Matrix product operator representations for the local conserved quantities of the Heisenberg chain

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Abstract

We present the explicit expressions for the matrix product operator (MPO) representation for the local conserved quantities of the Heisenberg chain. The bond dimension of the MPO grows linearly with the locality of the charges. The MPO has more simple form than the local charges themselves, and their Catalan tree patterns naturally emerge from the matrix products. The MPO representation of local conserved quantities is generalized to the integrable SU(N) invariant spin chain.

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1 Introduction

Quantum integrable models are special many-body systems that allow for exact solutions [1,2]. The Bethe Ansatz, with its origins tracing back to Hans Bethe's seminal work on the exact solution of the spin-1/2 Heisenberg spin chain [3], enables the exact calculation of energy spectrum and physical observables. Through various generalizations, the Bethe Ansatz has become the most renowned method for solving integrable models.

The defining feature of quantum integrable systems is the presence of an extensive number of local conserved quantities, denoted as $\{Q_k\}_{k=2,3,4,\ldots}$. They are local in the sense that they are a linear combination of operators that act on a finite range of local sites. In our notation here, Q_k is the site translation sum of the local operator that acts on the adjacent k sites. The existence of these local conserved quantities has been well established by the quantum inverse scattering method [4]: the local conserved quantities can be derived from the expansion of the transfer matrix $T(\lambda)$ with respect to the spectral parameter λ, given by $\log T(\lambda) \sim \sum_{k\geq 2} \lambda^{k-1} Q_k$, where Q_2 is usually the Hamiltonian itself. The commutativity of the transfer matrix, $[T(\lambda), T(\mu)] = 0$, ensures the mutual commutativity of the local conserved quantities, $[Q_k, Q_l] = 0$. Another way to obtain Q_k is the usage of the Boost operator, denoted by B, if it exists. Q_k can be calculated recursively by $[Q_k, B] = Q_{k+1}$.

Although the formal methodology for generating local conserved quantities Q_k, through the expansion of the transfer matrix and the usage of the Boost operator, has been known, determining their general expressions in practice still remains a formidable challenge. This difficulty stems not only from the exorbitant computational expense associated with higher-order charges but also from finding a general pattern within the vast data sets generated by these calculations. The general forms of local conserved quantities were firstly found for the spin-1/2 Heisenberg chain(XXX chain) independently by [5] and [6] and subsequently found for its SU(N) generalization [7]. For these models, the structure of the local charges has the Catalan tree pattern [8]: Q_k is constructed from the linear combination of the polynomial of spin operators with the coefficient of generalized Catalan number. More recently, the general forms of the local charges were found in the spin-1/2 XYZ chain [9], the Temperly-Lieb models [10], which include the spin-1/2 XXZ chain, and the one-dimensional Hubbard model [11]. Nonetheless, their expressions are still slightly complicated, even for these models where the general forms of the local charges are now known. A universal, more simple description of the general form of local conserved quantities is highly desirable.

Over the past two decades, there has been a growing trend to introduce tensor network techniques [12–14] to reformulate quantum integrability. The matrix product state(MPS) representation of the Bethe eigenstate of quantum integrable systems has been studied [15–22]. The symmetry of integrable systems was also investigated in terms of matrix product operator(MPO). In [23], the MPO commuting with the Hamiltonian of the Heisenberg chain was constructed, which was probed to be the product of two transfer matrices with different spectral parameters. More recently, the non-commutative symmetry of models with fragmented Hilbert space was obtained in the form of MPO, even for non-integrable cases [24]. The hidden symmetry of an integrable Lindblad system, which leads to multiple non-equilibrium steady states, was exactly given by MPO [25]. However, despite the transfer matrix, which is the source of Q_k, being defined by the MPO constructed from the Lax operator, there has yet to be an exploration of the MPO representation for local conserved quantities themselves.

In this work, we present the MPO representation of the local conserved quantities for the spin-1/2 Heisenberg spin chains. The local conserved quantity Q_k can be represented by the MPO whose bond dimension is $3k-1$. We found the Catalan tree pattern of the local conserved quantities [8] naturally emerges from the product of the MPO along with the identity of the generalized Catalan number. Unlike the local conserved quantities themselves, their MPO representation is only involved with the usual Catalan number, implying that the complexity of these expressions is folded within the product of the MPO. This MPO representation of the local conserved quantities can be immediately generalized for the integrable SU(N) invariant spin chains of fundamental representation. To our knowledge, this is the first study investigating the MPO representation for local conserved quantities of quantum integrable systems.

This paper consists of the following Sections: in Section 2, we review the local conserved quantities for the Heisenberg chain and the SU(N) integrable spin chain. In Section 3, we present the main result of the MPO for the Heisenberg chain. In section 4, we give the demonstration that the MPO introduced in section 2 actually reproduces the local conserved quantities of [5–7]. Section 5 contains the summary of our work and future outlooks.

2 Local conserved quantities of the Heisenberg chain

In this section, we review the result of the local conserved quantities of the Heisenberg chain [5, 6] and its SU(N) generalization [7].

2.1 spin-1/2 Heisenberg chain

The Hamiltonian of the spin-1/2 Heisenberg chain is given by:

$$H = \sum_{i=1}^{L} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1}, \tag{1}$$

where $\boldsymbol{\sigma}_i = (X_i, Y_i, Z_i)$ stands for the vector of the usual Pauli matrices acting non-trivially on i-th site, and L is the system size. We assume the periodic boundary condition: $\boldsymbol{\sigma}_{i+L} = \boldsymbol{\sigma}_i$. The Hamiltonian (1) is integrable [3] and has macroscopic number of local conserved quantities $\{Q_k\}_{k=2,3,4,\ldots}$. The key sign of its integrability is the mutual commutativity $[Q_k, Q_l] = 0$, and $Q_2 = H$ is the Hamiltonian itself.

To represent the expression of Q_k, we introduce some notations. A sequence of n sites $\mathcal{C} = \{i_1, i_2, \ldots, i_n\}$ with $i_1 < i_2 < \ldots < i_n$, will be called a *cluster* of order n. A cluster $\mathcal{C}$ can be further classified by *hole*, defined by $i_n - i_1 + 1 - n$, which is the number of the sites between i_1 and i_n that are not included in $\mathcal{C}$. For example, the cluster $\mathcal{C} = \{1, 3, 4, 7\}$ is the cluster of order 4, and whose hole is 3.

For a cluster $\mathcal{C} = \{i_1, i_2, \ldots, i_n\}$ of order n, we define the nested products of Pauli matrices $f_n(\mathcal{C})$ by:

$$f_n(\mathcal{C}) := \boldsymbol{\sigma}_{i_1} \cdot \left(\boldsymbol{\sigma}_{i_2} \times \left(\boldsymbol{\sigma}_{i_3} \times \left(\cdots \times \left(\boldsymbol{\sigma}_{i_{n-1}} \times \boldsymbol{\sigma}_{i_n}\right) \cdots\right)\right)\right). \tag{2}$$

Then we define the components of the local conserved quantities:

$$F_{n,m} = \sum_{\mathcal{C} \in \mathcal{C}^{(n,m)}} f_n(\mathcal{C}), \tag{3}$$

where $\mathcal{C}^{(n,m)}$ denotes the set of clusters of order n with m holes, satisfying $1 \leq i_1 \leq L$.

