]

The equation (2.23) does not hold if $\Delta$ takes a finite value; it holds only if $|\Delta| = \infty$.

### III. PROOF OF THE LIMIT OF FORMAL BETHE STATES

In this section we prove the theorem in the following.

**Theorem III.1** Let $|R\rangle$ be a regular Bethe ansatz eigenstate with $R$ down-spins and rapidities $v_1, \ldots, v_R$. We recall that the symbol $||R, K; \Lambda\rangle$ denotes the formal Bethe state with $R + K$ down-spins, which has the $R$ rapidities $v_1, \ldots, v_R$ of $|R\rangle$ together with additional rapidities $v_{R+1}(\Lambda) \ldots, v_{R+K}(\Lambda)$. Then, the non-regular eigenstate $|R, K\rangle$, which is a descendant of $R$, is equivalent to the limit of the formal Bethe state $||R, K; \Lambda\rangle$ with $\Lambda$ sent to infinity:

\[
\lim_{\Lambda \rightarrow \infty} ||R, K; \Lambda\rangle = C_K|R, K\rangle \tag{3.1}
\]

**A. Derivation of the formula for amplitudes $A_M(P)$’s**

We now discuss the derivation of the formula (2.10), which rewrites the amplitudes $A_M(P)$’s defined in (1.3). Let us recall that the symbol $H(x)$ denote the Heaviside step function defined by $H(x) = 1$ for $x > 0$, and $H(x) = 0$ otherwise. We now show the following proposition.

**Lemma III.1** Let $P$ be an element of $S_M$, and $v_1, v_2, \ldots, v_M$ be generic parameters. Then, the following identity holds.
\[
\prod_{1 \leq j < k \leq M} \frac{v_{P_j} - v_{P_k} + 2i}{v_j - v_k + 2i} = \prod_{1 \leq j < k \leq M} \left( \frac{v_k - v_j + 2i}{v_j - v_k + 2i} \right)^{H(P^{-1}j - P^{-1}k)}.
\] (3.2)

(Proof) Let us take a pair of integers \(j \) and \(k\) with \(j < k\), and consider the factor \(v_j - v_k + 2i\) in the denominator of LHS of eq. (3.2). For the pair, there exist two integers \(\ell\) and \(m\) such that \(P\ell = j\), \(Pm = k\). There are two cases either \(\ell < m\) or \(\ell > m\). If \(\ell < m\), then we have the factor \(v_{P\ell} - v_{Pm} + 2i\) in the enumerator of LHS of eq. (3.2). Thus, the factors associated with the rapidities \(v_j\) and \(v_k\) cancel each other. On the other hand, if \(\ell > m\), we have \(v_{Pm} - v_{P\ell} + 2i\) in the enumerator of LHS of eq. (3.2), and we have

\[
\frac{v_{Pm} - v_{P\ell} + 2i}{v_j - v_k + 2i} = \frac{v_k - v_j + 2i}{v_j - v_k + 2i}.
\] (3.3)

We can express these results by the following

\[
\left( \frac{v_k - v_j + 2i}{v_j - v_k + 2i} \right)^{H(\ell - m)}.
\]

Considering all the pairs \(j, k\) with \(j < k\), we establish the equality (3.2).

Q.E.D.

**Proposition III.1** The amplitude \(A_M(P)\) defined by eq. (1.3) for \(P \in S_M\) can be expressed as follows.

\[
A_M(P) = \prod_{1 \leq j < k \leq M} \left( \frac{v_j - v_k - 2i}{v_j - v_k + 2i} \right)^{H(P^{-1}j - P^{-1}k)}.
\] (3.4)

(Proof) The amplitude \(A_M(P)\) defined by eq. (1.3) is written in terms of rapidities as follows

\[
A_M(P) = \epsilon(P) \prod_{1 \leq j < k \leq M} \frac{v_{Pj} - v_{Pk} + 2i}{v_j - v_k + 2i}.
\] (3.5)

In Appendix C, we show the following identity in Prop. C.1

\[
\epsilon_M(P) = \prod_{1 \leq j < k \leq M} (-1)^{H(P^{-1}j - P^{-1}k)}.
\] (3.6)

Thus, making use of Lem. III.1 and Prop. C.1, we obtain
\[ A_M(P) = \epsilon(P) \prod_{1 \leq j < k \leq M} \frac{v_{Pj} - v_{Pk} + 2i}{v_j - v_k + 2i} \]
\[ = \epsilon(P) \prod_{1 \leq j < k \leq M} \left( \frac{v_k - v_j + 2i}{v_j - v_k + 2i} \right)^{H(P^{-1}j - P^{-1}k)} \]
\[ = \prod_{1 \leq j < k \leq M} \left( \frac{v_j - v_k - 2i}{v_j - v_k + 2i} \right)^{H(P^{-1}j - P^{-1}k)} \]  
(3.7)

\[ Q.E.D. \]

We give a remark. Using Prop. III.1, we can explicitly prove that the Bethe states (and also the formal Bethe states) should vanish when there are two momenta of the same value. The proof is given in Appendix D.

B. Proof of the limit

Let us take a permutation \( P \) on \( R + K \) letters (\( P \in S_{R+K} \)). We consider the following set

\[ P^{-1}\{1, 2, \ldots, R\} = \{P^{-1}j \mid \text{for } j = 1, 2, \ldots, R\}. \]  
(3.8)

Let us denote the elements of the set by \( a_1, a_2, \ldots, a_R \), where \( a_j \)'s are set in increasing order: \( a_1 < a_2 < \cdots < a_R \). For the permutation \( P \), we introduce permutation \( P_R \) on \( R \) letters by

\[ P_Rm = Pa_m \quad \text{for} \quad m = 1, \ldots, R. \]  
(3.9)

Then, we have the following.

Lemma III.2 Let \( P_R \) denote the permutation on \( R \) letters defined by (3.9) for a given permutation \( P \) on \( R + K \) letters. For two integers \( j_1 \) and \( j_2 \) with \( 1 \leq j_1, j_2 \leq R \), the inequality \( P^{-1}j_1 < P^{-1}j_2 \) holds if and only if \( P_R^{-1}j_1 < P_R^{-1}j_2 \). Equivalently, we have

\[ H(P^{-1}j_1 - P^{-1}j_2) = H(P_R^{-1}j_1 - P_R^{-1}j_2) \quad \text{for} \quad 1 \leq j_1, j_2 \leq R. \]  
(3.10)
(proof) Let us denote $P^{-1}j_1$ and $P^{-1}j_2$ by $a_{m_1}$ and $a_{m_2}$, respectively. Then, by definition, we have $m_1 = P_R^{-1}j_1$ and $m_2 = P_R^{-1}j_2$. Here we recall that $a_j$’s are set in increasing order. Thus, we see that $a_{m_1} < a_{m_2}$ if and only if $m_1 < m_2$, which gives the proof.

Similarly, let us introduce a permutation on $K$ letters. We consider the following set
\begin{equation}
P^{-1}\{R+1, R+2, \ldots, R+K\} = \{P^{-1}j \mid \text{for } j = R+1, R+2, \ldots, R+K\}. \tag{3.11}
\end{equation}
We denote by $b_1, b_2, \ldots, b_K$, the elements of the above set. Here we assume that $b_j$’s are in increasing order: $b_1 < b_2 < \cdots < b_K$. We define permutation $P_K$ on $K$ letters by the following
\begin{equation}
P_Km = Pb_m \quad \text{for } m = 1, 2, \ldots, K. \tag{3.12}
\end{equation}
Then, we can show the following.

**Lemma III.3** Let $P_K$ denote the permutation on $K$ letters defined by (3.12) for a given permutation $P$ on $R+K$ letters. For two integers $j_1$ and $j_2$ with $R+1 \leq j_1, j_2 \leq R+K$, the inequality $P^{-1}j_1 < P^{-1}j_2$ holds if and only if $P_K^{-1}(j_1-R) < P_K^{-1}(j_2-R)$. Equivalently, we have
\begin{equation}
H(P^{-1}j_1 - P^{-1}j_2) = H(P_K^{-1}(j_1-R) - P_K^{-1}(j_2-R)) \quad \text{for } R+1 \leq j_1, j_2 \leq R+K.
\end{equation}
\(3.13\)

Making use of Lemmas III.1, III.2 and III.3, we now show the following proposition

**Proposition III.2** Let us consider two positive integers $R$ and $K$ satisfying $0 < K \leq L - 2R$. Let $v_1, v_2, \ldots, v_R$ be the rapidities of a given regular eigenvector $|R\rangle$ with $R$ down-spins, and $v_{R+1}(\Lambda), \ldots, v_{R+K}(\Lambda)$ be additional $K$ rapidities which are given by $v_{R+j}(\Lambda) = \Lambda + \delta_j$ for $j = 1, 2, \ldots, K$. Here $\delta_j$’s are arbitrary constants. For the Bethe ansatz wavefunction $f_{R+K}$ with its amplitudes $A_{R+K}(P)$’s given by (1.3), we have the following limit.
\begin{equation}
\lim_{\Lambda \to \infty} f_{R+K}(x_1, \ldots, x_{R+K}; k_1, \ldots, k_R, k_{R+1}(\Lambda), \ldots, k_{R+K}(\Lambda)) = C_K \sum_{1 \leq j_1 < \cdots < j_R \leq R+K} f_R(x_{j_1}, \ldots, x_{j_R}, k_1, \ldots, k_R) \tag{3.14}
\end{equation}
Here $k_j$’s are related to the rapidities $v_j$’s through the relation: $\exp ik_j = (v_j + i)/(v_j - i)$, and the constant $C_K$ is given by

$$C_K = \sum_{P \in S_K} A_K(P) [\delta_1, \ldots, \delta_K]$$  \hspace{1cm} (3.15)

(Proof) We recall that the Bethe ansatz wavefunction $f_{R+K}$ is given by

$$f(x_1, \ldots, x_{R+K}) = \sum_{P \in S_{R+K}} A_{R+K}(P) \exp \left( i \sum_{j=1}^{R+K} k_{Pj} x_j \right)$$  \hspace{1cm} (3.16)

Let us take a permutation $P$ in $S_{R+K}$. By Lemma III.2 we can show that the amplitude $A_{R+K}(P)$ of the formal Bethe state is given by

$$A_{R+K}(P) [v_1, \ldots, v_R, v_{R+1}(A), \ldots, v_{R+K}(A)] = \prod_{1 \leq j < \ell \leq R+K} \left( \frac{v_j - v_\ell - 2i}{v_j - v_\ell + 2i} \right)^{H(P^{-1}j - P^{-1}\ell)}$$  \hspace{1cm} (3.17)

The above product can be decomposed into the three parts in the following

$$\prod_{1 \leq j < \ell \leq R+K} \left( \frac{v_j - v_\ell - 2i}{v_j - v_\ell + 2i} \right)^{H(P^{-1}j - P^{-1}\ell)} = \prod_{1 \leq j < \ell \leq R} \left( \frac{v_j - v_\ell - 2i}{v_j - v_\ell + 2i} \right)^{H(P^{-1}j - P^{-1}\ell)} \times \prod_{1 \leq j \leq R} \prod_{R+1 \leq \ell \leq R+K} \left( \frac{v_j - v_\ell - 2i}{v_j - v_\ell + 2i} \right)^{H(P^{-1}j - P^{-1}\ell)}$$

$$\times \prod_{R+1 \leq j < \ell \leq R+K} \left( \frac{v_j - v_\ell - 2i}{v_j - v_\ell + 2i} \right)^{H(P^{-1}j - P^{-1}\ell)}$$  \hspace{1cm} (3.18)

First, we consider the third part of RHS of (3.18). Making use of Lemma III.3, we have

$$\prod_{R+1 \leq j < \ell \leq R+K} \left( \frac{v_j - v_\ell - 2i}{v_j - v_\ell + 2i} \right)^{H(P^{-1}j - P^{-1}\ell)} = \prod_{1 \leq j < \ell \leq R+K} \left( \frac{v_{j+R} - v_{\ell+R} - 2i}{v_{j+R} - v_{\ell+R} + 2i} \right)^{H(P_K^{-1}j - P_K^{-1}\ell)}$$

$$\times \prod_{1 \leq j < \ell \leq R+K} \left( \frac{\delta_j - \delta_\ell - 2i}{\delta_j - \delta_\ell + 2i} \right)^{H(P_K^{-1}j - P_K^{-1}\ell)}$$  \hspace{1cm} (3.19)

We note that RHS of (3.19) is nothing but $A_K(P_K) [\delta_1, \ldots, \delta_K]$. Second, it is clear that the second part of RHS of (3.18) becomes 1 under the limit: $\Lambda \to \infty$. In fact, putting the additional rapidities into the second part of RHS of (3.18), we have

$$\prod_{1 \leq j \leq R} \prod_{R+1 \leq \ell \leq R+K} \left( \frac{v_j - v_\ell - 2i}{v_j - v_\ell + 2i} \right)^{H(P^{-1}j - P^{-1}\ell)}$$

$$\times \prod_{R+1 \leq j < \ell \leq R+K} \left( \frac{v_j - v_\ell - 2i}{v_j - v_\ell + 2i} \right)^{H(P^{-1}j - P^{-1}\ell)} = \prod_{1 \leq j \leq R} \prod_{R+1 \leq \ell \leq R+K} \left( \frac{v_j - \Lambda - \delta_\ell - 2i}{v_j - \Lambda - \delta_\ell + 2i} \right)^{H(P^{-1}j - P^{-1}\ell)}$$  \hspace{1cm} (3.20)
Third, we consider the first part of RHS of (3.18). We recall that \( P_R \) is defined for the given permutation \( P \) by the relation (3.9). Then, from Lemma III.2, we have

\[
\prod_{1 \leq j < \ell \leq R} \left( \frac{v_j - v_\ell - 2i}{v_j - v_\ell + 2i} \right)^{H(P^{-1}_{\ell-j} - P^{-1}_\ell)} = \prod_{1 \leq j < \ell \leq R} \left( \frac{v_j - v_\ell - 2i}{v_j - v_\ell + 2i} \right)^{H(P^{-1}_{R-j} - P^{-1}_R)}
\]

