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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 has been 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 is possible. In this paper, we discuss it explicitly at 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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1. Introduction

The one-dimensional Heisenberg model (*XXX* model) under the periodic boundary conditions is one of the fundamental models of integrable quantum spin systems [1]. 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 [2] that any regular Bethe ansatz eigenstate of the *XXX* model gives a highest weight vector [3, 4]. Let us consider the *XXX* Hamiltonian under the periodic boundary conditions,

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

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

Let us introduce some notation of the coordinate Bethe ansatz [1, 5, 6]. We denote by $x_1, x_2, \ldots, x_M$ the coordinates of the M down-spins set in increasing order: $1 \leqslant x_1 < x_2 < \cdots < x_M \leqslant L$. Then, we define the Bethe ansatz wavefunction with M parameters $k_1, k_2, \ldots, k_M$ by the following:

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

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 $\mathcal{S}_M$ denotes the permutation group of M letters. We define the amplitudes $A_M(P)$'s of the Bethe ansatz wavefunction by

$$A_M(P) = C\,\epsilon(P) \prod_{1 \leqslant j < \ell \leqslant M} \frac{\exp[\mathrm{i}(k_{Pj} + k_{P\ell})] + 1 - 2\ \exp(\mathrm{i}k_{Pj})}{\exp[\mathrm{i}(k_j + k_\ell)] + 1 - 2\ \exp(\mathrm{i}k_j)} \qquad \text{for} \quad P \in \mathcal{S}_M. \tag{1.3}$$

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:

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

Here, the summation is over all the possible values of x_j's given in increasing order. We call the vector $||M\rangle$ (1.4) with the amplitudes defined by equatoin (1.3), 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) 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,

$$\exp(\mathrm{i}Lk_j) = (-1)^{M-1} \prod_{\ell=1, \ell \neq j}^{M} \frac{\exp[\mathrm{i}(k_j + k_\ell)] + 1 - 2\ \exp(\mathrm{i}k_j)}{\exp[\mathrm{i}(k_j + k_\ell)] + 1 - 2\ \exp(\mathrm{i}k_\ell)} \quad \text{for} \quad j = 1, \ldots, M. \tag{1.5}$$

If all the parameters $k_1, k_2, \ldots, k_M$ satisfy the Bethe ansatz equations, then the formal Bethe vector $||M\rangle$ becomes an eigenvector of the *XXX* Hamiltonian. Furthermore, if the k_j's satisfy the conditions that $k_j \neq 0 \,(\mathrm{mod}\, 2\pi)$ 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 $S_{tot}^z = L/2 - R$. Here we assume that the number R should satisfy the condition $0 \leqslant R \leqslant L/2$ 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* and denote them by

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

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 [7] 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_{tot}^- by sending the rapidity v to infinity (see also [8–11]). We note that for the parameter k, the rapidity v has been defined by the relation $\exp(\mathrm{i}k) = (v + \mathrm{i})/(v - \mathrm{i})$; rapidity v is finite if and only if $k \neq 0 \pmod{2\pi}$. 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 [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 non-trivial. 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 briefly explain our derivation of non-regular eigenvectors from the formal Bethe states. 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 equation (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:

$$v_{R+j}(\Lambda) = \Lambda + \delta_j \qquad \text{for} \quad j = 1, \ldots, K. \tag{1.7}$$

Here we call the parameter Λ the 'centre' of the additional K rapidities $v_{R+1}, \ldots, v_{R+K}$. We assume that the δ_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 equation (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 Λ to infinity:

$$\lim_{\Lambda\to\infty} ||R, K; \Lambda\rangle = C\,|R, K\rangle. \tag{1.8}$$

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, 11, 15, 16]. 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 *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 discuss in section 4.

The contents of the paper consist 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. In section 4, we briefly discuss two related topics. First, we remark that 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. Then, we show that the infinite limits of formal Bethe states should be useful when we analyse the spectral flow of the *XXX* model under the twisted boundary conditions. Finally, we give some discussions in section 5. 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. Some fundamental properties of the symmetric group are given in appendix B, which are important in section 3. The 'Pauli principle' of the Bethe ansatz wavefunction is explicitly proven in appendix C.

2. Formal Bethe states and non-regular eigenstates

2.1. Non-regular eigenstates

Let us explicitly discuss the action of spin-lowering operator on arbitrary vectors with M down-spins. For an illustration we consider the case of $M=1$. Let $|1)$ denote a vector with one down-spin,

$$|1) = \sum_{x_1=1}^{L} g(x_1)\sigma_{x_1}^-|0\rangle \tag{2.1}$$

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

$$\begin{aligned}
S_{tot}^-|1) &= \sum_{x_2=1}^{L}\sigma_{x_2}^-\sum_{x_1}^{L} g(x_1)\sigma_{x_1}^-|0\rangle = \sum_{x_1=1}^{L}\sum_{x_2=1}^{L} g(x_1)\sigma_{x_1}^-\sigma_{x_2}^-|0\rangle \\
&= \left(\sum_{1\leqslant x_1<x_2\leqslant L} + \sum_{1\leqslant x_2<x_1\leqslant L}\right) g(x_1)\sigma_{x_1}^-\sigma_{x_2}^-|0\rangle \\
&= \sum_{1\leqslant x_1<x_2\leqslant L} (g(x_1)+g(x_2))\sigma_{x_1}^-\sigma_{x_2}^-|0\rangle \\
&= \sum_{1\leqslant x_1<x_2\leqslant L}\left(\sum_{1\leqslant j\leqslant 2} g(x_j)\right)\sigma_{x_1}^-\sigma_{x_2}^-|0\rangle.
\end{aligned} \tag{2.2}$$

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

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

$$|M) = \sum_{1\leqslant x_1<x_2<\cdots<x_M\leqslant L} g(x_1, x_2, \ldots, x_M)\, \sigma_{x_1}^- \sigma_{x_2}^- \cdots \sigma_{x_M}^-\, |0\rangle \tag{2.3}$$

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 $|M)$ with some function $g(x_1, x_2, \ldots, x_M)$. Now, we introduce the formula

$$\frac{1}{K!}\left(S_{tot}^-\right)^K |M) = \sum_{1\leqslant x_1<\cdots<x_{M+K}\leqslant L} \left(\sum_{1\leqslant j_1<\cdots<j_M\leqslant M+K} g(x_{j_1}, \ldots, x_{j_M}) \right) \sigma_{x_1}^- \cdots \sigma_{x_{M+K}}^- |0\rangle. \tag{2.4}$$

We note that the expression (2.2) corresponds to the case $M = K = 1$. An explicit proof of formula (2.4) is given in appendix A. In section 2.3, we consider the special case of $K = 2$ and $M = 1$, which is given in the following:

$$\begin{aligned}\frac{1}{2}\left(S_{tot}^-\right)^2 |1) &= \sum_{1\leqslant x_1<x_2<x_3\leqslant L} \sum_{1\leqslant j\leqslant 3} g(x_j)\sigma_{x_1}^- \sigma_{x_2}^- \sigma_{x_3}^- |0\rangle \\ &= \sum_{1\leqslant x_1<x_2<x_3\leqslant L} (g(x_1) + g(x_2) + g(x_3))\, \sigma_{x_1}^- \sigma_{x_2}^- \sigma_{x_3}^- |0\rangle.\end{aligned} \tag{2.5}$$