The general expression of Q_k is given by [5, 6]:

$$Q_k = F_{k,0} + \sum_{\substack{1 \leq n+m < \lfloor k/2 \rfloor \\ 0 \leq n, 1 \leq m}} C_{n+m-1,n} F_{k-2(n+m),m}, \tag{4}$$

where $C_{k,n} \equiv \binom{k+n}{n} - \binom{k+n}{n-1}$ is the generalized Catalan number.

2.2 SU(N) generalization

The structure of the local conserved quantities of the isotropic SU(N) version of the spin-1/2 Heisenberg chain in the fundamental representation is the same as that of the spin-1/2 Heisenberg chain [7]. The Hamiltonian of SU(N) invariant chain is given by [26]:

$$H=\sum_{i=1}^{L}\sum_{a=1}^{N^2-1} t_i^a t_{i+1}^a, \tag{5}$$

where $t_i^a, a=1,\ldots,N^2-1$ are the $su(N)$ generators in the fundamental representation. For the $N=2$ case, (5) reduces to the Hamiltonian of the spin-1/2 Heisenberg chain. We choose the normalization of the generators so that t_a's are the $su(N)$ Gell-Mann matrix, satisfying the following algebra:

$$\left[t^a,t^b\right]=2if^{abc}t^c, \tag{6}$$

$$t^a t^b+t^b t^a=\frac{4}{N}\delta_{ab}+2d^{abc}t^c, \tag{7}$$

where f^{abc} is the structure constant of $su(N)$, and d^{abc} is a completely symmetric tensor, which is non-trivial for $N>2$.

For the SU(N) case, $f_n(\mathcal{C})$ for a cluster $\mathcal{C}=\{i_1,i_2,\ldots,i_n\}$ is defined by:

$$f_n(\mathcal{C}):=\mathbf{t}_{i_1}\cdot\left(\mathbf{t}_{i_2}\times\left(\mathbf{t}_{i_3}\times\left(\cdots\times\left(\mathbf{t}_{i_{n-1}}\times\mathbf{t}_{i_n}\right)\cdots\right)\right)\right), \tag{8}$$

where $\mathbf{t}_i=\left(t_i^1,\ldots,t_i^{N^2-1}\right)$ stands for the vector of the $su(N)$ Gell-Mann matrices acting non-trivially on i-th site. The outer product of the vector $\mathbf{A},\mathbf{B}$ with N^2-1 components is defined by $(\mathbf{A}\times\mathbf{B})^c\equiv f^{abc}A^aB^b$.

The local conserved quantities of the SU(N) invariant chain are expressed in the same form as (4), with $f_n(\mathcal{C})$ defined in (8).

2.3 Doubling-product representation for SU(2) case

For the SU(2) case, the local conserved quantities can be represented using the *doubling-product* notation, which was initially introduced in the proof of the non-integrability of the spin-1/2 XYZ chain in a magnetic field [27], and subsequently employed to construct the local conserved quantities of the spin-1/2 XYZ chain without a magnetic field [9].

A doubling-product is a notation for the product of the Pauli matrices, defined by:

$$\overline{A_1A_2\cdots A_n}:=\sum_{i=1}^{L}(A_1)_i(A_1A_2)_{i+1}(A_2A_3)_{i+2}\cdots(A_{n-1}A_n)_{i+n-1}(A_n)_{i+n}, \tag{9}$$

where $A_i\in\{X,Y,Z\}$ and A_lA_{l+1} is the product of A_l and A_{l+1}. $(\cdot)_i$ denotes the operator acting on the i-th site. The hole is equal to the number of j that satisfies $A_j=A_{j+1}$. We define the support of an operator as the range of sites on which it acts. The support of the doubling-product of (9) is $n+1$.

With the doubling-product notation, the component of local conserved quantities for the spin-1/2 Heisenberg chain (3) can be rewritten by:

$$F_{n,m}=i^n\sum_{\overline{A}\in\mathcal{S}_{n+m,m}}\overline{A}, \tag{10}$$

where $\mathcal{S}_{l,m}$ is the set of all doubling-products with $(\text{support},\text{hole})=(l,m)$. The local conserved quantities constructed from (10) differ from those constructed from (3) by the factor i^k.

3 MPO representation for the local conserved quantities

In this section, we present the matrix product operator (MPO) representation for the local conserved quantities of the spin-1/2 Heisenberg chain and its SU(N) generalizations. Given an operator as a sum of finite-range interactions, it is possible to construct the MPO representation for such a local operator using entirely upper (or lower) triangular matrices [28]. We show the MPO representation for the local conserved quantities with the upper triangular matrix Γ_k^i.

3.1 MPO for the Hamiltonian

The MPO component for the Hamiltonian of the spin-1/2 Heisenberg chain (1) has been known as the matrix with bond dimension 5, the element of which are local operators acting on the physical Hilbert space [29]:

$$\Gamma_2^i := \begin{pmatrix} I & X_i & Y_i & Z_i & O \\ O & O & O & O & X_i \\ O & O & O & O & Y_i \\ O & O & O & O & Z_i \\ O & O & O & O & I \end{pmatrix} = \left(\begin{array}{c:c} I \;\; \boldsymbol{\sigma}_i & O \\ \hdashline O_{4,4} & \begin{matrix} \boldsymbol{\sigma}_i^\top \\ I \end{matrix} \end{array}\right), \tag{11}$$

where $\boldsymbol{\sigma}_i = (X_i, Y_i, Z_i)$ is treated as a row vector and $\boldsymbol{\sigma}_i^\top$ is its transpose and I is the identity operator. O denotes the zero-operator, and $O_{m,n}$ is an $m \times n$ matrix whose entries are all O.

The Hamiltonian is reproduced by the MPO constructed from Γ_2^i:

$$\Gamma_2^1 \Gamma_2^2 \cdots \Gamma_2^L = \left(\begin{array}{c:c} I \;\; \boldsymbol{\sigma}_L & H^{\mathrm{c}} \\ \hdashline O_{4,4} & \begin{matrix} \boldsymbol{\sigma}_1^\top \\ I \end{matrix} \end{array}\right), \tag{12}$$

where the $(1,5)$ component of the RHS, $H^{\mathrm{c}} = \sum_{i=1}^{L-1} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1}$, is the bulk term of the Hamiltonian, that misses the boundary term, $h^{\mathrm{B}} = \boldsymbol{\sigma}_L \cdot \boldsymbol{\sigma}_1 = \boldsymbol{\sigma}_L \boldsymbol{\sigma}_1^\top$. The Hamiltonian under the periodic boundary condition (1) is reproduced by the sum of the bulk term and boundary term: $H = H^{\mathrm{c}} + h^{\mathrm{B}}$. In the following, we generalize this result to the higher-order local conserved quantities Q_k.