(3.21)

We note again that RHS of (3.21) is equal to \( A_{R+K}(P_R) [v_1, \ldots, v_R] \). Thus, we have

\[
\lim_{\Lambda \to \infty} A_{P+K}(P) [v_1, \ldots, v_R, v_{R+1}(\Lambda), \ldots, v_{R+K}(\Lambda)] = A_R(P_R) [v_1, \ldots, v_R] \times A_K(P_K) [\delta_1, \ldots, \delta_K]
\]

(3.22)

Let us now consider the exponential part of (3.16). We note the following

\[
\sum_{j=1}^{R+K} k_{P_j} x_j = \sum_{\ell=1}^{R+K} k_{\ell} x_{P^{-1}_\ell}
\]

\[
= \sum_{\ell=1}^{R} k_{\ell} x_{P^{-1}_\ell} + \sum_{\ell=R+1}^{R+K} k_{\ell} x_{P^{-1}_\ell}.
\]

(3.23)

Since \( k_{R+1} \ldots k_{R+K} \) are approaching to 0 (mod 2\( \pi \)) in the limit of sending \( \Lambda \) to infinity, we have

\[
\lim_{\Lambda \to \infty} \sum_{\ell=R+1}^{R+K} k_{\ell}(\Lambda) x_{P^{-1}_\ell} = 0 \pmod{2\pi}.
\]

(3.24)

Making use of the relation \( P_{Rm} = Pa_m \), we have

\[
\sum_{\ell=1}^{R} k_{\ell} x_{P^{-1}_\ell} = \sum_{m=1}^{R} k_{P_{Rm}} x_{P^{-1}_{P_{Rm}}} = \sum_{m=1}^{R} k_{P_{Rm}} x_{a_m}
\]

(3.25)

Thus, we have

\[
\lim_{\Lambda \to \infty} A_{R+K}(P) \exp(\sum_{j=1}^{R+K} k_{P_j} x_j)
\]

\[
= A_K(P_K) [\delta_1, \ldots, \delta_K] \times A_R(P_R) [v_1, \ldots, v_R] \exp(\sum_{m=1}^{R} k_{P_{Rm}} x_{a_m}) \text{ for } P \in S_{R+K}
\]

(3.26)

Finally, we give a remark. To pick up a permutation \( P \) on \( R + K \) letters is equivalent to do the procedures in the following: we take a subset \( \{a_1, a_2, \ldots, a_R\} \) of the set of \( R + K \) letters 1, 2, \ldots, \( R + K \), and specify \( P_R \) on \( R \) letters and \( P_K \) on \( K \) letters by (3.3) and (3.12), respectively. Therefore, we have
\[
\sum_{P \in S_{R+K}} = \sum_{\{a_1, \ldots, a_R\} \subset \{1, 2, \ldots, R+K\}} \sum_{P_R \in S_R} \sum_{P_K \in S_K}
\]

Thus, we have the relation (3.14), where \(a_m\)'s correspond to \(j_m\)'s.

\[Q.E.D.\]

It is now clear that we obtain Theorem III.1 from Proposition III.2.

IV. FORMAL BETHE STATE FROM THE ALGEBRAIC BETHE ANSATZ

A. The algebraic Bethe ansatz for the XXX model under the P.B.C.s

The formal Bethe state has been formulated in terms of the coordinate Bethe ansatz method in sec. 1. However, in this section, we show that it is also important in the context of the algebraic Bethe ansatz method. In fact, we show that the formal Bethe state \(\mid M \rangle\) with \(M\) rapidities corresponds to the state created by the \(B\) operators with the same set of rapidities. In the derivation, we use the method of the generalized two-site model first discussed by Izergin and Korepin [18,19].

Let us formulate some notation for the algebraic Bethe ansatz of the XXX model under the periodic boundary conditions. We define the \(L\) operator acting on the \(n\)th site of the one-dimensional lattice by

\[
L_n(\lambda) = \begin{pmatrix}
\lambda I_n + \eta \sigma_n^z & 2\eta \sigma_n^- \\
2\eta \sigma_n^+ & \lambda I_n - \eta \sigma_n^z
\end{pmatrix}
\]

(4.1)

Here we recall that the \(\sigma_n^z\)'s are the Pauli matrices acting on the \(n\)th site. The monodromy matrix is defined by the product of \(L\) operators

\[
T(\lambda) = L_L(\lambda - q_L)L_{L-1}(\lambda - q_{L-1}) \cdots L_1(\lambda - q_1)
\]

(4.2)

Here the free variables \(q_k\)'s are called inhomogeneous parameters. Let us denote the operator-valued matrix elements of the monodromy matrix by
The transfer matrix of the XXX model is given by the trace of the monodromy matrix

\[ \tau(\lambda) = \text{tr} (T(\lambda)) = A(\lambda) + D(\lambda) \] (4.4)

The Hamiltonian of the XXX model is derived from the logarithmic derivative of the homogeneous transfer matrix where all the inhomogeneous parameters are given by zero. We note that when \( q_k = 0 \) for \( k = 1, \ldots, L \), we call the transfer matrix homogeneous. Explicitly, we have

\[ \tau(\eta) \left. \left( \frac{d}{d\lambda} \tau(\lambda) \right) \right|_{\lambda = \eta; q_1 = \cdots = q_L = 0} = \frac{1}{4\eta} \sum_{j=1}^{L} (\hat{\sigma}_j \cdot \hat{\sigma}_{j+1} + 1) \] (4.5)

Let us consider the Yang-Baxter equations. With the \( R \) matrix

\[ R(\lambda) = \frac{1}{\lambda} \begin{pmatrix} \lambda + 2\eta & 0 & 0 & 0 \\ 0 & 2\eta & \lambda & 0 \\ 0 & \lambda & 2\eta & 0 \\ 0 & 0 & 0 & \lambda + 2\eta \end{pmatrix} \] (4.6)

we can show the Yang-Baxter equations for the \( L \) operators

\[ R(\lambda - \mu) (L_n(\lambda) \otimes L_n(\mu)) = (L_n(\mu) \otimes L_n(\lambda)) R(\lambda - \mu) \] (4.7)

Here the symbol \( \otimes \) denotes the direct product of matrices. Applying eq. (4.7) to each site, we can derive the Yang-Baxter equations for the monodromy matrix

\[ R(\lambda - \mu) (T(\lambda) \otimes T(\mu)) = (T(\mu) \otimes T(\lambda)) R(\lambda - \mu) \] (4.8)

The Yang-Baxter equations for the monodromy matrices give the set of commutation relations among the operators \( A(\lambda), B(\lambda), C(\lambda), D(\lambda) \). For instance, we have

\[ A(\lambda_1)B(\lambda_2) = f_{12}B(\lambda_2)A(\lambda_1) - g_{12}B(\lambda_1)A(\lambda_2) \] (4.9)

\[ D(\lambda_1)B(\lambda_2) = f_{21}B(\lambda_2)C(\lambda_1) - g_{21}B(\lambda_1)D(\lambda_2) \] (4.10)
Here the symbols $f_{12}$ and $g_{12}$ denote the following

\[ f_{12} = \frac{\lambda_1 - \lambda_2 - 2\eta}{\lambda_1 - \lambda_2}, \quad g_{12} = -\frac{2\eta}{\lambda_1 - \lambda_2} \]  

(4.11)

The operators $A(\lambda)$ and $D(\lambda)$ act on the vacuum $|0\rangle$ as

\[ A(\lambda)|0\rangle = a(\lambda)|0\rangle, \quad D(\lambda)|0\rangle = d(\lambda)|0\rangle \] 

(4.12)

where $a(\lambda)$ and $d(\lambda)$ are given by

\[ a(\lambda) = \prod_{k=1}^{L} (\lambda - q_k + \eta), \quad d(\lambda) = \prod_{k=1}^{L} (\lambda - q_k - \eta) \] 

(4.13)

B. The Bethe ansatz wavefunction from the generalized two-site model

Let us explicitly calculate the entries (or matrix elements) of the vector $B(\lambda_1) \cdots B(\lambda_M)|0\rangle$. Let us consider two sub-lattices of the one-dimensional lattice with sites 1 to $L$: one consisting of sites 1 to $n$ and the other of $n+1$ to $L$. The monodromy matrix $T(\lambda)$ for the total lattice is given by the product of two monodromy matrices for the sub-lattices

\[ T(\lambda) = T^{(2)}(\lambda)T^{(1)}(\lambda) \] 

(4.14)

where $T^{(1)}(\lambda)$ and $T^{(2)}(\lambda)$ are given by

\[ T^{(1)}(\lambda) = L_n(\lambda - q_n)L_{n-1}(\lambda - q_{n-1}) \cdots L_1(\lambda - q_1) \]

\[ T^{(2)}(\lambda) = L_L(\lambda - q_L)L_{L-1}(\lambda - q_{L-1}) \cdots L_{n+1}(\lambda - q_{n+1}) \] 

(4.15)

Let us denote the elements of the monodromy matrices of the sub-chains by the following

\[ T^{(\alpha)}(\lambda) = \begin{pmatrix} A^{(\alpha)}(\lambda) & B^{(\alpha)}(\lambda) \\ C^{(\alpha)}(\lambda) & D^{(\alpha)}(\lambda) \end{pmatrix} \quad \text{for} \quad \alpha = 1, 2. \] 

(4.16)

Then, the product is given by
\[
\begin{pmatrix}
A(\lambda) & B(\lambda) \\
C(\lambda) & D(\lambda)
\end{pmatrix} = \begin{pmatrix}
A^{(2)}(\lambda) & B^{(2)}(\lambda) \\
C^{(2)}(\lambda) & D^{(2)}(\lambda)
\end{pmatrix} \begin{pmatrix}
A^{(1)}(\lambda) & B^{(1)}(\lambda) \\
C^{(1)}(\lambda) & D^{(1)}(\lambda)
\end{pmatrix}
\]
(4.17)

It gives four relations. Among them, we consider the following

\[ B(\lambda) = A^{(2)}(\lambda)B^{(1)}(\lambda) + B^{(2)}(\lambda)D^{(1)}(\lambda) \]
(4.18)

By applying the formula (4.18) extensively, we can show the following [18,20]

\[
\prod_{j=1}^{M} B(\lambda_j)|0\rangle = \sum_{S_1,S_2}^{(2)} \left( \prod_{k \in S_1} B^{(1)}_k \prod_{m \in S_2} B^{(2)}_m \right) |0\rangle \left( \prod_{k \in S_1} \prod_{m \in S_2} f_{km} \right) \left( \prod_{k \in S_1} a^{(2)}_k \right) \left( \prod_{m \in S_2} d^{(1)}_m \right)
\]
(4.19)

Here the symbol \(\sum_{S_1,S_2}^{(2)}\) denotes the sum over all the combination of sets \(S_1\) and \(S_2\) satisfying the condition: \(S_1 \cup S_2 = \{1, \ldots, M\}\). Here we have denoted \(B(\lambda_k)\) by \(B_k\), briefly. The symbol \(a^{(2)}_k\) has been defined by the relation: \(A^{(2)}(\lambda_k)|0\rangle = a^{(2)}_k\), and so on. We can prove the formula (4.19) by induction on \(M\).

Let us consider the case where the total lattice of 1 to \(L\) is divided into \(r\) parts. Then, applying the formula (4.19), we can show the following [18,20]

\[
\prod_{j=1}^{M} B(\lambda_j)|0\rangle = \sum_{S_1,\ldots,S_r}^{(r)} \left( \prod_{a=1}^{r} \prod_{m \in S_a} B^{(a)}_{m} \right) |0\rangle \times \prod_{1 \leq \alpha < \beta \leq r} \left\{ \left( \prod_{k \in S_\alpha} \prod_{m \in S_\beta} f_{km} \right) \left( \prod_{k \in S_\alpha} a^{(\beta)}_k \right) \left( \prod_{m \in S_\beta} d^{(\alpha)}_m \right) \right\}
\]
(4.20)

Here the symbol \(\sum_{S_1,\ldots,S_r}^{(r)}\) denotes the sum over all the sets \(S_1,\ldots,S_r\) which satisfy the condition: \(S_1 \cup S_2 \cup \cdots \cup S_r = \{1, 2, \ldots, M\}\). The formula (4.20) can be proven by induction on \(r\).