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 equation (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, it is explicitly expressed in terms of the Bethe ansatz wavefunctions,

$$|R, K\rangle = \sum_{1\leqslant x_1<\cdots<x_{R+K}\leqslant L} \left(\sum_{1\leqslant j_1<\cdots<j_R\leqslant R+K} f_R^{(B)}(x_{j_1}, \ldots, x_{j_R}) \right) \sigma_{x_1}^- \cdots \sigma_{x_{R+K}}^- |0\rangle. \tag{2.6}$$

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

2.2. Amplitudes of formal Bethe states

Let us recall the relation between rapidity v_j and parameter k_j:

$$\exp(\mathrm{i}k_j) = \frac{v_j + \mathrm{i}}{v_j - \mathrm{i}} \qquad \text{for} \quad j = 1, \ldots, M. \tag{2.7}$$

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

$$\left(\frac{v_j + \mathrm{i}}{v_j - \mathrm{i}}\right)^L = \prod_{\ell=1,\ell\neq j}^{M} \left(\frac{v_j - v_\ell + 2\mathrm{i}}{v_j - v_\ell - 2\mathrm{i}}\right) \qquad \text{for} \quad j = 1, \ldots, M. \tag{2.8}$$

The amplitudes $A_M(P)$'s defined in equation (1.3) are given by

$$A_M(P)\,[v_1, \ldots, v_M] = \epsilon(P) \prod_{1\leqslant j<k\leqslant M} \frac{v_{Pj} - v_{Pk} + 2\mathrm{i}}{v_j - v_k + 2\mathrm{i}}. \tag{2.9}$$

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

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 equation (2.9) are expressed by

$$A_M(P) = \prod_{1 \leqslant j < k \leqslant M} \left(\frac{v_j - v_k - 2\mathrm{i}}{v_j - v_k + 2\mathrm{i}} \right)^{H(P^{-1}j - P^{-1}k)}. \tag{2.10}$$

We prove the expression (2.10) in section 3.

For an illustration, we consider the amplitudes $A_M(P)$'s for the case $M = 3$. Let us express $A_M(P)$ by $A_{P1P2\cdots PM}$. Then, they are given as follows:

$$\begin{aligned}
&A_{123} = 1 \qquad A_{132} = \frac{v_2 - v_3 - 2\mathrm{i}}{v_2 - v_3 + 2\mathrm{i}} \qquad A_{213} = \frac{v_1 - v_2 - 2\mathrm{i}}{v_1 - v_2 + 2\mathrm{i}} \\
&A_{231} = \left(\frac{v_1 - v_2 - 2\mathrm{i}}{v_1 - v_2 + 2\mathrm{i}} \right) \left(\frac{v_1 - v_3 - 2\mathrm{i}}{v_1 - v_3 + 2\mathrm{i}} \right) \\
&A_{312} = \left(\frac{v_1 - v_3 - 2\mathrm{i}}{v_1 - v_3 + 2\mathrm{i}} \right) \left(\frac{v_2 - v_3 - 2\mathrm{i}}{v_2 - v_3 + 2\mathrm{i}} \right) \\
&A_{321} = \left(\frac{v_1 - v_2 - 2\mathrm{i}}{v_1 - v_2 + 2\mathrm{i}} \right) \left(\frac{v_1 - v_3 - 2\mathrm{i}}{v_1 - v_3 + 2\mathrm{i}} \right) \left(\frac{v_2 - v_3 - 2\mathrm{i}}{v_2 - v_3 + 2\mathrm{i}} \right).
\end{aligned} \tag{2.11}$$

2.3. 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 equation (1.7): $v_2 = \Lambda + \delta_1$, $v_3 = \Lambda + \delta_2$. We assume that δ_1 and δ_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 Δ. 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

$$\begin{aligned}
&A_{123}(\Lambda) = 1 \qquad A_{132}(\Lambda) = \frac{\Delta - 2\mathrm{i}}{\Delta + 2\mathrm{i}} \qquad A_{213}(\Lambda) = \frac{v_1 - \Lambda - \Delta/2 - 2\mathrm{i}}{v_1 - \Lambda - \Delta/2 + 2\mathrm{i}} \\
&A_{231}(\Lambda) = \left(\frac{v_1 - \Lambda - \Delta/2 - 2\mathrm{i}}{v_1 - \Lambda - \Delta/2 + 2\mathrm{i}} \right) \left(\frac{v_1 - \Lambda + \Delta/2 - 2\mathrm{i}}{v_1 - \Lambda + \Delta/2 + 2\mathrm{i}} \right) \\
&A_{312}(\Lambda) = \left(\frac{v_1 - \Lambda + \Delta/2 - 2\mathrm{i}}{v_1 - \Lambda + \Delta/2 + 2\mathrm{i}} \right) \left(\frac{\Delta - 2\mathrm{i}}{\Delta + 2\mathrm{i}} \right) \\
&A_{321}(\Lambda) = \left(\frac{v_1 - \Lambda - \Delta/2 - 2\mathrm{i}}{v_1 - \Lambda - \Delta/2 + 2\mathrm{i}} \right) \left(\frac{v_1 - \Lambda + \Delta/2 - 2\mathrm{i}}{v_1 - \Lambda + \Delta/2 + 2\mathrm{i}} \right) \left(\frac{\Delta - 2\mathrm{i}}{\Delta + 2\mathrm{i}} \right).
\end{aligned} \tag{2.12}$$

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

$$\begin{aligned}
f_{1,2}^{(B)}(x_1, x_2, x_3; k_1, k_2(\Lambda), k_3(\Lambda)) &= A_{123} \exp \mathrm{i}(k_1 x_1 + k_2(\Lambda) x_2 + k_3(\Lambda) x_3) \\
&+ A_{132} \exp \mathrm{i}(k_1 x_1 + k_3(\Lambda) x_2 + k_2(\Lambda) x_3) \\
&+ A_{213} \exp \mathrm{i}(k_2(\Lambda) x_1 + k_1 x_2 + k_3(\Lambda) x_3) \\
&+ A_{312} \exp \mathrm{i}(k_3(\Lambda) x_1 + k_1 x_2 + k_2(\Lambda) x_3) \\
&+ A_{231} \exp \mathrm{i}(k_2(\Lambda) x_1 + k_3(\Lambda) x_2 + k_1 x_3) \\
&+ A_{321} \exp \mathrm{i}(k_3(\Lambda) x_1 + k_2(\Lambda) x_2 + k_1 x_3) \quad \text{for} \quad 1 \leqslant x_1 < x_2 < x_3 \leqslant L
\end{aligned} \tag{2.13}$$

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

$$\exp(\mathrm{i}k_2(\Lambda)) = \left(\frac{\Lambda + \Delta/2 + \mathrm{i}}{\Lambda + \Delta/2 - \mathrm{i}}\right) \qquad \exp(\mathrm{i}k_3(\Lambda)) = \left(\frac{\Lambda - \Delta/2 + \mathrm{i}}{\Lambda - \Delta/2 - \mathrm{i}}\right). \tag{2.14}$$

Sending the centre Λ to infinity, $\Lambda \to \infty$, we have $k_2 = k_3 = 0\,(\mathrm{mod})2\pi$ and

$$\begin{aligned} &A_{123}(\infty) = A_{213}(\infty) = A_{231}(\infty) = 1 \\ &A_{132}(\infty) = A_{312}(\infty) = A_{321}(\infty) = \frac{\Delta - 2\mathrm{i}}{\Delta + 2\mathrm{i}}. \end{aligned} \tag{2.15}$$

