

Tensor product representation of a topological ordered phase: Necessary symmetry conditionsXie Chen,¹ Bei Zeng,^{2,3,4} Zheng-Cheng Gu,⁵ Isaac L. Chuang,¹ and Xiao-Gang Wen¹¹*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*²*Institute for Quantum Computing, University of Waterloo, Waterloo, Ontario, Canada*³*Department of Combinatorics and Optimization, University of Waterloo, Waterloo, Ontario, Canada*⁴*Department of Mathematics and Statistics, University of Guelph, Guelph, Ontario, Canada*⁵*Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA*

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The tensor product representation of quantum states leads to a promising variational approach to study quantum phase and quantum phase transitions, especially topological ordered phases which are impossible to handle with conventional methods due to their long-range entanglement. However, an important issue arises when we use tensor product states (TPSs) as variational states to find the ground state of a Hamiltonian: can arbitrary variations in the tensors that represent ground state of a Hamiltonian be induced by local perturbations to the Hamiltonian? Starting from a tensor product state which is the exact ground state of a Hamiltonian with \mathbb{Z}_2 topological order, we show that, surprisingly, not all variations in the tensors correspond to the variation in the ground state caused by local perturbations of the Hamiltonian. Even in the absence of any symmetry requirement of the perturbed Hamiltonian, one necessary condition for the variations in the tensors to be physical is that they respect certain \mathbb{Z}_2 symmetry. We support this claim by calculating explicitly the change in topological entanglement entropy with different variations in the tensors. This finding will provide important guidance to numerical variational study of topological phase and phase transitions. It is also a crucial step in using TPS to study universal properties of a quantum phase and its topological order.

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I. INTRODUCTION

The central task in the study of quantum many-body systems is the classification of possible phases of matter and the understanding of phase transitions between them. Of particular interest is the study of systems at zero temperature, where a whole distinct realm of quantum effects emerge, and that is what we will focus on in this paper. Landau's general principle for understanding continuous phase transitions based on symmetry breaking and local order parameter¹ does not apply to all phases and phase transitions. Topological order,^{2,3} in particular, is not related to any symmetry properties and topological phase transitions may happen between systems with the same⁴⁻⁷ or incompatible⁸ symmetries. It has been the subject of intensive research and will be the central topic of this paper. Aside from the lack of a qualitative understanding, what makes the problem harder is the fact that for quantum systems whose components strongly interact with each other, direct numerical approach is limited due to strong entanglement among the particles. Generically, the space required for description of a quantum system grows exponentially with system size, hence limiting direct numerical simulations to systems usually too small for any practical purpose.

Recently, insights into quantum many-body systems from both condensed-matter physics and quantum information science have led to the discovery of the tensor product representation of quantum states (also called the projected entangled pair states),⁹⁻¹³ which provides a promising variational approach to study zero-temperature quantum phase and phase transitions. Representing quantum many-body states with a network of tensors, tensor product states (TPSs) are proven to be efficient for the study of one-

dimensional quantum systems.¹⁴⁻¹⁶ The higher-dimensional generalization of this approach may not be as efficient, yet study has shown that it reproduces many known results and may be used to study systems not solvable in any conventional way.¹⁷⁻¹⁹ The strength of the approach lies in the fact TPS can describe long-range entanglement that are present in a large class of topologically ordered states.^{20,21} So the variational approach based on TPS can include both topologically ordered states and symmetry-breaking states and can produce a phase diagram that contains both types of states. In contrast, the conventional mean-field/variational approaches are based on states with no long-range entanglement, which exclude the topologically ordered states from the very beginning. We also note that the entanglement of a simple TPS satisfies an area law,²² which coincides with the scaling of entanglement in the ground state of most known noncritical systems.²³

In the variational approach based on TPS, we try to find a TPS which minimizes the average energy of a local Hamiltonian. As we change the Hamiltonian by adding perturbation, the tensors in the TPS are also changed in order to minimize the average energy for the new Hamiltonian. While local physical perturbations can always be reflected by variations in the tensors, the other direction of this problem remains unclear: can an arbitrary variation in the tensor be induced by a local perturbation of the Hamiltonian?

This is a very important question if we want to discuss phase based on states. Because phase is defined as a region in Hamiltonian space, where any two points H_1, H_2 within the region can be connected by a smooth path without encounter singularities (i.e., phase transitions). So the question about tensor and phase becomes, which set of states in Hilbert space correspond to such a region in Hamiltonian space and which set of tensors in the tensor space represent these states.

Starting from one point in the phase region, we would like to know what kind of variations in the tensors corresponds to local perturbations to the Hamiltonian.

We can discuss this important question in more concrete setting. Assume a TPS Ψ_T minimizing the average energy of a Hamiltonian H has a property. We would like to ask if the property is a universal property of a phase, or just a special property of H . If the property is a universal property of a phase, then the ground state $\Psi_{T+\Delta\Psi_T}$ for the perturbed Hamiltonian $H+\Delta H$ still has the same property. If the property is a special property of H , the ground state for the perturbed Hamiltonian will lose this property. It is the collection of universal properties that defines a phase. So a study of universal properties is a study of phases. If all the variations in the tensors can be induced by local perturbations of the Hamiltonian, then we can study the stability of a property against local perturbation ΔH of the Hamiltonian by studying the stability of a property against variations in the tensors. This will give us a powerful tool to study phases using TPS.

Unfortunately, it turns out that not all variations in the tensors can be induced by local perturbations of the Hamiltonian, as we show in this paper. For a generic TPS, which satisfies a condition called injectivity,²⁴ tensor variations indeed correspond to Hamiltonian perturbations. However, this is not true in the general case, as we show in this paper with a special system with topological order. So it is not easy to study universal properties and phases using TPS. In order to use TPS to study phases and phases transitions, we need to find the subset of variations in tensors that are physical, i.e., corresponding to local perturbations of the Hamiltonian.