Let us consider the case of \(r = L\) where each of the sub-lattices is consisting of only one site. Then, we can show \(B^{(a)}_k B^{(a)}_m|0\rangle = 0\), for any \(k, m \in S_\alpha\). Thus, if any one of the sets \(S_1,\ldots,S_L\) contains more than one integer, then the contribution for the sets vanishes in eq. (4.20). Therefore, we may consider only such partitions of \(\{1, \ldots, M\}\) into \(L\) sets: \(S_1,\ldots,S_L\) where each of \(S_j\)’s contains at most one integer. Let us take one such partition and assume that the symbols \(S_{x_1},\ldots,S_{x_M}\) denote the non-empty sets with \(1 \leq x_1 < x_2 < \cdots < x_M \leq L\).
Then, there exists an element of the permutation group $S_M$ such that $S_{x_j} = \{P_j\}$ for $j = 1, \ldots, M$. Now we can derive the following expression from eq. (4.20).

$$
\prod_{j=1}^{M} B(\lambda_j)|0\rangle = (2\eta)^M \sum_{P \in S_M} \sum_{1 \leq x_1 < \cdots < x_M \leq L} \prod_{j=1}^{M} \sigma_{x_j}^{-}|0\rangle
\times \left( \prod_{1 \leq \alpha, \beta \leq M} f_{P_k P_m}^{(k)} \prod_{\alpha=1}^{M} \prod_{1 \leq k < j_{\alpha}}^{\lambda_{P_\alpha} - \eta} \prod_{j_{\alpha} < k \leq L}^{\lambda_{P_\alpha} + \eta} \right) \quad (4.21)
$$

Here we have used the following

$$
\prod_{j=1}^{M} B_{P_j}^{(x_j)}|0\rangle = (2\eta)^M \prod_{j=1}^{M} \sigma_{x_j}^{-}|0\rangle \quad (4.22)
$$

which is valid when each of the $L$ sub-lattices consists of one site. Here we note that the product $\prod_{1 \leq j < k \leq M} f_{P_j P_k}$ is related to the amplitudes of the Bethe ansatz wavefunctions

$$
\prod_{1 \leq j < k \leq M} f_{P_j P_k} = \left( \prod_{1 \leq j < k \leq M} f_{j_k} \right) \prod_{1 \leq j < k \leq M} \left( \frac{\lambda_j - \lambda_k + 2\eta}{\lambda_j - \lambda_k - 2\eta} \right)^{H(P^{-1} j - P^{-1} k)} \quad (4.23)
$$

For the homogeneous case where $q_k = 0$ for $k = 1, \ldots, L$, we have

$$
\prod_{\alpha=1}^{M} \left( \prod_{1 \leq k < j_{\alpha}}^{d_{P_\alpha}^{(k)}} \prod_{j_{\alpha} < k \leq L}^{a_{P_\alpha}^{(k)}} \right) = \prod_{\alpha=1}^{M} \left\{ \frac{(\lambda_{P_\alpha} + \eta)^L}{\lambda_{P_\alpha} - \eta} \right\} \quad (4.24)
$$

Putting $\eta = -i$, we have

$$
\prod_{j=1}^{M} B(\lambda_j)|0\rangle = F_1(\{\lambda_j\}) \sum_{P \in S_M} \sum_{1 \leq x_1 < \cdots < x_M \leq L} \prod_{j=1}^{M} \sigma_{x_j}^{-}|0\rangle \left( \prod_{1 \leq \alpha, \beta \leq M} f_{P_k P_m}^{(k)} \right) \exp \left( i \sum_{j=1}^{M} k_{P_j} x_j \right) \quad (4.25)
$$

where the factor $F_1(\{\lambda_j\})$ has been given by

$$
F_1(\{\lambda_j\}) = (2\eta)^M \prod_{j=1}^{M} \frac{\lambda_j - i)^L}{\lambda_j + i} \quad (4.26)
$$

Noting the relation (4.23) we obtain

$$
\prod_{j=1}^{M} B(\lambda_j)|0\rangle = F_1(\{\lambda_j\}) F_2(\{\lambda_j\})
\times \sum_{P \in S_M} \sum_{1 \leq x_1 < \cdots < x_M \leq L} \left( \prod_{j=1}^{M} \sigma_{x_j}^{-}|0\rangle \right) A_M(P)[\lambda_1, \cdots, \lambda_M] \exp \left( i \sum_{j=1}^{M} k_{P_j} x_j \right) \quad (4.27)
$$

22
where the factor $F_2$ has been given by $F_2(\{\lambda_j\}) = \prod_{1 \leq j < k \leq M} f_{jk}$. In terms of the notation of the formal Bethe state $|M\rangle$, we have

$$B(\lambda_1) \cdots B(\lambda_M)|0\rangle = |M\rangle \times f_1(\{\lambda_j\})F_2(\{\lambda_j\})$$

(4.28)

Thus, we have shown that the formal Bethe state $|M\rangle$ is nothing but the vector $B(\lambda_1) \cdots B(\lambda_M)|0\rangle$ where all the rapidities are given by free parameters. Here we remark that the derivation of (4.21) for the cases of $M = 1$ and $M = 2$ has already been given explicitly such as in Refs. [4,11].

We give some remarks. The expression (4.21) also holds for the XXZ model, where $f_{jk}$, $a(\lambda)$ and $d(\lambda)$ are replaced by

$$f_{jk} = \frac{\sinh(\lambda_j - \lambda_k - 2\eta)}{\sinh(\lambda_j - \lambda_k)}, \quad g_{jk} = -\frac{\sinh(2\eta)}{\sinh(\lambda_j - \lambda_k)}$$

$$a(\lambda) = L \prod_{k=1}^{L} \sinh(\lambda - q_k + \eta), \quad d(\lambda) = L \prod_{k=1}^{L} \sinh(\lambda - q_k - \eta).$$

(4.29)

Corresponding to eq. (4.23), for the XXZ model we have

$$\prod_{1 \leq j < k \leq M} f_{P_j P_k} = \left( \prod_{1 \leq j < k \leq M} f_{jk} \right) \prod_{1 \leq j < k \leq M} \left( \frac{f_{kj}}{f_{jk}} \right)^{H(P^{-1} j - P^{-1} k)}$$

(4.30)

A similar relation with (4.21) has also been derived for the algebraic Bethe ansatz of the elliptic quantum group [21], where $f_{jk}$ are expressed in terms of the elliptic theta functions.

V. THE SPECTRAL FLOW UNDER THE TWISTED B.C.S

A. Formal Bethe states under P.B.C.s

Let us discuss the formal Bethe state from the viewpoint of the ground-state solution of the XXZ model given by Yang-Yang [4]. We consider the case of the anti-ferromagnetic Heisenberg model. In this section we assume that $L$ is even. We note that the relation between momentum and rapidity is slightly different from that of sec.1 and sec. 2 due to the gauge transformation [4].
The Hamiltonian of the XXZ model is given by

$$\mathcal{H} = -J \sum_{\ell=1}^{L} \left( S_\ell^x S_{\ell+1}^x + S_\ell^y S_{\ell+1}^y + \Delta S_\ell^z S_{\ell+1}^z \right).$$

(5.1)

where $\Delta$ is called the anisotropy parameter. Let us discuss the anti-ferromagnetic XXX model. Hereafter we assume $\Delta = -1$. Under the periodic boundary condition: $\vec{S}_{L+1} = \vec{S}_1$, we have the Bethe ansatz equations

$$\exp(iLk_j) = (-1)^{M-1} \prod_{\ell=1, \ell \neq j}^{M} \frac{\exp[i(k_j + k_\ell)] + 1 - 2(-1)^{\exp(i(k_j + k_\ell))}}{\exp[i(k_j + k_\ell)] + 1 - 2(-1)^{2\exp(i(k_\ell))}},$$

for $j = 1, \ldots, M$. (5.2)

We consider the case where all the momenta $k_j$’s are real. Taking the logarithm of the Bethe ansatz eqs. (5.2), we have

$$Lp_j = 2\pi I_j - \sum_{\ell=1, \ell \neq j}^{M} \Theta(p_j, p_\ell), \quad \text{for} \quad j = 1, \ldots, M. \quad (5.3)$$

Here $I_j = (M - 1)/2 \pmod{1}$. The function $\Theta(p, q)$ has been given by [5]

$$\Theta(p, q) = 2 \tan^{-1}\left( \frac{-1}{\cos((p + q)/2) - (1) \cos((p - q)/2)} \right). \quad (5.4)$$

In Ref. [5], some important analytic properties of the function $\Theta(p, q)$ have been given. In particular, we notice the following: When $-\pi < p < \pi$ and $-\pi < q < \pi$, we have

$$\lim_{\epsilon \to 0, 0 < \epsilon \ll 1} \Theta(p - \epsilon, q) = -\pi, \quad \lim_{\epsilon \to 0, 0 < \epsilon \ll 1} \Theta(p + \epsilon, q) = \pi, \quad (5.5)$$

$$\Theta(p, q) = -\Theta(q, p). \quad (5.6)$$

Here we note that $\epsilon$ should be positive in the limits. In Ref. [5], the function is mainly discussed within the range $(-\pi, \pi)$ for $p$ and $q$.

Let us first show that the limit: $p \to -\pi$ under $p > -\pi$ corresponds to the limit of infinite rapidity: $\Lambda \to \infty$ discussed in the previous sections. Let us introduce the transformation between momentum $k$ and rapidity $v$ for the anti-ferromagnetic case $(\Delta = -1)$

$$\exp(iv) = (-1)^{\frac{v + i}{v - i}}. \quad (5.7)$$
Here the extra $(-1)$ factor corresponds to the gauge transformation, which is consistent with the periodic boundary condition if $L$ is even. By taking the logarithm of the relation (5.7) and choosing the branch of the logarithmic function such that is consistent with the function $\Theta(p, q)$, we have

$$k = -2 \tan^{-1} v. \quad (5.8)$$

It is clear that momentum $k$ is in the range $(-\pi, \pi)$ if $v$ is finite. If we take the limit $v \to \infty$, then the momentum $k$ approaches to $-\pi$ from the above ($k > -\pi$). Thus, we can extend the range of real momenta as follows

$$-\pi \leq k < \pi. \quad (5.9)$$

Let us call momentum $k_j$ regular if it satisfies the condition: $-\pi < k_j < \pi$. We now introduce a symbol $T_1$ for $(L - M - 1)/2$. From the viewpoint of the string-hypothesis, it is shown that the integer (or half-odd integer) $I_j$ for a regular real momentum $k_j$ satisfies the condition: $|I_j| < T_1$ [1,3,13,22].

We now consider such a solution to the Bethe ansatz equations that has the momentum $k_0 = -\pi$. Suppose that the set of $R$ regular momenta $k_1, \ldots, k_R$ and one non-regular momentum $k_0 = -\pi$ gives a solution to the Bethe ansatz equations (5.3) with $M = R + 1$ down-spins. We have the following equations.

$$Lk_j = 2\pi I_j - \sum_{\ell=0,\ell\neq j}^{R} \Theta(k_j, k_\ell), \quad \text{for } j = 1, \ldots, R, \quad (5.10)$$

$$Lk_0 = 2\pi I_0 - \sum_{\ell=1}^{R} \Theta(k_0, k_\ell). \quad (5.11)$$

Here we have defined the equation for the momentum $k_0 = -\pi$ by taking the limit of $k$ to $-\pi$ under the condition $k > -\pi$. We also assume that $I_j = R/2 \pmod 1$ and $|I_j| \leq T_1 = (L - R)/2 - 1$ for $j = 1, \ldots, R$. ($M - 1 = R.$)

Let us construct solutions to eqs. (5.10) and (5.11). Making use of the limit (5.5), we can easily show that $k_0 = -\pi$ gives a solution to the equation (5.11) with $I_0 = -T_1 - 1$, where $T_1 = (L - R)/2 - 1$. Recall that for $k_0 = -\pi$, we assume the limit: $k_0 \to -\pi$ under the
condition: \( k_0 > -\pi \). From the property (5.3), we can show that the eq. (5.10) is equivalent to
\[
Lk_j = 2\pi (I_j + \frac{1}{2}) - \sum_{\ell=1,\ell\neq j}^R \Theta(k_j, k_\ell), \quad \text{for } j = 1, \ldots, R. \tag{5.12}
\]
We note that the set of equations (5.12) is equivalent to the standard Bethe ansatz equations (5.3) for \( R \) down-spins, where their numbers \( (I_j + 1/2) \)'s satisfy the parity with \( R \) down-spins: \( I_j + 1/2 = (R - 1)/2 \) (mod 1).

Let us summarize the construction of solutions to (5.10) and (5.11). We first consider the standard Bethe ansatz equations (5.3) (or (5.12)) with \( R \) down-spins where their quantum numbers \( \hat{I}_j \)'s are given by \( \hat{I}_j = I_j + 1/2 \) for \( j = 1, \ldots, R \). We denote the solutions by \( \hat{k}_1, \ldots, \hat{k}_R \) for \( \hat{I}_1, \ldots, \hat{I}_R \), respectively. Then, the solutions to eqs. (5.10) and (5.11) are given by
\[
k_j = \hat{k}_j, \quad \text{for } j = 1, \ldots, R,
\]
\[
k_0 = -\pi, \tag{5.13}
\]
where \( I_0 = -(L - R)/2 \).

It is interesting to note that the set of momenta \( k_0, \ldots, k_R \), constructed in the above corresponds to such a solution of the Bethe ansatz equations that gives the non-regular eigenstate \( |R, 1 \rangle \). In fact, we obtain the non-regular eigenstate \( |R, 1 \rangle \), by taking the limit of the formal Bethe state \( ||R, 1; \Lambda \rangle \) with the momenta \( k_0, \ldots, k_R \), where \( k_0 \) corresponds to the infinite rapidity.

**B. Bethe states under the twisted B.C.s with a small twist**

Let us now consider the twisted boundary conditions
\[
S_{L+1}^\pm = S_1^\pm \exp(\pm i\Phi), \quad S_{L+1}^z = S_1^z. \tag{5.14}
\]
Here we call the variable \( \Phi \) the twisting parameter. The Bethe ansatz equations under the twisted boundary conditions are given by \[23\ 29\]
\[ \exp(iLp_j) = (-1)^{M-1} \exp(i\Phi) \prod_{\ell=1,\ell\neq j}^{M} \exp[i(p_j + p_\ell)] + 1 - 2(-1) \exp(ip_j) \]

for \( j = 1, \ldots, M. \) \hfill (5.15)

Let us assume that all the momenta \( p_j \)'s are real. Taking the logarithms of eqs. (5.15), we have

\[ Lp_j = 2\pi I_j + \Phi - \sum_{\ell=1,\ell\neq j}^{M} \Theta(p_j, p_\ell), \quad \text{for } j = 1, \ldots, M. \] \hfill (5.16)

where \( I_j = (M - 1)/2 \) (mod 1).