3.2 Building blocks of MPO

We introduce a 3×3 matrix M_i, the element of which are local operators acting on the physical Hilbert space. M_i serves as the building block of the MPO for the local conserved quantities of the spin-1/2 Heisenberg chain. M_i is defined by:

$$M_i := \begin{pmatrix} O & -Z_i & Y_i \\ Z_i & O & -X_i \\ -Y_i & X_i & O \end{pmatrix}, \tag{13}$$

where the off-diagonal elements are the Pauli matrices acting on the i-th site. Note that M_i has the form of the $so(3)$ generator assigned with the Pauli matrices. The nested product of (2) is represented with these building blocks by:

$$\begin{aligned} f_n(i_1, i_2, \ldots, i_n) &= \boldsymbol{\sigma}_{i_1} \cdot \left(\boldsymbol{\sigma}_{i_2} \times \left(\boldsymbol{\sigma}_{i_3} \times \left(\cdots \times \left(\boldsymbol{\sigma}_{i_{n-1}} \times \boldsymbol{\sigma}_{i_n}\right) \cdots\right)\right)\right) \\ &= \boldsymbol{\sigma}_{i_1} M_{i_2} M_{i_3} \cdots M_{i_{n-1}} \boldsymbol{\sigma}_{i_n}^\top, \end{aligned} \tag{14}$$

where in the second line, $\boldsymbol{\sigma}_i = (X_i, Y_i, Z_i)$ is treated as a row vector, and $\boldsymbol{\sigma}_i^\top$ is its transpose.

For the more general SU(N) invariant chain, the building block for the MPO becomes the N^2-1 by N^2-1 matrix defined by:

$$\left(M_i^{(N)}\right)_{ac} := \sum_{b=1}^{N^2-1} f^{abc} t_i^b, \tag{15}$$

where the indices run $a, c = 1, 2, \ldots, N^2-1$. We note that $M_i^{(N=2)} = M_i$. The nested product (8) for the SU(N) case is represented by:

$$f_n(i_1, i_2, \ldots, i_n) = \mathbf{t}_{i_1} M_{i_2} M_{i_3} \cdots M_{i_{n-1}} \mathbf{t}_{i_n}^\top, \tag{16}$$

where $\mathbf{t}_i = (t_i^1, \ldots, t_i^{N^2-1})$ is treated as a row vector, and $\mathbf{t}_i^\top$ is its transpose.

We introduce another building block for the MPO, the 3 by 3 diagonal matrix e for the SU(2) case and the N^2-1 by N^2-1 diagonal matrix $e^{(N)}$ for the general SU(N) cases, the diagonal elements of which are the identity operators:

$$e := \begin{pmatrix} I & O & O \\ O & I & O \\ O & O & I \end{pmatrix}, \quad e^{(N)} := \overbrace{\begin{pmatrix} I & & & \\ & I & & \\ & & \ddots & \\ & & & I \end{pmatrix}}^{N^2-1}, \tag{17}$$

where the non-diagonal elements are all O. We note that $e^{(2)} = e$.

3.3 Explicit expressions of MPO

Next, we construct the MPO for the local conserved quantities from the building block defined above. While we focus on the spin-1/2 Heisenberg chain (SU(2) case) here, the scenario for the more general SU(N) case is similar as well: simply replace $M_i, e, \boldsymbol{\sigma}_i$ with $M_i^{(N)}, e^{(N)}, \mathbf{t}_i$, respectively.

The MPO component for k-th local conserved quantity Q_k for $k > 2$ is the upper triangle square matrix with bond dimension $3k-1$:

$$\Gamma_k^i := \left(\begin{array}{cc:c:c} I & \boldsymbol{\sigma}_L & & \\ \hdashline & & \mathcal{M}_k^i + \Theta_k & \\ \hdashline & & & \boldsymbol{\sigma}_1^\top \\ & & & I \end{array}\right), \tag{18}$$

where $\mathcal{M}_k^i$ and Θ_k are the square matrices of size $3(k-2)$, and the blank blocks are entirely filled with zero-operators. $\mathcal{M}_k^i$ is defined by:

$$\mathcal{M}_k^i := \overbrace{\begin{pmatrix} M_i & & & \\ & M_i & & \\ & & \ddots & \\ & & & M_i \end{pmatrix}}^{k-2}, \tag{19}$$

where the diagonal 3 by 3 block elements are all M_i and the non-diagonal elements are all $O_{3,3}$. Θ_k is defined by:

$$(\Theta_k)_{a,b} := \begin{cases} C_n e & (\exists n \in \mathbb{N} : b - a = 2n+1) \\ O_{3,3} & (\text{otherwise}) \end{cases}, \tag{20}$$

where a and b ($1 \leq a, b \leq k-2$) indicate the coordinate for the 3 by 3 block matrices in Θ_k, and $\mathbb{N} = \{0, 1, 2, \dots\}$ is the set of all natural numbers and $C_n = \binom{2n}{n} - \binom{2n}{n-1}$ is n-th Catalan number, which is the special case of the generalized Catalan number $C_{n,n} = C_n$. Θ_k can also be obtained from a simple recursion equation, which will be shown in the appendix C.

One can calculate the k-th local conserved quantity Q_k by taking the product of Γ_i^k over all the sites and doing some boundary treatment. To be specific, for $L \geq k$ one can write the explicit form of the matrix product as:

$$\Gamma_k^1 \Gamma_k^2 \cdots \Gamma_k^L = \left(\begin{array}{cc:c} I & \mathbf{u}_{k,L} & Q_k^{\mathrm{c}} \\ \hdashline \multicolumn{2}{c:}{\multirow{2}{*}{$O_{m,m}$}} & \mathbf{v}_{k,1}^\top \\ & & I \end{array}\right), \tag{21}$$

where $m \equiv 3k-2$ and $\mathbf{u}_{k,L} = (u_{k,L}^1, \dots, u_{k,L}^{3(k-1)})$ and $\mathbf{v}_{k,1} = (v_{k,1}^1, \dots, v_{k,1}^{3(k-1)})$ is the row vector of $3(k-1)$ dimension with its elements being the operator localized at the boundary. $u_{k,L}^j$ has non-trivial action on the sites from the $(L-k+1)$-th site to the L-th site, and $v_{k,1}^j$ has non-trivial action from the 1-st site to the k-th site. The local conserved quantity Q_k under the periodic boundary condition is given by:

$$Q_k = Q_k^{\mathrm{c}} + q_k^{\mathrm{B}}, \tag{22}$$

where Q_k^{c} is the bulk term of Q_k. and $q_k^{\mathrm{B}} \equiv \mathbf{u}_{k,L} \mathbf{v}_{k,1}^\top$ is the boundary term of Q_k. The boundary term q_k^{B} is constructed from the operators that jump over the boundary, i.e. the linear combination of the operators that act across the boundary from the L-th site to the 1-st site. In the periodic boundary case considered here, the structure of the boundary terms is the same as that of the bulk term.

When taking products of Γ_k^i, we can treat each building block as if it was a non-commutative scalar because the building blocks appearing in the MPO are conformable for multiplication. Therefore, in the following, we denote the zero-operator block matrix $O_{n,m}$ just simply as O.