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

$$\lim_{\Lambda\to\infty} f_{1,2}^{(B)}(x_1, x_2, x_3; k_1, k_2(\Lambda), k_3(\Lambda)) = C_2\left(\mathrm{e}^{\mathrm{i}k_1x_1} + \mathrm{e}^{\mathrm{i}k_1x_2} + \mathrm{e}^{\mathrm{i}k_1x_3}\right). \tag{2.16}$$

where the constant C_2 is given by

$$C_2 = \left(1 + \frac{\Delta - 2\mathrm{i}}{\Delta + 2\mathrm{i}}\right). \tag{2.17}$$

Combining equations (2.16) and (2.5), we obtain the following result:

$$\begin{aligned} \lim_{\Lambda\to\infty} ||1, 2; \Lambda\rangle &= C_2 \sum_{1\leqslant x_1<x_2<x_3\leqslant L} \left(\mathrm{e}^{\mathrm{i}k_1x_1} + \mathrm{e}^{\mathrm{i}k_1x_2} + \mathrm{e}^{\mathrm{i}k_1x_3}\right)\sigma_{x_1}^-\sigma_{x_2}^-\sigma_{x_3}^-|0\rangle \\ &= C_2\,\tfrac{1}{2!}\left(S_{tot}^-\right)^2|1\rangle = C_2\,|1, 2\rangle. \end{aligned} \tag{2.18}$$

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 prove this equivalence for the general case in section 3.

Let us give some remarks on equation (2.18). We see that the limiting procedure depends on the difference Δ. If $\Delta = -2\mathrm{i}$, 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.

2.4. The PBCs for the limits of the formal Bethe states

The formal Bethe state $||R, K; \Lambda\rangle$ satisfies the periodic boundary conditions (PBCs) 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 PBCs. Here we note that the total spin operator $\vec{S}_{tot}$ 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 Λ sent to infinity. We see that it satisfies the PBCs $f_{1,2}^{(\infty)}(x_1, x_2, x_3) = f_{1,2}^{(\infty)}(x_2, x_3, x_1 + L)$ for $1 \leqslant x_1 < x_2 < x_3 \leqslant L$. Explicitly we have

$$f_{1,2}^{(\infty)}(x_2, x_3, x_1 + L) = \frac{2\Delta}{\Delta + 2\mathrm{i}}\left(\mathrm{e}^{\mathrm{i}k_1x_2} + \mathrm{e}^{\mathrm{i}k_1x_3} + \mathrm{e}^{\mathrm{i}k_1(x_1+L)}\right). \tag{2.19}$$

Thus, it satisfies the PBCs if and only if the following holds:

$$\exp(\mathrm{i}k_1L) = 1. \tag{2.20}$$

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 PBCs. Let us consider the Bethe ansatz equations for three rapidities v_1, v_2 and v_3

$$\begin{aligned}\left(\frac{v_1+\mathrm{i}}{v_1-\mathrm{i}}\right)^L &= \left(\frac{v_1-v_2+2\mathrm{i}}{v_1-v_2-2\mathrm{i}}\right)\left(\frac{v_1-v_3+2\mathrm{i}}{v_1-v_3-2\mathrm{i}}\right)\\ \left(\frac{v_2+\mathrm{i}}{v_2-\mathrm{i}}\right)^L &= \left(\frac{v_2-v_1+2\mathrm{i}}{v_2-v_1-2\mathrm{i}}\right)\left(\frac{v_2-v_3+2\mathrm{i}}{v_2-v_3-2\mathrm{i}}\right)\\ \left(\frac{v_3+\mathrm{i}}{v_3-\mathrm{i}}\right)^L &= \left(\frac{v_3-v_1+2\mathrm{i}}{v_3-v_1-2\mathrm{i}}\right)\left(\frac{v_3-v_2+2\mathrm{i}}{v_3-v_2-2\mathrm{i}}\right).\end{aligned} \tag{2.21}$$

Taking the limit $\Lambda \to \infty$, the three equations are reduced to

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

$$\left(\frac{\Delta+2\mathrm{i}}{\Delta-2\mathrm{i}}\right) = 1. \tag{2.23}$$

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

3. Proof of the limit of formal Bethe states

In this section we prove the theorem in the following.

Theorem 3.1. *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 Λ sent to infinity:*

$$\lim_{\Lambda\to\infty} ||R, K; \Lambda\rangle = C_K |R, K\rangle. \tag{3.1}$$

3.1. Derivation of the formula for amplitudes $A_M(P)$'s

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

Lemma 3.1. *Let P be an element of S_M and $v_1, v_2, \ldots, v_M$ be generic parameters. Then, the following identity holds:*

$$\prod_{1\leqslant j<k\leqslant M} \frac{v_{Pj}-v_{Pk}+2\mathrm{i}}{v_j-v_k+2\mathrm{i}} = \prod_{1\leqslant j<k\leqslant M}\left(\frac{v_k-v_j+2\mathrm{i}}{v_j-v_k+2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}k)}. \tag{3.2}$$

Proof. Let us take a pair of integers j and k with $j < k$ and consider the factor $v_j - v_k + 2\mathrm{i}$ in the denominator of LHS of equation (3.2). For the pair, there exist two integers ℓ and m such that $P\ell = j$, $Pm = k$. There are two cases either $\ell < m$ or $\ell > m$. If $\ell < m$, we have the factor $v_{P\ell} - v_{Pm} + 2\mathrm{i}$ in the enumerator of the LHS of equation (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 $v_{Pm} - v_{P\ell} + 2\mathrm{i}$ in the enumerator of the LHS of equation (3.2) and

$$\frac{v_{Pm}-v_{P\ell}+2\mathrm{i}}{v_j-v_k+2\mathrm{i}} = \frac{v_k-v_j+2\mathrm{i}}{v_j-v_k+2\mathrm{i}}. \tag{3.3}$$

We can express these results by

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

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

□

Proposition 3.1. *The amplitude $A_M(P)$ defined by equation (1.3) for $P \in S_M$ can be expressed as*

$$A_M(P) = \prod_{1\leqslant j<k\leqslant M} \left(\frac{v_j - v_k - 2\mathrm{i}}{v_j - v_k + 2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}k)} \tag{3.4}$$

Proof. The amplitude $A_M(P)$ defined by equation (1.3) is written in terms of rapidities as

$$A_M(P) = \epsilon(P) \prod_{1\leqslant j<k\leqslant M} \frac{v_{Pj} - v_{Pk} + 2\mathrm{i}}{v_j - v_k + 2\mathrm{i}}. \tag{3.5}$$

In appendix B, we show the following identity in proposition B.1.

$$\epsilon_M(P) = \prod_{1\leqslant j<k\leqslant M} (-1)^{H(P^{-1}j-P^{-1}k)}. \tag{3.6}$$

Thus, making use of lemma 3.1 and proposition B.1, we obtain

$$\begin{aligned} A_M(P) = \epsilon(P) \prod_{1\leqslant j<k\leqslant M} \frac{v_{Pj} - v_{Pk} + 2\mathrm{i}}{v_j - v_k + 2\mathrm{i}} &= \epsilon(P) \prod_{1\leqslant j<k\leqslant M} \left(\frac{v_k - v_j + 2\mathrm{i}}{v_j - v_k + 2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}k)} \\ &= \prod_{1\leqslant j<k\leqslant M} \left(\frac{v_j - v_k - 2\mathrm{i}}{v_j - v_k + 2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}k)}. \end{aligned} \tag{3.7}$$

□

We give a remark. Using proposition 3.1, 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 C.

3.2. Proof of the limit

Let us take a permutation P on $R + K$ letters ($P \in \mathcal{S}_{R+K}$). We consider the following set:

$$P^{-1}\{1, 2, \ldots, R\} = \{P^{-1}j| \quad \text{for} \quad j = 1, 2, \ldots, R\}. \tag{3.8}$$

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

$$P_R m = P a_m \qquad \text{for} \quad m = 1, \ldots, R. \tag{3.9}$$

Then, we have the following.

