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Derivation of the matrix product ansatz for the Heisenberg chain from the algebraic Bethe ansatz

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Abstract

We derive a matrix product representation of the Bethe ansatz state for the XXX and XXZ spin- $\frac{1}{2}$ Heisenberg chains using the algebraic Bethe ansatz. In this representation, the components of the Bethe eigenstates are expressed as traces of products of matrices which act on $\tilde{\mathcal{H}}$, the tensor product of auxiliary spaces. By changing the basis in $\tilde{\mathcal{H}}$, we derive explicit finite-dimensional representations for the matrices. These matrices are the same as those appearing in the recently proposed matrix product ansatz by Alcaraz and Lazo (2006 *J. Phys. A: Math. Gen.* **39** 11335) apart from normalization factors. We also discuss the close relation between the matrix product representation of the Bethe eigenstates and the six-vertex model with domain wall boundary conditions (Korepin 1982 *Commun. Math. Phys.* **86** 391) and show that the change of basis corresponds to a mapping from the six-vertex model to the five-vertex model.

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1. Introduction

Matrix product states (MPS) have attracted considerable interest in the interdisciplinary field of condensed matter physics and quantum information science [1, 2]. The archetype of MPS can be traced back to the seminal work of Affleck, Kennedy, Lieb and Tasaki [3–5], which is aimed at understanding the ground state properties of Haldane gap systems [6, 7]. It was then formalized in more generalized and abstract ways [8–10]. After those works, the density matrix renormalization group (DMRG) method, a powerful numerical method to study one-dimensional strongly correlated systems, was introduced by White [11, 12] and its connection to MPS formulation was discussed by Rommer and Östlund [13]. A common feature of mathematically rigorous and numerical approaches is that both have failed to describe quantum critical ground states which exhibit quasi-long range order. In the context of quantum information theory, Vidal *et al* have attempted to characterize the

quantitative difference between non-critical and critical ground states in one dimension in terms of entanglement entropy [14]. However, a natural question to ask is whether or not there are quantum critical ground states expressed in the form of MPS. Surprisingly, the answer is *yes*. In [15] and the subsequent work [16], Alcaraz and Lazo have actually shown that the eigenstates of the spin- $\frac{1}{2}$ Heisenberg chain can be expressed as MPS. It has been well known that this model is gapless and the quasiparticles, so-called spinons, have a linear dispersion relation since the pioneering work of Bethe in 1931 [17]. The method to solve this model used by Bethe is called the coordinate Bethe ansatz and there are several variants (algebraic, functional, etc) of it. Alcaraz and Lazo proposed another alternative formulation of the Bethe ansatz in terms of MPS, which they call the matrix product ansatz (MPA). In this formulation, one can obtain the spectrum conditions, i.e. Bethe equations, imposing algebraic relations between matrices consisting of MPS. The physical meaning of those matrices is interpreted as the generators of the Zamolodchikov–Faddeev algebra in (1+1)-dimensional field theories [18]. In [19], Alcaraz and Lazo applied MPA to other integrable models such as the Hubbard model [20], fermionic supersymmetric t - J model [21] and Fateev–Zamolodchikov model [22], and obtained the correct Bethe equations.

In this paper, we show that MPA is essentially equivalent to the algebraic Bethe ansatz (ABA) in the XXX and XXZ spin- $\frac{1}{2}$ Heisenberg chains. The ABA is an elegant method for solving the eigenvalue problem of quantum integrable models developed in the late 1970s [23–25]. So far, the relation between the MPS and ABA has been discussed in a completely different context, i.e. stochastic Markovian models in one dimension [26]. One of the simplest examples of the models is the asymmetric simple exclusion process (ASEP), which plays an important role in non-equilibrium statistical mechanics. This model was first exactly solved *not* using the Bethe ansatz [27], while the relation to the integrable quantum spin chains was then clarified by Alcaraz *et al* [28]. It was first discovered in [26] that the MPA for ASEP can be derived from the ABA. The authors have also constructed the explicit finite-dimensional matrices for the MPA. The key ingredient is the change of basis in \mathcal{H} , the tensor product of auxiliary spaces. Since the MPS are defined as traces over \mathcal{H} , they are invariant under the change and hence one can take an appropriate basis in which the matrices have very simple expressions. Along the same lines as their approach, we derive the MPA for the XXX and XXZ spin- $\frac{1}{2}$ Heisenberg chains. The explicit expressions for the matrices are also obtained.

The organization of this work is as follows. In section 2, we review the ABA method for solving the eigenvalue problem of the Heisenberg chain. In section 3, we derive the MPS representations for the Bethe eigenstates from the ABA by preparing $\tilde{\mathcal{H}}$, the tensor product of the auxiliary spaces. In section 4, the explicit expressions for the matrices appearing in the MPA are obtained by solving the recursion relations for the matrices. In section 5, the relation between the MPA and the six-vertex model with domain wall boundary conditions [29] is discussed. Conclusions and future perspectives are given in the last section. In the appendices, we provide graphical representations for the matrices in the main text and discuss the mapping from the six-vertex model to a five-vertex model.

2. Algebraic Bethe ansatz for the XXZ spin- $\frac{1}{2}$ Heisenberg chain

The XXZ spin- $\frac{1}{2}$ Heisenberg model with the periodic boundary condition is described by the following Hamiltonian:

$$\mathbf{H}_{\text{XXZ}} = \sum_{i=1}^L \left\{ \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta (\sigma_i^z \sigma_{i+1}^z - 1) \right\}, \quad (1)$$

where L denotes the total number of sites and σ_i^α ($\alpha = x, y, z$) are the Pauli matrices defined on the i th site. Here Δ is the anisotropy parameter and the particular cases $\Delta = 1$ and $\Delta = 0$ correspond to the XXX and XY chains, respectively.

The eigenstates of this model can be constructed using the ABA [23–25, 30]. We shall briefly review this construction. In the ABA, the central object is the quantum R -matrix which is the solution of the Yang–Baxter equation. For the XXZ model, the R -matrix acting on $\mathbb{C}^2 \otimes \mathbb{C}^2$ is given by

$$R(\lambda) = \frac{1}{\sinh(\lambda + \eta)} \begin{pmatrix} \sinh(\lambda + \eta) & 0 & 0 & 0 \\ 0 & \sinh \lambda & \sinh \eta & 0 \\ 0 & \sinh \eta & \sinh \lambda & 0 \\ 0 & 0 & 0 & \sinh(\lambda + \eta) \end{pmatrix}, \quad (2)$$

where λ is the spectral parameter and the relation between η and the anisotropy Δ is given by $\Delta = \cosh \eta$. Next, we introduce the quantum L -operator represented by a matrix acting on the tensor product of two-dimensional vector spaces $\bar{V}_j \otimes V_i$. The auxiliary space \bar{V}_j introduced here is spanned by two orthonormal states labeled as $|\leftarrow\rangle$ and $|\rightarrow\rangle$ while the physical Hilbert space at the i th site V_i is spanned by $|\uparrow\rangle$ and $|\downarrow\rangle$. For the XXZ model, the L -operator $\mathcal{L}_{ji}(\lambda)$ is defined by the R -matrix as

$$\mathcal{L}_{ji}(\lambda) = R_{ji} \left(\lambda - \frac{\eta}{2} \right), \quad (3)$$

where \mathcal{L}_{ji} acts on $\bar{V}_j \otimes V_i$. Note that the operator $\mathcal{L}_{ji}(\lambda)$ acts trivially on all the sites other than V_i . More explicitly, the L -operator is written as

$$\mathcal{L}_{ji}(\lambda) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(\lambda) & c(\lambda) & 0 \\ 0 & c(\lambda) & b(\lambda) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (4)$$

where

$$b(\lambda) = \frac{\sinh \left(\lambda - \frac{\eta}{2} \right)}{\sinh \left(\lambda + \frac{\eta}{2} \right)}, \quad c(\lambda) = \frac{\sinh \eta}{\sinh \left(\lambda + \frac{\eta}{2} \right)} \quad (5)$$

for the XXZ chain and

$$b(\lambda) = \frac{\lambda - \frac{i}{2}}{\lambda + \frac{i}{2}}, \quad c(\lambda) = \frac{i}{\lambda + \frac{i}{2}} \quad (6)$$

for the XXX chain. The latter can be obtained by taking the scaling limit of the former, i.e. $\lambda_{\text{XXZ}} = \epsilon \lambda_{\text{XXX}}$ and $\eta = i\epsilon$ with the limit of $\epsilon \rightarrow 0$. It is useful to note the relation between $b(\lambda)$, $c(\lambda)$ and the physical quasi-momentum k . For both the XXZ and XXX cases, $b(\lambda) = z$ with $z = e^{-ik}$ [15]. By a straightforward calculation, one can verify the following relation:

$$c(\lambda)^2 = 1 - 2\Delta z + z^2. \quad (7)$$

In particular, $c(\lambda) = 1 - z$ when $\Delta = 1$ corresponding to the XXX chain. The following identity can then be shown as a direct consequence of the Yang–Baxter equation:

$$R_{01}(\lambda - \mu) \mathcal{L}_{0i}(\lambda) \mathcal{L}_{1i}(\mu) = \mathcal{L}_{1i}(\mu) \mathcal{L}_{0i}(\lambda) R_{01}(\lambda - \mu). \quad (8)$$

Here, R_{01} acts nontrivially on $\bar{V}_0 \otimes \bar{V}_1$ and trivially on V_i . Note that \mathcal{L}_{1i} acts nontrivially on $\bar{V}_1 \otimes V_i$ and trivially on \bar{V}_0 and the other spatial sites.

