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Modular matrices as topological order parameter by a gauge-symmetry-preserved tensor renormalization approach

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Topological order has been proposed to go beyond Landau symmetry breaking theory for more than 20 years. But it is still a challenging problem to generally detect it in a generic many-body state. In this paper, we will introduce a systematic numerical method based on tensor network to calculate modular matrices in two-dimensional systems, which can fully identify topological order with gapped edge. Moreover, it is shown numerically that modular matrices, including S and T matrices, are robust characterization to describe phase transitions between topologically ordered states and trivial states, which can work as topological order parameters. This method only requires local information of one ground state in the form of a tensor network, and directly provides the universal data (S and T matrices), without any nonuniversal contributions. Furthermore, it is generalizable to higher dimensions. Unlike calculating topological entanglement entropy by extrapolating, in which numerical complexity is exponentially high, this method extracts a much more complete set of topological data (modular matrices) with much lower numerical cost.

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I. INTRODUCTION

The most basic question in condensed matter is to classify all different states and phases. Landau symmetry breaking theory is the first successful step to classify all phases [1–3]. However, the experimental discovery of integer quantum Hall effect [4] and fractional quantum Hall effect [5] led condensed matter physics to a new era that goes beyond Landau theory, in which the most fundamental concept is topological order [6–8]. Topological order is characterized by a new kind of “topological order parameter”: (a) the topology-dependent ground state degeneracy [6,7] and (b) the non-Abelian geometric phases S and T of the degenerate ground states [8–10], where both of them are robust against any local perturbations that can break any symmetries [7]. This is just like superfluid order being characterized by zero viscosity and quantized vorticity that are robust against any local perturbations that preserve the U(1) symmetry.

Recently, it was found that, microscopically, topological order is related to long-range entanglement [11,12]. In fact, we can regard topological order as a pattern of long-range entanglement [13] defined through local unitary (LU) transformations [14–16]. Chiral spin liquids [17,18], integral/fractional quantum Hall states [4,5,19], Z2 spin liquids [20–22], and non-Abelian fractional quantum Hall states [23–26] are examples of topologically ordered phases. Topological order and long-range entanglement are truly new phenomena, which require new mathematical language to describe them. It appears that tensor category theory [13,14,27–29] and simple current algebra [23,30–32] (or pattern of zeros [33–41]) may be part of the new mathematical language. For (2+1)-dimensional topological orders (with gapped or gapless edge) that have only Abelian statistics, we find that we can use integer K matrices to classify them [42–47].

As proposed in Refs. [8–10], the non-Abelian geometric phases of the degenerate ground states, i.e., the modular matrices generated by Dehn twist and 90° rotation, are effective topological order parameters that can be used to characterize topological order. References [48–51] make the first step to calculate numerically modular matrices using various methods. Actually, the calculation of tensor network states (TNS) and topological order has already been investigated by several papers [52,53]. References [54–57] concluded that gauge-symmetry structure of TNS will give rise to information of topological order. Unlike calculating topological entanglement entropy by extrapolating, in which numerical complexity is exponentially high computational cost, extracting topological data through the gauge-symmetry structure of TNS has acceptable lower cost.

In this paper, we will give a systematic approach to calculate modular matrices, using the wave-function overlap method proposed in Refs. [58,59]. Our approach is based on TNS and gauge-symmetry preserved tensor renormalization group. Gauge-symmetry preserved RG differs from original tensor RG (TRG) in the sense that every step of TRG will keep the gauge-symmetry structure invariant and manifest. The paper is organized as follows: (I) we will first review the basic ideas of modular matrices and TRG; (II) we will explain the systematic method to calculate modular matrices based on TRG; (III) we will show the numerical results of modular matrices for the toric code and double-semion topological orders [14,20–22,27], which clearly identifies the correct topological order and characterizes phase transitions.

II. REVIEW OF MODULAR MATRICES

Modular matrices, or T and S matrices, are generated respectively by Dehn twist (twist) and 90° rotation on torus. The operation of twist can be defined by cutting up a torus along one axis, twisting the edge by 360°, and gluing the two edges back.

The elements of the universal T and S matrices are given by [58,59]

\[
\langle \psi_i | \hat{T} | \psi_j \rangle = e^{-A/|\xi|^2 + i \alpha^2/|\xi|^2} T_{ij},
\]

\[
\langle \psi_i | \hat{S} | \psi_j \rangle = e^{-A/|\xi|^2 + i \alpha^2/|\xi|^2} S_{ij},
\]

(1)
where $|\psi_i\rangle$ form a set of orthonormal basis for degenerate ground space; and $\hat{T}$ and $\hat{S}$ are the operators that generate the twist and the rotation on torus. $\Lambda$ is the area of the system and $\xi$ is of the order of correlation length which is not universal.