Lemma 3.2. *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 $1 \leqslant j_1, j_2 \leqslant R$, 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*

$$H\left(P^{-1}j_1 - P^{-1}j_2\right) = H\left({P_R}^{-1}j_1 - {P_R}^{-1}j_2\right) \qquad \text{for} \quad 1 \leqslant j_1, j_2 \leqslant R. \tag{3.10}$$

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:

$$P^{-1}\{R+1, R+2, \ldots, R+K\} = \{P^{-1}j \,| \qquad \text{for} \quad j = R+1, R+2, \ldots, R+K\}. \tag{3.11}$$

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:

$$P_K m = P b_m - R \qquad \text{for} \quad m = 1, 2, \ldots, K. \tag{3.12}$$

Then, we can show the following.

Lemma 3.3. *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 $R+1 \leqslant j_1, j_2 \leqslant R+K$, 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*

$$H\left(P^{-1}j_1 - P^{-1}j_2\right) = H\left({P_K}^{-1}(j_1 - R) - {P_K}^{-1}(j_2 - R)\right) \qquad \text{for} \quad R+1 \leqslant j_1, j_2 \leqslant R+K. \tag{3.13}$$

Making use of lemmas 3.1–3.3, we now show the following proposition.

Proposition 3.2. *Let us consider two positive integers R and K satisfying $0 < K \leqslant L - 2R$. 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 δ_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 limit*

$$\lim_{\Lambda\to\infty} f_{R+K}(x_1, \ldots, x_{R+K}; k_1, \ldots, k_R, k_{R+1}(\Lambda), \ldots, k_{R+K}(\Lambda)) = C_K \sum_{1\leqslant j_1<\cdots<j_R\leqslant R+K} f_R(x_{j_1}, \ldots, x_{j_R}, k_1, \ldots, k_R). \tag{3.14}$$

Here k_j's are related to the rapidities v_j's through the relation $\exp \mathrm{i}k_j = (v_j + \mathrm{i})/(v_j - \mathrm{i})$, and the constant C_K is given by

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

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

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

Let us take a permutation P in S_{R+K}. By lemma 3.2 we can show that the amplitude $A_{R+K}(P)$ of the formal Bethe state is given by

$$A_{R+K}(P)\,[v_1, \ldots, v_R, v_{R+1}(\Lambda), \ldots, v_{R+K}(\Lambda)] = \prod_{1\leqslant j<\ell\leqslant R+K} \left(\frac{v_j - v_\ell - 2\mathrm{i}}{v_j - v_\ell + 2\mathrm{i}}\right)^{H(P^{-1}j - P^{-1}\ell)}. \tag{3.17}$$

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

$$\prod_{1\leqslant j<\ell\leqslant R+K}\left(\frac{v_j-v_\ell-2\mathrm{i}}{v_j-v_\ell+2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}\ell)}=\prod_{1\leqslant j<\ell\leqslant R}\left(\frac{v_j-v_\ell-2\mathrm{i}}{v_j-v_\ell+2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}\ell)}$$
$$\times\prod_{1\leqslant j\leqslant R}\ \prod_{R+1\leqslant\ell\leqslant R+K}\left(\frac{v_j-v_\ell-2\mathrm{i}}{v_j-v_\ell+2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}\ell)}$$
$$\times\prod_{R+1\leqslant j<\ell\leqslant R+K}\left(\frac{v_j-v_\ell-2\mathrm{i}}{v_j-v_\ell+2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}\ell)}. \tag{3.18}$$

First, we consider the third part of the RHS of (3.18). Making use of lemma 3.3, we have

$$\prod_{R+1\leqslant j<\ell\leqslant R+K}\left(\frac{v_j-v_\ell-2\mathrm{i}}{v_j-v_\ell+2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}\ell)}=\prod_{1\leqslant j<\ell\leqslant K}\left(\frac{v_{j+R}-v_{\ell+R}-2\mathrm{i}}{v_{j+R}-v_{\ell+R}+2\mathrm{i}}\right)^{H(P_K^{-1}j-P_K^{-1}\ell)}$$
$$=\prod_{1\leqslant j<\ell\leqslant K}\left(\frac{\delta_j-\delta_\ell-2\mathrm{i}}{\delta_j-\delta_\ell+2\mathrm{i}}\right)^{H(P_K^{-1}j-P_K^{-1}\ell)}. \tag{3.19}$$

We note that the 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 the RHS of (3.18) becomes 1 under the limit $\Lambda\to\infty$. In fact, putting the additional rapidities into the second part of the RHS of (3.18), we have

$$\prod_{1\leqslant j\leqslant R}\ \prod_{R+1\leqslant\ell\leqslant R+K}\left(\frac{v_j-v_\ell-2\mathrm{i}}{v_j-v_\ell+2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}\ell)}$$
$$=\prod_{1\leqslant j\leqslant R}\ \prod_{R+1\leqslant\ell\leqslant R+K}\left(\frac{v_j-\Lambda-\delta_\ell-2\mathrm{i}}{v_j-\Lambda-\delta_\ell+2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}\ell)}. \tag{3.20}$$

Third, we consider the first part of the RHS of (3.18). We recall that P_R is defined for the given permutation P by the relation (3.9). Then, from lemma 3.2, we have

$$\prod_{1\leqslant j<\ell\leqslant R}\left(\frac{v_j-v_\ell-2\mathrm{i}}{v_j-v_\ell+2\mathrm{i}}\right)^{H(P^{-1}j-P^{-1}\ell)}=\prod_{1\leqslant j<\ell\leqslant R}\left(\frac{v_j-v_\ell-2\mathrm{i}}{v_j-v_\ell+2\mathrm{i}}\right)^{H({P_R}^{-1}j-{P_R}^{-1}\ell)}. \tag{3.21}$$

We note again that the RHS of (3.21) is equal to $A_R(P_R)\,[v_1,\ldots,v_R]$. Thus, we have

$$\lim_{\Lambda\to\infty}A_{P+K}(P)\,[v_1,\ldots,v_R,v_{R+1}(\Lambda),\ldots,v_{R+K}(\Lambda)]$$
$$=A_R(P_R)\,[v_1,\ldots,v_R]\times A_K(P_K)\,[\delta_1,\ldots,\delta_K]\,. \tag{3.22}$$

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

$$\sum_{j=1}^{R+K}k_{Pj}x_j=\sum_{\ell=1}^{R+K}k_\ell x_{P^{-1}\ell}=\sum_{\ell=1}^{R}k_\ell x_{P^{-1}\ell}+\sum_{\ell=R+1}^{R+K}k_\ell x_{P^{-1}\ell}. \tag{3.23}$$

Since $k_{R+1},\cdots,k_{R+K}$ are approaching to 0 (mod 2π) in the limit of sending Λ to infinity, we have

$$\lim_{\Lambda\to\infty}\sum_{\ell=R+1}^{R+K}k_\ell(\Lambda)x_{P^{-1}\ell}=0\quad(\mathrm{mod}\ 2\pi). \tag{3.24}$$

Making use of the relation $P_Rm=Pa_m$, we have

$$\sum_{\ell=1}^{R}k_\ell x_{P^{-1}\ell}=\sum_{m=1}^{R}k_{P_Rm}x_{P^{-1}P_Rm}=\sum_{m=1}^{R}k_{P_Rm}x_{a_m}. \tag{3.25}$$

Thus, we have

$$\lim_{\Lambda\to\infty} A_{R+K}(P)\exp\left(\sum_{j=1}^{R+K} k_{Pj}x_j\right) = A_K(P_K)\,[\delta_1,\ldots,\delta_K]$$
$$\times A_R(P_R)\,[v_1,\ldots,v_R]\exp\left(\sum_{m=1}^{R} k_{P_R m}x_{a_m}\right) \qquad \text{for} \quad P\in S_{R+K}. \tag{3.26}$$

Finally, we give a remark. To pick up a permutation P on $R+K$ letters is equivalent to doing 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 (3.9) and (3.12), respectively. Therefore, we have

$$\sum_{P\in S_{R+K}} = \sum_{\{a_1,\ldots,a_R\}\subset\{1,2,\ldots,R+K\}} \sum_{P_R\in S_R}\sum_{P_K\in S_K}. \tag{3.27}$$

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

□

It is now clear that we obtain theorem 3.1 from proposition 3.2.