The monodromy matrix is then constructed as the following ordered matrix product:

$$\mathcal{T}_0(\lambda) = \mathcal{L}_{01}(\lambda) \mathcal{L}_{02}(\lambda) \dots \mathcal{L}_{0L}(\lambda). \quad (9)$$

In the basis of \bar{V}_0 , the monodromy matrix can be represented as a 2×2 matrix:

$$\mathcal{T}_0(\lambda) = \begin{pmatrix} \mathbf{A}(\lambda) & \mathbf{B}(\lambda) \\ \mathbf{C}(\lambda) & \mathbf{D}(\lambda) \end{pmatrix}, \quad (10)$$

where the matrix elements $\mathbf{A}(\lambda)$, $\mathbf{B}(\lambda)$, $\mathbf{C}(\lambda)$ and $\mathbf{D}(\lambda)$ are themselves operators acting on the total Hilbert space $\mathcal{H} = \otimes_{i=1}^L V_i$. Using relation (8), one can show the following relation for the monodromy matrix:

$$R_{01}(\lambda - \mu) \mathcal{T}_0(\lambda) \mathcal{T}_1(\mu) = \mathcal{T}_1(\mu) \mathcal{T}_0(\lambda) R_{01}(\lambda - \mu). \quad (11)$$

The commutation relations among \mathbf{A} , \mathbf{B} , \mathbf{C} and \mathbf{D} can be obtained from this relation. Taking the trace of the monodromy matrix over \bar{V}_0 , one obtains a one-parameter family of transfer matrices acting on \mathcal{H} :

$$\mathbf{T}(\lambda) = \text{Tr}_{\bar{V}_0} \mathcal{T}_0(\lambda) = \mathbf{A}(\lambda) + \mathbf{D}(\lambda). \quad (12)$$

The Hamiltonian equation (1) can then be obtained from $\mathbf{T}(\lambda)$ by the trace identity

$$\mathbf{H}_{\text{XXZ}} = 2 \sinh \eta \frac{\partial}{\partial \lambda} \log \mathbf{T}(\lambda) \Big|_{\lambda=\eta/2} + \text{const.} \quad (13)$$

Since the Hamiltonian commutes with the monodromy matrix, one can construct a simultaneous eigenstate of both \mathbf{H}_{XXZ} and \mathbf{T} . The eigenstate of this operator is constructed by $\mathbf{B}(\lambda)$'s as

$$|\lambda_1, \lambda_2, \dots, \lambda_n\rangle = \mathbf{B}(\lambda_n) \dots \mathbf{B}(\lambda_1) \Phi_0, \quad (14)$$

where Φ_0 denotes the reference ferromagnetic state, i.e. $\Phi_0 = |\uparrow\rangle \equiv |\uparrow, \uparrow \dots \uparrow\rangle$ and n denotes the number of down spins. We call the above state a Bethe state. Since one can show that $\mathbf{B}(\lambda_i)$'s commute with each other from relation (11), this state is invariant under permutations of λ_i 's. The spectrum conditions, i.e. the Bethe equations, are then obtained using the commutation relations between \mathbf{A} , \mathbf{D} and \mathbf{B} [23–25]. For the XXZ model, those equations are given by

$$\left(\frac{\sinh(\lambda_j - \frac{\eta}{2})}{\sinh(\lambda_j + \frac{\eta}{2})} \right)^L \prod_{\substack{k=1 \\ k \neq j}}^n \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)} = 1, \quad j = 1, 2, \dots, n. \quad (15)$$

3. Derivation of the matrix product state representation from the algebraic Bethe ansatz

In the previous section, we outlined the construction of the eigenstates of \mathbf{H}_{XXZ} using the ABA. In this section, we derive the matrix product state representations for the eigenstates from the ABA. Let $|\leftarrow\rangle$ and $|\rightarrow\rangle$ be the two orthonormal states spanning \bar{V} . Then the Bethe state is expressed as

$$\begin{aligned} |\lambda_1, \lambda_2, \dots, \lambda_n\rangle &= \mathbf{B}(\lambda_n) \dots \mathbf{B}(\lambda_2) \mathbf{B}(\lambda_1) \Phi_0 \\ &= \langle \leftarrow | \mathcal{T}(\lambda_n) | \rightarrow \rangle \dots \langle \leftarrow | \mathcal{T}(\lambda_2) | \rightarrow \rangle \langle \leftarrow | \mathcal{T}(\lambda_1) | \rightarrow \rangle \Phi_0 \\ &= \text{Tr}_{\bar{V}^{\otimes n}} (Q_n \mathcal{T}(\lambda_n) \otimes \dots \otimes \mathcal{T}(\lambda_2) \otimes \mathcal{T}(\lambda_1) \Phi_0) \\ &= \text{Tr}_{\bar{V}^{\otimes n}} \left(Q_n \left[\prod_{i=1}^L \mathcal{L}_i(\lambda_1, \dots, \lambda_n) \right] \Phi_0 \right) \end{aligned} \quad (16)$$

with $Q_n = |\rightarrow, \rightarrow \dots \rightarrow\rangle \langle \leftarrow, \leftarrow \dots \leftarrow| \equiv |\Rightarrow\rangle \langle \Leftarrow|$ and $\mathcal{L}_i(\lambda_1, \dots, \lambda_n) \equiv \mathcal{L}_i(\lambda_n) \otimes \dots \otimes \mathcal{L}_i(\lambda_1)$ which acts on the vector space V_i only in \mathcal{H} . Here, we have omitted the indices for the auxiliary spaces. It would be helpful to note that the following identity for tensor products holds: $(AB) \otimes (CD) = (A \otimes C)(B \otimes D)$.

We now introduce two matrices D_n and C_n via

$$\mathcal{L}_i(\lambda_1, \dots, \lambda_n)|\uparrow\rangle = D_n(\lambda_1, \dots, \lambda_n)|\uparrow\rangle + C_n(\lambda_1, \dots, \lambda_n)|\downarrow\rangle \quad (17)$$

or equivalently, $D_n(\lambda_1, \dots, \lambda_n) = \langle\uparrow|\mathcal{L}_i(\lambda_1, \dots, \lambda_n)|\uparrow\rangle$ and $C_n(\lambda_1, \dots, \lambda_n) = \langle\downarrow|\mathcal{L}_i(\lambda_1, \dots, \lambda_n)|\uparrow\rangle$. It should be noted that D_n , C_n , and Q_n are $2^n \times 2^n$ matrices acting on $\bar{V}^{\otimes n}$ with scalar elements. The first terms are, for example, given by

$$D_1(\lambda) = \begin{pmatrix} 1 & 0 \\ 0 & b(\lambda) \end{pmatrix}, \quad C_1(\lambda) = \begin{pmatrix} 0 & c(\lambda) \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad Q_1(\lambda) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (18)$$

Henceforth, we shall denote the n -fold tensor product of the auxiliary spaces as $\mathcal{H}^{\otimes n} \equiv \bigotimes_{j=1}^n \bar{V}_{n-j+1}$. Using D_n , C_n and Q_n , the Bethe state can be written as

$$|\lambda_1, \lambda_2, \dots, \lambda_n\rangle = \text{Tr}_{\mathcal{H}^{\otimes n}} \left[Q_n \prod_{i=1}^L (D_n(\lambda_1, \dots, \lambda_n)|\uparrow\rangle_i + C_n(\lambda_1, \dots, \lambda_n)|\downarrow\rangle_i) \right], \quad (19)$$

where $|\uparrow\rangle_i$ and $|\downarrow\rangle_i$ denote the up and down spin states at the i th site, respectively. This form can be regarded as the matrix product state in the usual sense except for the boundary matrix Q_n .