Let us discuss the adiabatic behaviors of solutions of the Bethe ansatz equations (5.16) under the twisted boundary conditions, where \( \Phi \) is a very small positive number, and is increased adiabatically. Here we assume that \( R + 1 \) momenta: \( p_0, p_1, \ldots, p_R \) are solutions of the Bethe ansatz equations where one momentum \( p_0 \) is close to \(-\pi \) \((p_0 \sim -\pi)\). We also assume that \( R < L/2 \). We consider the following equations.

\[ Lp_j = 2\pi I_j + \Phi - \sum_{\ell=0,\ell\neq j}^{R} \Theta(p_j, p_\ell), \quad \text{for } j = 1, \ldots, R, \] \hfill (5.17)

\[ Lp_0 = 2\pi I_0 + \Phi - \sum_{\ell=1}^{R} \Theta(p_0, p_\ell). \] \hfill (5.18)

Here, \( I_j = R/2 \) (mod 1) and \( |I_j| \leq T_1 = (L - R)/2 - 1 \) for \( j = 1, \ldots, R \). (Note \( M - 1 = R \).)

Now, let us introduce a small positive number \( \epsilon \) and express \( p_0 \) as \( p_0 = -\pi + \epsilon \). Then, we can expand the function \( \Theta(p, q) \) in the following

\[ \Theta(-\pi + \epsilon, q) = \pi - 2\epsilon + \epsilon^2 \tan \frac{q}{2} + O(\epsilon^3), \]

\[ \Theta(\pi - \epsilon, q) = -\pi + 2\epsilon + \epsilon^2 \tan \frac{q}{2} + O(\epsilon^3). \] \hfill (5.19)

Substituting the expansion into eq. (5.18) we have

\[ 2\pi I_0 + \Phi = -\pi(L - R) + \epsilon(L - 2R) + O(\epsilon^2). \] \hfill (5.20)

Let us consider the adiabatic change of the twisting parameter \( \Phi \). When we change the parameter \( \Phi \) infinitesimally, then the quantum number \( I_0 \) does not change at all. Thus, we obtain the following solutions
\[ I_0 = -L - R/2 = -T_1 - 1, \]
\[ \epsilon = \Phi/(L - 2R) + O(\epsilon^2). \quad (5.21) \]

The solution: \( p_0 = -\pi + \Phi/(L - 2R) + O(\epsilon^2) \) can be considered as a regular solution, since it satisfies the condition \(-\pi < p_0 < -\pi\). Furthermore, it is clear that \( p_0 \) approaches to \( k_0 \) under the limit \( \Phi \to 0 \) with \( \Phi > 0 \). Therefore, we conclude that the formal solution \( k_0 = -\pi \) under the periodic boundary conditions corresponds to the regular solution \( p_0 = -\pi + \Phi/(L - 2R) + O(\epsilon^2) \) under the twisted boundary conditions.

We make a remark on the number of solutions to eq. (5.16). Under the periodic boundary conditions, there are \( 2T_1 + 1 = L - M \) regular solutions. Under the twisted boundary conditions, however, we have one more regular solution and \( 2T_1 + 2 = L - M + 1 \) regular solutions in total.

**C. Analytic continuation of \( \Theta(p, q) \) and 2\( \pi \)-shift of momentum**

In the previous subsection we have considered the case where the twisting parameter \( \Phi \) is very small. Hereafter, we discuss how the ground-state solution changes with respect to the parameter \( \Phi \), and then we shall show that the spectral flow should have the period of \( 4\pi \), at the end of sec. 5.

Let us consider an extension of the function \( \Theta(p, q) \) of the variable \( p \) defined on the range \((-\pi, \pi)\) into a continuous function defined over \((-\infty, \infty)\). Taking into account the analytic property (5.5), we make the extension with respect to \( p \) as follows

\[
\Xi(p, q) = \begin{cases} 
-(2n + 1)\pi, & \text{if } p = (2n + 1)\pi, \text{ for an integer } n, \\
\Theta(p - 2\pi \left\lceil \frac{p + \pi}{2\pi} \right\rceil, q) - 2\pi \left\lceil \frac{p + \pi}{2\pi} \right\rceil, & \text{otherwise.}
\end{cases} \quad (5.22)
\]

Here the symbol \( \lceil x \rceil \) denotes the Gauss’ symbol. We recall that \( p \) is an arbitrary real number in eq. (5.22). We also extend the function \( \Theta(p, q) \) with respect to \( q \) by assuming the relation \( \theta(p, q) = -\theta(q, p) \).

In terms of the extended function, the Bethe ansatz equations are given by
\[ L \rho_j = 2\pi I_j + \Phi - \sum_{\ell=1, \ell \neq j}^M \Xi(p_j, p_\ell), \quad \text{for} \quad j = 1, \ldots, M, \] (5.23)

where \( I_j = (M - 1)/2 \) (mod 1). We recall that the range of \( p_j \)'s are given by the extended zone \((-\infty, \infty)\) in eqs. (5.23). We note that for regular solutions, eqs. (5.23) are equivalent to the standard Bethe ansatz equations (5.10). We recall that when \( p_j \)'s are regular, then they satisfy \(-\pi < p_j < \pi\).

Let us discuss the number of all the possible solutions to eqs. (5.23). We assume that \( p_1, \ldots, p_M \) are solutions to (5.23) with the quantum numbers \( I_1, \ldots, I_M \), respectively. Let us take a suffix \( j_1 \) from 1, \ldots, \( M \). We consider momenta \( \hat{p}_j \) given by

\[
\hat{p}_{j_1} = p_{j_1} + 2\pi \quad \text{and} \quad \hat{p}_j = p_j \quad \text{if} \quad j \neq j_1 \quad (1 \leq j \leq M).
\] (5.24)

Putting \( \hat{p}_j \)'s into the eq. (5.23), we see that they give solutions to eq. (5.23) with the quantum numbers \( \hat{I}_j \)'s where they are given by

\[
\hat{I}_{j_1} = I_{j_1} + L - M + 1, \quad \text{and} \quad \hat{I}_j = I_j + 1 \quad \text{for} \quad j \neq j_1 \quad (1 \leq j \leq M).
\] (5.25)

Thus, we may regard the number \( L - M + 1 \) as the period of the quantum numbers \( I_j \)'s. Therefore, we may consider only \( L - M + 1 \) different values for \( I_j \)'s such as \(-T_1 - 1, -T_1, \ldots, T_1\). This choice is consistent with the range of momentum \(-\pi \leq k < \pi\). \( (I_0 = -T_1 - 1 \) corresponds to \( k_0 = -\pi \) or \( v = \infty \) when \( \Phi = 0\).) Thus, if there is a one-to-one correspondence between \( k_j \)'s and \( I_j \)'s, then the number of solutions of the Bethe ansatz equations is given by \( L - M + 1 \). We note \( L - M + 1 = (2T_1 + 1) + 1 \), where \( 2T_1 + 1 \) is the number of regular solutions given by the string hypothesis.

Let us make a remark on the change in the total momentum \( P_{tot} \) induced by the shift: \( p_{j_1} \rightarrow p_{j_1} + 2\pi \). In fact, it is consistent with the shift of the quantum numbers \( \hat{I}_j \)'s. We denote by \( \hat{P}_{tot} \) the total momentum for the momenta \( \hat{p}_j \)'s and \( \hat{I}_j \)'s. Then, we have

\[
\hat{P}_{tot} = \sum_j \hat{p}_j = 2\pi + \sum_j p_j,
\]

\[
\frac{2\pi}{L} \sum_j \hat{I}_j = \frac{2\pi}{L} \sum_{j \neq j_1} (I_j - 1) + \frac{I_{j_1} + L - M + 1}{L} = 2\pi + \frac{2\pi}{L} \sum_j I_j.
\] (5.26)
Let us discuss how the ground-state solution changes when we increase the twisting parameter \( \Phi \) adiabatically from 0 to \( 4\pi \). In fact, it is known that the spectral flow of the ground-state energy has the period of \( 4\pi \) with respect to the twisting parameter \([23, 29]\). In the following paragraphs, we shall show that the shift \((5.25)\) on the \( I_j \)'s is consistent with the \( 4\pi \) period of the spectral flow of the ground-state energy.

We consider the half-filling case where \( M = L/2 \). Here, we have \( T_1 = (L/2 - 1)/2 \). Let symbols \( p_j(\Phi) \) for \( j = 1, \ldots, M \) denote the momenta satisfying the Bethe ansatz equations \((5.23)\) under the twisted boundary condition. We assume that when \( \Phi = 0 \), the momenta are given by those of the ground state, where \(-\pi < p_j(0) < \pi \) and \( I_j = -T_1 + (j - 1) \) for \( j = 1, \ldots, L/2 \). We may assume that \( p_1(0) < \cdots < p_{L/2}(0) \).

Let us recall the adiabatic hypothesis that when we change the parameter \( \Phi \) infinitesimally, then the quantum number \( I_j \) for momentum \( p_j(\Phi) \) does not change at all, while the momentum \( p_j(\Phi) \) changes proportionally to the infinitesimal change of \( \Phi \). We note that under the adiabatic hypothesis we have \( k_1(\Phi) < \cdots < k_{L/2}(\Phi) \). Now we consider the case when \( \Phi \) is very close to \( 2\pi \). We set \( \Phi = 2\pi - \delta \), where \( \delta \) is a small positive number. Making use the expansion \((5.19)\), we can solve the Bethe ansatz equations \((5.23)\), and we obtain the following

\[
p_{L/2}(2\pi - \delta) = \pi - \delta/2 + O(\delta^2). \tag{5.27}
\]

Thus, when \( \Phi = 2\pi \), we have momenta \( p_1(2\pi), \ldots, p_{L/2}(2\pi) \), where their quantum numbers are increased by 1 and they are given by

\[
I_j = -T_1 + (j - 1) + 1 \quad \text{for} \quad j = 1, \ldots, L/2. \tag{5.28}
\]

Here we note that \( p_{L/2}(2\pi) = \pi \) and \( I_{L/2} = T_1 + 1 \). Let us now apply the shift \((5.25)\) to the system of the solutions. We note that \( p_{L/2}(2\pi) - 2\pi = -\pi \) and \( T_1 + 1 - (L - M + 1) = -T_1 - 1 \). Thus, they are equivalent to the following set of solutions to \((5.23)\)

\[
p_{L/2}(2\pi) - 2\pi = -\pi, \quad p_1(2\pi), \ldots, p_{(L-2)/2}(2\pi)
\]
with their quantum numbers given by

\[ I_{L/2} = -T_1 - 1, \ I_1 = -T_1, \ldots, T_1 - 1, \]

respectively. We further increase the twist parameter \( \Phi \) until it becomes \( 4\pi \). Then, we see that the set of momenta

\[ p_{L/2}(4\pi) - 2\pi, \ p_1(4\pi), \ldots, p_{L/2-1}(4\pi) \]

satisfy the Bethe ansatz equations (5.23) with

\[ I_{L/2} = -T_1, \ I_1 = -T_1 + 1, \ldots, I_{(L-2)/2} = T_1. \]

Thus, we obtain

\[ p_{L/2}(4\pi) - 2\pi = p_1(0), \ p_1(4\pi) = p_2(0), \ldots, p_{(L-2)/2}(4\pi) = p_{(L-2)/2}. \]

The set of momenta for \( \Phi = 4\pi \) is equivalent to that of \( \Phi = 0 \). Therefore we conclude that the solutions to the Bethe ansatz equations which corresponds to the ground-state at \( \Phi = 0 \) has the period of \( 4\pi \).

VI. DISCUSSIONS

In this paper, we have explicitly shown that any non-regular eigenvector is derived from the Bethe ansatz wavefunction with infinite rapidities, for the one-dimensional XXX model under the periodic boundary conditions. The formula (2.10) for the amplitudes of the Bethe ansatz wavefunction has played a central role in the proof.

Let us discuss the string hypothesis, explicitly. It is based on the assumption that the Bethe ansatz equations (2.8) have complex solutions given in the following

\[ v^{n,j}_\alpha = v^n_\alpha + i(n + 1 - 2j) + \epsilon^{n,j}_\alpha \quad \text{for} \quad j = 1, \ldots, n. \]

\[ (6.1) \]

Here, it is also assumed that the absolute values of the correction terms \( |\epsilon^{n,j}_\alpha| \) should be very small. The set of complex rapidities \( v^{n,j}_\alpha \) for \( j = 1, \ldots, n \) is called an \( n \)-string solution.
The value \( v_\alpha^n \) is called the center of the string solution. The number \( n \) is called the length of the string solution.

Let us discuss the formula (2.10) of the amplitudes from the viewpoint of the string hypothesis. For any given \( n \)-string solution, we set the \( n \) rapidities in the string in such an order that \( v_\alpha^j - v_\alpha^k \approx 2i(k - j) \) for any \( j < k \) with \( 1 \leq j, k \leq n \). Then, the value of the amplitude \( A_M(P) \) given by eq. (2.10) becomes stabilized and well-defined, since we can avoid the appearance of any very small factor of \( O(\epsilon) \) in the denominator of eq. (2.10).

Let us discuss the number of solutions to the Bethe ansatz equations for the strings of length \( n \). Let us define number \( T_n \) by

\[
T_n = \frac{1}{2} \left( N - 1 - \sum_{m=1}^{\infty} t_{nm} M_m \right)
\]

Here \( M_m \) denotes the number of string solutions of length \( m \) and \( t_{nm} \) is given by

\[
t_{nm} = 2\min(n, m) - \delta_{nm}.
\]

Under the periodic boundary conditions (\( \Phi = 0 \)), it is discussed that the number of string solutions of length \( n \) is given by \( 2T_n + 1 \). We can show that if there are \( 2T_n + 2 \) different string solutions of length \( n \), then all the solutions to the Bethe ansatz equations correspond to a complete set of the eigenvectors of the XXX Hamiltonian under the twisted boundary conditions. The result of the present paper suggests that the \( K \) infinite rapidities of a non-regular eigenvector \( |R, K\rangle \) might correspond to a \( K \)-string solution under the twisted boundary conditions. Thus, we have a conjecture that any non-regular eigenvector under the P.B.C.s of the form \( |R, K\rangle \) should correspond to a regular eigenvector with a \( K \)-string solution under the twisted B.C.s. It seems that the conjecture should be consistent with the result of Ref. \( [17] \). However, a detailed numerical research on \( K \)-strings with large \( K \)'s should be performed such as studied in Ref. \( [30] \).