For clarity, we will always refer to small changes in the Hamiltonian as ‘‘perturbation’’ and to those in the tensors as ‘‘variation.’’ Without any efficient method to solve for exact TPS representation of ground states of quantum many-body systems, finding the subset of the variations in the tensors that can be induced by local perturbation of Hamiltonian is in general very difficult.

We want to, in particular, study this problem for topologically ordered phases. As TPS can give a simple description of a large class of topological ordered states, we expect that it might provide a powerful tool for studying topological phases in general. As we know, topologically ordered phases are proven to be stable against any local perturbations of the Hamiltonian.^{3,25,26} That is, the topological properties, such as ground state degeneracy³ and quasiparticle statistics,^{27,28} are robust under any local perturbation to the Hamiltonian. So in the TPS approach to topologically ordered phase, it is natural to ask: are those topological properties robust against any variation in tensors, that is, for any tensor which represents a topologically ordered state, is the topological order robust against arbitrary variation in the tensors? Surprisingly, we find that this is not true.

We focus on the \mathbb{Z}_2 topological order represented by an ideal TPS in this paper and study how the topological order of the state changes as we vary certain parameters in the representing tensors. We characterize topological order by calculating the topological entanglement entropy S_{tp} (Refs. 29 and 30) for the state and observe that topological order (i.e., the topological entanglement entropy S_{tp}) is stable only against variations in the tensors that preserve certain \mathbb{Z}_2 sym-

metry of the tensors. Since the topological order is robust against any local perturbations of Hamiltonian, this result shows that not all variations in the tensors correspond to local perturbations of Hamiltonian. For this \mathbb{Z}_2 model, we show that in the generic case \mathbb{Z}_2 symmetry is a necessary condition for the variations in tensors to correspond to physical perturbations of the Hamiltonian. This claim is further supported by checking stability of the topological Renyi entropy of TPS with \mathbb{Z}_2 symmetry-preserving variations and \mathbb{Z}_2 symmetry-breaking variations in the tensors, respectively.

While calculating S_{tp} for a general state is exponentially hard,³¹ we find efficient ways to do so for two sets of TPS near the ideal TPS with \mathbb{Z}_2 topological order. For a general TPS, we calculate the topological Renyi entropy by mapping it to the contraction of a two-dimensional (2D) tensor network, which is accomplished by using the tensor entanglement renormalization algorithm.³² Hence we are able to calculate topological entropy for regions much larger than was possible previously and determine the topological order of the state more accurately.

Our result on the stability of topological order will help us in the TPS-based variational approach to \mathbb{Z}_2 topological phase: we should only consider the variations in the tensors within the subspace of tensors with \mathbb{Z}_2 symmetry. The \mathbb{Z}_2 symmetry condition and possibly other conditions will help us to understand the physical variations in tensors in TPS. This is crucial in using TPS to study quantum phases and quantum phase transitions. It may even lead to a classification of topological order.

This paper is organized as follows. We start by introducing an ‘‘ideal’’ lattice spin model with \mathbb{Z}_2 topological order and show how the presence of topological order in the ground-state wave function can be understood nicely with a physical mechanism called ‘‘string-net condensation.’’ Such a physical picture naturally gives rise to a simple tensor product representation of the wave function, to which we then add two kinds of local variations, ‘‘string tension’’ and ‘‘end of strings.’’ By calculating topological entanglement entropy numerically for the first case and analytically for the second case, we show how topological order is stable against \mathbb{Z}_2 preserving variations (string tension) but breaks down immediately when \mathbb{Z}_2 symmetry is broken (by end of strings). We then randomly picked 200 tensors in the neighborhood of the ideal \mathbb{Z}_2 TPS and calculate the topological Renyi entropy of the corresponding states. Tensors with and without \mathbb{Z}_2 symmetry demonstrate totally different behavior as system size scales up. We discuss in the last section the implications of our findings in variational studies of topological phase and phase transitions. The details of the calculations are given in the appendices.

II. MODELS AND RESULT

A. Spin model with \mathbb{Z}_2 topological order

We start from an exactly solvable model which has \mathbb{Z}_2 topological order.^{33–35} In this section, we give the system Hamiltonian, find the ground-state wave function and explain its structure and how that leads to a nontrivial topological order which can be detected with topological entangle-

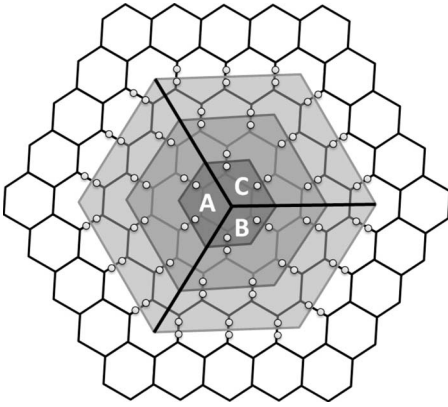


FIG. 1. Hexagonal lattice where each link is occupied by two qubits. The three gray regions are configurations used for calculating topological entanglement entropy. Qubits on the boundaries are drawn explicitly while others are omitted for clarity. Notice that regions are always separated by breaking links in half. For Z_2 model with string tension, numerical calculation for S_{tp} is done for the three gray regions while for Z_2 model with end of strings, analytical calculation is possible for any region.

ment entropy. With these insights about the state we then present a simple tensor product representation of this wave function.