We give the expressions up to Γ_8^i below:

$$\Gamma_2^i = \begin{pmatrix} I & \boldsymbol{\sigma}_i & O \\ & O & \boldsymbol{\sigma}_i^\top \\ & & I \end{pmatrix}, \qquad \Gamma_3^i = \begin{pmatrix} I & \boldsymbol{\sigma}_i & O & O \\ & O & M_i & O \\ & & O & \boldsymbol{\sigma}_i^\top \\ & & & I \end{pmatrix},$$

$$\Gamma_4^i = \begin{pmatrix} I & \boldsymbol{\sigma}_i & O & O & O \\ & O & M_i & C_0 e & O \\ & & O & M_i & O \\ & & & O & \boldsymbol{\sigma}_i^\top \\ & & & & I \end{pmatrix}, \qquad \Gamma_5^i = \begin{pmatrix} I & \boldsymbol{\sigma}_i & O & O & O & O \\ & O & M_i & C_0 e & O & O \\ & & O & M_i & C_0 e & O \\ & & & O & M_i & O \\ & & & & O & \boldsymbol{\sigma}_i^\top \\ & & & & & I \end{pmatrix},$$

$$
\Gamma_6^i = \begin{pmatrix} I & \boldsymbol{\sigma}_i & O & O & O & O & O \\ & O & M_i & C_0 e & O & C_1 e & O \\ & & O & M_i & C_0 e & O & O \\ & & & O & M_i & C_0 e & O \\ & & & & O & M_i & O \\ & & & & & O & \boldsymbol{\sigma}_i^\top \\ & & & & & & I \end{pmatrix}, \quad
\Gamma_7^i = \begin{pmatrix} I & \boldsymbol{\sigma}_i & O & O & O & O & O & O \\ & O & M_i & C_0 e & O & C_1 e & O & O \\ & & O & M_i & C_0 e & O & C_1 e & O \\ & & & O & M_i & C_0 e & O & O \\ & & & & O & M_i & C_0 e & O \\ & & & & & O & M_i & O \\ & & & & & & O & \boldsymbol{\sigma}_i^\top \\ & & & & & & & I \end{pmatrix},
$$

$$
\Gamma_8^i = \begin{pmatrix} I & \boldsymbol{\sigma}_i & O & O & O & O & O & O & O \\ & O & M_i & C_0 e & O & C_1 e & O & C_2 e & O \\ & & O & M_i & C_0 e & O & C_1 e & O & O \\ & & & O & M_i & C_0 e & O & C_1 e & O \\ & & & & O & M_i & C_0 e & O & O \\ & & & & & O & M_i & C_0 e & O \\ & & & & & & O & M_i & O \\ & & & & & & & O & \boldsymbol{\sigma}_i^\top \\ & & & & & & & & I \end{pmatrix},
$$

where the lower triangular elements are all zero operators and the O's in these expressions represent zero-operator block matrices, suitably shaped for the position of their respective blocks.

In the following section, we treat the building block elements of Γ_k^i such as M_i and $\boldsymbol{\sigma}$ and e and O as a symbol, and the indices indicate the positions of these building block elements. For example, $\left(\Gamma_k^i\right)_{1,2} = \boldsymbol{\sigma}_i$, and $\left(\Gamma_k^i\right)_{2,3} = M_i$ for $k \geq 3$, and $\left(\Gamma_8^i\right)_{2,8} = C_2 e$.

We note that the component of the MPO is only involved with the usual Catalan number, unlike the local conserved quantities themselves.

4 Proof of the MPO

In this section, we give the demonstration that the MPO introduced in the previous section actually reproduces the local conserved quantities of the spin-1/2 Heisenberg chain.

4.1 Catalan number identity

There is the useful identity of generalized Catalan numbers $C_{n+m,n}$ and usual Catalan numbers C_n for the proof of the MPO:

$$
C_{n+m,n} = \sum_{n_0+\cdots+n_m=n} C_{n_0} \cdots C_{n_m} = \sum_{\substack{\sum_{j=0}^m n_j = n \\ n_j \geq 0}} \prod_{j=0}^{m} C_{n_j}. \tag{23}
$$

One can prove this recurrence relation (23) by relating $C_{n+m,n}$ to the numbers of monotone lattice paths from $(x, y) = (0, 0)$ to $(n, n+m)$ that never crosses the line $y = x + m$.

Let $\Omega_{n+m,n}$ represent the set of monotone lattice paths that meet this condition. For each $P \in \Omega_{n+m,n}$, let $x_j(P)$ be the smallest x coordinate of the point on the path where the path reaches the line $y = x + j$ for the first time for $1 \leq j \leq m$. We define $x_0(P) \equiv 0$ and $x_{m+1}(P) \equiv n$. We define the subset of $\Omega_{n+m,n}$ as follows:

$$
\Omega_{n+m,n}^{n_0,\ldots,n_m} := \left\{ P \in \Omega_{n+m,n} \middle| \forall j \in \mathbb{N}, 0 \leq j \leq m : x_{j+1}(P) - x_j(P) = n_j \right\}. \tag{24}
$$

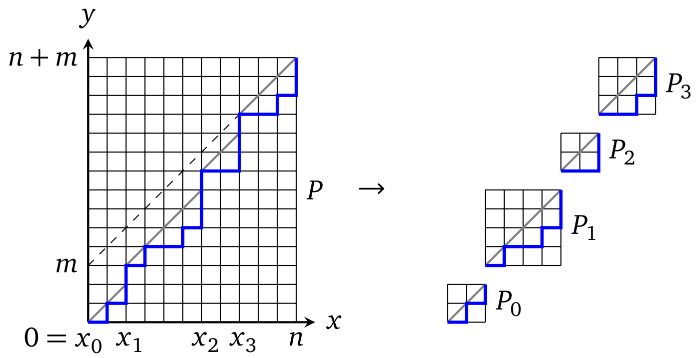

Figure 1: Graphical explanation of the proof of the recurrence relations of generalized Catalan numbers eq. (23). $n = 11$, $m = 3$ case is shown. $C_{n+m,n}$ equals the number of possible lattice paths from $(0,0)$ to $(n+m,n)$ that never crosses the line $y = x+m$. If one divides a path P into $(m+1)$ pieces $P_0, P_1, \dots, P_m$ by the point where P first reaches the line $y = x + j$, each P_j can be related one by one to a possible lattice path from $(0,0)$ to $(x_{j+1} - x_j, x_{j+1} - x_j)$ that never reaches the line $y = x$.