Let us consider the recursion relation between D_{n+1} , C_{n+1} and D_n , C_n . From the fact $\mathcal{L}_i(\lambda_1, \dots, \lambda_n, \lambda_{n+1}) = \mathcal{L}_i(\lambda_{n+1}) \otimes \mathcal{L}_i(\lambda_1, \dots, \lambda_n)$, one can derive the following relations:

$$\begin{aligned} D_{n+1}(\lambda_1, \dots, \lambda_n, \lambda_{n+1}) &= \begin{pmatrix} 1 & 0 \\ 0 & b(\lambda_{n+1}) \end{pmatrix} \otimes D_n(\lambda_1, \dots, \lambda_n) \\ &\quad + \begin{pmatrix} 0 & 0 \\ c(\lambda_{n+1}) & 0 \end{pmatrix} \otimes C_n(\lambda_1, \dots, \lambda_n) \\ &= \begin{pmatrix} D_n(\lambda_1, \dots, \lambda_n) & 0 \\ c(\lambda_{n+1})C_n(\lambda_1, \dots, \lambda_n) & b(\lambda_{n+1})D_n(\lambda_1, \dots, \lambda_n) \end{pmatrix} \end{aligned} \quad (20)$$

and

$$\begin{aligned} C_{n+1}(\lambda_1, \dots, \lambda_n, \lambda_{n+1}) &= \begin{pmatrix} 0 & c(\lambda_{n+1}) \\ 0 & 0 \end{pmatrix} \otimes D_n(\lambda_1, \dots, \lambda_n) \\ &\quad + \begin{pmatrix} b(\lambda_{n+1}) & 0 \\ 0 & 1 \end{pmatrix} \otimes C_n(\lambda_1, \dots, \lambda_n) \\ &= \begin{pmatrix} b(\lambda_{n+1})C_n(\lambda_1, \dots, \lambda_n) & c(\lambda_{n+1})D_n(\lambda_1, \dots, \lambda_n) \\ 0 & C_n(\lambda_1, \dots, \lambda_n) \end{pmatrix}. \end{aligned} \quad (21)$$

Here we have used the following identities:

$$\begin{aligned} {}_i\langle\uparrow|\mathcal{L}_i(\lambda_{n+1})|\uparrow\rangle_i &= \begin{pmatrix} 1 & 0 \\ 0 & b(\lambda_{n+1}) \end{pmatrix}, & {}_i\langle\uparrow|\mathcal{L}_i(\lambda_{n+1})|\downarrow\rangle_i &= \begin{pmatrix} 0 & 0 \\ c(\lambda_{n+1}) & 0 \end{pmatrix}, \\ {}_i\langle\downarrow|\mathcal{L}_i(\lambda_{n+1})|\uparrow\rangle_i &= \begin{pmatrix} 0 & c(\lambda_{n+1}) \\ 0 & 0 \end{pmatrix}, & {}_i\langle\downarrow|\mathcal{L}_i(\lambda_{n+1})|\downarrow\rangle_i &= \begin{pmatrix} b(\lambda_{n+1}) & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned}$$

The above matrices are understood to act on the auxiliary space \bar{V}_i (see appendix A.1 for a more detailed explanation). By definition, it is obvious that $Q_n(\lambda_1, \dots, \lambda_n, \lambda_{n+1})$ satisfies the following recursion relation:

$$Q_{n+1}(\lambda_1, \dots, \lambda_n, \lambda_{n+1}) = \begin{pmatrix} 0 & 0 \\ Q_n(\lambda_1, \dots, \lambda_n) & 0 \end{pmatrix} \quad (22)$$

and hence the explicit form of $Q_n(\lambda_1, \dots, \lambda_n)$ is given by

$$Q_n(\lambda_1, \dots, \lambda_n) = \bigotimes_{l=1}^n \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (23)$$

Therefore, one can construct a matrix product representation of the Bethe ansatz state using relations (20)–(22) recursively. The interesting point here is that the dimension of the matrix is finite even in the thermodynamic limit if the number of down spins is finite. On the other hand, if we consider the case of the fixed magnetization, i.e. the ratio n/L is fixed, the dimension of the matrix becomes infinite in the limit of $L \rightarrow \infty$.

4. Change of the basis in $\tilde{\mathcal{H}}$

In the previous section, we have derived the matrix product state representation for the Bethe states from the ABA. At that point, however, the matrices are defined by the recursion relations and the connection to another representation proposed by Alcaraz and Lazo [15, 16] is not clear. In this section, we clarify the direct relation between them by solving the recursion relations. We now try to rewrite the matrices D_n and C_n as diagonally as possible. For simplicity, we omit here the indeterminants of matrices, i.e. $\lambda_1, \dots, \lambda_n$. Furthermore, we will replace $b(\lambda_j)$ with $z_j = e^{-ik_j}$. Suppose that D_n is diagonalized by the invertible matrix F_n as $F_n^{-1}D_nF_n = \mathcal{D}_n$. In the new basis in $\tilde{\mathcal{H}}$, C_n and Q_n are transformed into $\mathcal{C}_n = F_n^{-1}C_nF_n$ and $\mathcal{Q}_n = F_n^{-1}Q_nF_n$, respectively. From the cyclic property of the trace, it is obvious that the Bethe state can be written by new matrices as

$$|\lambda_1, \lambda_2, \dots, \lambda_n\rangle = \text{Tr}_{\tilde{\mathcal{H}}} \left[\mathcal{Q}_n \prod_{i=1}^L (\mathcal{D}_n |\uparrow\rangle_i + \mathcal{C}_n |\downarrow\rangle_i) \right]. \quad (24)$$

We now decompose \mathcal{C}_n as a sum of n matrices:

$$\mathcal{C}_n = \sum_{i=1}^n \mathcal{C}_n^{(i)}, \quad (25)$$

and suppose that \mathcal{D}_n and $\mathcal{C}_n^{(i)}$ satisfy the following algebraic relations:

$$\mathcal{C}_n^{(i)}\mathcal{D}_n = z_i\mathcal{D}_n\mathcal{C}_n^{(i)} \quad (26)$$

$$\mathcal{C}_n^{(i)}\mathcal{C}_n^{(j)} = \tilde{S}_{ij}(z_i, z_j)\mathcal{C}_n^{(j)}\mathcal{C}_n^{(i)} \quad (27)$$

$$\mathcal{C}_n^{(i)}\mathcal{C}_n^{(i)} = 0. \quad (28)$$

Then we look for an appropriate $\tilde{S}_{ij}(z_i, z_j)$ by observation. Let us now consider the case of $n = 2$. In this case, D_2 and C_2 are given by

$$D_2 = \begin{pmatrix} D_1(\lambda_1) & 0 \\ 0 & z_2 D_1(\lambda_1) \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ c(\lambda_2)C_1(\lambda_1) & 0 \end{pmatrix}, \quad (29)$$

$$C_2 = \begin{pmatrix} 0 & c(\lambda_2)D_1(\lambda_1) \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} z_2 C_1(\lambda_1) & 0 \\ 0 & C_1(\lambda_1) \end{pmatrix}, \quad (30)$$

respectively, where $D_1(\lambda_1)$ and $C_1(\lambda_1)$ are defined in equation (18). By an explicit calculation, one can confirm that the matrix D_2 is diagonalized as

$$D_2 = F_2^{-1}D_2F_2 = \begin{pmatrix} D_1(\lambda_1) & 0 \\ 0 & z_2 D_1(\lambda_1) \end{pmatrix}, \quad (31)$$

where

$$F_2 = \begin{pmatrix} 1 & 0 \\ \mathcal{F}_1 & 1 \end{pmatrix} \tag{32}$$

with $\mathcal{F}_1 = \frac{c(\lambda_2)}{z_1 - z_2} C_1(\lambda_1)$. We note that the inverse of F_2 is given by

$$F_2^{-1} = \begin{pmatrix} 1 & 0 \\ -\mathcal{F}_1 & 1 \end{pmatrix}. \tag{33}$$

In the new basis defined by F_2 , the matrix C_2 becomes

$$C_2 = F_2^{-1} C_2 F_2 = \begin{pmatrix} z_2 C_1(\lambda_1) + c(\lambda_2) \mathcal{F}_1 & c(\lambda_2) D_1(\lambda_1) \\ 0 & -z_1 c(\lambda_2) \mathcal{F}_1 + C_1(\lambda_1) \end{pmatrix}. \tag{34}$$

We now divide the above matrix into two matrices as $C_2 = C_2^{(1)} + C_2^{(2)}$ with

$$C_2^{(1)} = \begin{pmatrix} z_2 C_1(\lambda_1) + c(\lambda_2) \mathcal{F}_1 & 0 \\ 0 & -c(\lambda_2) z_1 \mathcal{F}_1 + C_1(\lambda_1) \end{pmatrix}, \quad C_2^{(2)} = \begin{pmatrix} 0 & c(\lambda_2) D_1(\lambda_1) \\ 0 & 0 \end{pmatrix}. \tag{35}$$