The model is defined on a two-dimensional hexagonal lattice where each link is occupied by a qubit (spin-1/2). The Hamiltonian is a sum of commuting projection operators

$$H_{Z_2}^0 = - \sum_p \prod_{i \in p} X_i - \sum_v \prod_{j \in v} Z_j, \quad (1)$$

X and Z are qubit Pauli operators defined as $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. p stands for each hexagon plaquette in the lattice and $\prod_{i \in p} X_i$ is the tensor product of six X operators around the plaquette. v stands for each vertex and $\prod_{j \in v} Z_j$ is the tensor product of three Z operators connected to the vertex. The ground-state wave function has a nice interpretation using the ‘‘string-net’’ picture where state $|0\rangle$ corresponds to no string on a link and state $|1\rangle$ corresponds to the presence of a string. The vertex term $\prod_{j \in v} Z_j$ enforces that there are even number of strings connected to each vertex and hence the strings form closed loop while the plaquette term $\prod_{i \in p} X_i$ gives dynamics to the closed loops. The ground-state wave function is an equal weight superposition of all closed loop configurations on the lattice,

$$|\Phi_{Z_2}\rangle = \sum_{cl} |\phi_{cl}\rangle. \quad (2)$$

The normalization factor is omitted. If we refer to each closed loop configuration as a string-net, the appearance of Z_2 topological order in this system has then a natural interpretation as being due to the condensation of string-nets. We will refer to this model as the ideal Z_2 model.

For simplicity of discussion, we split each qubit on a link into two qubits as illustrated in Fig. 1. The string-net condensed Z_2 wave function on the original lattice can be naturally extended to a state on the new lattice by replacing a 0 link with 00 and a 1 link with 11. This new state is still an

equal weight superposition of all string-nets and hence maintains the Z_2 topological order. The new system Hamiltonian can be obtained from the old one by adding a $-ZZ$ term to each link and expand the plaquette term into a product of X operators on all twelve qubits around the plaquette,

$$H_{Z_2} = - \sum_p \prod_{i \in p} X_i - \sum_v \prod_{j \in v} Z_j - \sum_l Z_{l_1} Z_{l_2}, \quad (3)$$

where l denotes all the links and l_1, l_2 are the two qubits on the link. It is easy to see that the new Hamiltonian indeed has the new string-net condensed state as its ground state. The topological order of the system can be detected from the ground-state wave function by calculating the topological entanglement entropy of the state. The mapping to the new lattice allows this calculation to be carried out exactly in a few steps, as illustrated below.

According to the definition of topological entanglement entropy in Ref. 29 (or equivalently defined in Ref. 30), we take out a simply connected region from the whole lattice and divide it into three parts A, B , and C as shown in Fig. 1. By calculating the entanglement entropy for regions A, B, C, AB, AC, BC, ABC and combining them according to

$$S_{tp} = S_A + S_B + S_C - S_{AB} - S_{BC} - S_{AC} + S_{ABC}, \quad (4)$$

we arrive at the topological entanglement entropy S_{tp} of the state, where the entanglement entropy for region A , for example, is denoted as S_A . The above definition needs to be applied to regions much larger than the correlation length of the state. For the state in consideration, the correlation length is zero and the calculation gives the right result for whatever regions we take. We divide the regions by cutting through the pair of qubits on boundary links as illustrated in Fig. 1. For a region with n outgoing links on the boundary, there are 2^{n-1} orthogonal boundary configurations due to the closed-loop constraint of the wave function. Tracing out each boundary configuration contributes equally and independently to the entropy of the region and hence $S = n - 1$, which includes one term proportional to the length of the boundary n and one constant term -1 . The combination in the definition of S_{tp} makes sure that the boundary terms of different regions cancel out with each other, so topological entanglement entropy for the state is then $S_{tp} = -1$.

This globally entangled state has yet a surprisingly simple local representation using the tensor product language. A tensor product state of two-dimensional lattice model is represented by associating with each lattice site m a set of s tensors $T_{[k]}^m(\alpha\beta\gamma\cdots)$, $k=1, 2, \dots, s$, where s is the dimension of local Hilbert space at site m . k is called the physical index of the tensor. $\alpha\beta\gamma$, the inner indices of the tensors, connect to each other and form a graph. The wave function (unnormalized) is then given by

$$|\psi\rangle = \sum_{k_1, k_2, \dots, k_m, \dots} \mathcal{C}(T_{[k_1]}^1 T_{[k_2]}^2 \cdots T_{[k_m]}^m \cdots) |k_1 k_2 \cdots k_m \cdots\rangle, \quad (5)$$

where \mathcal{C} denotes tensor contraction of the inner indices according to the connection graph. We omit the inner indices here. (We will in most cases ignore normalization of wave

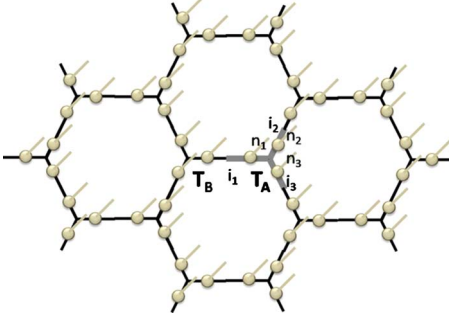


FIG. 2. (Color online) Tensor product representation of \mathbb{Z}_2 ground state. One tensor is assigned to every three qubits connected to the same vertex. Tensors T_A are on vertices in sublattice A and T_B are in sublattice B . The out-of-plane gray links represent the physical indices of the qubits. The tensors connect according to the underlying hexagonal lattice.

function in the following discussion and mention specifically when normalization is needed.) The tensors representing the ground state of the ideal \mathbb{Z}_2 model can be given as follows. We group every three qubits connected to the same vertex together and assign a rank-3 tensor to each of the eight physical basis states of the three qubits. Now every physical index k in Eq. (5) is represented with three bits $n_1 n_2 n_3$. The eight tensors are

$$\begin{aligned} T_{[000]}(000) = 1 \quad T_{[011]}(011) = 1, \\ T_{[101]}(101) = 1 \quad T_{[110]}(110) = 1, \end{aligned} \quad (6)$$

all other terms are zero.