$\Omega_{n+m,n}$ can be represented by the direct sum of $\Omega_{n+m,n}^{n_0,\dots,n_m}$:

$$\Omega_{n+m,n} = \bigsqcup_{\substack{n_0+\cdots+n_m=n \\ n_j \geq 0}} \Omega_{n+m,n}^{n_0,\dots,n_m}. \tag{25}$$

Let us denote P_j as the part of a path P from (x_j, x_j) to (x_{j+1}, x_{j+1}), corresponding to the element of Ω_{n_j,n_j}, that is, to a monotone lattice path from $(0,0)$ to (n_j, n_j) that never crosses the line $y = x$ (see Fig. 1). Because the number of elements in Ω_{n_j,n_j} equals C_{n_j}, one gets

$$\#\left[\Omega_{n+m,n}^{n_0,\dots,n_m}\right] = \prod_{j=0}^{m} C_{n_j}, \tag{26}$$

where $\#[\bullet]$ denotes the number of elements in a (finite) set. Using (25), we have

$$C_{n+m,n} = \#\left[\Omega_{n+m,n}\right] = \sum_{\substack{\sum_{j=0}^m n_j = n \\ n_j \geq 0}} \#\left[\Omega_{n+m,n}^{n_0,\dots,n_m}\right] = \sum_{\substack{\sum_{j=0}^m n_j = n \\ n_j \geq 0}} \prod_{j=0}^{m} C_{n_j}. \tag{27}$$

Thus, we have proved (23).

4.2 Demonstration of equivalence of MPO and Q_k

In this subsection, we demonstrate the MPO actually reproduces the local conserved quantities, taking the case of Q_{12} as an example. The rigorous proof is given in appendix A for the bulk term and in appendix B for the boundary term.

Considering Eq. (4), we can see the operator $\boldsymbol{\sigma}_1 M_2 M_4 \boldsymbol{\sigma}_6^\top$ is included in $F_{12-2(n+m),m} = F_{4,2}$ for $(n,m) = (2,2)$, and therefore included in Q_{12}, particularly being included in the bulk term Q_{12}^{c} for $L > 6$. The coefficient of $\boldsymbol{\sigma}_1 M_2 M_4 \boldsymbol{\sigma}_6^\top$ in Q_{12} is $C_{n+m-1,n} = C_{3,2}$. In the following, we demonstrate this coefficient and operator are reproduced by the MPO made from Γ_{12}^i.

Q_{12}^{c} is calculated as follows:

$$Q_{12}^{\mathrm{c}} = \left(\Gamma_{12}^1 \Gamma_{12}^2 \cdots \Gamma_{12}^L\right)_{1,13} = \sum_{\substack{1=a_1\leq a_2 \leq \cdots \\ \cdots \leq a_L \leq a_{L+1}=13}} \gamma^1_{a_1,a_2} \gamma^2_{a_2,a_3} \cdots \gamma^L_{a_L,a_{L+1}}, \tag{28}$$

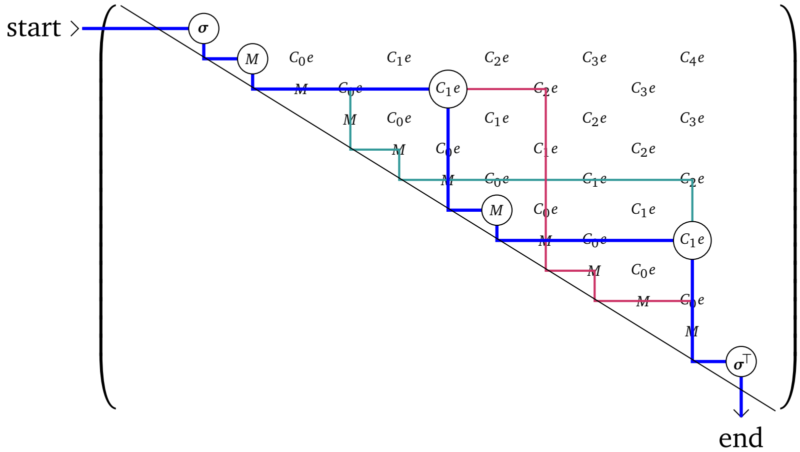

Figure 2: An intuitive method for calculating the coefficient of $\sigma_1 M_2 M_4 \sigma_6^\top$ in $Q_{12}^{\rm c}$, which is one of the components of $F_{4,2}$. The three paths depicted by the teal, the bold blue, and the purple line contribute to the coefficients. For example, the bold blue line represents the path that picks $\boldsymbol{\sigma}$, M, $C_1 e$, M, $C_1 e, \boldsymbol{\sigma}^\top$ in this order, and the contribution is ${C_1}^2 \sigma_1 M_2 M_4 \sigma_6^\top$. To obtain the coefficients of $F_{k-2(n+m),m}$ in more general $Q_k^{\rm c}$, we must take all the possible paths including $C_{n_1} e, \dots, C_{n_m} e$ in this order that satisfy $n_1 + \cdots + n_m = n$.

where the indices indicate the position of the building blocks, and $\gamma^p_{a_p,a_{p+1}}$ represents the (a_p, a_{p+1})-th block element of Γ^p_{12}, and the second equality holds from the fact that Γ^p_{12} is an upper triangular matrix. In the summation in (28), $\boldsymbol{\sigma}_1 M_2 M_4 \boldsymbol{\sigma}_6^\top$ is included in the restricted summation of (28) as follows:

$$\sum_{1=a_1 \le a_2 \le \cdots \le a_6 \le a_7 = 13} \gamma^1_{a_1,a_2} \gamma^2_{a_2,a_3} \gamma^3_{a_3,a_4} \gamma^4_{a_4,a_5} \gamma^5_{a_5,a_6} \gamma^6_{a_6,a_7}, \tag{29}$$

where the other variables in (28) is fixed as $a_p = 13$ for $p \ge 7$, and therefore $\gamma^p_{a_p,a_{p+1}} = I$ for $p \ge 7$.

Each term in (29) corresponds to the "path" from "start" to "end" traversing through the matrix in Figure 2, which has the same structure as Γ^i_{12}. A "path" is defined as follows: first, we pick up the element in the first row, where only $\boldsymbol{\sigma}$ is non-zero [1]. Thus we have to pick $\boldsymbol{\sigma}$ first, corresponding to $\gamma^1_{1,2} = \boldsymbol{\sigma}_1$. Every time we pick an element, we then vertically descend within the same column till we reach the diagonal line, after which we move horizontally to the right within the same row and pick up an element on the row. The element chosen in our p-th pick corresponds to $\gamma^p_{a_p,a_{p+1}}$ in equation (29). At the final (sixth) pick, we have to pick $\boldsymbol{\sigma}^\top$, corresponding to $\gamma^6_{a_6,a_7} = \boldsymbol{\sigma}_6^\top$, and finish the procedure for this path. By considering all possible paths, we can compute equation (29). For calculating the coefficient of $\boldsymbol{\sigma}_1 M_2 M_4 \boldsymbol{\sigma}_6^\top$ in $Q_{12}^{\rm c}$, we have to pick up the point of $\boldsymbol{\sigma}$, M, $C_{n_1} e$, M, $C_{n_2} e, \boldsymbol{\sigma}^\top$ in the matrix in Figure 2 in that order. There are three possible paths that generate $\boldsymbol{\sigma}_1 M_2 M_4 \boldsymbol{\sigma}_6^\top$ in $Q_{12}^{\rm c}$, which are depicted by the teal, the bold blue, and the purple line in Figure 2, corresponding to $(n_1, n_2) = (0, 2)$, $(1, 1)$, and $(2, 0)$ respectively. These paths all satisfy $n_1 + n_2 = 2$. All the contribution to the coefficient is

$$C_0 C_2 + C_1 C_1 + C_2 C_0 = C_{3,2}, \tag{30}$$

[1] Indeed, the $(1,1)$-component of Γ^i_k is I, presenting another non-zero component on the first row. Nevertheless, an initial pick of I does not yield $\boldsymbol{\sigma}_1 M_2 M_4 \boldsymbol{\sigma}_6^\top$ in $Q_{12}^{\rm c}$, thus these cases are not considered here.

where we used the Catalan number identity (23). Thus, we have demonstrated that the coefficients of $\boldsymbol{\sigma}_1 M_2 M_4 \boldsymbol{\sigma}_6^\top$ in the MPO is actually $C_{3,2}$, which is the same as the case of the local conserved quantity Q_{12}.