One can confirm that $C_2^{(1)}$ and $C_2^{(2)}$ satisfy the algebraic relations (26) and (28). Then we compare the commutation relation between $C_2^{(1)}$ and $C_2^{(2)}$ with equation (27) and find that $\tilde{S}_{12}(z_1, z_2)$ should be given by

$$\tilde{S}_{12}(z_1, z_2) = -\frac{z_1}{z_2} \cdot \frac{z_1 z_2 + 1 - 2\Delta z_2}{z_1 z_2 + 1 - 2\Delta z_1}. \tag{36}$$

From this observation, we take the coefficient $\tilde{S}_{ij}(z_i, z_j)$ to be

$$\tilde{S}_{ij}(z_i, z_j) = -\frac{z_i}{z_j} \cdot \frac{z_i z_j + 1 - 2\Delta z_j}{z_i z_j + 1 - 2\Delta z_i} \tag{37}$$

for general i and j . We shall prove the algebraic relations (26)–(28) with this $\tilde{S}_{ij}(z_i, z_j)$ by induction on n . For $n = 1$, the matrices $\mathcal{D}_1 = D_1$, $\mathcal{C}_1 = C_1$ trivially satisfy relations (26)–(28). Now, we suppose that we have already found the matrix F_n which diagonalizes \mathcal{D}_n as $\mathcal{D}_n = F_n^{-1} D_n F_n$ and have found a decomposition $\mathcal{C}_n = \sum_{i=1}^n C_n^{(i)}$ such that relations (26)–(28) are satisfied between \mathcal{D}_n and $C_n^{(i)}$'s. Then we show that it is possible to construct a matrix F_{n+1} which diagonalizes \mathcal{D}_{n+1} and can find a decomposition of \mathcal{C}_{n+1} . First, we take the matrix F_{n+1} to be of the following form:

$$F_{n+1} = \begin{pmatrix} F_n & 0 \\ F_n \mathcal{F}_n & F_n \end{pmatrix} \tag{38}$$

or equivalently

$$F_{n+1}^{-1} = \begin{pmatrix} F_n^{-1} & 0 \\ -\mathcal{F}_n F_n^{-1} & F_n^{-1} \end{pmatrix}. \tag{39}$$

We then obtain the following recursion relations using equations (20)–(22):

$$\mathcal{D}_{n+1} = \begin{pmatrix} \mathcal{D}_n & 0 \\ -\mathcal{F}_n \mathcal{D}_n + c(\lambda_{n+1}) \mathcal{C}_n + z_{n+1} \mathcal{D}_n \mathcal{F}_n & z_{n+1} \mathcal{D}_n \end{pmatrix}, \tag{40}$$

$$\mathcal{C}_{n+1} = \begin{pmatrix} z_{n+1} \mathcal{C}_n + c(\lambda_{n+1}) \mathcal{D}_n \mathcal{F}_n & c(\lambda_{n+1}) \mathcal{D}_n \\ \mathcal{C}_n \mathcal{F}_n - z_{n+1} \mathcal{F}_n \mathcal{C}_n - c(\lambda_{n+1}) \mathcal{F}_n \mathcal{D}_n \mathcal{F}_n & \mathcal{C}_n - c(\lambda_{n+1}) \mathcal{F}_n \mathcal{D}_n \end{pmatrix}, \tag{41}$$

$$\mathcal{Q}_{n+1} = \begin{pmatrix} 0 & 0 \\ \mathcal{Q}_n & 0 \end{pmatrix}, \tag{42}$$

where \mathcal{F}_n is an unknown matrix to be determined. Since one can take F_1 to be the 2×2 identity matrix, $\mathcal{Q}_1 = Q_1$ holds and hence $\mathcal{Q}_n = Q_n$ for $\forall n$. In other words, the change of basis preserves the domain wall boundary condition (DWBC) in \mathcal{H} . This property plays a crucial role when we interpret our results in terms of the six-vertex model as discussed in section 5. From equation (40), one can see that \mathcal{D}_{n+1} is a diagonal matrix if the matrix \mathcal{F}_n satisfies $-\mathcal{F}_n \mathcal{D}_n + c(\lambda_{n+1})\mathcal{C}_n + z_{n+1}\mathcal{D}_n \mathcal{F}_n = 0$. Using equation (26), such \mathcal{F}_n can be constructed as

$$\mathcal{F}_n = c(\lambda_{n+1})\mathcal{D}_n^{-1} \sum_{i=1}^n \frac{\mathcal{C}_n^{(i)}}{z_i - z_{n+1}}. \quad (43)$$

Next, we shall show that the (2,1)-component of \mathcal{C}_{n+1} is also zero if $\tilde{S}_{ij}(z_i, z_j)$ is given by equation (37). By a direct calculation, one obtains

$$\mathcal{C}_n \mathcal{F}_n - z_{n+1} \mathcal{F}_n \mathcal{C}_n - c(\lambda_{n+1})\mathcal{F}_n \mathcal{D}_n \mathcal{F}_n = c(\lambda_{n+1})\mathcal{D}_n^{-1} \sum_{i=1}^n \sum_{j=1}^n d_{ij} \mathcal{C}_n^{(i)} \mathcal{C}_n^{(j)} \quad (44)$$

with

$$\begin{aligned} d_{ij} &= z_i^{-1} \frac{1}{z_j - z_{n+1}} - z_{n+1} \frac{1}{z_i - z_{n+1}} - \frac{c(\lambda_{n+1})^2}{(z_i - z_{n+1})(z_j - z_{n+1})} \\ &= z_i^{-1} \frac{1}{z_j - z_{n+1}} - z_{n+1} \frac{1}{z_i - z_{n+1}} - \frac{1 - 2\Delta z_{n+1} + z_{n+1}^2}{(z_i - z_{n+1})(z_j - z_{n+1})} \\ &= -\frac{z_{n+1}}{z_i} \cdot \frac{z_i z_j + 1 - 2\Delta z_i}{(z_i - z_{n+1})(z_j - z_{n+1})}, \end{aligned} \quad (45)$$

where we have used relation (7). Using relations (27) and (28), equation (44) is zero if d_{ij} satisfies $d_{ij} + [\tilde{S}_{ij}(z_i, z_j)]^{-1} d_{ji} = 0$. Although this relation is highly nontrivial, one can confirm that it holds if $\tilde{S}_{ij}(z_i, z_j)$ is given by equation (37). The recursion relations (40) and (41) can now be written as

$$\mathcal{D}_{n+1} = \begin{pmatrix} 1 & 0 \\ 0 & z_{n+1} \end{pmatrix} \otimes \mathcal{D}_n, \quad (46)$$

$$\mathcal{C}_{n+1} = \begin{pmatrix} \sum_{i=1}^n \frac{z_i z_{n+1} + 1 - 2\Delta z_{n+1}}{z_i - z_{n+1}} \mathcal{C}_n^{(i)} & c(\lambda_{n+1})\mathcal{D}_n \\ 0 & -z_{n+1} \sum_{i=1}^n \frac{z_i z_{n+1} + 1 - 2\Delta z_i}{z_i - z_{n+1}} \mathcal{C}_n^{(i)} \end{pmatrix}. \quad (47)$$

From them we deduce the decomposition of $\mathcal{C}_{n+1} = \sum_{i=1}^{n+1} \mathcal{C}_{n+1}^{(i)}$ with

$$\mathcal{C}_{n+1}^{(i)} = \frac{1}{z_i - z_{n+1}} \begin{pmatrix} (z_i z_{n+1} + 1 - 2\Delta z_{n+1})\mathcal{C}_n^{(i)} & 0 \\ 0 & -z_{n+1}(z_i z_{n+1} + 1 - 2\Delta z_i)\mathcal{C}_n^{(i)} \end{pmatrix} \quad \text{for } i \leq n, \quad (48)$$

and

$$\mathcal{C}_{n+1}^{(n+1)} = \begin{pmatrix} 0 & c(\lambda_{n+1})\mathcal{D}_n \\ 0 & 0 \end{pmatrix}. \quad (49)$$

From the above expressions, it is shown that \mathcal{D}_{n+1} and $\mathcal{C}_{n+1}^{(i)}$ ($1 \leq i \leq n+1$) also satisfy the algebraic relations (26)–(28). Therefore, we have proved that there exists a decomposition of \mathcal{C}_n with algebraic relations (26)–(28) at any n .