The physical indices $[n_1 n_2 n_3]$ correspond to the out-of-plane gray links in Fig. 2. The inner indices $(i_1 i_2 i_3)$ correspond to the in-plane links in Fig. 2. The inner and physical indices all have dimension two and are given in the same order as shown in Fig. 2. Hence the inner indices truthfully reflect the configuration of the physical space and only configurations with even number of strings at each vertex are allowed. It can then be checked that only string-net configurations have nonzero amplitude in this representation and the amplitude are actually all equal. Therefore, the tensors given in Fig. 6 indeed represent a string-net condensed state—the ideal \mathbb{Z}_2 ground state.

This set of tensors serves as a starting point for our variational study of topological phase transitions and we wish to know what kind of variations in the tensors correspond to physical perturbations of the Hamiltonian. We will study first two specific cases in the following two sections.

B. \mathbb{Z}_2 model with string tension

Suppose that we want to know how magnetic field in the Z direction might affect topological order. The perturbed Hamiltonian reads

$$\begin{aligned} H &= H_{\mathbb{Z}_2} + \lambda \sum_k Z_k \\ &= - \sum_p \prod_{i \in p} X_i - \sum_v \prod_{j \in v} Z_j - \sum_l Z_{l_1} Z_{l_2} + \lambda \sum_k Z_k. \end{aligned} \quad (7)$$

The Z_k term commute with the vertex and link term $\prod_{j \in v} Z_j$, $Z_{l_1} Z_{l_2}$ in the unperturbed Hamiltonian, so the closed-loop constraint is maintained. The ground-state wave function is still a superposition of string-net configurations but with different weight. The magnetic field adds energy to each string segment, therefore one reasonable guess about the ground state is that each string-net configuration has weight exponential in its total length of string,

$$|\Phi_{\mathbb{Z}_2}^g\rangle = \sum_{cl} g^{-L(\phi_{cl})/2} |\phi_{cl}\rangle, \quad (8)$$

where the summation is over all string-net configurations and $L(\phi_{cl})$ is the total string length of a configuration. When g is positive, this variational wave function has been extensively studied in Refs. 36 and 37 by mapping to an Ising model where the corresponding Hamiltonian perturbation from the \mathbb{Z}_2 model is obtained and topological entropy of the state is calculated. It is found that topological order of the state is stable as g deviates from 1 and the perturbation in Hamiltonian can indeed be local. Here, we study this wave function from the tensor point of view and reach similar conclusions. The parameter g in our TPS can be complex in general.

This weighted superposition can still have a simple tensor product representation by locally modifying the tensors in Eq. (6) to

$$\begin{aligned} T_{[000]}(000) = g \quad T_{[011]}(011) = 1, \\ T_{[101]}(101) = 1 \quad T_{[110]}(110) = 1, \end{aligned} \quad (9)$$

all other terms are zero.

For $|g| > 1$, the weight of each string segment is smaller by a factor of $|g|^{-1/2}$ than that of no string, lowering the weight of string-net configurations exponentially. Physically, we can imagine this is due to some kind of tension in the strings. Therefore, we refer to this wave function as \mathbb{Z}_2 state with string tension (g). This state cannot be the exact ground state of the Hamiltonian given in Eq. (8) but it is possible that it gives a qualitatively right and quantitatively close approximation to the ground state and hence might be a good guess for variational study. One necessary condition for this conjecture to be true is that the topological order of the state remains stable with g close to 1, and this is indeed the case as we will show below by calculating topological entanglement entropy of the state. Our calculation can be done for any g and when g is positive, our result is consistent with Refs. 36 and 37.

In general, this computation is intractable. The equality in Eq. (4) holds only in the limit of infinitely large regions A , B , and C . Therefore the computation involves diagonalization of exponentially large matrices, each element of which takes exponential time to calculate. For \mathbb{Z}_2 state with string tension, we circumvent this difficulty by appealing to the spe-

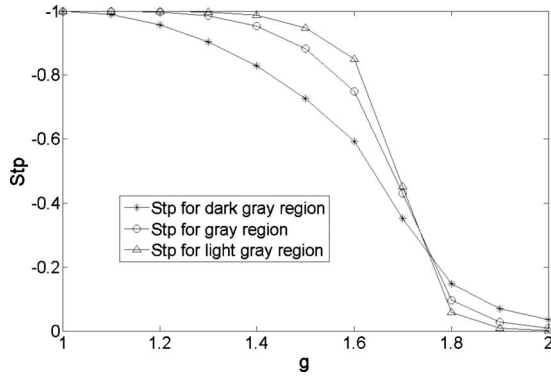


FIG. 3. Topological entanglement entropy S_{tp} of the \mathbb{Z}_2 model with string tension calculated for the three gray regions as shown in Fig. 1. $1/g$ is the weight of each string segment relative to vacuum. S_{tp} remains stable for a finite region away from the ideal \mathbb{Z}_2 model and goes sharply to zero at $g \sim 1.75$.

cial structure of the tensors in Eq. (9). In order to find the entanglement entropy of a region, we map the computation of the eigenvalues of the reduced density matrix to the contraction of a two dimensional tensor network. While contracting general two-dimensional tensor networks is $\#P$ -complete,^{38,39} the tensor networks we are dealing with turn out to be of a special type, called the “matchgate” tensor.⁴⁰ Matchgate tensors can be contracted efficiently, which leads to an efficient algorithm for determining the topological entanglement entropy of this state. The details of the procedure will be explained in Appendix A.