Let us consider a more general situation, leaving the rigorous proof to the appendix A. We calculate the coefficient of the operator $\boldsymbol{\sigma}_{i_1} M_{i_2} \cdots M_{i_{j-1}} \boldsymbol{\sigma}_{i_j}^\top$ in Q_k^{c} for $j = k - 2(n+m)$ and with m-holes, i.e. $i_j - i_1 + 1 - j = m$. The paths that generate $\boldsymbol{\sigma}_{i_1} M_{i_2} \cdots M_{i_{j-1}} \boldsymbol{\sigma}_{i_j}^\top$ have to pick up the elements of $C_{n_1} e, \dots, C_{n_m} e$, corresponding to the m-holes. Every time we pick up $C_n e$ on the paths, there is a horizontal move of $(2n+2)$ columns to the right, and every time we pick up M, there is a horizontal move of one column to the right. The number of the columns between $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}^\top$ of the matrix corresponding to Γ_k^i is $k-2$, thus we have the relation $\sum_{p=1}^m (2n_p + 2) + j - 2 = k - 2$. Solving this equation, we have $n_1 + \cdots + n_m = n$, and all the contributions to the coefficients become

$$\sum_{\substack{n_1+n_2+\cdots+n_m=n \\ n_j \geq 0}} C_{n_1} C_{n_2} \cdots C_{n_m} = C_{n+m-1,n}, \tag{31}$$

where we used the Catalan number identity (23), and we can see the coefficient of (4) is reproduced by the MPO.

5 Summary and Outlook

In this work, we show the matrix product operator(MPO) representation of the local conserved quantities for the spin-1/2 Heisenberg chain and its SU(N) generalization. In terms of our MPO representation, the local conserved quantities are more simply written: the pattern in the expression of the MPO is more straightforward than that of the local conserved quantities themselves. The Catalan tree pattern of the local conserved quantities naturally appears from the product of the MPOs. This means the complexity of the local conserved quantities is folded into the product of the MPO.

Investigating the MPO representation of local conserved quantities in other quantum integrable models is an intriguing future research direction. Especially the generalization of our result to the spin-1/2 XYZ chain [9], the anisotropic case of the Heisenberg chain is an interesting topic. And it would also be worthwhile to verify how the mutual commutativity of the local conserved quantities can be explained with our MPO representation.

Another potential direction is the investigation of the open boundary case. In the periodic boundary condition, the boundary term of the local conserved quantity is trivial: they have the same structure as the bulk term. However, the boundary term in the open boundary condition is non-trivial, and the expressions have yet to be elucidated even for the most famous spin-1/2 Heisenberg chain [30]. Using the MPO representation, we might infer the pattern of the boundary terms also in the open boundary case.

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A Rigorous proof for bulk term

In appendix A, we give the rigorous proof of the bulk part of (22).

In the following, the matrix indices indicate the position of the building blocks, i.e. treating the elements of Γ_k^i such as M_i and $\boldsymbol{\sigma}$ and e and O in Γ_k^i as a symbol.

Calculating the product of the MPO explicitly, we have:

$$Q_k^c = \left(\Gamma_k^1 \Gamma_k^2 \cdots \Gamma_k^L\right)_{1,k+1} = \sum_{1=a_1 \le a_2 \le \cdots \le a_{L-1} \le a_L = k+1} \overrightarrow{\prod_{1\le p\le L}} \gamma^p_{a_p,a_{p+1}}, \tag{32}$$

where the second equality holds from the fact that Γ_k^i is an upper triangular matrix and we denote the matrix element of Γ_k^i by $\left(\Gamma_k^i\right)_{a,b} \equiv \gamma^i_{a,b}$. Considering the first row and the last column of Γ_k^p is written by:

$$\gamma^p_{1,a} = \begin{cases} I & (a=1) \\ \boldsymbol{\sigma}_p & (a=2) \\ O & (\text{otherwise}) \end{cases}, \quad \gamma^p_{a,k+1} = \begin{cases} I & (a=k+1) \\ \boldsymbol{\sigma}_p^\top & (a=k) \\ O & (\text{otherwise}) \end{cases}, \tag{33}$$

and $\gamma^p_{a,a} = O$ for $2 \le a \le k$, the summation in (32) can be decomposed as:

$$\begin{aligned}
(32) &= \sum_{1\le i<j\le L} \sum_{2=a_{i+1}<a_{i+2}<\cdots<a_{j-1}<a_j=k} \boldsymbol{\sigma}_i \left(\overrightarrow{\prod_{i+1\le p\le j-1}} \gamma^p_{a_p,a_{p+1}} \right) \boldsymbol{\sigma}_j^\top \\
&= \sum_{1\le i<j\le L} \sum_{\substack{b_{i+1}+\cdots+b_{j-1}=k-2 \\ b_p>0}} \boldsymbol{\sigma}_i \left(\overrightarrow{\prod_{i+1\le p\le j-1}} \gamma^p_{b_p} \right) \boldsymbol{\sigma}_j^\top \\
&= \sum_{1\le i\le L-k+1} \boldsymbol{\sigma}_i \gamma_1^{i+1} \gamma_1^{i+2} \cdots \gamma_1^{i+k-2} \boldsymbol{\sigma}_{i+k-1}^\top \\
&\qquad + \sum_{1\le i<j\le L} \sum_{\substack{b_{i+1}+\cdots+b_{j-1}=k-2 \\ b_p>0,\ \exists p': b_{p'}>1}} \boldsymbol{\sigma}_i \left(\overrightarrow{\prod_{i+1\le p\le j-1}} \gamma^p_{b_p} \right) \boldsymbol{\sigma}_j^\top,
\end{aligned} \tag{34}$$

where the second summation on the first row is taken over $a_{i+2}, \ldots, a_{j-1}$ and the other a_p's are fixed by $a_1, \ldots, a_i = 1, a_{i+1} = 2, a_j = k, a_{j+1}, \ldots a_L = k+1$, and in the second equality we define $b_p \equiv a_{p+1} - a_p$ for $i < p < j$ and $\gamma^p_{b_p} \equiv \gamma^p_{a_p,a_{p+1}}$. $\gamma^p_{b_p}$ is well-defined because $\gamma^p_{a_p,a_{p+1}}$ depends only on the difference $a_{p+1} - a_p$. In the last equality, we decompose the summation to the case that all $b_p = 1$ for all p and the other cases that at least one b_p is greater than one. The explicit form of $\gamma^p_{b_p}$ is:

$$\gamma^p_{b_p} = \begin{cases} M_p & (b_p = 1) \\ C_{b_p/2-1} e & (b_p \text{ is even}) \\ O & (\text{otherwise}) \end{cases}. \tag{35}$$