Finally, we give a remark on a possible application of the result of the present paper to the XXZ and XYZ models. Recently, it has been shown that under the periodic boundary conditions, the one-dimensional XXZ Hamiltonian at the \( q \) root of unity conditions has the
sl\textsubscript{2} loop algebra symmetry \cite{31,33}. In fact, we can discuss the spectral degeneracy of the XXZ model at the root of unity conditions in terms of the algebraic Bethe ansatz method by applying some of the techniques developed in the paper \cite{34}: combining the expression (4.21) with the formula (4.30) of the amplitudes $A_M(P)$’s, we can construct singular solutions related to the sl\textsubscript{2} loop algebra. Thus, we can show the validity of the construction of the complete $N$-string solutions discussed in Ref. \cite{33} in the level of eigenvectors. We can also prove it by showing that the limits of the Bethe ansatz wavefunctions satisfy the sufficient conditions for the eigenvectors of the XXZ model, which are summarized in Appendix E. Surprisingly, a similar method can also be applied to the analysis of the spectral degeneracy of the XYZ model addressed in Ref. \cite{31}. The details will be discussed in subsequent papers.

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A. APPENDIX: FORMULA FOR THE ACTION OF SPIN-LOWERING OPERATOR

Let us introduce some symbols. First, we shall abbreviate the symbol $\sum_{1 \leq x_1 < \cdots < x_M \leq L}$ by $\sum_{\sim} x_1 < \cdots < x_M$, in short. Second, for a non-negative integer $K$, we denote by the symbol $\sum_{\{j_1,j_2,\ldots,j_M\} \subset \{1,\ldots,M+K\}}$ the summation over all the subsets $\{j_1,j_2,\ldots,j_M\}$ of $\{1,2,\ldots,M+K\}$, where $j_k$’s are set in increasing order $j_1 < \cdots < j_M$. Thus, the two symbols in the
following express the same sum.
\[
\sum_{\{j_1, \ldots, j_M\} \subset \{1, \ldots, M+K\}} = \sum_{1 \leq j_1 < \cdots < j_M \leq M+K} .
\] (A.1)

**Proposition A.1** Recall that \(|M|\) denotes an arbitrary vector with \(M\) down-spins defined by eq. (2.3). We denote by \(|M, K\|\) the vector obtained from \(|M|\) multiplied by the power of the spin-lowering operator
\[
|M, K\rangle = \frac{1}{K!} \left(S_{\text{tot}}^{-}\right)^K |M\rangle
\] (A.2)

Then, we can show the following formula
\[
|M, K\rangle = \sum x_1 < \cdots < x_{M+K} \left( \sum_{\{j_1, \ldots, j_M\} \subset \{1, \ldots, M+K\}} g(x_{j_1}, \ldots, x_{j_M}) \sigma_{x_1}^- \sigma_{x_2}^- \cdots \sigma_{x_{M+K}}^- |0\rangle \right)
\] (A.3)

**Proof** We prove the formula (A.3) by induction on \(K\).

(i) We show (A.3) for the case of \(K = 1\). Applying \(S_{\text{tot}}^{-}\) to \(|M|\), we have
\[
S_{\text{tot}}^{-} |M\rangle = \sum_{y=1}^L \sum_{x_1 < \cdots < x_M} g(x_1, \ldots, x_M) \sigma_{x_1}^- \cdots \sigma_{x_M}^- |0\rangle
\]
\[
= \sum x_1 < \cdots < x_M \left( \sum_{y=1}^{x_1} + \sum_{y>x_1} \cdots + \sum_{y>x_M} \right) g(x_1, \ldots, x_M) \sigma_{x_1}^- \cdots \sigma_{x_M}^- |0\rangle.
\] (A.4)

We note the following calculation.
\[
\sum x_1 < \cdots < x_{M+1} \sum_{y>x_{j+1}} g(x_1, \ldots, x_M) \sigma_{x_1}^- \cdots \sigma_{x_M}^- \sigma_{y}^- \sigma_{x_{j+1}}^- \cdots \sigma_{x_{M+1}}^{-}
\]
\[
= \sum x_1 < \cdots < x_{M+1} \sum_{y>x_{j+1}} g(x_1, \ldots, x_M) \sigma_{x_1}^- \cdots \sigma_{x_j}^- \sigma_{y}^- \sigma_{x_{j+1}}^- \cdots \sigma_{x_{M+1}}^{-}
\]
\[
= \sum x_1 < \cdots < x_{M+1} g(x_1, \ldots, x_j, x_{j+2}, \ldots, x_{M+1}) \sigma_{x_1}^- \cdots \sigma_{(j+1)\text{th}, \ldots, M\text{th}}^{-} \] (A.5)

In the last line, we have replaced the symbols \(y, x_{j+1}, \ldots, x_M\) by \(x_{j+1}, x_{j+2}, \ldots, x_{M+1}\), respectively. Substituting (A.3) into (A.4), we have
Let us assume the expression (A.3) for the case of 
respectively. Substituting (A.8) into (A.7), we have

\[ S_{\text{tot}}^{-} | M \] = \sum_{x_1 < \cdots < x_{M+1}} \left( g(x_2, \ldots, x_{M+1}) + g(x_1, x_3, \ldots, x_{M+1}) + \cdots \right.
\]
\[ + \cdots + g(x_1, x_2, \ldots, x_M) \sigma_{x_1}^{-} \cdots \sigma_{x_{M+1}}^{-} | 0 \left. \right) \]
\[ = \sum_{x_1 < \cdots < x_{M+1}} \left( \sum_{\{j_1, \ldots, j_M\} \subset \{1, 2, \ldots, M+1\}} g(x_{j_1}, \ldots, x_{j_M}) \sigma_{x_1}^{-} \cdots \sigma_{x_{M+1}}^{-} | 0 \right). \]

(A.6)

Thus, we have the expression (A.3) for the case of \( K = 1 \).

(ii) Let us assume the expression (A.3) for the case of \( K \). Then, we show the case of \( K + 1 \) in the following.

\[ S_{\text{tot}}^{-} | M, K \] = \sum_{y=1}^{L} \sigma_{y}^{-} \left( \sum_{x_1, \ldots, x_{M+K} \{j_1, \ldots, j_M\} \subset \{1, \ldots, M+K\}} g(x_{j_1}, \ldots, x_{j_M}) \sigma_{x_1}^{-} \cdots \sigma_{x_{M+K}}^{-} | 0 \right) \]
\[ = \sum_{x_1 < \cdots < x_{M+K}} \left( \sum_{y=x_1}^{x_{M+K}} \sum_{y>x_1}^{x_{M+K}} + \cdots + \sum_{y>1}^{L} \right) \times \sum_{\{j_1, \ldots, j_M\} \subset \{1, \ldots, M+K\}} g(x_{j_1}, \ldots, x_{j_M}) \sigma_{x_1}^{-} \cdots \sigma_{x_{M+K}}^{-} | 0 \right). \]

(A.7)

By a similar method for the case (i), we can show the following

\[ S_{\text{tot}}^{-} | M, K \]
\[ = \sum_{x_1 < \cdots < x_{M+K+1}} \left( \sum_{y=x_1}^{x_{M+K+1}} \sum_{y>x_1}^{x_{M+K+1}} + \cdots + \sum_{y>1}^{L} \right) \times g(x_{j_1}, \ldots, x_{j_M}) \sigma_{x_1}^{-} \cdots \sigma_{x_{M+K+1}}^{-} | 0 \right) \]
\[ = (K + 1) \sum_{x_1 < \cdots < x_{M+K+1}} \left( \sum_{\{j_1, \ldots, j_M\} \subset \{1, 2, \ldots, M+K+1\}} g(x_{j_1}, \ldots, x_{j_M}) \sigma_{x_1}^{-} \cdots \sigma_{x_{M+K+1}}^{-} | 0 \right). \]

(A.9)
In the derivation of the last line, we note that after selecting $M$ integers $j_1, j_2, \ldots, j_M$ from the set $\{1, 2, \ldots, M + K + 1\}$, there are $(K + 1)$ ways for choosing one more element from the remaining $K + 1$ integers. Thus, we have the factor $(K + 1)$.

Q.E.D.

B. APPENDIX: FORMAL BETHE STATE WITH THREE INFINITE RAPIDITIES

Let us discuss the infinite limit of the formal Bethe state $| 0, 3; \Lambda \rangle$ of the case $R = 0$ and $K = 3$. Here, $v_1, v_2$ and $v_3$ are additional rapidities given by $v_1 = \Lambda + \delta_1$, $v_2 = \Lambda + \delta_2$ and $v_3 = \Lambda + \delta_3$. Let us denote $\delta_1 - \delta_2$ and $\delta_2 - \delta_3$ by $\Delta_{12}$ and $\Delta_{23}$, respectively. After taking the limit of sending $\Lambda$ to infinity, we have

$$A_{123}(\infty) = 1, \quad A_{132}(\infty) = \frac{\Delta_{23} - 2i}{\Delta_{23} + 2i}, \quad A_{213}(\infty) = \frac{\Delta_{12} - 2i}{\Delta_{12} + 2i},$$

$$A_{231}(\infty) = \left( \frac{\Delta_{12} - 2i}{\Delta_{12} + 2i} \right) \left( \frac{\Delta_{12} + \Delta_{23} - 2i}{\Delta_{12} + \Delta_{23} + 2i} \right),$$

$$A_{312}(\infty) = \left( \frac{\Delta_{12} + \Delta_{23} - 2i}{\Delta_{12} + \Delta_{23} + 2i} \right) \left( \frac{\Delta_{23} - 2i}{\Delta_{23} + 2i} \right),$$

$$A_{321}(\infty) = \left( \frac{\Delta_{12} - 2i}{\Delta_{12} + 2i} \right) \left( \frac{\Delta_{12} + \Delta_{23} - 2i}{\Delta_{12} + \Delta_{23} + 2i} \right) \left( \frac{\Delta_{23} - 2i}{\Delta_{23} + 2i} \right).$$

(B.1)

The limit of the Bethe ansatz wavefunction for the formal Bethe state $| 0, 3; \Lambda \rangle$ is given by

$$\lim_{\Lambda \to \infty} f^{(B)}_{0,3}(x_1, x_2, x_3; k_1(\Lambda), k_2(\Lambda), k_3(\Lambda)) = C_3$$

(B.2)

where the constant $C_3$ is given by

$$C_3 = \sum_{P \in S_3} A_3(P)[\delta_1, \delta_2, \delta_3]$$

$$= 1 + \frac{\Delta_{23} - 2i}{\Delta_{23} + 2i} + \frac{\Delta_{12} - 2i}{\Delta_{12} + 2i} + \left( \frac{\Delta_{12} - 2i}{\Delta_{12} + 2i} \right) \left( \frac{\Delta_{12} + \Delta_{23} - 2i}{\Delta_{12} + \Delta_{23} + 2i} \right)$$

$$+ \left( \frac{\Delta_{12} + \Delta_{23} - 2i}{\Delta_{12} + \Delta_{23} + 2i} \right) \left( \frac{\Delta_{23} - 2i}{\Delta_{23} + 2i} \right) + \left( \frac{\Delta_{12} - 2i}{\Delta_{12} + 2i} \right) \left( \frac{\Delta_{12} + \Delta_{23} - 2i}{\Delta_{12} + \Delta_{23} + 2i} \right) \left( \frac{\Delta_{23} - 2i}{\Delta_{23} + 2i} \right).$$

(B.3)

Thus, we have
\[
\lim_{\Lambda \to \infty} |0, 3; \Lambda \rangle = C_3 \sum_{1 \leq x_1 < x_2 < x_3 \leq L} \sigma_{x_1}^{-} \sigma_{x_2}^{-} \sigma_{x_3}^{-} |0\rangle \\
= C_3 \frac{1}{3!} (S_{\text{tot}}^{-})^3 |0\rangle \\
= C_3 |0, 3\rangle
\]  

(C.4)

C. APPENDIX: SOME USEFUL PROPERTIES OF THE SYMMETRIC GROUP

We introduce some notation of the symmetric group [36]. Let \( M \) be a positive integer. We consider the permutation group \( S_M \) of integers \( 1, 2, \ldots, M \). Take an element \( P \) of \( S_M \). We denote the action of \( P \) on \( j \) by \( P_j \) for \( j = 1, \ldots, M \). Let us introduce the symbol \((i_1 i_2 \cdots i_r)\) of the cyclic permutation where \( i_j \) is sent to \( i_{j+1} \) for \( j = 1, \ldots, r - 1 \), and \( i_r \) is sent to \( i_1 \). It is known [36] that any permutation \( P \) can be decomposed into a product of disjoint cycles such as follows

\[
P = (i_1 i_2 \cdots i_r)(j_1 j_2 \cdots j_s) \cdots (\ell_1 \ell_2 \cdots \ell_u). \tag{C.1}
\]

Here, any two of the cycles share no letter (or integer) in common. The factorization (C.1) is unique except for order of the factors [36].