In the computation, we take the total system size to be large enough such that it does not affect the result of the computation. Taking the size of regions A , B , and C to infinity is hard. We manage to carry out the computation for progressively larger regions as shown in Fig. 1, with 18, 72, and 162 qubits inside, respectively. The resulting topological entanglement entropy for $g \in [1, 2]$ is plotted in Fig. 3. We do see a trend of sharper transition of S_{tp} from -1 to 0 as the size of the region is increased. At g close to zero or g very large when the correlation length is small compared to the size of the region, the calculated value for S_{tp} is reliable and we find that it remains stable within a finite range of the ideal \mathbb{Z}_2 TPS and goes to zero beyond certain critical string tension g_c . We can decide from the plot the critical point g_c to be around 1.75. We would like to comment that the tensor network representing the norm of the \mathbb{Z}_2 state with string tension g is the same as that representing the partition function of classical Ising model on triangular lattice with coupling constant J at inverse temperature $\beta = \ln g / (2J)$.^{36,37} A phase transition at $g = \sqrt{3}$ is known for this classical model. Our calculation for the quantum model confirms this observation and shows that the quantum phase transition is in fact topological.

The stability of topological order at $g \geq 1$ is a necessary condition for string tension to correspond to local Hamiltonian perturbations. In this particular case, we can actually find the corresponding perturbations explicitly. The relation we mentioned above between the \mathbb{Z}_2 state with string tension and 2D classical Ising model at finite temperature allows the construction of a continuous family of parent Hamiltonian

$H(g)$ for the quantum states.^{22,41–43} The Hamiltonian $H(g)$ is local, has the state $|\Phi_{\mathbb{Z}_2}^g\rangle$ as its exact ground state and remains gapped for $g < g_c$. The Hamiltonian for this variational wave function is also given in Refs. 36 and 37. Therefore we can conclude that string tension can be induced by local perturbations of the Hamiltonian and hence is an allowed variation in the \mathbb{Z}_2 tensors.

C. \mathbb{Z}_2 model with end of strings

Another simple model one might want to study is the \mathbb{Z}_2 model with magnetic field perturbation in the X direction,

$$H = H_{\mathbb{Z}_2} + \lambda \sum_k X_k$$

$$= - \sum_p \prod_{i \in p} X_i - \sum_v \prod_{j \in v} Z_j - \sum_l Z_{l_1} Z_{l_2} + \lambda \sum_k X_k. \quad (10)$$

The action of the perturbation operator X_k on \mathbb{Z}_2 ground state will flip a link from no string to having a string (or back) and hence break one or more closed loops. The perturbed ground state would contain configurations with end of strings. In tensor language, this seems to allow some odd configurations to be nonzero. However, as we will see, this is actually not true. Even though the physical configuration contains end of strings, the tensor variation could never have odd terms. As shown by the following example, the appearance of odd terms in the tensor destroys topological order immediately and hence cannot be induced by any local Hamiltonian perturbation.

Taking the translational and rotational symmetries of the Hamiltonian into consideration, one might expect that the following tensors which assign a small and equal weight ϵ to all odd configurations might represent a good trial wave function for the ground state,

$$T_{[000]}(000) = 1 \quad T_{[011]}(011) = 1,$$

$$T_{[101]}(101) = 1 \quad T_{[110]}(110) = 1,$$

$$T_{[001]}(001) = \epsilon \quad T_{[010]}(010) = \epsilon,$$

$$T_{[100]}(100) = \epsilon \quad T_{[111]}(111) = \epsilon, \quad (11)$$

all others are zero.

Again the inner indices $(i_1 i_2 i_3)$ truthfully reflect the configurations of the physical indices $[n_1 n_2 n_3]$. When $\epsilon = 0$, this is reduced to the tensors in the ideal \mathbb{Z}_2 TPS. When ϵ is nonzero, the wave function contains all possible string configurations, closed loop or open string. The weight of each string configuration is exponentially small in the number of end of strings contained,

$$|\Phi_{\mathbb{Z}_2}^\epsilon\rangle = \sum_{sc} \epsilon^{q(\phi_{sc})} |\phi_{sc}\rangle, \quad (12)$$

where the summation is over all possible string configurations and $q(\phi_{sc})$ is the number of end of strings in a particular configuration.

To see how topological order of the state changes as ϵ varies from 0, we again calculate the topological entangle-

ment entropy of the state. In this case, it turned out that analytical calculation is possible. The detailed procedure is given in Appendix B. The entanglement entropy and topological entropy of this variational wave function has been computed in Ref. 36 and our calculation in terms of the tensors agrees with this result. We find that for any finite value of ϵ , when system size goes to infinity, S_{gp} goes to zero. Hence topological order is unstable under this kind of variation. At first sight this may be a surprising result, as we are only changing the tensors locally and we are not expected to change the global entanglement pattern of the state. However, when we write out the wave function explicitly we will see that we have actually induced global changes to the state. The wave function in Eq. (12) can be expanded in powers of ϵ as

$$|\Phi_{Z_2}^\epsilon\rangle = |\Phi_{Z_2}\rangle + \epsilon^2 \sum_{v_i, v_j} |\Phi_{Z_2}^{v_i, v_j}\rangle + \dots, \quad (13)$$

where the v 's are any vertices in the lattice. $|\Phi_{Z_2}^{v_i, v_j}\rangle$ is an excited eigenstate of the Z_2 Hamiltonian [Eq. (3)] which minimizes energy of all local terms except the vertex terms at v_i, v_j and is hence an equal-weight superposition of all configurations with end of strings at v_i and v_j . Note that end of strings always appear in pairs. We will call such a pair a defect in the string-net condensate. v_i, v_j can be separated by any distance and the number of local operations needed to take $|\Phi_{Z_2}\rangle$ to $|\Phi_{Z_2}^{v_i, v_j}\rangle$ scale with this distance.