4. Some related topics

4.1. Formal Bethe state and the algebraic Bethe ansatz

Let us explicitly review the connection of the formal Bethe state to the algebraic Bethe ansatz: the formal Bethe state $||M\rangle$ corresponds to the vector $B(\lambda_1)\cdots B(\lambda_M)|0\rangle$ with generic rapidities $\lambda_1, \ldots, \lambda_M$. We can define the formal Bethe state also by the algebraic Bethe ansatz method. Here $B(\lambda)$ denotes the creation operator of the algebraic Bethe ansatz [18, 19].

Let us introduce the symbol $f_{jk} = (\lambda_j - \lambda_k - 2\eta)/(\lambda_j - \lambda_k)$ with $\eta = -\mathrm{i}$. Then, applying the method of the generalized two-site model [18–20], we can show

$$\prod_{j=1}^{M} B(\lambda_j)|0\rangle = F_1(\{\lambda_j\}) \sum_{P\in\mathcal{S}_M}\sum_{1\leqslant x_1<\cdots<x_M\leqslant L}\prod_{j=1}^{M}\sigma_{x_j}^{-}|0\rangle$$
$$\times\left(\prod_{1\leqslant\alpha<\beta\leqslant M} f_{Pk\,Pm}\right)\exp\left(i\sum_{j=1}^{M}k_{Pj}x_j\right). \tag{4.1}$$

where $F_1(\{\lambda_j\})$ is given by $F_1(\{\lambda_j\}) = (2\eta)^M\prod_{j=1}^{M}(\lambda_j-\mathrm{i})^L/(\lambda_j+\mathrm{i})$. We note that the factors $\prod_{1\leqslant j<k\leqslant M} f_{Pj\,Pk}$ are related to the amplitudes of the Bethe ansatz wavefunctions as

$$\prod_{1\leqslant j<k\leqslant M} f_{Pj\,Pk} = \left(\prod_{1\leqslant j<k\leqslant M} f_{jk}\right)\prod_{1\leqslant j<k\leqslant M}\left(\frac{\lambda_j-\lambda_k+2\eta}{\lambda_j-\lambda_k-2\eta}\right)^{H(P^{-1}j-P^{-1}k)}. \tag{4.2}$$

Making use of (4.2), we have the connection

$$B(\lambda_1)\cdots B(\lambda_M)|0\rangle = ||M\rangle \times F_1(\{\lambda_j\})F_2(\{\lambda_j\}) \tag{4.3}$$

where $F_2(\{\lambda_j\}) = \prod_{1\leqslant j<k\leqslant M} f_{jk}$. Thus, the formal Bethe state introduced in equation (1.4) in terms of the coordinate Bethe ansatz method is equivalent to the Bethe vector with generic rapidities of the algebraic Bethe ansatz.

We note that the derivation of (4.1) for the cases $M = 1$ and $M = 2$ has been discussed explicitly in [9, 11]. A similar relation with (4.1) has also been derived for the algebraic Bethe ansatz of the elliptic quantum group [21].

4.2. Spectral flow under the twisted BCs

We show briefly that the infinite limit of the formal Bethe state is closely related to the spectral flow under the twisted boundary conditions (TBCs).

Let us consider the *XXX* Hamiltonian (1.1) for the antiferromagnetic case ($J < 0$) under the twisted boundary conditions $\sigma_{L+1}^{\pm} = \sigma_1^{\pm}\ \exp(\pm \mathrm{i}\Phi), \sigma_{L+1}^{z} = \sigma_1^{z}$. Here the variable Φ is called the twisting parameter. The Bethe ansatz equations under the TBCs [22–28] for real momenta p_j's are given by

$$Lp_j = 2\pi I_j + \Phi - \sum_{\ell=1,\ell\neq j}^{M} \Theta(p_j, p_\ell) \qquad \text{for} \quad j = 1, \ldots, M. \tag{4.4}$$

Here $I_j = (M-1)/2 \pmod 1$, and the function $\Theta(p, q)$ is given by [5]

$$\Theta(p, q) = 2\tan^{-1}\left(\frac{(-1)\sin((p-q)/2)}{\cos((p+q)/2) - (-1)\cos((p-q)/2)}\right). \tag{4.5}$$

When $-\pi < p_j < \pi$ for $j = 1, \ldots, M$, we may assume that the I_j's satisfy $|I_j| \leqslant T_1 = (L - M - 1)/2$ for $j = 1, \ldots, M$. The inequalities have been derived under some physical assumptions [13, 29]. Here we note that for the antiferromagnetic case, we call momentum k *regular* when $-\pi < k < \pi$.

Let us now consider the case where one of the momenta is very close to $-\pi$, i.e., we assume that $p_0 = -\pi + \epsilon$ with a very small positive number ϵ. Then, through the expansion

$$\Theta(-\pi + \epsilon, q) = \pi - 2\epsilon + \epsilon^2 \tan\frac{q}{2} + O(\epsilon^3) \tag{4.6}$$

we can show that $I_0 = -(L - M + 1)/2 = -T_1 - 1$ and $\epsilon = \Phi/(L - 2M + 2) + O(\epsilon^2)$. The solution $p_0 = -\pi + \Phi/(L - 2M + 2) + O(\epsilon^2)$ can be considered as a regular solution, since it satisfies the condition $-\pi < p_0 < \pi$. Furthermore, it is clear that p_0 comes close to $-\pi$ when $\Phi \to 0$ with $\Phi > 0$. Thus, the formal solution $p_0 = -\pi$ for $\Phi = 0$ corresponds to the regular solution $p_0 = -\pi + \Phi/(L - 2M + 2) + O(\epsilon^2)$ when $0 < \Phi \ll 1$.

We observe the increase by one for the number of solutions to equations (4.4): there are $2T_1 + 1$ regular solutions under the PBCs, while we have $2T_1 + 2$ regular solutions under the TBCs.

Let us introduce an extension of the function $\Theta(p, q)$ of the variable p defined on the range $(-\pi, \pi)$ into a continuous function defined over $(-\infty, \infty)$ as follows:

$$\Xi(p, q) = \begin{cases} -(2n+1)\pi & \text{if} \quad p = (2n+1)\pi \quad \text{for an integer } n \\ \Theta\left(p - 2\pi\left[\frac{p+\pi}{2\pi}\right], q\right) - 2\pi\left[\frac{p+\pi}{2\pi}\right] & \text{otherwise.} \end{cases} \tag{4.7}$$

Here the symbol [,] denotes the Gauss symbol. We also extend the function $\Theta(p, q)$ with respect to q through the relation $\Theta(p, q) = -\Theta(q, p)$. In terms of the extended function, the Bethe ansatz equations are given by

$$Lp_j = 2\pi I_j + \Phi - \sum_{\ell=1,\ell\neq j}^{M} \Xi(p_j, p_\ell) \qquad \text{for} \quad j = 1, \ldots, M \tag{4.8}$$

where I_j's satisfy $I_j = (M-1)/2 \pmod 1$. We note that for regular solutions which satisfy $-\pi < p_j < \pi$, equations (4.8) are equivalent to the standard Bethe ansatz equations (4.4).