We now write down the explicit expressions for \mathcal{D}_n and $\mathcal{C}_n^{(i)}$ using the recursion relations (46)–(49). From equation (46), we first obtain

$$\mathcal{D}_n = \bigotimes_{l=1}^n \begin{pmatrix} 1 & 0 \\ 0 & z_{n-l+1} \end{pmatrix}. \tag{50}$$

Then, from equation (49), we obtain

$$\mathcal{C}_n^{(n)} = c(\lambda_n) \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \bigotimes_{l=2}^n \begin{pmatrix} 1 & 0 \\ 0 & z_{n-l+1} \end{pmatrix}. \tag{51}$$

We finally find the explicit form of $\mathcal{C}_n^{(i)}$ with $1 \leq i \leq n$. Relation (48) can be recast as

$$\mathcal{C}_{n+1}^{(i)} = -\frac{z_i z_{n+1} + 1 - 2\Delta z_i}{z_i - z_{n+1}} \begin{pmatrix} S_{i,n+1}(z_i, z_{n+1}) & 0 \\ 0 & z_{n+1} \end{pmatrix} \otimes \mathcal{C}_n^{(i)}, \tag{52}$$

where

$$S_{ij}(z_i, z_j) = -\frac{z_i z_j + 1 - 2\Delta z_j}{z_i z_j + 1 - 2\Delta z_i}. \tag{53}$$

Therefore, we obtain the explicit expression for $\mathcal{C}_n^{(i)}$ as

$$\begin{aligned} \mathcal{C}_n^{(i)} &= f(z_i, \dots, z_n) c(\lambda_i) \bigotimes_{l=1}^{n-i} \begin{pmatrix} S_{i,n-l+1}(z_i, z_{n-l+1}) & 0 \\ 0 & z_{n-l+1} \end{pmatrix} \\ &\quad \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \bigotimes_{l=n-i+2}^n \begin{pmatrix} 1 & 0 \\ 0 & z_{n-l+1} \end{pmatrix}. \end{aligned} \tag{54}$$

with

$$f(z_i, \dots, z_n) = \prod_{l=i+1}^n \left(-\frac{z_i z_l + 1 - 2\Delta z_i}{z_i - z_l} \right) \tag{55}$$

for $i = 1, \dots, n - 1$. We note $f(z_n) = 1$. The action of the matrix $\mathcal{C}_n^{(i)}$ is almost diagonal in \mathcal{H} except in the single auxiliary space \tilde{V}_i . Therefore, it is now quite trivial to confirm the algebraic relations (26)–(28) using equations (50), (51) and (54).

Let us now clarify the relations between the ABA and the MPA explicitly. Keeping the notations as close as possible to those in [15, 16], the Bethe eigenstate in the MPA is written in the form

$$|\psi_n\rangle = \sum_{\{x_1, x_2, \dots, x_n\}} \text{Tr}(E_n^{x_1-1} A_n E_n^{x_2-x_1-1} A_n \dots E_n^{x_n-x_{n-1}-1} A_n E_n^{L-x_n} \Omega_n) |x_1, x_2, \dots, x_n\rangle, \tag{56}$$

where $|x_1, x_2, \dots, x_n\rangle$ ($1 \leq x_1 < x_2 < \dots < x_n \leq L$) denote the configurations with down spins at (x_1, x_2, \dots, x_n) and the subscript n indicates the total number of down spins. Note that in the original papers by Alcaraz and Lazo [15, 16], (x_1, x_2, \dots, x_n) are the locations of up spins. The matrix A_n is decomposed by n matrices as

$$A_n = \sum_{i=1}^n A_{k_i, n} E_n, \tag{57}$$

where the matrices $A_{k_i, n}$ obey the commutation relations

$$A_{k_i, n} E_n = z_i E_n A_{k_i, n}, \tag{58}$$

$$A_{k_i, n} A_{k_j, n} = S_{ij}(z_i, z_j) A_{k_j, n} A_{k_i, n}, \tag{59}$$

$$E_n \Omega_n = e^{-iP} \Omega_n E_n, \tag{60}$$

with $P = \sum_{i=1}^n k_i$. The above relations assure that $|\psi_n\rangle$ is the eigenstate of the Heisenberg Hamiltonian \mathbf{H}_{XXZ} . From equation (59), one can derive $A_{k_i,n}^2 = 0$. Relations (58)–(59) together with $A_{k_i,n}^2 = 0$ look very similar to equations (26)–(28). We now try to find a one-to-one correspondence between the matrices in equations (26)–(28) and those in equations (58)–(59). To reproduce the correct commutation relations, the following relations are required:

$$E_n = \alpha \mathcal{D}_n, \quad \Omega_n = \beta \mathcal{Q}_n = \beta \mathcal{Q}_n \quad \text{and} \quad A_{k_i,n} E_n = \gamma_i \mathcal{C}_n^{(i)}, \tag{61}$$

where α , β and γ_i ($i = 1, \dots, n$) can be the arbitrary numbers. Here we have used the fact that $z_j \tilde{S}_{ij}(z_i, z_j) = z_i S_{ij}(z_i, z_j)$. For simplicity, let us fix $\alpha = \beta = 1$. Then, from the above correspondence, we obtain $A_{k_i,n} = \gamma_i \mathcal{C}_n^{(i)} \mathcal{D}_n^{-1}$ and find

$$E_n = \bigotimes_{l=1}^n \begin{pmatrix} 1 & 0 \\ 0 & z_{n-l+1} \end{pmatrix} \tag{62}$$

$$A_{k_i,n} = \gamma_i \frac{c(\lambda_i)}{z_i} f(z_i, \dots, z_n) \bigotimes_{l=1}^{n-i} \begin{pmatrix} S_{i,n-l+1}(z_i, z_{n-l+1}) & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \bigotimes_{l=n-i+2}^n \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{63}$$

which are indeed equivalent to the matrices found in [16] if we change the ordering of quasi-momenta from (k_1, k_2, \dots, k_n) to (k_n, \dots, k_2, k_1) and take an appropriate set of γ_i 's. In this way, we have derived the matrices appearing in the MPA using the ABA. Therefore, the matrix product Bethe ansatz is equivalent to the algebraic Bethe ansatz. We note here that if we take the XY limit ($\Delta = 0$), $S(z_i, z_j) = -1$, and hence equation (63) can be regarded as the Jordan–Wigner transformation in the *auxiliary* space \mathcal{H} .

We remark on the coefficient γ_i in the proportional relation between $A_{k_i,n} E_n$ and $\mathcal{C}_n^{(i)}$. In the original work by Alcaraz and Lazo, A_n is defined by $\sum_{i=1}^n A_{k_i,n} E_n = \sum_{i=1}^n \gamma_i \mathcal{C}_n^{(i)}$, while \mathcal{C}_n is defined by equation (25). Therefore, one may think that there is a constraint on the proportionality coefficients γ_i 's. However, they can be arbitrary. Let us explain the reason for it. Since $A_{k_i,n}$'s are nilpotent ($A_{k_i,n}^2 = 0$), only the following products appear in equation (56):

$$\Omega_n E_n^{x_1-1} A_{k_{\sigma(1)},n} E_n^{x_2-x_1} A_{k_{\sigma(2)},n} \dots E_n^{x_n-x_{n-1}} A_{k_{\sigma(n)},n} E_n^{L-x_n+1} \tag{64}$$

where σ are the permutations of $(1, 2, \dots, n)$. Therefore, if we take an arbitrary set of γ_i 's, the matrix product equation (64) for any σ has the same prefactor and hence the state is uniquely determined apart from an overall factor.

We also remark on the relation between equations (24) and (56). Using the correspondence (61), we can rewrite equation (24) as

$$|\lambda_1, \lambda_2, \dots, \lambda_n\rangle = \text{Tr}_{\mathcal{H}} \left[\Omega_n \prod_{i=1}^L (E_n |\uparrow\rangle_i + A_n |\downarrow\rangle_i) \right], \tag{65}$$

where we have set $\alpha = \beta = \gamma_i = 1$. It is easy to show $|\lambda_1, \lambda_2, \dots, \lambda_n\rangle = |\psi_n\rangle$, where $|\psi_n\rangle$ is defined in equation (56). One may think that in the expansion of the rhs of equation (65) there are traces of the following matrix products:

$$\Omega_n E_n^{x_1-1} A_{k_{\sigma(i_1)},n} E_n^{x_2-x_1} A_{k_{\sigma(i_2)},n} \dots E_n^{x_m-x_{m-1}} A_{k_{\sigma(i_m)},n} E_n^{L-x_m+1}, \quad (m < n) \tag{66}$$

where (i_1, i_2, \dots, i_m) are subsets of $(1, 2, \dots, n)$. Such terms do not appear in equation (56). In fact, they are forbidden since $\text{Tr}_{\mathcal{H}} [\Omega_n M_n]$ is nonzero only when the matrix M_n is written

as $M_n = \Omega_n^T + \dots$, where T denotes the matrix transpose. Let us explain it in more detail. From equation (63), it is obvious that only a single arrow which is one of the orthonormal vectors in \tilde{V}_i is flipped by the action of $A_{k_i, n}$. On the other hand, $\text{Tr}_{\mathcal{H}} [\Omega_n M_n]$ can be recast as $\langle \leftarrow | M_n | \rightarrow \rangle$. This matrix element is nonzero only when all the arrows are flipped by the action of M_n . This proves that the trace of (66) is zero when $m < n$.