On the other hand, with arbitrary local perturbation to the dynamics, the Hamiltonian reads

$$H' = H_{Z_2} + \eta \sum_u h_u, \quad (14)$$

where h_u 's are any local operator and η is small. The perturbed ground-state wave function will contain terms like $|\Phi_{Z_2}^{v_i, v_j}\rangle$ but only with weight $\eta^{\text{distance}(v_i, v_j)}$. When v_i, v_j are separated by a global distance, the weight will be exponentially small. Hence a constant, finite weight ϵ^2 for all $|\Phi_{Z_2}^{v_i, v_j}\rangle$ as required in Eq. (13) is not possible. Therefore, while we are only modifying the tensors locally, we introduce global “defects” to the state, which cannot be the result of any local perturbation to the Hamiltonian. We can, of course, design a Hamiltonian H_ϵ which has $|\Phi_{Z_2}^\epsilon\rangle$ as its exact ground state using the method introduced in Ref. 24 or Refs. 41–43. However, H_ϵ will not be able to smoothly connect to H_{Z_2} as $\epsilon \rightarrow 0$.

D. Necessary symmetry condition

The two kinds of tensor variations we have studied have drastically different effects on the topological order of the state. While the first type corresponds to local perturbations of the Hamiltonian and keeps topological order intact, the second type does not have a physical correspondence and destroys the topological order completely. What leads to such a difference? Given a general variation in Z_2 tensor, how can we tell if it is allowed?

We observe that the tensor representing the ideal Z_2 state [Eq. (6)] has certain inner symmetry, that is, the tensor is

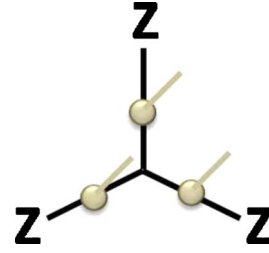


FIG. 4. (Color online) Symmetry of the Z_2 tensor. The tensor representing the ideal Z_2 state is invariant under the action of $Z \otimes Z \otimes Z$ to its inner indices. The variation in string tension [Eq. (9)] does not break this symmetry and topological order is stable. The variation with end of strings [Eq. (11)] breaks this symmetry and destroys topological order

invariant under some nontrivial operations on the inner indices, as shown in Fig. 4.

Z does nothing to the tensor when the index is 0 and changes the sign of the tensor when the index is 1. In the ideal Z_2 tensor, only even configurations of the inner indices are nonzero. Hence applying Z at the same time to all three inner indices does not change the tensor. That is, $Z \otimes Z \otimes Z$ is a symmetry of the tensor. As $Z \otimes Z \otimes Z$ squares to identity, we will say that the tensor has Z_2 symmetry. Note that we can insert a set of unitary operators U, U^\dagger between any connected links in a tensor network without affecting the result of tensor contraction and hence the quantity represented by the tensor network. Therefore, the Z_2 symmetry could take any form which is local unitary equivalent to $Z \otimes Z \otimes Z$. This Z_2 symmetry is closely related to the closed-loop constraint of the state. Due to this symmetry, the tensor network cannot be “injective” as defined in Ref. 24.

Adding string tension to the Z_2 tensor [Eq. (9)] does not violate this symmetry, as all the odd terms of inner indices are still zero. We found that topological order of the state is stable with small string tension. On the other hand, adding end of strings [Eq. (11)] breaks this symmetry for any finite ϵ . In general, assume the variation in the tensor T contains a Z_2 symmetry-breaking term dT of magnitude δ . Such a term would represent an end of string in the tensor network. To the leading order in δ , the wave function would contain terms on the order of $O(\delta^2)$ with dT on two of the sites and T on the others. In the physical space, this would correspond to an open string configuration (up to local unitaries at the ends). The weight of such a term is $O(\delta^2)$ even though the two sites with dT may be globally apart, hence introducing global defects to the wave function and breaking topological order. Such defect terms cannot be created by local perturbation to the Hamiltonian. Therefore, Z_2 symmetry breaking variations to the tensors are not allowed and preserving Z_2 symmetry of the tensor is shown to be a necessary condition for any variation in the ideal Z_2 tensor to be physical. This argument is valid for a generic Z_2 breaking variation. There can be specially designed cases where Z_2 breaking variations does not lead to breakdown of topological order, e.g., when such variations only occur within a finite region of the system or different contributions to the global defects exactly cancel each other. However, for a random Z_2 breaking variation, topological order will be lost and it cannot correspond to local perturbation of Hamiltonian.

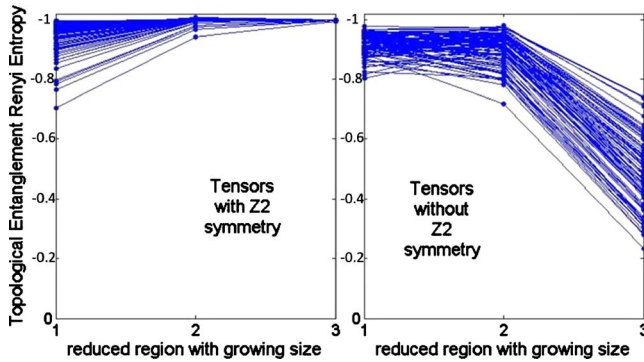


FIG. 5. (Color online) Topological entanglement Renyi entropy (S_{tpr}) calculated for the three gray regions as shown in Fig. 1. Size of regions grow from region 1 to 3. The calculation is done for 200 random tensors in the neighborhood of \mathbb{Z}_2 tensor. 100 of them have \mathbb{Z}_2 symmetry (plotted on the left hand side) while the other 100 have not (plotted on the right hand side). For tensors with \mathbb{Z}_2 symmetry, S_{tpr} approach -1 very quickly as we include more and more qubits in the reduced region while for tensors without \mathbb{Z}_2 symmetry, S_{tpr} goes toward 0 as the region gets larger.