The $T$ and $S$ matrices encode all the information of quasiparticles statistics and their fusion [60,61]. It was also conjectured that the $T$ and $S$ matrices form a complete and one-to-one characterization of topological orders with gapped quasiparticles statistics and their fusion [60,61]. It was also lost. So that in order to reproduce all topological data, the here is that during TRG, the gauge symmetry information is happening. Another reason that normal TRG is not suitable is that some wrong fixed point tensors. Gauge-symmetry-preserved modular matrices could be calculated. However, it is difficult to determine singular values will be kept. Figure 1(d) is coarse graining. The four tensors on the small square will form a new double tensor $T'$. Note that $T_1$ and $T_4$ are outcoming tensors that are cut in another direction.

### III. Review of Tensor Renormalization Group

To be specific, TRG here means double tensor renormalization group [62]. Essentially, a translation invariant TNS can be written by definition as

$$|\psi\rangle = \sum_{m_1,m_2,...} tTr(T^{m_1}:T^{m_2}... T^{m_N})|m_1\rangle|m_2\rangle...|m_N\rangle,$$

where $T^{m_j}$'s are local tensors with physical index $m_j$ defined either on links or vertices; and $m_1$'s are local Hilbert space basis. (Sometimes $m_1$ is not written out explicitly if there is no ambiguity.) $tTr$ means contracting over all internal indices of local tensors pair by pair. The norm of the state is given by

$$\langle \psi | \psi \rangle = tTr(TT...T),$$

where $T$ is the local double tensor, which is formed by $T^*$ and $T$ tracing out a physical degree of freedom:

$$T = \sum_{m_i} T^{m_i*}T^{m_i}.$$  

The essence of double TRG is to find fewer double tensors $T'$, which keeps the norm approximately invariant. That is,

$$\langle \psi | \psi \rangle \simeq tTr(T'T'...T').$$

This approximation can be done nonuniquely. And SVD TRG approach shall be utilized in this paper for its convenience and low cost. The procedure of SVD RG approach is graphically explained in Figs. 1(c) and 1(d). Step (c) is to perform local SVD to decompose double tensor $T$ into $T_1$ and $T_2$. In order to prevent the bond dimension of internal indices from growing exponentially, only a finite number $D_{cut}$ of singular values are kept. Step (d) is to do coarse graining; the tensors on new smaller squares will form a new double tensor $T'$. After steps (c) and (d), half of the tensors will be contracted. For a translation invariant TNS, after enough steps of SVD TRG, the double tensor will flow to the fixed point double tensor, $T_{fp}$, which plays an essential role in the next section. Topological data can be extracted from $T_{fp}$.

Note that the above TRG approach suffers from the necessary symmetry condition [54]. If the gauge symmetry is not preserved in each step of TRG, the approach will be ruined by errors. And, more importantly, the RG flow will arrive at some wrong fixed point tensors. Gauge-symmetry-preserved TRG is introduced in the next section in order to prevent this happening. Another reason that normal TRG is not suitable here is that during TRG, the gauge symmetry information is lost. So that in order to reproduce all topological data, the gauge symmetry should be preserved.

### IV. Modular Matrices by Gauge-Symmetry-Preserved Tensor Renormalization Group

In Refs. [55–57], the gauge structure of TNS is analyzed. It was concluded that by inserting gauge transformation tensors to TNS, a set of bases for the degenerate ground space will be obtained. More specifically, the ground states could be labeled as $|\psi(g,h)\rangle$, where $g,h$ are gauge tensors acting on internal indices in two directions. Different ground states can be transformed to each other by applying gauge tensors on internal indices of a TNS. Therefore, it is natural to think that since all ground states could be obtained, by calculating all overlaps $\langle \psi_i|\hat{T}^x|\psi_j\rangle$ and $\langle \psi_i|\hat{S}^x|\psi_j\rangle$, the whole modular matrices could be calculated. However, it is difficult to compute the overlap directly and keep track of the nonuniversal contributions. See Eq. (1).