We now show that the number $L–M + 1$ gives the period of the quantum numbers I_j's. If we increase by 2π the value of a momentum, say p_{j_1}, then through equations (4.8) we can show the changes of I_j's in the following

$$I_{j_1} \to I_{j_1} + L - M + 1 \quad \text{and} \quad I_j \to I_j + 1 \qquad \text{for} \quad j \neq j_1 \ (1 \leqslant j \leqslant M). \tag{4.9}$$

Thus, we may consider only $L - M + 1$ different values for I_j's such as $-T_1 - 1,\ -T_1, \ldots, T_1$.

Let us derive the 4π period of the spectral flow under the TBCs with respect to the twisting parameter Φ for the state which gives the ground state at $\Phi = 0$. Here we note that the 4π period of the spectral flow has been numerically shown in several papers [24–28]. We first recall that under zero magnetic field, the ground state under the PBCs is given by the half-filling case: $M = L/2$. Then, we have $2T_1 + 1 = L/2$, and we have a unique set of real solutions $k_1, \ldots, k_{L/2}$ corresponding to $I_1, \ldots, I_{L/2}$ with $I_j = -T_1 + j - 1$ for $j = 1, \ldots, L/2$. Let us assume that $p_j(\Phi)$'s are solutions to equations (4.8) where $p_j(0) = k_j$ for $j = 1, \ldots, L/2$. Then, increasing the parameter Φ adiabatically from 0 to 4π, using equations (4.8), (4.6) and (4.9), we can show that $p_{L/2}(4\pi) - 2\pi = p_1(0),\ p_1(4\pi) = p_2(0), \ldots, p_{(L-2)/2}(4\pi) = p_{L/2}(0)$. For an illustration, let us consider the case of $L = 6$ and $M = 3$. When $\Phi = 0$, we have $I_1 = -1$, $I_2 = 0$, and $I_3 = 1$. Increasing the parameter Φ from 0 to 4π, we have $I_1 = 1$, $I_2 = 2$ and $I_3 = 3$. Replacing p_3 with $p_3 - 2\pi$, we have the changes of I_j's such as those shown in equations (4.9), and we obtain $I_3 = -1$, $I_1 = 0$ and $I_2 = 1$. Here we note that the period $L - M + 1$ is given by $6 - 3 + 1 = 4$. Thus, the set of momenta for $\Phi = 4\pi$ is equivalent to that of $\Phi = 0$. Therefore, we conclude that the set of momenta $p_j(\Phi)$'s, which gives the ground state solutions at $\Phi = 0$, has the period of 4π for its spectral flow with respect to the parameter Φ.

5. 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. Formula (2.10) for the amplitudes of the Bethe ansatz wavefunction has played a central role in the proof.

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

$$v_\alpha^{n,j} = v_\alpha^n + \mathrm{i}(n + 1 - 2j) + \epsilon_\alpha^{n,j} \qquad \text{for} \quad j = 1, \ldots, n. \tag{5.1}$$

Here, it is also assumed that the absolute values of the correction terms $|\epsilon_\alpha^{n,j}|$ should be very small. The set of complex rapidities $v_\alpha^{n,j}$ for $j = 1, \ldots, n$ is called an n-string solution [1, 13, 14]. The value v_α^n is called the *centre* of the string solution. The number n is called the length of the string solution.

Let us discuss 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 $v_\alpha^{n,j} - v_\alpha^{n,k} \approx 2\mathrm{i}(k - j)$ for any $j < k$ with $1 \leqslant j, k \leqslant n$. Then, the value of the amplitude $A_M(P)$ given by equation (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 equation (2.10).

Let us discuss the number of solutions to the Bethe ansatz equations for the strings of length n [1, 13, 14, 29]. Let us define number T_n by

$$T_n = \frac{1}{2}\left(N - 1 - \sum_{m=1}^{\infty} t_{nm} M_m\right). \tag{5.2}$$

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 $2T_n + 1$ [13, 14]. 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 PBCs of the form $|R, K\rangle$ should correspond to a regular eigenvector with a K-string solution under the twisted BCs. It seems that the conjecture should be consistent with the result of [17]. However, a detailed numerical research on K-string with large K's should be performed such as that studied in [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_2 loop algebra symmetry [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: combining the expression analogous to equation (4.1) with the formula of the amplitudes $A_M(P)$'s similar to equation (4.2), we can construct singular solutions related to the sl_2 loop algebra [34]. Thus, we can show the validity of the construction of the complete N-string solutions discussed in [33] in the level of eigenvectors. We can also prove it by showing that the limits of the Bethe ansatz wavefunctions satisfy sufficient conditions for the eigenvectors of the *XXZ* model. Surprisingly, a similar method can also be applied to the analysis of the spectral degeneracy of the *XYZ* model addressed in [31]. The details will be discussed in subsequent papers [34].

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Appendix A. Formula for the action of spin-lowering operator

Let us introduce some symbols. First, we abbreviate the symbol $\sum_{1\leqslant x_1<\cdots<x_M\leqslant L}$ as $\sum^{\sim}_{x_1<\cdots<x_M}$. 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:

$$\sum_{\{j_1,\ldots,j_M\}\subset\{1,\ldots,M+K\}} = \sum_{1\leqslant j_1<\cdots<j_M\leqslant M+K} . \tag{A.1}$$

Proposition A.1. *Recall that $|M)$ denotes an arbitrary vector with M down-spins defined by equation (2.3). We denote by $|M, K)$ the vector obtained from $|M)$ multiplied by the power of the spin-lowering operator:*

$$|M, K) = \frac{1}{K!}\left(S^{-}_{tot}\right)^{K}|M). \tag{A.2}$$

Then, we can show the following formula:

$$|M,K\rangle = \widetilde{\sum_{x_1<\cdots<x_{M+K}}} \left(\sum_{\{j_1,\ldots,j_M\}\subset\{1,\ldots,M+K\}} g(x_{j_1},\ldots,x_{j_M}) \right) \sigma_{x_1}^-\sigma_{x_2}^-\cdots\sigma_{x_{M+K}}^-|0\rangle. \tag{A.3}$$

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

(i) We show (A.3) for the case $K=1$. Applying S_{tot}^- to $|M\rangle$, we have

$$\begin{aligned} S_{tot}^-|M\rangle &= \sum_{y=1}^{L}\sigma_y^- \sum_{x_1<\cdots<x_M} g(x_1,\ldots,x_M)\sigma_{x_1}^-\cdots\sigma_{x_M}^-|0\rangle \\ &= \widetilde{\sum_{x_1<\cdots<x_M}} \left(\sum_{y=1}^{y<x_1} + \sum_{y>x_1}^{y<x_2} + \cdots + \sum_{y>x_M}^{L} \right) g(x_1,\ldots,x_M)\sigma_y^-\sigma_{x_1}^-\cdots\sigma_{x_M}^-|0\rangle. \end{aligned} \tag{A.4}$$