The necessity of \mathbb{Z}_2 symmetry in the generic case is clearly reflected in the following calculation. We randomly pick tensors in the neighborhood of the ideal \mathbb{Z}_2 tensor and find the topological order of the corresponding state numerically. To do this, we make use of a generalization of topological entanglement entropy, the topological entanglement Renyi entropy.⁴⁴ Renyi entropy for a reduced density matrix ρ of order α , where $\alpha \geq 0$

$$S_\alpha(\rho) = \frac{1}{1-\alpha} \log[\text{Tr}(\rho^\alpha)] \quad (15)$$

is a valid measure of entanglement. In the limit of $\alpha \rightarrow 1$, it reduces to the usual von Neumann entropy. It was shown in Ref. 44 that we can replace von Neumann entropy with Renyi entropy in the definition of topological entanglement entropy [Eq. (4)] and still have a valid characterization of topological order. The resulting quantity, topological entanglement Renyi entropy S_{tpr} , does not depend on α . We are hence free to choose α for the ease of computation and we take it to be 2. The calculation of Renyi entropy is mapped to the contraction of a two-dimensional tensor network which can be computed approximately using the tensor entanglement renormalization algorithm.³² We take the same geometry of regions as in Fig. 1 and the Renyi entropies of different regions are then combined in the same way as in Eq. (4) to yield S_{tpr} . The details of the computation will be described in Appendix C. Here we present our result. We restrict ourselves to a small neighborhood near the \mathbb{Z}_2 tensor

$$|T_{[n_1 n_2 n_3]}(i_1 i_2 i_3) - T_{\mathbb{Z}_2[n_1 n_2 n_3]}(i_1 i_2 i_3)| < 0.1. \quad (16)$$

We pick 100 tensors with \mathbb{Z}_2 symmetry and plot how their topological entanglement Renyi entropy scales with reduced region size in the left half of Fig. 5 and do the same for 100 tensors without \mathbb{Z}_2 symmetry in the right half of Fig. 5. We see that for tensors with \mathbb{Z}_2 symmetry, S_{tpr} approach -1 very quickly as we include more and more qubits in the reduced

region while for tensors without \mathbb{Z}_2 symmetry, S_{tpr} goes toward 0 as the region gets larger. This confirms our statement that \mathbb{Z}_2 symmetry is a necessary condition for any generic variation in \mathbb{Z}_2 tensor to correspond to physical perturbations of the Hamiltonian and hence characterize variations within the topological ordered phase. The plot also suggests that \mathbb{Z}_2 symmetry might be a sufficient condition.

III. CONCLUSION AND DISCUSSION

Our result on \mathbb{Z}_2 topological order provides useful perspective on the general relation between tensor variation and Hamiltonian perturbation. First, it is shown that not all variations in tensor correspond to perturbations to the Hamiltonian. For the \mathbb{Z}_2 model in particular, based on our calculation of topological entanglement (Renyi) entropy for tensors in the neighborhood of the ideal \mathbb{Z}_2 tensor [see Eq. (6)], we show that, one necessary condition is that the tensor is invariant under \mathbb{Z}_2 symmetry operation $Z \otimes Z \otimes Z$ (or any local unitary equivalent operator) on its inner indices. A generic variation which breaks this symmetry cannot be induced by local perturbation of the Hamiltonian and the tensors no longer represent state with \mathbb{Z}_2 topological order. This gives partial answer to the question of what kind of variations in the \mathbb{Z}_2 tensor corresponds to physical perturbations to the Hamiltonian and hence represents states within the same topological ordered phase. Note that we start with a particular Hamiltonian in order to better explain the property of the state. Our result does not depend on this particular form of this Hamiltonian and remains valid for any local Hamiltonian of the \mathbb{Z}_2 topological ordered state. (Certain uniformity condition of the Hamiltonian must be satisfied, as pointed out in Ref. 25.) Moreover for simplicity of calculation, we restricted ourselves to hexagonal lattice in the above discussion. However, the \mathbb{Z}_2 symmetry requirement is generally true for any lattice structure and the symmetry operation would take the form $Z \otimes Z \otimes \dots \otimes Z$ on all inner indices (or any local unitary equivalent operator). We expect that similar necessary symmetry condition also holds for other quantum double model with gauge symmetry.³⁵ The generalization to other gauge symmetries are discussed in more detail in Appendix D.

This understanding will provide important guidance for variational studies of topological order using tensor product states. Suppose that, for example, we want to find a tensor product state which is the approximate ground state of a Hamiltonian with \mathbb{Z}_2 topological order. It is then very important to search within the set of variational tensors that have \mathbb{Z}_2 symmetry. If the numerical calculation does not carefully preserve this symmetry, we might result in a tensor without \mathbb{Z}_2 invariance. As the \mathbb{Z}_2 breaking term can be arbitrarily small, the corresponding tensor product state might still give good approximation to local properties such as energy, but will have totally wrong global properties such as topological order. Then any attempt to decide the phase diagram based on the state would be misleading.

We would like to comment that, the tensor product approach allows us to study wave function variation in a general setting. While the models we studied, \mathbb{Z}_2 model with

string tension or end of string, are well understood in the “wave-function deformation”^{36,43} formalism where the wave function amplitudes have to be positive, the wave function variations that can be studied using tensors can be negative and complex in general. In Sec. II D, the random variations we tested are complex and can be studied with the tensor entanglement renormalization algorithm with no extra complexity.