For a given permutation \( P \) with a factorization of disjoint cycles such as eq. (C.1), we denote by \( N(P) \) the sum \( (r - 1) + (s - 1) + \cdots + (u - 1) \). Then, we can show that the parity of the permutation \( P \) is equal to that of \( N(P) \). Hereafter, we shall write by the symbol \( a \equiv b \pmod{2} \) that integers \( a \) and \( b \) have the same parity. We first recall that the cycle \((i_1 i_2 \cdots i_r)\) can be written as the product of \( r - 1 \) transposition such as

\[
(i_1 i_2 \cdots i_r) = (i_1 i_r)(i_1 i_{r-1}) \cdots (i_1 i_2).
\]

Thus, the parity of the cycle is given by that of \( r - 1 \). Let us denote by the symbol \( \epsilon(P) \) the sign of permutation \( P \). Then, we have [36]

\[
\epsilon(P) = (-1)^{(r-1)+(s-1)+\cdots+(u-1)} = (-1)^{N(P)} \tag{C.2}
\]
Let us introduce ordered pairs of integers. We take two different integers \( j \) and \( k \), and consider an ordered pair \(< j, k >\). We distinguish \(< j, k >\) from \(< k, j >\). Let us consider the action of a permutation on ordered pairs. We take a permutation \( P \) of \( S_M \) and two integers \( j \) and \( k \) satisfying \( 1 \leq j < k \leq M \). We denote by \(< P_j, Pk >\) the action of \( P \) on the pair \(< j, k >\). If \( Pj > Pk \), we call the pair \(< j, k >\) is transposed by \( P \).

Let the symbol \( T(P) \) denote the number of all such pairs \(< j, k >\) that are transposed by \( P \) among all the ordered pairs \(< j, k >\) with the condition \( 1 \leq j < k \leq M \). Then, we can show the following.

**Lemma C.1** The parity of an element \( P \) of \( S_M \) is equivalent to that of the number \( T(P) \):

\[
N(P) \equiv T(P) \pmod{2}.
\]  

(C.3)

*(Proof)* We now prove the lemma based on induction on \( M \) of \( S_M \). It is easy to see that when \( M = 2 \) the statement is true. Let us now assume that eq. (C.3) holds for all permutations \( P \) of \( S_R \) if \( R < M \). Let us take an element \( P \) of \( S_M \). Then, we may assume that the permutation \( P \) has a factorization of disjoint cycles such as shown in eq. (C.1). Suppose that \( P \) has the same factorization with eq. (C.1). We take a cycle \((i_1i_2\cdots i_r)\), which is one of the disjoint cycles, and we denote by \( B \) the set \( \{i_1, i_2, \ldots, i_r\} \). We also denote by \( \Sigma_M \) the set of \( M \) integers: \( \Sigma_M = \{1, 2, \ldots, M\} \). We now consider the subset \( A \) of the set \( \Sigma_M \) that is complementary to the set \( B \): \( A = \Sigma_M - B \). We define permutation \( P_A \) by

\[
P_A = (j_1j_2\cdots j_s)(\ell_1\ell_2\cdots \ell_u). \tag{C.4}
\]

Note that \( P_A \) is a permutation of \( A \) and it does not change any letter in \( B \): \( P_Ai_j = i_j \) for \( j = 1, \ldots, r \). Thus, we see that \( T(P) \) and \( T(P_A) + (r - 1) \) have the same parity. Here, we note that \( T((i_1i_2\cdots i_r)) = r - 1 \), i.e., \( r - 1 \) pairs of the elements in \( B \) are transposed by \((i_1i_2\cdots i_r)\), and therefore by \( P \). On the other hand, since \( P_A \) is a permutation of \( A \), it is equivalent to an element of \( S_{M-r} \). From the induction hypothesis, we have that \( N(P_A) \) and \( T(P_A) \) have the same parity. Thus, we have
\[ T(P) \equiv T(P_A) + (r - 1) \pmod{2} \]  
\[ \equiv N(P_A) + (r - 1) \pmod{2} \]  
\[ = N(P) \]  

Therefore, \( T(P) \) and \( N(P) \) have the same parity.

\[ Q.E.D. \]

We now have the following.

**Proposition C.1** Let \( P \) be an element of \( S_M \). Then, we have the following identity.

\[ \epsilon(P) = \prod_{1 \leq j < k \leq M} (-1)^{H(P^{-1}j - P^{-1}k)} \]  
(C.5)

**(Proof)** Let us note the following

\[ T(P) = \sum_{1 \leq j < k \leq M} H(P^{-1}j - P^{-1}k) \]  
(C.6)

Then, we can show eq. \((C.5)\) from the previous lemma and eq. \((C.2)\).

**D. APPENDIX: PROOF OF THE “PAULI PRINCIPLE”**

We give a simple proof for the “Pauli principle” of the Bethe ansatz that when there are two rapidities of the same value, then the Bethe ansatz wavefunction of the XXX model vanishes. We note that it is also proven by the algebraic Bethe ansatz method in Ref. \[20\]. However, the proof in this appendix is much more elementary; it is only based on the expression \((2.10)\) of the amplitudes \( A_M(P) \)'s. In this appendix, we assume that rapidities \( v_1, \ldots, v_M \) are free parameters.

Let us take a pair of integers \( a \) and \( b \) such that \( 1 \leq a < b \leq M \). Then, we show that the Bethe ansatz wavefunction \( f_M^{(P)} \) with the amplitudes defined by eq. \((1.3)\) (equivalently by eq. \((2.10)\)) vanishes if \( k_a = k_b \) (i.e., \( v_a = v_b \)). Let the symbol \((ab)\) denote the permutation between \( a \) and \( b \). Then, we have
\[ f_M^{(B)}(x_1, \ldots, x_M; k_1, \ldots, k_M) = \sum_{P \in S_M} A_M(P) \exp(i \sum_{j=1}^{M} k_{Pj}x_j) \]
\[ = \frac{1}{2} \sum_{P \in S_M} A_M(P) \exp \left( i \sum_{j=1}^{M} k_{Pj}x_j \right) + \frac{1}{2} \sum_{P \in S_M} A((ab)P) \exp \left( i \sum_{j=1}^{M} k_{((ab)P)j}x_j \right) \]  
(D.1)

Here we have replaced \( P \) by \((ab)P\) in the second term. Considering the cases when \( j = P^{-1}a \) and \( j = P^{-1}b \), we can show

\[ \sum_{j=1}^{M} k_{Pj}x_j = k_ax_{P^{-1}a} + k_bx_{P^{-1}b} + \sum_{j=1; j \neq P^{-1}a,P^{-1}b}^{M} k_{Pj}x_j \]  
(D.2)

\[ \sum_{j=1}^{M} k_{((ab)P)j}x_j = k_{(ab)a}x_{P^{-1}a} + k_{(ab)b}x_{P^{-1}b} + \sum_{j=1; j \neq P^{-1}a,P^{-1}b}^{M} k_{(ab)Pj}x_j \]
\[ = k_bx_{P^{-1}a} + k_ax_{P^{-1}b} + \sum_{j=1; j \neq P^{-1}a,P^{-1}b}^{M} k_{Pj}x_j \]  
(D.3)

When \( k_a = k_b = k \), we have

\[ f_M^{(B)}(x_1, \ldots, x_M; k_1, \ldots, k_M) = \frac{1}{2} \sum_{P \in S_M} \left( A_M(P) + A_M((ab)P) \right) \times \exp \left( ik(x_{P^{-1}a} + x_{P^{-1}b}) + i \sum_{j=1; j \neq P^{-1}a,P^{-1}b}^{M} k_{Pj}x_j \right) \]  
(D.4)

We now show that \( A_M(P) + A_M((ab)P) = 0 \) for any \( P \in S_M \). Here we introduce the following symbols

\[ e(j, k) = \frac{v_j - v_k - 2i}{v_j - v_k + 2i}, \quad H(j, k; P) = H(P^{-1}j - P^{-1}k) \]  
(D.5)

Then, the amplitude \( A_M(P) \) given by eq.(2.10) is expressed as

\[ A_M(P) = \prod_{1 \leq j < k \leq M} e(j, k)^{H(j,k;P)} \]  
(D.6)

Let us consider the six cases for the integers \( j \) and \( k \) in the above product: \( j = a \) and \( k = b \); \( j < a \) and \( k = a \); \( j < b \) and \( k = b \) where \( j \neq a \); \( j = b \) and \( k > b \); \( j = a \) and \( k > a \) where \( k \neq b \); \( j \neq a \) and \( k \neq b \). We have the following

\[ A_M(P) = e(a,b)^{H(a,b;P)} \prod_{j=1}^{a-1} e(j,a)^{H(j,a;P)} \prod_{j=1; j \neq a}^{b-1} e(j,b)^{H(j,b;P)} \]
\[ \times \prod_{k=b+1}^M e(b, k)^{H(b,k;P)} \prod_{k=a+1; k \neq b}^M e(a, k)^{H(a,k;P)} \prod_{1 \leq j < k \leq M; j,k \neq a,b}^1 e(j, k)^{H(j,k;P)} \]

\[ = e(a, a)^{H(a,a;P)} \prod_{j=1}^{a-1} e(j, a)^{H(j,a;P)+H(j,a;P)} \prod_{j=a+1}^{b-1} e(j, a)^{H(j,a;P)} \prod_{1 \leq j < k \leq M; j,k \neq a,b}^1 e(j, k)^{H(j,k;P)} \]

\[ \times \prod_{j=b+1}^M e(a, j)^{H(b,j;P)+H(a,j;P)} \prod_{j=a+1}^{b-1} e(a, j)^{H(a,j;P)} \prod_{1 \leq j < k \leq M; j,k \neq a,b}^1 e(j, k)^{H(j,k;P)} \]

\[ = (-1)^{H(a,b;P)} \prod_{j=a+1}^{b-1} e(a, j)^{H(j,a;P) - H(j,b;P)} \prod_{j=b+1}^M e(a, j)^{H(b,j;P) + H(a,j;P)} \]

Here we have used the relations \( e(j, a) = e(j, b), e(a, j) = 1/e(j, a), e(a, b) = e(a, a) = -1 \), and so on. In a similar way, we have

\[ A_M((ab)P) = (-1)^{H(b,a;P)} \prod_{j=a+1}^{b-1} e(a, j)^{H(b,j;P) - H(j,a;P)} \prod_{1 \leq j < k \leq M; j,k \neq a,b}^1 e(j, k)^{H(j,k;P)} \]

\[ \times \prod_{j=1}^{a-1} e(j, a)^{H(j,a;P) + H(j,b;P)} \prod_{j=b+1}^M e(a, j)^{H(b,j;P) + H(a,j;P)} \]

(D.7)

Noting the relation: \( H(j, k; P) - 1/2 = - (H(k, j; P) - 1/2) \), we can show

\[ H(a, j; P) - H(j, b; P) = H(P^{-1}a - P^{-1}j) - H(P^{-1}j - P^{-1}b) \]

\[ = -H(-P^{-1}a + P^{-1}j) + H(-P^{-1}j + P^{-1}b) \]

\[ = -H(j, a; P) + H(b, j; P). \]

(D.9)

Thus, we have

\[ A_M(P) + A_M((ab)P) = \left( (-1)^{H(a,b;P)} + (-1)^{H(b,a;P)} \right) \prod_{j=a+1}^{b-1} e(a, j)^{H(a,j;P) - H(j,b;P)} \]

\[ \times \prod_{j=1}^{a-1} e(j, a)^{H(j,a;P) + H(j,b;P)} \prod_{j=b+1}^M e(a, j)^{H(a,j;P) + H(b,j;P)} \prod_{1 \leq j < k \leq M; j,k \neq a,b}^1 e(j, k)^{H(j,k;P)}, \]

(D.10)

and we obtain

\[ A_M(P) + A_M((ab)P) = 0 \quad \text{for any} \quad P \in S_M. \]

(D.11)

Here we note the following: \( H(b, a; P) = 0 \) when \( H(a, b; P) = 1 \); \( H(b, a; P) = 1 \) when \( H(a, b; P) = 0 \).
Following the discussion in the appendix, we can show the Pauli principle of the Bethe ansatz also for the XXZ model; we redefine $e(j, k)$ by $e(j, k) = \frac{\sinh(v_j - v_k + 2\eta)}{\sinh(v_j - v_k - 2\eta)}$, where $\eta$ is related to $\Delta$ in eq. (5.1) by $\Delta = \cosh 2\eta$.

E. APPENDIX: RIGOROUS DERIVATION OF THE COORDINATES BETHE ANSATZ

A. Secular equations of the XXZ model

The coordinate Bethe ansatz was introduced by Bethe for the one-dimensional XXX model in Ref. [1]. In this appendix, we derive rigorously some sets of sufficient conditions for a vector to be an eigenvector of the XXZ model under the twisted boundary conditions. The derivation should be useful for discussing singular eigenvectors of the model such as shown in Refs. [31–33]. We note that when the twisting parameter is zero: $\Phi = 0$, the twisted boundary conditions reduces into the periodic boundary conditions, and also that when $\Delta = 1$ the XXZ Hamiltonian (5.1) becomes the XXX Hamiltonian.

Let us consider the action of the XXZ Hamiltonian $H_{XXZ}$ (5.1) on any given vector. We recall that the symbol $|M\rangle$ in eq. (2.3) denotes a vector with $M$ down-spins where the amplitude $g(x_1, x_2, \ldots, x_M)$ is given by any function. Then, the action of $H_{XXZ}$ on the vector $|M\rangle$ can be calculated rigorously. The result is given in the following

\[
\left( H_{XXZ} - J \Delta (M - L) \right) |M\rangle = -\frac{J}{2} \sum_{1 \leq x_1 < \cdots < x_M \leq L} \left\{ \sum_{j=1}^{M} \sum_{s=\pm 1} g(x_1, \ldots, x_j + s, \ldots, x_M) \right. \\
- \sum_{j=1}^{M-1} \delta_{x_{j+1}, x_{j+1}} \left( g(x_1, \ldots, x_{j+1}, x_j, \ldots, x_M) + g(x_1, \ldots, x_j + 1, x_j + 1, \ldots, x_M) - 2\Delta g(x_1, \ldots, x_M) \right) \\
- \delta_{x_1, L} g(0, x_2, \ldots, x_M) + g(x_1, \ldots, x_M, L + 1) - 2\Delta g(1, x_2, \ldots, x_M, L + 1) \left\} \times \prod_{k=1}^{M} \sigma_{x_k}^{-} |0\rangle \\
- \frac{J}{2} \sum_{1 < x_1 < \cdots < x_M < L} \left\{ \left( -g(0, x_1, \ldots, x_{M-1}) + g(x_1, \ldots, x_{M-1}, L) e^{-i\Phi} \right) \sigma_{x_1}^{-} \right. \\
\left. \prod_{k=1}^{M-1} \sigma_{x_k}^{-} |0\rangle + \left( g(1, x_1, \ldots, x_{M-1}) - g(x_1, \ldots, x_{M-1}, L + 1) e^{-i\Phi} \right) \sigma_{L}^{-} \right. \\
\left. \prod_{k=1}^{M-1} \sigma_{x_k}^{-} |0\rangle \right\} \quad (E.1)
\]
Here, we have assumed the twisted boundary conditions for the spin operators: $\sigma^\pm_{L+1} = e^{\pm i\Phi} \sigma^\pm_1; \sigma^z_{L+1} = \sigma^z_1$, while any boundary conditions have been assigned on the function $g(x_1, \ldots, x_M)$.