5. Relation to the six-vertex model with domain wall boundary conditions

In this section, we shall clarify the relation between the matrix product Bethe ansatz and the six-vertex model with domain wall boundary conditions. The six vertex model is a two-dimensional statistical mechanics model in which the Boltzmann weights are assigned to the six different configurations of arrows around a vertex. If the Boltzmann weights satisfy the Yang–Baxter relation, the model is exactly solvable by the Bethe ansatz. The partition function of this model on an $n \times L$ rectangle is defined as

$$\mathcal{Z} = \left[\prod_{j=1}^n \sinh \left(\lambda_j + \frac{\eta}{2} \right) \right]^L Z \quad \text{with} \quad Z = \sum_{\text{config}} \prod_{v=(i,j)} [\mathcal{L}_i(\lambda_j)]_{\nu_v \rho_v}^{\mu_v \sigma_v}, \quad (67)$$

where the summation is taken over all the possible configurations satisfying the *ice rule*, and $v = (i, j)$ denotes the vertex which is the intersection of the i th vertical and j th horizontal lines. In the definition of Z , the product is taken over all the vertices. The Boltzmann weights are related to the six nonzero matrix elements of the L -operator and $\mathcal{L}_i(\lambda_j)$ is assigned to the vertex v . The indices μ and ν correspond to arrows on the horizontal edges, while σ and ρ correspond to spins on the vertical edges (see figure 1(a)). The model with periodic boundary conditions was first solved by Lieb [31]. The model with domain wall boundary conditions (see figure 1(b)), which is relevant to our study, was first discovered by Korepin in the context of the norm of the Bethe state [29]. For a finite ($n \times n$) lattice, the partition function apart from an overall factor is given by a component of the Bethe state as

$$Z_n^{\text{DWBC}} = \langle \Downarrow | \lambda_1, \dots, \lambda_n \rangle, \quad (68)$$

where $\langle \Downarrow | = \bigotimes_{i=1}^n \langle \downarrow |$. In [29], the recursion relation for Z_n^{DWBC} was derived, and then later it was solved by a determinant formula [32]. Note that in the original papers, an inhomogeneous generalization of the six-vertex model was studied. Not only the component of the state $\langle \Downarrow |$ but also the other components of the Bethe state can be interpreted as partition functions of the six-vertex model. The coefficient of the state $|\sigma_1^{[V_1]}, \dots, \sigma_L^{[V_L]}\rangle$, i.e.

$$\langle \sigma_1^{[V_1]}, \dots, \sigma_L^{[V_L]} | \lambda_1, \dots, \lambda_n \rangle, \quad (69)$$

corresponds to the partition function with the boundary conditions shown in figure 1(c) (a more detailed discussion is provided in appendix A.1). Here, σ_i ($i = 1, 2, \dots, L$) denotes the spin state, i.e. \uparrow or \downarrow . In this sense, to obtain the Bethe state is equivalent to obtaining the partition function of the six-vertex model with various boundary conditions. It appears to be a formidable combinatorial task. However, if we construct a vertex model corresponding to the new basis in \mathcal{H} , this complexity is greatly reduced as shown in appendices A.2 and A.3. It corresponds exactly to the similarity transformation from the triangular matrices D_n and C_n to the matrices \mathcal{D}_n and $\mathcal{C}_n^{(i)}$ whose actions are diagonal and almost diagonal except for the single space \tilde{V}_i , respectively. It is important to stress here that this change of basis does not alter Q_n , i.e. the domain wall boundary condition in \mathcal{H} . In the corresponding vertex model, the Boltzmann weight of one of six vertices becomes zero. We henceforth call this model a *five-vertex model*. Note that since the partition function itself is the same after the

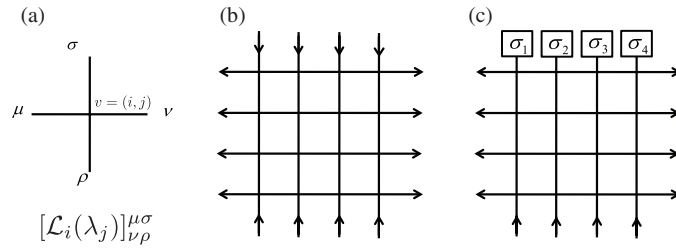


Figure 1. (a) L -operator associated with the vertex which is the intersection of the i th vertical line and j th horizontal line. (b) Domain wall boundary conditions. (c) Other boundary conditions. Each σ_i is \uparrow or \downarrow .

transformation, the statistical model is unchanged. Compared with the six-vertex model, however, the combinatorial complexity has been already resolved in the five-vertex model and hence the possible number of configurations involved in the calculation of Z is greatly reduced.

A similar reduction has been known as F -matrices in the context of the Drinfel'd twist and triangular Hopf algebras [33, 34], which have been used to calculate the correlation functions in the Heisenberg chain [35–38]. The F -matrix is named after a factorization of the R -matrix and defines a transformation from \mathbf{A} , \mathbf{B} , \mathbf{C} and \mathbf{D} to the new operators. By this transformation, \mathbf{A} and \mathbf{D} are transformed into diagonal matrices. On the other hand, \mathbf{B} and \mathbf{C} are transformed into the matrices whose actions are almost diagonal in \mathcal{H} . By expanding the physical spin operators in terms of those diagonal and almost diagonal operators, it is able to handle calculations of various correlation functions. Compared with this approach, the matrix F_n we found is a counterpart of the F -matrix in \mathcal{H} . Note that the original F -matrix is defined in the physical space \mathcal{H} while our F_n acts on \mathcal{H} . It is surprising that the connection between the MPA and the ABA we found turns out to be related to the F -matrices. It would be interesting to bridge over these two approaches more concretely.

6. Conclusion

In conclusion, we have derived the matrix product representation of the Bethe ansatz state for the XXX and XXZ spin- $\frac{1}{2}$ Heisenberg chains from the algebraic Bethe ansatz. We have also shown that the finite-dimensional representations for the matrices appearing in the matrix product ansatz proposed by Alcaraz and Lazo are equivalent to those obtained from the algebraic Bethe ansatz by use of the nontrivial change of basis in \mathcal{H} , which is related to the F -matrices. In the new basis, the matrices have a quite simple structure and the algebraic relations between matrices can be shown very easily. The relation between the MPA and the six-vertex model with domain wall boundary conditions has also been discussed. It would be of great interest to apply the obtained explicit matrices to calculations of static and dynamical correlation functions [34, 36–42] and entanglement properties [43–45] in the Heisenberg spin chains. The first step should be a calculation of the norm of the Bethe eigenstate [46], which has been obtained and is related to the determinant expression for the partition function of the six-vertex model with domain wall boundary conditions [29, 32, 47]. It would also be interesting to find a relation between the matrix product ansatz and the hidden Grassmann structure in the XXZ model discussed in the context of mathematically rigorous approaches [48–50]. Another interesting direction is a systematic construction of the matrix product state representation of the Bethe states for other integrable models, especially for correlated electron

systems such as the Hubbard model [20, 51–53]. Our discussion in section 2 indicates that it can be obtained if the model is exactly solvable by the algebraic Bethe ansatz. However, it is highly nontrivial whether or not we can obtain explicit expressions for the matrices since we need to find a new basis in which the matrices are almost diagonal.