TRG will help reduce the difficulty, since one fixed point double tensor essentially represents the whole lattice. Calculating on one double tensor is much easier and size effects do not appear. However, normal TRG is not suitable here since gauge symmetry needs to be preserved through every tensor RG step in order to insert gauge transformation tensors. To be more specific, let us consider the case of $Z_2$ topological order, which also makes it clear in the next section. As already known in Refs. [55–57], tensor network representation for $Z_2$ topological state has $Z_2$ gauge symmetry. The double tensor $T_{\alpha\alpha'\beta\beta' \gamma \gamma'}$ will have a $Z_2 \times Z_2$ gauge symmetry, where $\alpha, \alpha', \beta, \beta', \gamma, \gamma' ,\delta, \delta'$, and $\alpha, \beta, \gamma, \delta$ are indices coming from $T$, while $\alpha, \beta, \gamma', \delta'$ are indices coming from $T^*$. So the double tensor with $Z_2$ gauge symmetry.
FIG. 2. (Color online) Modular matrices from the fixed point double tensor $T_{\text{fp}}$. Eight legs of $T_{\text{fp}}$ will all be traced over because of torus geometry. (a) By inserting gauge tensors into a double tensor; (b) after several steps of GSPTRG (cf. Fig. 3), double tensor ~$g\delta$~ needs to be block diagonalized; (c) represents twist.

where repeated indices imply summation and tensor $A, B \in \{I, \sigma_z\}$ generates the $Z_2 \times Z_2$ gauge symmetry on both layers of double tensor, which only act on internal indices. If a double tensor has such a gauge symmetry, its elements are nonzero only when $\alpha + \beta + \gamma + \delta$ and $\alpha^* + \beta^* + \gamma^* + \delta^*$ are both even [63].

In order to keep $Z_2 \times Z_2$ gauge symmetry manifest at each RG step, we develop gauge-symmetry-preserved tensor RG (GSPTRG). Essentially, it differs from normal TRG only when we do SVD. The double tensor needs to be block diagonalized by even or odd of its indices, and then SVD is performed in each block and recombinates the tensors coming out of SVD into one tensor, just as the way to block diagonalize it. In each block, the tensor elements have the same even or odd indices, which therefore is key to preserving $Z_2$ symmetry manifest. The procedures are also explained in Fig. 1.

After several steps of GSPTRG (cf. Fig. 3), double tensor will flow to the gauge-symmetry-preserved fixed point tensor. Equivalent to calculating the overlap by brute force, we can obtain the modular matrices by the following three steps: (1) inserting gauge symmetry tensors into a double tensor; (2) performing rotation and twist on one layer of a fixed point double tensor; (3) tracing out rest indices.

The procedures are also explained in Fig. 2. Actually the inner product of ground states $\langle \psi(g',h')|\psi(g,h)\rangle$ (each ground state is obtained by inserting gauge tensors on boundary) in topological phase will be diagonal with each element modulo 1. The elements of $T$ and $S$ matrices are just reshuffling of elements $\langle \psi(g',h')|\psi(g,h)\rangle$. More explicitly for the $Z_2$ topological state

$$\langle \psi(g',h')|\hat{T}|\psi(g,h)\rangle = \langle \psi(g',h')|\psi(g,h)\rangle,$$

$$\langle \psi(g',h')|\hat{S}|\psi(g,h)\rangle = \langle \psi(g',h')|\psi(h,g^{-1})\rangle.$$

V. MODULAR MATRICES FOR $Z_2$ TOPOLOGICAL ORDER

Toric code model [64] is the simplest model that realizes the $Z_2$ topological order [20,21]. Local physical states are defined on every link with spin up and down. In the notation of string-net states, spin up represents a string while spin down represents no string. Essentially, the $Z_2$ topological state can be written as equal superposition of all closed string loops:

$$|\psi_{\text{TC}}\rangle = \sum_{X} |X\rangle,$$

where $X$ represents a closed loop, and the normalization factor is implicit in the above equation.

When putting the $Z_2$ topologically ordered state on a torus, the ground state degeneracy is four and the quasiparticles are usually labeled by $\{1,e,m,em\}$. $T$ and $S$ matrices in the twist basis [59] are given in Fig. 3(c) for $g > 0.802$.

It is easy to represent $|\psi_{\text{TC}}\rangle$ in terms of a tensor network. For the sake of convenience, we replace local physical states $|1\rangle$ and $|0\rangle$ with $|1\rangle$ and $|0\rangle$, respectively. And combine each $|1\rangle$ and $|0\rangle$ to its nearest sites. So local physical states now are on vertices without extending Hilbert space. Here we choose the parametrization of $Z_2$ topological state utilized in Ref. [13]

$$T_{\alpha\beta\gamma\delta}^{a\beta\gamma\delta} = g^{a+\beta+\gamma+\delta}$$

Rest elements of $T$ are zeros.

When $g = 1$, it is $|\psi_{\text{TC}}\rangle$ while when $g = 0$, it is a trivial state $|0000\ldots0\rangle$. Of course, when $g$ is driven from zero to 1, it must undergo a phase transition.