Let us discuss sufficient conditions for vector $|M\rangle$ to be an eigenvector of the XXZ Hamiltonian, explicitly. Considering the last part of eq. (E.1) we have the twisted boundary conditions on the function $g(x_1, \ldots, x_M)$:

$$g(0, x_1, \ldots, x_{M-1}) = g(x_1, \ldots, x_{M-1}, L)e^{-i\Phi} \quad \text{for } 1 < x_1 < \cdots < x_{M-1} < L,$$

$$g(1, x_1, \ldots, x_{M-1}) = g(x_1, \ldots, x_{M-1}, L+1)e^{-i\Phi} \quad \text{for } 1 < x_1 < \cdots < x_{M-1} < L. \quad (E.2)$$

Considering the second part of eq. (E.1), we have the following conditions.

$$g(x_1, \ldots, x_j, x_j, \ldots, x_M) + g(x_1, \ldots, x_j + 1, x_j + 1, \ldots, x_M) - 2\Delta g(x_1, \ldots, x_j, x_j + 1, \ldots, x_M) = 0$$

for $1 \leq x_1 < \cdots < x_j, x_j + 1 < x_{j+2} < \cdots < x_M \leq L$ and $x_{j+1} = x_j + 1$. \quad (E.3)

where $j$ is given by $j = 1, \ldots, M - 1$. And we also have

$$g(0, x_2, \ldots, x_{M-1}, L) + g(1, x_2, \ldots, x_{M-1}, L+1) - 2\Delta g(1, x_2, \ldots, x_{M-1}, L) = 0$$

for $1 < x_2 < \cdots < x_{M-1} < L$. \quad (E.4)

Under the twisted boundary conditions (E.2), the conditions (E.4) correspond to the special cases of the conditions (E.3), where $j = M - 1$ and $x_{M-1} = L$, or $j = 1$ and $x_1 = 0$.

Let us now assume that the function $g(x_1, \ldots, x_M)$ is given by $f(x_1, \ldots, x_M)$ defined by a general linear combination of the planewave-type solutions

$$f(x_1, \ldots, x_M) = \sum_{P \in S_M} B(P) \exp(i \sum_{j=1}^M k_{Pj} x_j) . \quad (E.5)$$

Here $k_1, \ldots, k_M$ are free parameters, $S_M$ denotes the symmetric group on $M$ letters, and the amplitudes $B(P)$’s are arbitrary. The amplitudes $B(P)$’s in (E.3) are $M!$ independent parameters, and we shall determine them so that the function $f(x_1, \ldots, x_M)$ satisfies the conditions (E.2), (E.3) and (E.4). The function $f(x_1, \ldots, x_M)$ has the following property
\[
\sum_{j=1}^{M} \left( f(x_1, \ldots, x_{j-1}, x_j - 1, x_{j+1}, \ldots, x_M) + f(x_1, \ldots, x_{j-1}, x_j + 1, x_{j+1}, \ldots, x_M) \right)
= \left( \sum_{j=1}^{M} 2 \cos k_j \right) f(x_1, \ldots, x_M), \quad \text{for} \quad 1 \leq x_1 < \cdots < x_M \leq L.
\] (E.6)

In fact, we see explicitly
\[
\sum_{j=1}^{M} \left( f(x_1, \ldots, x_{j-1}, x_j - 1, x_{j+1}, \ldots, x_M) + f(x_1, \ldots, x_{j-1}, x_j + 1, x_{j+1}, \ldots, x_M) \right)
\]
\[
= \sum_{j=1}^{M} \sum_{P \in S_M} \left( B(P) \exp(i \sum_{\ell=1}^{M} k_{P\ell} x_{\ell} - i k_{Pj}) + B(P) \exp(i \sum_{\ell=1}^{M} k_{P\ell} x_{\ell} + i k_{Pj}) \right)
\]
\[
= \sum_{P \in S_M} \sum_{j=1}^{M} B(P) \exp(i \sum_{\ell=1}^{M} k_{P\ell} x_{\ell}) (\exp(-i k_{Pj}) + \exp(i k_{Pj}))
\]
\[
= \left( \sum_{j=1}^{M} 2 \cos k_j \right) f(x_1, \ldots, x_M).
\] (E.7)

Let us summarize the discussion given in the above. Assuming that the function \( g(x_1, \ldots, x_M) \) is given by \( f(x_1, \ldots, x_M) \) defined by eq. (E.5), the vector \( |M \rangle \) is an eigenfunction of the Hamiltonian if the conditions (E.2), (E.3) and (E.4) are satisfied.

We now show that the conditions (E.3) are satisfied if the following relations hold for the amplitudes \( B(P) \)'s:
\[
B(Q) \left( 1 + \exp(i k_{Qj} + i k_{Q(j+1)}) \right) - 2 \Delta \exp(i k_{Q(j+1)})
+ B(Q \pi_j) \left( 1 + \exp(i k_{Qj} + i k_{Q(j+1)}) \right) - 2 \Delta \exp(i k_{Qj}) = 0
\]
for \( Q \in S_M \) and \( j = 1, \ldots, M - 1. \) (E.8)

Here the symbol \( \pi_j \) denotes the permutation of \( j \) and \( j+1: \pi_j = (j, j+1) \) for \( j = 1, \ldots, M - 1. \)

Explicitly we have
\[
f(x_1, \ldots, x_{j-1}, x_j, x_{j+1}, \ldots, x_M) + f(x_1, \ldots, x_{j-1}, x_j + 1, x_{j+1}, \ldots, x_M)
- 2 \Delta f(x_1, \ldots, x_{j-1}, x_j, x_{j+1}, \ldots, x_M)
\]
\[
= \sum_{P \in S_M} \left[ B(P) \exp \left( \sum_{\ell=1; \ell \neq j, j+1}^{M} i k_{P\ell} x_{\ell} + i k_{Pj} x_j + i k_{P(j+1)} x_j \right) \right]
+ B(P) \exp \left( \sum_{\ell=1; \ell \neq j, j+1}^{M} i k_{P\ell} x_{\ell} + i k_{Pj}(x_j + 1) + i k_{P(j+1)}(x_j + 1) \right)
\]
\[-2\Delta B(P) \exp \left( \sum_{\ell=1; \ell\neq j,j+1}^{M} ik_{p_{\ell}} x_{\ell} + ik_{p_{j}} x_{j} + ik_{p_{(j+1)}} (x_{j} + 1) \right) \right] \} \\
= \sum_{P \in S_{M}} B(P) \exp \left( \sum_{\ell=1; \ell\neq j,j+1}^{M} ik_{p_{\ell}} x_{\ell} + i(k_{p_{j}} + k_{p_{(j+1)}}) x_{j} \right) \\
\quad \times \left( 1 + \exp(ik_{p_{j}} + ik_{p_{(j+1)}}) - 2\Delta \exp(ik_{p_{(j+1)}}) \right) \\
= \frac{1}{2} \sum_{Q \in S_{M}} \exp \left( \sum_{\ell=1; \ell\neq j,j+1}^{M} ik_{q_{\ell}} x_{\ell} + i(k_{q_{j}} + k_{q_{(j+1)}}) x_{j} \right) \\
\quad \times \left\{ B(Q) \left( 1 + \exp(ik_{q_{j}} + ik_{q_{(j+1)}}) - 2\Delta \exp(ik_{q_{(j+1)}}) \right) \\
\quad + B(Q_{\pi_{j}}) \left( 1 + \exp(ik_{q_{j}} + ik_{q_{(j+1)}}) - 2\Delta \exp(ik_{q_{j}}) \right) \right\}. \quad (E.9)

Here, we have made use of the following relation

$$\sum_{P \in S_{M}} F(P) = \frac{1}{2} \sum_{Q \in S_{M}} F(Q) + \frac{1}{2} \sum_{Q \in S_{M}} F(Q_{\pi_{j}}). \quad (E.10)$$

There are \((M-1)M!/2\) independent relations in eq. \((E.8)\). If they hold, then the terms involving \(B(Q)\)'s and \(B(Q_{\pi_{j}})\)'s in RHS of eq. \((E.9)\) vanish. Thus, LHS of \((E.9)\) becomes zero, and the conditions \((E.3)\) are satisfied for the case of \(j\). Thus, we have shown that the relations \((E.8)\) are sufficient for the conditions \((E.3)\). Hereafter, we shall call the conditions \((E.8)\) the vanishing conditions.

Let us discuss the number \(W\) of independent relations given by eqs. \((E.3)\) and \((E.4)\). It is given by the number of configurations where \(x_{1}, \ldots, x_{M}\) satisfy the conditions: \(1 \leq x_{1} < \cdots < x_{j}, x_{j} + 1 < x_{j+2} < \cdots < x_{M} \leq L\) and \(x_{j+1} = x_{j} + 1\) for \(j = 1, \ldots, M - 1\) and also those of \((E.4)\). The number \(W\) is given by

$$W = L \times L-2 \times C_{M-2} = \frac{L(L-2)!}{(L-M)!(M-2)!} \quad (E.11)$$

We recall that the number \(V\) of the relations of \((E.8)\) is given by \(M!\).

Let us now consider the ratio \(W/V\). We recall that the vanishing conditions \((E.8)\) are sufficient for the conditions \((E.3)\) and \((E.4)\) to hold. If the ratio \(W/V\) is larger than 1, then the vanishing conditions \((E.8)\) are also necessary conditions for \((E.3)\) and \((E.4)\). Here we recall that the variables \(k_{1}, \ldots, k_{M}\) are assumed to be free parameters in this subsection. Let us calculate the ratio \(W/V\), explicitly. It is given by

45
\[ W/V = \frac{2L(L-2)!}{(L-M)!M!(M-1)!} \]  
(E.12)

For example, we have \( W/V = L \) for \( M = 2 \); \( W/V = L(L-2)/6 \) for \( M = 3 \); \( W/V = L(L-2)(L-3)/72 \) for \( M = 4 \). Thus, when \( L \) is large enough with respect to the number of down-spins \( M \), then the ratio \( W/V \) is larger than one. When \( W/V > 1 \), the vanishing conditions (E.8) are necessary for the relations (E.3) and (E.4). However, we should note that the ratio \( W/V \) is not always larger than 1. For instance, when \( L = 16 \) and \( M = 8 \), we have \( W/V = 143/420 \). For the half-filling case, we have \( W/V < 1 \) for \( M = L/2 \geq 8 \), in general. If \( W/V < 1 \), then the vanishing conditions (E.8) for the amplitudes are not necessary for the relations (E.3) and (E.4).

Let us make a conclusion of Appendix E.A. Assuming that the function \( g(x_1, \ldots, x_M) \) is given by \( f(x_1, \ldots, x_M) \) defined by eq. (E.5), the vector \( |M\rangle \) is an eigenvector of the XXZ Hamiltonian, if the vanishing conditions (E.8) and the twisted boundary conditions (E.2) hold.

We give remarks. Let us consider the case of \( |\Delta| < 1 \), where \( \Delta = \cosh 2\eta \). When all the momenta are generic, or \( k_{Qj} \neq \pm 2|\eta| (\text{mod } 2\pi) \) or \( k_{Q(j+1)} \neq \pm 2|\eta| (\text{mod } 2\pi) \), the relations (E.8) can be expressed as follows

\[
\frac{B(Q)}{B(Q\pi_j)} = (-1)^j \frac{1 + \exp(i k_{Qj} + i k_{Q(j+1)}) - 2\Delta \exp(i k_{Qj})}{1 + \exp(i k_{Qj} + i k_{Q(j+1)}) - 2\Delta \exp(i k_{Q(j+1)})},
\]

for \( Q \in S_M \) and \( j = 1, \ldots, M - 1 \).  
(E.13)

For the singular solutions of the XXZ model such as discussed in Ref. [31–33], some of them satisfy the sufficient conditions (E.8) and (E.24), but their amplitudes \( B(P) \)'s do not satisfy the factorization property (E.13). Some details will be discussed elsewhere.

**B. Amplitudes of the Bethe ansatz wavefunction**

We show that the amplitudes \( A_M(P) \)'s defined by eq. (1.3) satisfy the vanishing conditions (E.8), where the parameters \( k_1, \ldots, k_M \) are generic. Let us introduce the following notation

\[ g(Q) = \frac{B(Q)}{B(Q\pi_j)} \]
(E.14)
\[ F_{j\ell}(P) = \exp[i(k_{P_j} + k_{P_\ell})] + 1 - 2\Delta \exp(i k_{P_j}) \]  

(E.14)

Then, the expression (1.3) of the amplitude \( A_M(P) \) is given by

\[ A_M(P) = \epsilon(P) \prod_{1 \leq j < \ell \leq M} \frac{F_{j\ell}(P)}{F_{j\ell}(e)} \quad \text{for} \quad P \in S_M. \]  

(E.15)

Here \( e \) denotes the unit element of the permutation group \( S_M \), and we put \( C = 1 \) in (1.3).