The first term of (34) becomes

$$\begin{aligned}
\text{First term of (34)} &= \sum_{1\le i\le L-k+1} \boldsymbol{\sigma}_i \gamma_1^{i+1} \gamma_1^{i+2} \cdots \gamma_1^{i+k-2} \boldsymbol{\sigma}_{i+k-1}^\top \\
&= \sum_{1\le i\le L-k+1} \boldsymbol{\sigma}_i M_{i+1} M_{i+2} \cdots M_{i+k-2} \boldsymbol{\sigma}_{i+k-1}^\top \\
&= \sum_{\mathcal{C}\in\mathcal{C}^{k,0}_{\text{bulk}}} f_k(\mathcal{C}) = F^{\text{bulk}}_{k,0},
\end{aligned} \tag{36}$$

where $\mathcal{C}^{n+m,m}_{\text{bulk}}$ denotes the set of clusters $\mathcal{C} = \{i_1, \dots, i_n\}$ of order n with m holes, satisfying $1 \le i_1 < i_n \le L$, and we can see $F^{\text{bulk}}_{k,0}$ is the bulk term of $F_{k,0}$.

We denote the number of p's that satisfies $b_p > 1$ in the variable $\{b_{i+1}, \dots, b_{j-1}\}$ of the second summation of (34) by m. Then the second term of (34) becomes:

$$
\begin{aligned}
&\text{Second term of (34)}\\
&= \sum_{1\le i<j\le L} \sum_{\substack{b_{i+1}+\cdots+b_{j-1}=k-2\\ b_p>0,\ \exists p': b_{p'}>1}} \boldsymbol{\sigma}_i \left(\overrightarrow{\prod_{i<p<j}} \gamma^p_{b_p} \right) \boldsymbol{\sigma}_j^\top \\
&= \sum_{1\le i<j\le L} \sum_{m=1}^{w-2} \sum_{i<i_1<\cdots<i_{w-2-m}<j} \sum_{\substack{b_{i'_1}+\cdots+b_{i'_m}=k-2-(w-2-m)\\ b_{i'_{m'}}>1}} \boldsymbol{\sigma}_i \left(\prod_{r=1}^{m} \gamma^{i'_r}_{b_{i'_r}} \right) \left(\overrightarrow{\prod_{1\le r\le w-2-m}} \gamma^{i_r}_{b_{i_r}} \right) \boldsymbol{\sigma}_j^\top \\
&= \sum_{1\le i<j\le L} \sum_{m=1}^{w-2} \Big(\sum_{\substack{b_{i'_1}+\cdots+b_{i'_m}=k-w+m\\ b_{i'_{m'}}>1}} \prod_{r=1}^{m} \gamma_{b_{i'_r}} \Big) \sum_{i<i_1<\cdots<i_{w-2-m}<j} \boldsymbol{\sigma}_i M_{i_1} M_{i_2} \cdots M_{i_{w-2-m}} \boldsymbol{\sigma}_j^\top \\
&= \sum_{w=2}^{k} \sum_{m=1}^{w-2} \left(\sum_{\substack{c_1+\cdots+c_m=k-w+m\\ c_r>1}} \prod_{r=1}^{m} \gamma_{c_r} \right) \sum_{i=1}^{L-w-1} \sum_{i<i_1<\cdots<i_{w-2-m}<i+w-1} \boldsymbol{\sigma}_i M_{i_1} M_{i_2} \cdots M_{i_{w-2-m}} \boldsymbol{\sigma}_{i+w-1}^\top \\
&= \sum_{w=2}^{k} \sum_{m=1}^{w-2} \left(\sum_{\substack{c_1+\cdots+c_m=k-w+m\\ c_r>1}} \prod_{r=1}^{m} \gamma_{c_r} \right) \sum_{\mathcal{C}\in\mathcal{C}^{w-m,m}_{\text{bulk}}} f_{w-m}(\mathcal{C}) \\
&= \sum_{w=2}^{k} \sum_{m=1}^{w-2} \left(\sum_{\substack{2(d_1+\cdots+d_m)=k-w+m\\ d_r>1}} \prod_{r=1}^{m} \gamma_{2d_r} \right) \sum_{\mathcal{C}\in\mathcal{C}^{w-m,m}_{\text{bulk}}} f_{w-m}(\mathcal{C}) \\
&= \sum_{n=0}^{\lfloor k/2\rfloor} \sum_{m=1}^{\lfloor k/2\rfloor-n} \left(\sum_{\substack{d_1+\cdots+d_m=n+m\\ d_r\ge1}} \prod_{r=1}^{m} C_{d_r-1} \right) \sum_{\mathcal{C}\in\mathcal{C}^{k-2(n+m),m}_{\text{bulk}}} f_{k-2(n+m)}(\mathcal{C}) \\
&= \sum_{\substack{0<n+m<\lfloor k/2\rfloor\\ n\ge0,m\ge1}} \left(\sum_{\substack{d_1+\cdots+d_m=n\\ d_r\ge0}} \prod_{r=1}^{m} C_{d_r} \right) F^{\text{bulk}}_{k-2(n+m),m} \\
&= \sum_{\substack{0<n+m<\lfloor k/2\rfloor\\ n\ge0,m\ge1}} C_{n+m-1,n} F^{\text{bulk}}_{k-2(n+m),m},
\end{aligned}
\tag{37}
$$

where we denote $w \equiv j-i+1$ and we decompose the summation $\sum_{b_{i+1}+\cdots+b_{j-1}=k-2,b_p>0}$, after fixing m, to the summation over $\{i_1, \dots, i_{w-1-m}\}$ where i_r satisfies $b_{i_r} = 1$ and the summation over $\{b_{i'_1}, \dots, b_{i'_{w_m}}\}$ where i'_r satisfies $b_{i'_r} > 1$. Note that $\{i'_1, \dots, i'_m\} \bigcup \{i_1, \dots, i_{w-2-m}\} = \{i+1, \dots, j-1\}$. In the third equality, we used the following relation:

$$
\boldsymbol{\sigma}_i \left(\prod_{r=1}^{m} \gamma^{i'_r}_{b_{i'_r}} \right) \left(\overrightarrow{\prod_{1\le r\le w-2-m}} \gamma^{i_r}_{b_{i_r}} \right) \boldsymbol{\sigma}_j^\top = \left(\prod_{r=1}^{m} \gamma_{b_{i'_r}} \right) \boldsymbol{\sigma}_i M_{i_1} M_{i_2} \cdots M_{i_{w-2-m}} \boldsymbol{\sigma}_{i+w-1}^\top,
$$