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Appendix A. Graphical representation

A.1. Definitions of graphs

The L -operator $\mathcal{L}_{ji}(\lambda_j)$ given by equation (4) is a 4×4 matrix acting on a vector space $\bar{V}_j \otimes V_i$. The space \bar{V}_j is spanned by $|\leftarrow\rangle_j$ and $|\rightarrow\rangle_j$ while V_i is by $|\uparrow\rangle_i$ and $|\downarrow\rangle_i$. We hereafter denote it as $\mathcal{L}_i(\lambda_j)$. The order of the basis in $\bar{V}_j \otimes V_i$ is fixed as $|\leftarrow\uparrow\rangle, |\leftarrow\downarrow\rangle, |\rightarrow\uparrow\rangle, |\rightarrow\downarrow\rangle$. In a graphical representation, we denote a matrix element as

$$\langle\mu\sigma|\mathcal{L}_i(\lambda_j)|\nu\rho\rangle = [\mathcal{L}_i(\lambda_j)]_{\nu\rho}^{\mu\sigma} = \mu - \begin{array}{c} \sigma \\ | \\ \rho \end{array}, -\nu$$

where μ and ν are \leftarrow or \rightarrow while σ and ρ are \uparrow or \downarrow . The space V_i (or \bar{V}_j) is denoted by a black thick line (a bold dashed line). There are $2^4 = 16$ possible configurations of vertices. However, six of them are nonzero as we have seen in equation (4), which corresponds to the six-vertex model. The correspondence between the vertices and the ‘Boltzmann weights’ is summarized as follows:

$$\begin{array}{c} \uparrow \\ | \\ \leftarrow \end{array} = \begin{array}{c} \downarrow \\ | \\ \rightarrow \end{array} = 1, \quad \begin{array}{c} \downarrow \\ | \\ \leftarrow \end{array} = \begin{array}{c} \uparrow \\ | \\ \rightarrow \end{array} = b, \quad \begin{array}{c} \downarrow \\ | \\ \leftarrow \end{array} = \begin{array}{c} \downarrow \\ | \\ \rightarrow \end{array} = c.$$

Note that the weights b and c depend on j and can be complex. We should stress here that the above correspondence is not unique but depends on an order of basis. We now introduce a graphical representation for the L -operator. The L -operator acting on $\bar{V}_j \otimes V_i$ is drawn as a vertex without arrows:

$$\mathcal{L}_i(\lambda_j) = \begin{array}{c} \text{j} \\ | \\ \text{i} \end{array} \begin{array}{c} \text{---} \\ | \\ \text{---} \end{array}.$$

Next we describe four kinds of operators acting on V_i from the L -operator. They are defined by decomposing the 4×4 matrix into equation (4) into 2×2 sub-matrices:

$$\mathcal{L}_i(\lambda_j) = \left(\begin{array}{c} \begin{array}{c} \text{j} \\ | \\ \text{i} \end{array} \begin{array}{c} \text{---} \\ | \\ \text{---} \end{array} \\ \begin{array}{c} \text{j} \\ | \\ \text{i} \end{array} \begin{array}{c} \text{---} \\ | \\ \text{---} \end{array} \end{array} \right)_{[\bar{V}_j]}. \tag{A.1}$$

Here, the index $[\bar{V}]$ denotes the space in which the L -operator is represented as a 2×2 matrix. In addition, we can define the operators acting on \bar{V}_j by a decomposition of the 4×4 matrix:

$$\mathcal{L}_i(\lambda_j) = \left(\begin{array}{cc} \begin{array}{c} \uparrow \\ j \\ \hline j \\ \downarrow \\ i \end{array} & \begin{array}{c} \uparrow \\ j \\ \hline j \\ \downarrow \\ i \end{array} \\ \begin{array}{c} \uparrow \\ j \\ \hline j \\ \downarrow \\ i \end{array} & \begin{array}{c} \uparrow \\ j \\ \hline j \\ \downarrow \\ i \end{array} \end{array} \right)_{[V_i]} . \tag{A.2}$$

Here, the index $[V]$ denotes the space in which the 4×4 matrix is represented as a 2×2 matrix. Although the 4×4 matrix appearing in the above equation is exactly the same as $\mathcal{L}_i(\lambda_j)$, i.e. the matrix in equation (4), the order of basis has been changed and hence the graphical representations for the matrix elements of equation (A.2) are different from equation (A.1). The reason why the 4×4 matrices themselves are the same is related to the fact that the Boltzmann weights of the six-vertex model are invariant under the simultaneous reversal of all arrows when there is no external field. Two operators out of the four operators acting on \bar{V}_j are defined in equation (18), and graphs of them are given by

$$D_1(\lambda_j) = \begin{array}{c} \uparrow \\ j \\ \hline \downarrow \\ i \end{array} , \quad C_1(\lambda_j) = \begin{array}{c} \downarrow \\ j \\ \hline \uparrow \\ i \end{array} .$$

Note that the absence of arrows on the horizontal (dashed) line indicates that the above operators act on the space \bar{V}_j .

We are now ready to introduce a graphical representation of the Bethe state. As was seen in the main text, the Bethe state can be defined through the monodromy matrix $\mathcal{T}(\lambda_j)$ or $\mathcal{L}_i(\lambda_1, \dots, \lambda_n)$. These operators are drawn as

$$\mathcal{T}(\lambda_j) = \bigotimes_{i=1}^L \mathcal{L}_i(\lambda_j) = \prod_{i=1}^L \left(\begin{array}{cc} \begin{array}{c} \leftarrow \\ j \\ \hline \rightarrow \\ i \end{array} & \begin{array}{c} \leftarrow \\ j \\ \hline \rightarrow \\ i \end{array} \\ \begin{array}{c} \leftarrow \\ j \\ \hline \rightarrow \\ i \end{array} & \begin{array}{c} \leftarrow \\ j \\ \hline \rightarrow \\ i \end{array} \end{array} \right)_{[V_j]} = \begin{array}{c} j \\ \hline | \\ 1 \\ \hline | \\ 2 \\ \hline | \\ L \end{array} , \tag{A.3}$$

$$\mathcal{L}_i(\lambda_1, \dots, \lambda_n) = \bigotimes_{l=0}^{n-1} \mathcal{L}_i(\lambda_{n-l}) = \prod_{\substack{l=0 \\ (j=n-l)}}^{n-1} \left(\begin{array}{cc} \begin{array}{c} \uparrow \\ j \\ \hline \downarrow \\ i \end{array} & \begin{array}{c} \uparrow \\ j \\ \hline \downarrow \\ i \end{array} \\ \begin{array}{c} \uparrow \\ j \\ \hline \downarrow \\ i \end{array} & \begin{array}{c} \uparrow \\ j \\ \hline \downarrow \\ i \end{array} \end{array} \right)_{[V_i]} = \begin{array}{c} \mathbf{n} \\ \hline \mathbf{2} \\ \hline \mathbf{1} \\ \hline i \end{array} . \tag{A.4}$$

Here, each bond connecting two vertices represents summation over two possible arrows. The monodromy matrix is represented as a horizontal object while $\mathcal{L}_i(\lambda_1, \dots, \lambda_n)$ is a vertical one. The connection between nearest vertices can be easily interpreted as the multiplication of 2×2 matrices. A creation operator for the Bethe state ($\mathbf{B}(\lambda_j)$) corresponds to the (1,2)-component

The DWBC in \mathcal{H} corresponds to the case where $\forall \sigma_i = \downarrow$ as shown in figure 1(b). In particular, if $L = n$, it is shown that the partition function is expressed as

$$Z_n^{\text{DWBC}} = \langle \downarrow | \prod_{l=0}^{n-1} \mathbf{B}(\lambda_{n-l}) | \uparrow \rangle = \langle \leftarrow | C_n(\lambda_1, \dots, \lambda_n)^n | \Rightarrow \rangle \tag{A.6}$$

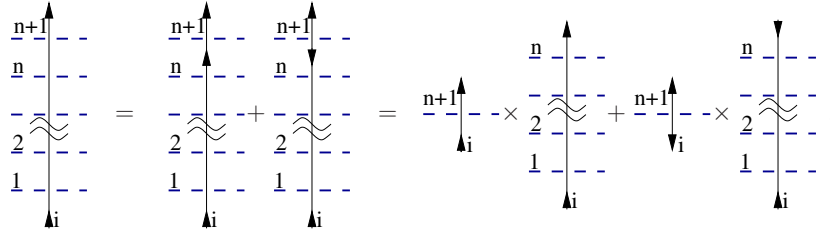
$$= \text{Tr}_{\mathcal{H}} [Q_n C_n(\lambda_1, \dots, \lambda_n)^n]. \tag{A.7}$$

A.2. Recursion relations in terms of graphs

In section 3, we have derived the recursion relations for the matrices D_n and C_n . Those recursions are easy to understand if we use graphical representations. The recursion relation for D_n (see equation (20)),

$$D_{n+1} = \begin{pmatrix} 1 & 0 \\ 0 & b(\lambda_{n+1}) \end{pmatrix}_{[\bar{V}_{n+1}]} \otimes D_n + \begin{pmatrix} 0 & 0 \\ c(\lambda_{n+1}) & 0 \end{pmatrix}_{[\bar{V}_{n+1}]} \otimes C_n,$$

can be expressed as



Here, for simplicity, we have abbreviated the indeterminants $\lambda_1, \dots, \lambda_n$ and λ_{n+1} . One can also express the recursion for C_n , equation (21), in a similar manner. The matrix D_n is a lower triangular matrix while C_n is an upper triangular one. This can be easily seen by representing them 2×2 matrices on \bar{V}_{n+1} whose elements are graphs:

$$D_{n+1} = \begin{pmatrix} \text{graph} & 0 \\ \text{graph} & \text{graph} \end{pmatrix}_{[\bar{V}_{n+1}]}, \quad C_{n+1} = \begin{pmatrix} \text{graph} & \text{graph} \\ 0 & \text{graph} \end{pmatrix}_{[\bar{V}_{n+1}]} \tag{A.8}$$

A.3. Mapping to five-vertex model

As we have seen in section 4, the triangular matrices D_n and C_n are transformed into \mathcal{D}_n and \mathcal{C}_n by the invertible matrix F_n . This similarity transformation corresponds to a mapping from the six-vertex model to a five-vertex model. This relation can be easily understood using graphs.