We note the following calculation:

$$\begin{aligned} &\widetilde{\sum_{x_1<\cdots<x_M}} \sum_{y>x_j}^{y<x_{j+1}} g(x_1,\ldots,x_M)\sigma_y^-\sigma_{x_1}^-\cdots\sigma_{x_M}^- \\ &\quad= \widetilde{\sum_{x_1<\cdots<x_j<y<x_{j+1}<\cdots>x_M}} g(x_1,\ldots,x_M)\sigma_{x_1}^-\cdots\sigma_{x_j}^-\sigma_y^-\sigma_{x_{j+1}}^-\cdots\sigma_{x_M}^- \\ &\quad= \widetilde{\sum_{x_1<\cdots<x_{M+1}}} g(x_1,\ldots,x_j,\underbrace{x_{j+2},\ldots,x_{M+1}}_{(j+1)\mathrm{th},\ldots,M\mathrm{th}})\sigma_{x_1}^-\cdots\sigma_{x_{M+1}}^-. \end{aligned} \tag{A.5}$$

In the last line, we have replaced the symbols y, $x_{j+1},\ldots$ and x_M by x_{j+1}, $x_{j+2},\ldots$ and x_{M+1}, respectively. Substituting (A.5) into (A.4), we have

$$\begin{aligned} S_{tot}^-|M\rangle &= \widetilde{\sum_{x_1<\cdots<x_{M+1}}} \big(g(x_2,\ldots,x_{M+1}) + g(x_1,x_3,\ldots,x_{M+1}) \\ &\qquad + \cdots + g(x_1,x_2,\ldots,x_M)\big)\sigma_{x_1}^-\cdots\sigma_{x_{M+1}}^-|0\rangle \\ &= \widetilde{\sum_{x_1<\cdots<x_{M+1}}} \left(\sum_{\{j_1,\ldots,j_M\}\subset\{1,2,\ldots,M+1\}} g(x_{j_1},\ldots,x_{j_M}) \right)\sigma_{x_1}^-\cdots\sigma_{x_{M+1}}^-|0\rangle. \end{aligned} \tag{A.6}$$

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

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

$$\begin{aligned} S_{tot}^-|M,K\rangle &= \sum_{y=1}^{L}\sigma_y^- \left(\sum_{x_1<\cdots<x_{M+K}} \sum_{\{j_1,\ldots,j_M\}\subset\{1,\ldots,M+K\}} g(x_{j_1},\ldots,x_{j_M})\sigma_{x_1}^-\cdots\sigma_{M+K}^- \right)|0\rangle \\ &= \widetilde{\sum_{x_1<\cdots<x_{M+K}}} \left(\sum_{y=1}^{y<x_1} + \sum_{y>x_1}^{y<x_2} + \cdots + \sum_{y>x_{M+K}}^{L} \right) \\ &\quad \times \sum_{\{j_1\cdots j_M\}\subset\{1,\ldots,M+K\}} g(x_{j_1},\ldots,x_{j_M})\sigma_y^-\sigma_{x_1}^-\cdots\sigma_{x_{M+K}}^-|0\rangle. \end{aligned} \tag{A.7}$$

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

$$\sum_{x_1<\cdots<x_{M+K}}^{\sim} \sum_{y>x_\ell}^{y<x_{\ell+1}} \sum_{\{j_1,\ldots,j_M\}\subset\{1,\ldots,M+K\}} g(x_{j_1},\ldots,x_{j_M}) \quad \sigma_y^- \sigma_{x_1}^- \cdots \sigma_{x_M}^-$$
$$= \sum_{x_1<\cdots<x_\ell<y<x_{\ell+1}<\cdots<x_{M+K}}^{\sim} \sum_{\{j_1,\ldots,j_M\}\subset\{1,\ldots,M+K\}} g(x_{j_1},\ldots,x_{j_M}) \sigma_{x_1}^- \cdots \sigma_{x_\ell}^- \sigma_y^- \sigma_{x_{\ell+1}}^- \cdots \sigma_{x_M}^-$$
$$= \sum_{x_1<\cdots<x_{M+K+1}}^{\sim} \sum_{\{j_1,\ldots,j_M\}\subset\{1,\ldots,\ell,\ell+2,\ldots,M+K+1\}} g(x_{j_1},\ldots,x_{j_M}) \sigma_{x_1}^- \cdots \sigma_{x_{M+1}}^-. \tag{A.8}$$

In the last line, we have replaced the symbol y by $x_{\ell+1}$ and $\ell+1,\ldots,M$ by $\ell+2,\ldots,M+1$. Substituting (A.8) into (A.7), we have

$$S_{tot}^- |M, K\rangle$$
$$= \sum_{x_1<\cdots<x_{M+K+1}}^{\sim} \left(\sum_{\{j_1,\ldots,j_M\}\subset\{2,3,\ldots,M+K+1\}} + \sum_{\{j_1,\cdots,j_M\}\subset\{1,3,\ldots,M+K+1\}} + \cdots + \sum_{\{j_1,\ldots,j_M\}\subset\{1,2,\ldots,M+K\}} \right)$$
$$\times g(x_{j_1},\ldots,x_{j_M}) \sigma_{x_1}^- \cdots \sigma_{x_{M+K+1}}^- |0\rangle$$
$$= (K+1) \sum_{x_1<\cdots<x_{M+K+1}}^{\sim} \left(\sum_{\{j_1,\ldots,j_M\}\subset\{1,2,\ldots,M+K+1\}} g(x_{j_1},\ldots,x_{j_M}) \right) \sigma_{x_1}^- \cdots \sigma_{x_{M+1}}^- |0\rangle. \tag{A.9}$$

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 of choosing one more element from the remaining $K+1$ integers. Thus, we have the factor $(K+1)$.

□

Appendix B. 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 Pj 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*,

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

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

For a given permutation P with a factorization of disjoint cycles such as equation (B.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 denote by the expression $a \equiv b$ (mod 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 transpositions,

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

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

$$\epsilon(P) = (-1)^{(r-1)+(s-1)+\cdots+(u-1)} = (-1)^{N(P)}. \tag{B.2}$$

Let us introduce ordered pairs of integers. We take two different integers j and k and consider an ordered pair $\langle j, k\rangle$. We distinguish $\langle j, k\rangle$ from $\langle k, j\rangle$. 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 $1 \leqslant j < k \leqslant M$. We denote by $\langle Pj, Pk\rangle$ the action of P on the pair $\langle j, k\rangle$. If $Pj > Pk$, we call that the pair $\langle j, k\rangle$ is transposed by P.

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

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

$$N(P) \equiv T(P) \pmod 2. \tag{B.3}$$

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 equation (B.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 that shown in equation (B.1). Suppose that P has the same factorization with equation (B.1). We take a cycle $(i_1 i_2 \cdots i_r)$, 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 Σ_M the set of M integers: $\Sigma_M = \{1, 2, \ldots, M\}$. We now consider the subset A of the set Σ_M that is complementary to the set B: $A = \Sigma_M - B$. We define permutation P_A by

$$P_A = (j_1 j_2 \cdots j_s) \cdots (\ell_1 \ell_2 \cdots \ell_u). \tag{B.4}$$

Note that P_A is a permutation of A and it does not change any letter in B: $P_A i_j = i_j$ for $j = 1, \ldots, r$. Thus, we see that $T(P)$ and $T(P_A) + (r-1)$ have the same parity. Here, we can show that $T((i_1 i_2 \cdots i_r)) \equiv r - 1 \pmod 2$ by noting that $T((ab)) = 2(b - a - 1) + 1$ when $a < b$. 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

$$\begin{aligned} T(P) &\equiv T(P_A) + (r-1) \quad (\mathrm{mod} 2) \\ &\equiv N(P_A) + (r-1) \quad (\mathrm{mod} 2) \\ &= N(P). \end{aligned}$$

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

□

We now have the following.