We calculate $T$ and $S$ matrices along $g$. We find that when $0 \leq g < 0.802$, all components of $T$ and $S$ matrices are 1, because the gauge twisting does not produce other ground states in the trivial phase. When $0.802 \leq g < 1$, it belongs to $Z_2$ topological phase, since the $T$ and $S$ matrices for each $g \in (0.802,1]$ agree with that of $Z_2$ topological phase [59] [see Fig. 3(c)].

VI. MODULAR MATRICES FOR DOUBLE-SEMION MODEL

The double-semion model [14,27,65] is another topologically ordered state with two semions of statistics $\pm \pi/2$. In the notation of string-net states, the double-semion ground state can also be written as superposition of all closed string loops:

$$|\psi_{\text{DS}}\rangle = \sum_{X} (-1)^{N_{\text{loops}}}|X\rangle,$$

where $X$ represents a closed loop, and $N_{\text{loops}}$ the number of loops. The above double-semion state can be described by a TNS with the following tensors $T$ and $G^n$ at $g = 1$. 

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FIG. 3. (Color online) Trace of modular matrices $S$ and $T$ as functions of $g$ display a very sharp phase transition at critical point $g_c$ as increasing RG steps, for both $Z_2$ and double-semion topological order. The $Z_2$ topological order transition point coincides exactly with the results in Ref. [13] by another characterization.

\[
S = \begin{pmatrix}
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1
\end{pmatrix}
\]
\[
T = \begin{pmatrix}
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1
\end{pmatrix}
\]

(11)

Note that if we view $\alpha = \beta'$, $\beta = \gamma$, $\gamma' = \delta$, and $\delta' = \alpha'$ as indices that label “virtual qubits” in the squares, then the strings can be viewed as domain wall between the “0” and “1” states of the qubits. Also if we choose $t_{ab'y'y'} = 1$, the above tensors will describe the $Z_2$ topologically ordered state discussed previously.

The $Z_2$ gauge symmetry is generated by $\sigma^x \otimes \sigma^x$ acting on each internal indices $(\alpha\alpha')$ followed by a transformation generated by $u^i_{\alpha\alpha'}$, $i = t,l,b,r$ acting on the links of the four orientations. Here $u^i_{\alpha\alpha'}$ must satisfy

\[
f_{ab'y'y'} = u^b_{y'y'} u^b_{a\delta} u^r_{\alpha a} u^r_{y'y'},
\]

(12)

where

\[
f_{1000} = f_{0111} = f_{0010} = f_{1101} = -1, \quad \text{other} \quad f_{ab'y'y'} = 1.
\]

(13)

Furthermore, $u^i_{\alpha\alpha'}$ must also satisfy

\[
g^m_{\alpha\alpha'} = (u^r_{\alpha\alpha'})^g m_{\alpha\alpha'} (u^l_{\alpha\alpha'})^*,
\]

\[
g^m_{\alpha\alpha'} = (u^l_{\alpha\alpha'})^g m_{\alpha\alpha'} (u^r_{\alpha\alpha'})^*.
\]

(14)
We find that
\[ u' = u^b = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad u'' = u'^b = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}. \] (15)

See [57] for a general analysis of twisted gauge structures.

After the GSPTRG calculation, we find a phase transition at \( g_\epsilon = 0.802 \). The \( S \) and \( T \) matrices for the nontrivial phase with \( g \in (0,0.802,1) \) are given by Fig. 3(f), which agrees with the modular matrices for the double semion model in string basis [66]. For the trivial phase near \( g = 0 \), the modular matrices become \( T_{\alpha\beta} = S_{\alpha\beta} = \delta_\alpha \delta_\beta \).

VII. CONCLUSION

We have developed a systematic approach, gauge-symmetry-preserved tensor renormalization, to calculate modular matrices from a generic many-body wave function described by a tensor network. The modular matrices can be viewed as a very robust topological order parameter that only changes at a phase transition. The tensor network approach gives rise to \( S \) and \( T \) matrices in a particular basis which is different from the standard quasiparticle basis [8–10,48–51,60,61]. The trivial phase will result in modular matrices \( S = 1 \) and \( T = 1 \) (since there is no degeneracy on a torus), and the topological phase will give rise to nontrivial modular matrices, which contain topological information, such as quasiparticle information, like statistic angle, fusion rule, quantum dimension, etc.