where γ_{b_p} is defined by $\gamma_{b_p} \equiv C_{b_p/2-1}(0)$ for b_p is even(odd), and the factor on the left hand side $\left(\prod_{r=1}^{m} \gamma_{b_{i'_r}}^{i'_r}\right)$ can be treat as a c-number, and factored out on the right hand side because $\gamma_{b_{i'_r}}^{i'_r}$ is O or is proportional to e for $b_{i'_r>1}$, and e behave as identity operator: $eM_p = M_p e = M_p$ and $\boldsymbol{\sigma}_i e = \boldsymbol{\sigma}_i$. In the fourth equality, we replace the variable by $c_r = b_{i'_r}$. If c_r is odd for some r, we can see $\gamma_{c_r} = 0$. Thus the non-zero contribution comes from the case that all c_r is even, and in the sixth equality, we rewrite c_r by $c_r = 2d_r$. For $k - w + m$ being an even integer, w and m have to satisfy the relation $w = k - 2n - m$ with $\exists n \in \mathbb{N}$. In the seventh equality, we change the variable by $d_r - 1 \to d_r$, and in the ninth equality, we used the Catalan number identity (23). $F^{\text{bulk}}_{k-2(n+m),m}$ is the bulk term of $F_{k-2(n+m),m}$.

Therefore, with (36) and (37), we have proved Q^{c}_k becomes:

$$Q^{\text{c}}_k = F^{\text{bulk}}_{k,0} + \sum_{\substack{0<n+m<\lfloor k/2 \rfloor \\ n\geq 0, m\geq 1}} C_{n+m-1,n} F^{\text{bulk}}_{k-2(n+m),m}, \tag{38}$$

and we can see this is actually the bulk term of Q_k.

B Boundary treatment

We prove the boundary terms of the local conserved quantities Q_k are given by $q^{\text{B}}_k \equiv \mathbf{u}_{k,L} \mathbf{v}^{\top}_{k,1}$.

We write the k-th matrix product operator from i-th site to j-th site ($j - i \geq k$) by:

$$\Gamma^i_k \Gamma^{i+1}_k \cdots \Gamma^j_k = \left(\begin{array}{cc:c} I & \mathbf{u}_{k,j} & Q^{c}_{k,[i:j]} \\ \hdashline & & \mathbf{v}^{\top}_{k,i} \\ & O & I \end{array}\right), \tag{39}$$

where $\mathbf{u}_{k,j}$ and $\mathbf{v}_{k,i}$ are the row vectors of dimension $3(k-1)$, whose elements are independent of i and j, respectively, and are constructed from the local operators that act on at most k adjacent sites between the $(j-k+1)$-th site and j-th site and between the i-th site and $(i+k-1)$-th site, respectively. $\mathbf{u}_{k,j}(\mathbf{v}_{k,i})$ is independent of $i(j)$. $Q^{c}_{k,[i:j]}$ is constructed from the local operators that act on at most k adjacent sites between the i-th site and the j-th site.

We can decompose the products in the MPO for the k-th local conserved quantities as:

$$\begin{aligned} \Gamma^1_k \Gamma^2_k \cdots \Gamma^{L+N}_k &= \Gamma^1_k \Gamma^2_k \cdots \Gamma^L_k \times \Gamma^{L+1}_k \Gamma^{L+2}_k \cdots \Gamma^{L+N}_k \\ &= \left(\begin{array}{cc:c} I & \mathbf{u}_{k,L} & Q^{\text{c}}_{k,[1:L]} \\ \hdashline & & \mathbf{v}^{\top}_{k,1} \\ & O & I \end{array}\right) \left(\begin{array}{cc:c} I & \mathbf{u}_{k,L+N} & Q^{\text{c}}_{k,[L+1:L+N]} \\ \hdashline & & \mathbf{v}^{\top}_{k,L+1} \\ & O & I \end{array}\right), \end{aligned} \tag{40}$$

and we have

$$Q^{\text{c}}_{k,[1:L+N]} = Q^{\text{c}}_{k,[1:L]} + Q^{\text{c}}_{k,[L+1:L+N]} + \mathbf{u}_{k,L} \mathbf{v}^{\top}_{k,L+1}. \tag{41}$$

Now, we can see the term in $Q^{\text{c}}_{k,[1:L+N]}$ whcih acts across the L-site and the $L+1$-site is $\mathbf{u}_{k,L} \mathbf{v}^{\top}_{k,L+1}$. Consequently, the boundary term q^{B}_k in system size L for periodic boundary condition is given by $\mathbf{u}_{k,L} \mathbf{v}^{\top}_{k,1}$.

C Recursion equation for Θ_k

Θ_k can be obtained from the following recursion equation:

$$\Theta_{k+1} = \begin{pmatrix} O_{3(k-2),3} & (\Theta_k)^2 \\ O_{3,3} & O_{3,3(k-2)} \end{pmatrix} + E_{k+1}, \tag{42}$$

where E_k is a square matrix of order $3(k-2)$, defined by:

$$(E_k)_{a,b} := \begin{cases} e & (b-a=1) \\ O_{3,3} & (\text{otherwise}) \end{cases}, \tag{43}$$

where a and b $(1 \leq a, b \leq k-2)$ indicate the coordinate for the 3 by 3 block matrices in E_k.

In the following, we prove (42). We first calculate the $(\Theta_k)^2$ is the RHS of (42) for $k \geq 3$. Substituting the expression of Θ_k of (20), we have

$$\left[(\Theta_k)^2\right]_{a,b} = \sum_{n=1}^{k-2} (\Theta_k)_{a,n} (\Theta_k)_{n,b} = \begin{cases} \sum_{n=a+1}^{b-1} (\Theta_k)_{a,n} (\Theta_k)_{n,b} & (b-a>1) \\ O_{3,3} & (\text{otherwise}) \end{cases}, \tag{44}$$

where a and b $(1 \leq a, b \leq k-2)$ indicate the coordinate for the 3 by 3 block matrices in Θ_k. For the case of $b-a \equiv 1 \pmod 2$, there do not exist any integers n that satisfy both $n-a \equiv 1 \pmod 2$ and $b-n \equiv 1 \pmod 2$ simultaneously. Thus one gets:

$$\begin{aligned} \left[(\Theta_k)^2\right]_{a,b} &= \begin{cases} \sum_{l=0}^{m} (\Theta_k)_{a,a+2l+1} (\Theta_k)_{a+2l+1,b} & (\exists m \in \mathbb{N} : b-a=2m+2) \\ O_{3,3} & (\text{otherwise}) \end{cases} \\ &= \begin{cases} \sum_{l=0}^{m} C_l C_{m-l} e & (\exists m \in \mathbb{N} : b-a=2m+2) \\ O_{3,3} & (\text{otherwise}) \end{cases} \\ &= \begin{cases} C_{m+1} e & (\exists m \in \mathbb{N} : b-a=2m+2) \\ O_{3,3} & (\text{otherwise}) \end{cases}. \end{aligned} \tag{45}$$

From (45), we can see the RHS of (42) is equal to the Θ_{k+1} of (20). Then we have proved eq. (20) satisfies the recursion equation (42).

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