Proposition B.1. *Let P be an element of S_M. Then, we have the following identity:*

$$\epsilon(P) = \prod_{1 \leqslant j < k \leqslant M} (-1)^{H(P^{-1}j - P^{-1}k)}. \tag{B.5}$$

Proof. Let us note the following:

$$T(P) = \sum_{1 \leqslant j < k \leqslant M} H(P^{-1}j - P^{-1}k). \tag{B.6}$$

Then, we can show equation (B.5) from the previous lemma and equation (B.2).

□

Appendix C. 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 [19]. 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 $1 \leqslant a < b \leqslant M$. Then, we show that the Bethe ansatz wavefunction $f_M^{(B)}$ with the amplitudes defined by equation (1.3) (equivalently by equation (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

$$\begin{aligned} f_M^{(B)}(x_1, \ldots, x_M; k_1, \ldots, k_M) &= \sum_{P\in\mathcal{S}_M} A_M(P)\ \exp\left(\mathrm{i}\sum_{j=1}^{M} k_{Pj}x_j\right) \\ &= \frac{1}{2}\sum_{P\in\mathcal{S}_M} A_M(P)\ \exp\left(\mathrm{i}\sum_{j=1}^{M} k_{Pj}x_j\right) \\ &\quad + \frac{1}{2}\sum_{P\in\mathcal{S}_M} A((ab)P)\ \exp\left(\mathrm{i}\sum_{j=1}^{M} k_{((ab)P)j}x_j\right). \end{aligned} \tag{C.1}$$

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 that

$$\sum_{j=1}^{M} k_{Pj}x_j = k_a x_{P^{-1}a} + k_b x_{P^{-1}b} + \sum_{j=1;\,j\neq P^{-1}a,P^{-1}b}^{M} k_{Pj}x_j \tag{C.2}$$

$$\begin{aligned} \sum_{j=1}^{M} k_{((ab)P)j}x_j &= k_{(ab)a}x_{P^{-1}a} + k_{(ab)b}x_{P^{-1}b} + \sum_{j=1;\,j\neq P^{-1}a,P^{-1}b}^{M} k_{(ab)Pj}x_j \\ &= k_b x_{P^{-1}a} + k_a x_{P^{-1}b} + \sum_{j=1;\,j\neq P^{-1}a,P^{-1}b}^{M} k_{Pj}x_j \end{aligned} \tag{C.3}$$

When $k_a = k_b = k$, we have

$$\begin{aligned} f_M^{(B)}(x_1, \ldots, x_M; k_1, \ldots, k_M) &= \frac{1}{2}\sum_{P\in\mathcal{S}_M} (A_M(P) + A_M((ab)P))) \\ &\quad \times\ \exp\left(\mathrm{i}k(x_{P^{-1}a} + x_{P^{-1}b}) + \mathrm{i}\sum_{j=1;\,j\neq P^{-1}a,P^{-1}b}^{M} k_{Pj}x_j\right). \end{aligned} \tag{C.4}$$

We now show that $A_M(P) + A_M((ab)P) = 0$ for any $P \in \mathcal{S}_M$. Here we introduce the following symbols:

$$e(j,k) = \frac{v_j - v_k - 2\mathrm{i}}{v_j - v_k + 2\mathrm{i}} \qquad H(j,k;\,P) = H(P^{-1}j - P^{-1}k). \tag{C.5}$$

Then, the amplitude $A_M(P)$ given by equation (2.10) is expressed as

$$A_M(P) = \prod_{1\leqslant j<k\leqslant M} e(j,k)^{H(j,k;P)}. \tag{C.6}$$

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:

$$\begin{aligned}
A_M(P) &= e(a,b)^{H(a,b;P)} \prod_{j=1}^{a-1} e(j,a)^{H(j,a;P)} \prod_{j=1;\, j\neq a}^{b-1} e(j,b)^{H(j,b;P)} \prod_{k=b+1}^{M} e(b,k)^{H(b,k;P)} \\
&\quad \times \prod_{k=a+1;\, k\neq b}^{M} e(a,k)^{H(a,k;P)} \prod_{1\leqslant j<k\leqslant M;\, j,k\neq a,b} e(j,k)^{H(j,k;P)} \\
&= e(a,a)^{H(a,b;P)} \prod_{j=1}^{a-1} e(j,a)^{H(j,a;P)+H(j,b;P)} \prod_{j=a+1}^{b-1} e(j,a)^{H(j,b;P)} \\
&\quad \times \prod_{j=b+1}^{M} e(a,j)^{H(b,j;P)+H(a,j;P)} \prod_{j=a+1}^{b-1} e(a,j)^{H(a,j;P)} \\
&\quad \times \prod_{1\leqslant j<k\leqslant M;\, j,k\neq a,b} e(j,k)^{H(j,k;P)} = (-1)^{H(a,b;P)} \prod_{j=a+1}^{b-1} e(a,j)^{H(a,j;P)-H(j,b;P)} \\
&\quad \times \prod_{1\leqslant j<k\leqslant M;\, j,k\neq a,b} e(j,k)^{H(j,k;P)} \prod_{j=1}^{a-1} e(j,a)^{H(j,a;P)+H(j,b;P)} \\
&\quad \times \prod_{j=b+1}^{M} e(a,j)^{H(b,j;P)+H(a,j;P)}. \qquad \text{(C.7)}
\end{aligned}$$

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

$$\begin{aligned}
A_M((ab)P) &= (-1)^{H(b,a;P)} \prod_{j=a+1}^{b-1} e(a,j)^{H(b,j;P)-H(j,a;P)} \times \prod_{1\leqslant j<k\leqslant M;\, j,k\neq a,b} e(j,k)^{H(j,k;P)} \\
&\quad \times \prod_{j=1}^{a-1} e(j,a)^{H(j,a;P)+H(j,b;P)} \prod_{j=b+1}^{M} e(a,j)^{H(b,j;P)+H(a,j;P)}. \qquad \text{(C.8)}
\end{aligned}$$

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

$$\begin{aligned}
H(a,j;P) - H(j,b;P) &= H(P^{-1}a - P^{-1}j) - H(P^{-1}j - P^{-1}b) \\
&= -H(-P^{-1}a + P^{-1}j) + H(-P^{-1}j + P^{-1}b) \\
&= -H(j,a;P) + H(b,j;P). \qquad \text{(C.9)}
\end{aligned}$$

Thus, we have

$$\begin{aligned}
A_M(P) + A_M((ab)P) &= \left((-1)^{H(a,b;P)} + (-1)^{H(b,a;P)}\right) \prod_{j=a+1}^{b-1} e(a,j)^{H(a,j;P)-H(j,b;P)} \\
&\quad \times \prod_{j=1}^{a-1} e(j,a)^{H(j,a;P)+H(j,b;P)} \prod_{j=b+1}^{M} e(a,j)^{H(a,j;P)+H(b,j;P)} \\
&\quad \times \prod_{1\leqslant j<k\leqslant M;\, j,k\neq a,b} e(j,k)^{H(j,k;P)} \qquad \text{(C.10)}
\end{aligned}$$

and we obtain

$$A_M(P) + A_M((ab)P) = 0 \qquad \text{for any} \quad P \in S_M. \qquad \text{(C.11)}$$

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 $e(j, k) = \sinh(v_j - v_k + 2\eta)/\sinh(v_j - v_k - 2\eta)$, where η is related to the anisotropy parameter Δ by $\Delta = \cosh 2\eta$.

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