In particular, a general algorithm can be developed: the tensor network ansatz can be imposed with gauge symmetry \( G \) (or MPO symmetry, see below) in the beginning, and the corresponding update algorithm, which is used to find ground states, also preserves such a gauge symmetry. Therefore, if the topological phase indeed has such a gauge theory description, the ansatz obviously is better than the normal tensor network ansatz. In Appendix B we perform such a benchmark computation using the \( Z_2 \) phase of the Kitaev honeycomb model [67]. There we prepare an arbitrary tensor with \( Z_2 \) symmetry, find the ground state (locally) numerically by gauge-symmetry-preserved update, and from there compute the modular matrices. A similar tensor network computation of the Kitaev honeycomb model is developed in Ref. [68] where \( Z_2 \) gauge structure is also imposed but expressed by Grassmann tensor network. The energy and nearest neighbor correlation are computed there.

After the completion of this paper, the notion of (twisted) \( G \) injectivity of [56,57] was generalized to the matrix product operator (MPO) case in [69] and it was shown that any string-net model is included with this generalization. The method developed in this paper can thus similarly be generalized to any MPO symmetry and does not need any group structure (and thus is not restricted to twisted discrete gauge theories).

The universal wave function overlap [59] (1) applies to any dimension and has already been investigated in exactly solvable models in 3+1 dimensions (3+1D) [70–72]. The method outlined in this paper can similarly be generalized to higher dimensions to extract universal topological information from generic gapped ground states.

Finally, we note that although the universal wave function overlap [59] works for any topological order, the machinery developed in this paper in 2+1D only works for nonchiral topological order (gapped boundaries) as formulated here. This is only because the tensor network techniques used are best understood for nonchiral topological order, but a generalization for chiral topological order would be both interesting and important.

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APPENDIX A: ROBUSTNESS OF MODULAR MATRICES UNDER \( Z_2 \) PERTURBATIONS

In the phase diagram Fig. 3, it is already demonstrated that \( T \) and \( S \) matrices are very robust characterizations of topological order, which only depend on the phase. In order to address this issue more explicitly, we will perturb \( Z_2 \) topological state at \( g = 1 \), while the perturbation also respects internal \( Z_2 \) gauge symmetry, i.e., the perturbation tensor \( T' \) is written as
\[ T'_{\alpha'\beta'\gamma'\delta'} = \epsilon r \text{ when } \alpha + \beta + \gamma + \delta \text{ even}, \] (A1)
where \( r \) is a uniform distributed random number ranging from \([-1,1]\) depending on \( \alpha', \beta', \gamma', \delta', \alpha, \beta, \gamma, \delta \) and \( \epsilon \) represents perturbation strength starting from zero. The initial tensor before RG will be \( T + T' \).

As already shown in Ref. [13], \( Z_2 \) topological phase is robust under tensor perturbations which respect the \( Z_2 \) gauge symmetry, while fragile under perturbations breaking the \( Z_2 \) gauge symmetry. Here we start from perturbed tensor \( T + T' \) and calculate modular matrices for different \( \epsilon 's \), which will demonstrate the robustness of this topological characterization (Fig. 5).

Numerically it demonstrates that when \( 0 \leq \epsilon \leq 0.35 \), \( T \) and \( S \) matrices are always Eq. (10). However, when \( \epsilon > 0.35 \), the perturbations will possibly break the topological phase (and possibly not). In this case, \( T \) and \( S \) matrices
have three possibilities as shown in the figure. Anyway, this calculation clearly demonstrates modular matrices are robust characterizations of topological phase.

**APPENDIX B: GAUGE-SYMMETRY-PRESERVED UPDATE**

For a typical tensor network algorithm, there are two main steps: updating local tensors to lower the energy to ground state energy and contracting all local tensors to compute physical quantities and norms. Here we only point out some details in the gauge-symmetry-preserved update algorithm, since the details in contraction have already been reviewed in the main text to some extent.

We choose a Kitaev honeycomb model as a benchmark. Kitaev honeycomb model is defined on the honeycomb lattice with spins on each site and different interactions along the three different links connected to each site,

\[
H = -J_x \sum_{\text{links}} \sigma_x^i \sigma_x^j - J_y \sum_{\text{links}} \sigma_y^i \sigma_y^j - J_z \sum_{\text{links}} \sigma_z^i \sigma_z^j.
\]

\(J_x\) are coupling constants along the \(x\) link. For simplicity we will assume they are all positive. For the coupling constants \(J_y\), \(J_z\) satisfying \(J_x + J_y < J_z\) (or other permutations), a gapped phase will be acquired that indeed is a toric code phase by perturbation analysis [67].

We impose \(Z_2\) gauge symmetry on our tensor network ansatz. That is, local tensors should satisfy

\[
T^{\text{even}}_{ijk} = 0, \quad \text{if} \quad i + j + k \text{ odd}. \quad (B1)
\]

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