In the new basis, the matrix \mathcal{D}_n is diagonal and its recursion equation (46) can be represented as

$$\mathcal{D}_{n+1} = \begin{pmatrix} \begin{array}{c} \uparrow \\ \text{n+1} \\ \uparrow \\ \text{n} \\ \text{---} \\ \uparrow \\ \text{1} \\ \text{---} \\ \uparrow \\ \text{i} \end{array} & 0 \\ 0 & \begin{array}{c} \uparrow \\ \text{n+1} \\ \uparrow \\ \text{n} \\ \text{---} \\ \uparrow \\ \text{1} \\ \text{---} \\ \uparrow \\ \text{i} \end{array} \end{pmatrix}_{[\bar{V}_{n+1}]} \quad \text{with } \mathcal{D}_n = \begin{array}{c} \uparrow \\ \text{n} \\ \text{---} \\ \uparrow \\ \text{2} \\ \text{---} \\ \uparrow \\ \text{1} \\ \text{---} \\ \uparrow \\ \text{i} \end{array}, \quad (\text{A.9})$$

where the vertical lines are modified to indicate the transformed operators. Since the recursion (46) uniquely determines the graphical representation for \mathcal{D}_n , all the arrows on the vertical line are \uparrow . Note that a horizontal dashed line without arrows acts on the space (\bar{V}) diagonally. In the main text, the matrix \mathcal{C}_n is decomposed as $\mathcal{C}_n = \sum_{j=1}^n \mathcal{C}_n^{(j)}$. From equation (54), we see that $\mathcal{C}_n^{(j)}$ flips only the state in \bar{V}_j from $|\rightarrow\rangle$ to $|\leftarrow\rangle$. Therefore, $\mathcal{C}_n^{(j)}$ can be written as $\mathcal{C}_n^{(j)} = |\leftarrow\rangle_j \langle\leftarrow| \mathcal{C}_n^{(j)} |\rightarrow\rangle_j \langle\rightarrow|$. Since the action of $\mathcal{C}_n^{(j)}$ is diagonal in \mathcal{H} except for \bar{V}_j , the arrows on the vertical line are specified as follows:

$${}_j \langle\leftarrow| \mathcal{C}_n^{(j)} |\rightarrow\rangle_j = \begin{array}{c} \uparrow \\ \text{n} \\ \text{---} \\ \uparrow \\ \text{j} \\ \text{---} \\ \uparrow \\ \text{1} \\ \text{---} \\ \uparrow \\ \text{i} \end{array} = \begin{array}{c} \uparrow \\ \text{n} \\ \text{---} \\ \uparrow \\ \text{j} \\ \text{---} \\ \uparrow \\ \text{1} \\ \text{---} \\ \uparrow \\ \text{i} \end{array}. \quad (\text{A.10})$$

From the graphical representation, $\mathcal{C}_n^{(j)}$ can be regarded as a kink in \mathcal{H} . It is consistent with the picture that $A_{k_j,n}$ becomes a Jordan–Wigner fermion in \mathcal{H} when $\Delta = 0$ as we discussed in section 4. Again we note that the horizontal line without arrows acts diagonally on the space. In equations (A.9) and (A.10), the vertex $\begin{array}{c} \uparrow \\ \text{---} \\ \uparrow \\ \text{---} \\ \uparrow \end{array}$ does not appear, which means that the original six-vertex model becomes a five-vertex model after the similarity transformation. Comparing the graphs with equations (50) and (54), we find the weights for six vertices:

$$\begin{array}{c} \uparrow \\ \text{---} \\ \uparrow \\ \text{---} \\ \uparrow \end{array} = 1, \quad \begin{array}{c} \uparrow \\ \text{---} \\ \downarrow \\ \text{---} \\ \uparrow \end{array} = z_j, \quad \begin{array}{c} \uparrow \\ \text{---} \\ \uparrow \\ \text{---} \\ \downarrow \end{array} = z_j, \quad \begin{array}{c} \uparrow \\ \text{---} \\ \downarrow \\ \text{---} \\ \downarrow \end{array} = S_{k,j}(z_k, z_j),$$

$$\begin{array}{c} \uparrow \\ \text{---} \\ \downarrow \\ \text{---} \\ \downarrow \end{array} = f(z_j, \dots, z_n) c(\lambda_j), \quad \begin{array}{c} \uparrow \\ \text{---} \\ \uparrow \\ \text{---} \\ \uparrow \end{array} = 0,$$

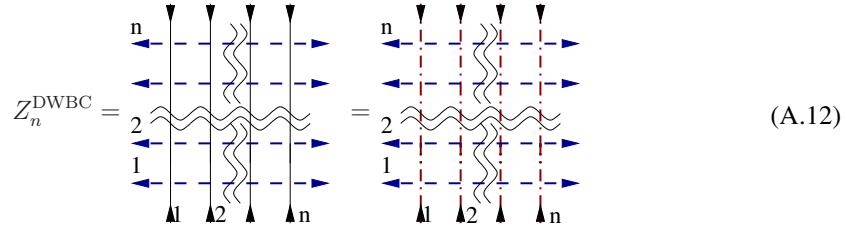
where j and k denote the horizontal line and the index for $\mathcal{C}_n^{(k)}$, respectively. Note that the weight of the fourth vertex is determined in a non-local way, i.e. if the intersection of the vertical line and k th horizontal line is $\begin{array}{c} \uparrow \\ \text{---} \\ \downarrow \\ \text{---} \\ \downarrow \end{array}$, then the weight for the intersection of the vertical

line and the j th horizontal line with $j > k$ is given by $S_{k,j}(z_k, z_j)$ when both the arrows on the horizontal edges are \leftarrow . The weight for the fifth vertex also depends non-locally on $j + 1, j + 2, \dots, n$. In exchange for this non-locality, the combinatorial complexity is greatly reduced in the five-vertex model. In the original matrices D_n and C_n , there are 2^{n-1} possible configurations of arrows (\uparrow and \downarrow) on the vertical line. After the similarity transformation, however, the configuration for \mathcal{D}_n is uniquely determined as seen in equation (A.9). The number of possible configurations of arrows for \mathcal{C}_n is n since each $\mathcal{C}_n^{(j)}$ is uniquely determined (see equation (A.10)).

Finally, we represent Z_n^{DWBC} in terms of the transformed graphs. Recalling that the DWBC is not altered after the similarity transformation, i.e. $Q_n = |\Rightarrow\rangle\langle\Leftarrow| = \mathcal{Q}_n$, and $F_n F_n^{-1} = 1$, equation (A.7) is written as

$$\begin{aligned} Z_n^{\text{DWBC}} &= \text{Tr}_{\mathcal{H}}[Q_n C_n(\lambda_1, \dots, \lambda_n)^n] \\ &= \text{Tr}_{\mathcal{H}}[F_n^{-1} Q_n F_n (F_n^{-1} C_n(\lambda_1, \dots, \lambda_n) F_n)^n] \\ &= \text{Tr}_{\mathcal{H}}[\mathcal{Q}_n \mathcal{C}_n(\lambda_1, \dots, \lambda_n)^n] \\ &= \langle\Leftarrow| C_n(\lambda_1, \dots, \lambda_n)^n |\Rightarrow\rangle. \end{aligned} \tag{A.11}$$

In short, what we have shown is graphically represented as



$$Z_n^{\text{DWBC}} = \text{Diagram 1} = \text{Diagram 2} \tag{A.12}$$

with $\begin{matrix} \uparrow \\ \downarrow \\ \leftarrow \\ \rightarrow \end{matrix} = 0$. Again it should be stressed here that a merit of the five-vertex model introduced is the reduction of possible configurations involved in the calculation of Z_n^{DWBC} .

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