Let us calculate the ratio of \( A_M(Q\pi_a) \) and \( A_M(Q) \), explicitly. Here \( a \) is taken to be an integer satisfying \( 1 \leq a \leq M - 1 \). We note that integers \( j \) and \( \ell \) satisfy the condition: \( 1 \leq j < \ell \leq M \) in (E.15). We consider the four cases: (1) \( j = a \) and \( \ell = a + 1 \); (2) \( j = a \) and \( \ell > a + 1 \); (3) \( j = a + 1 \) and \( \ell > a + 1 \); (4) \( j, \ell \neq a, a + 1 \). Then we have

\[ A_M(Q) \prod_{j < \ell} F_{j\ell}(e) = \epsilon(Q) F_{aa+1}(Q) \prod_{\ell > a+1} F_{a\ell}(Q) \prod_{\ell > a+1} F_{a+1\ell}(Q) \prod_{1 \leq j < \ell \leq M: j, \ell \neq a,a+1} F_{j\ell}(Q) \]  

(E.16)

When \( P = Q\pi_a \), we have

\[ A_M(Q\pi_a) \prod_{j < \ell} F_{j\ell}(e) = \epsilon(Q\pi_a) F_{aa+1}(Q\pi_a) \prod_{\ell > a+1} F_{a\ell}(Q\pi_a) \prod_{\ell > a+1} F_{a+1\ell}(Q\pi_a) \times \prod_{j < \ell, j, \ell \neq a,a+1} F_{j\ell}(Q\pi_a) \]  

(E.17)

Through an explicit calculation, we have

\[ F_{aa+1}(Q\pi_a) = F_{a+1,a}(Q), \quad F_{a+1a}(Q\pi_a) = F_{a,a+1}(Q) \]

\[ F_{a\ell}(Q\pi_a) = F_{a+1,\ell}(Q), \quad F_{a+1\ell}(Q\pi_a) = F_{a,\ell}(Q) \]  

(E.18)

Thus, the ratio is given by

\[ \frac{A_M(Q)}{A_M(Q\pi_a)} = (-1)^\frac{F_{a,a+1}(Q)}{F_{a+1,a}(Q)} \]  

(E.19)

It is nothing but the relation (E.13), which is equivalent to the vanishing conditions (E.8) for the case of \( a \). Here we recall that all the momenta are given generic in Appendix E.B.

Let us now discuss the uniqueness or well-definedness of the amplitudes \( A_M(P) \)'s. First we note that any permutation \( P \) can be written in terms of a product of generators \( \pi_j \)'s. For example, cyclic permutation \((213)\) corresponds to \((23)(12) = \pi_2\pi_1\). Thus, we can calculate \( A_M(P) \) by using the relations (E.13). For example, let us take \( P = (213) \). We have
\[
A(\pi_2 \pi_1) = \frac{A(\pi_2 \pi_1) A(\pi_2)}{A(\pi_2)} A(e) \\
= \frac{F_{21}(\pi_2)}{F_{12}(\pi_2)} \frac{F_{32}(e)}{F_{23}(e)}
\]  

(E.20)

However, different products of generators can correspond to the same permutation. For instance, we have \((213) = (23)(12) = (12)(23)(12)(23)\). The amplitude \(A(\pi_2 \pi_1)\) should be equivalent to \(A(\pi_1 \pi_2 \pi_1 \pi_2)\).

In fact, we can prove the uniqueness of amplitudes \(A_M(P)'s\), explicitly. We note that the defining relations \([37]\) of the symmetric group \(S_M\) given by the following:

\[
\pi_j^2 = 1 \quad \text{for} \quad j = 1, \ldots, M - 1, \\
\pi_j \pi_{j+1} \pi_j = \pi_{j+1} \pi_j \pi_{j+1} \quad \text{for} \quad j = 1, \ldots, M - 2
\]  

(E.21) (E.22)

Thus, for a given permutation \(P\), any given two products of generators expressing the same \(P\) can be transformed into one another, by using the defining relations given in eqs. (E.21) and (E.22). Therefore, the uniqueness of the amplitudes is proven if we show that the amplitudes \(A_M(P)\)'s satisfy the following relations:

\[
\frac{A_M(Q)}{A_M(Q \pi_j)} \cdot \frac{A_M(Q \pi_j)}{A_M((Q \pi_j) \pi_j)} = 1 \quad \text{for} \quad j = 1, \ldots, M - 1, \\
\frac{A_M(Q)}{A_M(Q \pi_j)} \cdot \frac{A_M(Q \pi_j)}{A_M((Q \pi_j) \pi_{j+1})} \cdot \frac{A_M(Q \pi_j \pi_{j+1})}{A_M(Q \pi_{j+1} \pi_j)} \\
= \frac{A_M(Q)}{A_M(Q \pi_{j+1})} \cdot \frac{A_M(Q \pi_{j+1})}{A_M((Q \pi_{j+1} \pi_j) \pi_j)} \cdot \frac{A_M(Q \pi_{j+1} \pi_j)}{A_M((Q \pi_{j+1} \pi_j) \pi_{j+1})} \quad \text{for} \quad j = 1, \ldots, M - 2.
\]  

(E.23) (E.24)

Here \(Q \in S_M\). In fact, it is easy to check the relations (E.23) and (E.24).

C. Derivation of the Bethe ansatz equations

The twisted boundary conditions (E.2) for the wavefunction are given by the following

\[
f(x_1, \ldots, x_M) = \exp(-i\Phi) f(x_2, \ldots, x_M, x_1 + L) \quad \text{for} \quad 0 \leq x_1 < \cdots < x_M \leq L
\]  

(E.25)

In terms of the amplitudes \(B(P)'s\), RHS of (E.25) is given by
\[
\sum_{P \in S_M} B(P) \exp\left(-i\Phi + i(k_{P1}x_2 + \cdots + k_{P(M-1)}x_M + k_{PM}(x_1 + N))\right)
= \sum_{P \in S_M} B(P) \exp\left(-i\Phi + ik_{PM}N + i(k_{PM}x_1 + k_{P1}x_2 + \cdots + k_{P(M-1)}x_M)\right)
= \sum_{Q \in S_M} B(Q(12 \cdots M)) \exp\left(-i\Phi + i{k_Q}_1N + i\sum_{j=1}^M {k_Q}_jx_j\right).
\] (E.26)

Here we note that for \(Q(12 \cdots M) = P\) we have
\[
Q1 = PM, \quad Q2 = P1, \ldots, \quad QM = P(M - 1).
\] (E.27)

In order for RHS (E.26) to be equivalent to LHS of (E.25), we have
\[
\exp(ik_{Q1}N) = \exp(i\Phi) B(Q) B(Q(12 \cdots M)), \quad \text{for} \quad Q \in S_M.
\] (E.28)

Let us now derive the Bethe ansatz equations from the eqs. (E.28). Here, we assume that the amplitudes \(B(P)\)'s are given by \(A_M(P)\)’s satisfying the vanishing conditions (E.8) (or (E.13)). Then, we have the following
\[
\frac{A(Q)}{A(Q(12 \cdots M))} = \frac{A(Q)}{A(Q\pi_1)} \cdot \frac{A(Q\pi_1\pi_2)}{A(Q\pi_1\pi_2\pi_{M-1})} \cdots \frac{A_M(Q\pi_1 \cdots \pi_{M-2})}{A_M((\pi_1 \cdots \pi_{M-2})\pi_{M-1})}
= (-1)^{M-1} \prod_{m=2}^M \left(\frac{1 + \exp(i(k_{Q1} + k_{Qm}) - 2\Delta \exp(ik_{Q1}))}{1 + \exp(i(k_{Q1} + k_{Qm})) - 2\Delta \exp(ik_{Qm})}\right)
\] (E.29)

Here we note that \(Q\pi_1 \cdots \pi_{r-1}r = Q1\) and \(Q\pi_1 \cdots \pi_{r-1}(r + 1) = Q(r + 1)\). Thus, we have
\[
\exp(iLk_{Q1}) = (-1)^{M-1} \exp(i\Phi) \prod_{m=2}^M \left(\frac{1 + \exp(i(k_{Q1} + k_{Qm}) - 2\Delta \exp(ik_{Q1}))}{1 + \exp(i(k_{Q1} + k_{Qm})) - 2\Delta \exp(ik_{Qm})}\right)
\] for \(Q \in S_M\). (E.30)

Let us write \(Q1\) by \(j\). Then, \(Q2, \ldots, QM\) are given by all the integers from 1 to \(M\) except \(j\). We may write \(Qm\) by \(\ell\) which runs from 1 to \(M\) except \(j\). Thus, we obtain the standard form of the Bethe ansatz equations.

Finally, we summarize the rigorous formulation of the coordinate Bethe ansatz. Assuming that the function \(g(x_1, \ldots, x_M)\) is given by \(f(x_1, \ldots, x_M)\) defined by eq. (E.3), we have shown in Appendix E.A that the vector \(|M\) is an eigenvector of the XXZ Hamiltonian, if
the vanishing conditions (E.8) and the twisted boundary conditions (E.2) hold. In Appendix E.B, we have shown that the amplitudes $A_M(P)$’s defined by eq. (1.3) are well-defined and also that they indeed satisfy the vanishing conditions (E.8). In Appendix E.C, we have shown that the twisted boundary conditions (E.2) are satisfied when the Bethe ansatz equations (E.30) hold. Therefore, if $k_1, \ldots, k_M$ satisfy the Bethe ansatz equations, with the amplitudes $A_M(P)$’s constructed by the momenta via eq. (1.3), the vector $|M\rangle$ becomes an eigenvector of the XXZ model under the twisted boundary conditions.
REFERENCES

[1] H. Bethe, Z. Phys. 71 (1931) 205.

[2] L. Takhtajan and L. Faddeev, Russ. Math. Survey 34(5) (1979) 11.

[3] L. Takhtajan and L. Faddeev, J. Sov. Math. 24 (1984) 241.

[4] L.A. Takhtajan, Lect. Notes in Physics, Vol. 242, (Springer-Verlag, Berlin, 1985) pp. 175-219; L.D. Faddeev, “How Algebraic Bethe Ansatz works for integrable model”, hep-th/9605187.

[5] C.N. Yang and C.P. Yang, Phys. Rev. 150(1966) 321.

[6] C.N. Yang, Phys. Rev. Lett. 19(1967) 1312.

[7] M. Gaudin, La fonction d’onde de Bethe, (Masson, Paris, 1983).

[8] F. Woynarovich, J. Phys. C 15 (1982) 85.

[9] F.H.L. Essler, V.E. Korepin and K. Schoutens, Nucl. Phys. B 372 (1992) 559.

[10] B. Sutherland, Phys. Rev. Lett. 74 (1995) 816.

[11] T. Deguchi, F.H.L. Essler, F. Göhmann, A.Klümper, V.E. Korepin, and K. Kusakabe, Phys. Reports 331 (2000) 197.

[12] R. Siddharthan, cond-mat/9804210.

[13] M. Takahashi, Prog. Theor. Phys. 46 (1971) 401.

[14] A.N. Kirillov, J. Sov. Math., 30 (1985) 2298.

[15] F.H.L. Essler, V.E. Korepin and K. Schoutens, J. Phys. A: Math. Gen. 25(1992) 4115.

[16] F.H.L. Essler, V. Korepin and K. Schoutens, Nucl Phys. B 384 (1992) 431.

[17] V. Tarasov and A. Varchenko, Bases of Bethe Vectors and Difference Equations with Regular Singular Points, Kyoto-Math 95-04.
A.G. Izergin and V.E. Korepin, Comm. Math. Phys. 94 (1984) 67.

A.G. Izergin, V.E. Korepin and N.Y. Reshetikhin, J. Phys. A 20 (1987) 4799.

V.E. Korepin, N.M. Bogoliubov and A.G. Izergin, Quantum Inverse Scattering Method and Correlation Functions, Cambridge University Press (1993).

G. Felder and A. Varchenko, Nucl. Phys. B 480 (1996) 485.

M. Takahashi, Lecture Notes in Physics, Vol. 498, Springer, Berlin, 1997, p.204.

N. Byers and C.N. Yang, Phys. Rev. Lett. 7 (1961) 46.

H.J. de Vega, Nucl Phys. B 240 (1984) 495.

F.C. Alcaraz, M.N. Barber and M.T. Batchelor, Ann. Phys. 182 (1988) 280.

B.S. Shastry and B. Sutherland, Phys. Rev. Lett. 65 (1990) 243.

N. Yu and M. Fowler, Phys. Rev. 45 (1992) 11795.

K. Kusakabe and H. Aoki, J. Phys. Soc. Jpn. 65 (1996) 2772.

T. Fukui and N. Kawakami, Nucl. Phys. B 519 (1988) 715.

A. Dhar and B.S. Shastry, Phys. Rev. Lett. 85 (2000) 2813.

T. Deguchi, K. Fabricius and B.M. McCoy, cond-mat/9912141 (to appear in J. Stat. Phys.).

K. Fabricius and B.M. McCoy, cond-mat/0009279 (to appear in J. Stat. Phys.).

K. Fabricius and B.M. McCoy, cond-mat/0012501 (to appear in J. Stat. Phys.).

T. Deguchi, a talk in the conference “MATHPHYS ODYSSEY 2001– Integrable Models and Beyond”, Feb. 2001, Okayama and Kyoto.

T. Deguchi, R. Yue and K. Kusakabe, J. Phys. A 31 (1998) 7315.
[36] N. Jacobson, *Basic Algebra I*, (W.H. Freeman and Co., New York, 1985).

[37] W. Magnus, A. Karrass, and D. Solitar, *Combinatorial Group Theory* (Dover, New York, 1976).