Finally we would like to note that the symmetry conditions might not be sufficient. A complete understanding of the correspondence between Hamiltonian perturbation and tensor variation would be very much desired as it might lead to full classification of quantum states and quantum phases using the tensor language.

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APPENDIX A: CALCULATING S_{ip} FOR Z_2 MODEL WITH STRING TENSION

In this section, we give detailed procedure of how topological entanglement entropy S_{ip} of Z_2 model with string tension can be calculated using the matchgate tensor technique. Following the definition in Ref. 29, we take out a region (as in Fig. 1) from the hexagonal lattice by breaking the m outgoing links in half. Due to the closed-loop constraint on the wave function, the boundary qubits have only 2^{m-1} possible configurations c_i . Regrouping terms in the wave function according to different boundary configurations, we have (up to normalization)

$$|\Phi_{Z_2}^g\rangle = \sum_{c_i} \alpha_i |\phi_{c_i}^{out}\rangle |\phi_{c_i}^{in}\rangle. \quad (\text{A1})$$

This wave function is automatically in Schmidt-decomposition form because for different boundary configurations c_i , $|\phi_{c_i}^{out}\rangle$'s are orthogonal to each other, and so are $|\phi_{c_i}^{in}\rangle$'s. Knowing the norm and all the α_i 's would enable us to calculate entropy of the reduced density matrix of the region.

Define rank-3 tensors T , T_0 , and T_1 with inner dimension two as

$$\begin{aligned} T(000) &= g^2 & T(011) &= 1 & T(101) &= 1 & T(110) &= 1, \\ T_0(000) &= g^2 & T_0(011) &= 1, \\ T_1(101) &= 1 & T_1(110) &= 1, \end{aligned} \quad (\text{A2})$$

all others are 0.

It can be verified that the contraction of T on all vertices of the hexagonal lattice gives the norm of $|\Phi_{Z_2}^g\rangle$. To calculate

α_i for a particular boundary condition c_i , replace tensors at the boundary with T_0 if the boundary qubit is 0 and with T_1 if the qubit is 1 and make sure the first inner index is on the boundary link. Contraction of the new tensor network will give $|\alpha_i|^2$. These three tensors satisfy the conditions as defined in Ref. 40 and are called matchgate tensors. The contraction of a tensor network of N matchgate tensors can be done efficiently (in time N^3). Therefore, for a fixed reduced region with boundary length m in a system of total size N , the computation of entanglement entropy takes time polynomial in N but exponential in m .

We start from a small reduced region (dark gray region in Fig. 1) with a small m , calculate S_{ip} and increase the total system size N until the change in S_{ip} is negligible (<0.01). We repeat this process for different values of g and for progressively larger reduced regions (lighter gray in Fig. 1). The result is plotted in Fig. 3.

APPENDIX B: CALCULATING S_{ip} FOR Z_2 MODEL WITH END OF STRINGS

Now we show how the calculation of S_{ip} can be carried out for Z_2 model with end of strings, analytically. We start again with the division of the lattice into sections A , B , and C as in Fig. 1. Without the closed loop constraint, a region with m boundary links has 2^m different boundary configurations. Rewriting the wave function according to different boundary configurations c_i as

$$|\Phi_{Z_2}^\epsilon\rangle = \sum_{c_i} \beta_i |\phi_{c_i}^{out}\rangle |\phi_{c_i}^{in}\rangle, \quad (\text{B1})$$

we have obtained the Schmidt-decomposed form of the wave function and all we need to know to calculate entropy are the β_i 's and the norm.

Define rank-3 tensors S , S_0 , and S_1 with inner dimension two as

$$\begin{aligned} S(000) &= 1 & S(011) &= 1 & S(101) &= 1 & S(110) &= 1, \\ S(001) &= \epsilon^2 & S(010) &= \epsilon^2 & S(100) &= \epsilon^2 & S(111) &= \epsilon^2, \\ S_0(000) &= 1 & S_0(011) &= 1 & S_0(001) &= \epsilon^2 & S_0(010) &= \epsilon^2, \\ S_1(101) &= 1 & S_1(110) &= 1 & S_1(100) &= \epsilon^2 & S_1(111) &= \epsilon^2, \end{aligned} \quad (\text{B2})$$

all others are 0.

Contraction of tensor S on every vertex of the lattice gives the norm of $|\Phi_{Z_2}^\epsilon\rangle$. To calculate β_i for a particular boundary condition c_i , replace tensors at the boundary with S_0 if the boundary qubit is 0 and with S_1 if the qubit is 1 and make sure the first inner index is on the boundary link. Contraction of the new tensor network will give $|\beta_i|^2$. The contraction of these two-dimensional tensor networks can be made efficient by applying a Hadamard transformation $(|0\rangle \rightarrow (|0\rangle + |1\rangle)/\sqrt{2}, |1\rangle \rightarrow (|0\rangle - |1\rangle)/\sqrt{2})$ to each of the three inner indices of the tensors and transforming them into

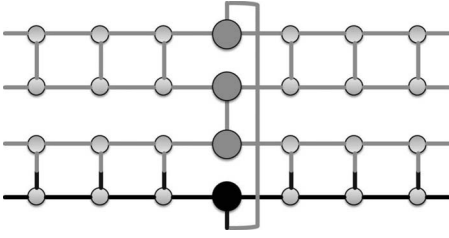


FIG. 6. Tensor network for calculating Renyi entropy ($\alpha=2$) of the big site in a one-dimensional tensor product state. The contraction of the tensor network gives $\text{Tr}(\rho^2) = \exp[-S_2(\rho)]$, where ρ is the reduced density matrix. The lowest level represents the state, where horizontal links represent inner indices along the one-dimensional chain and vertical links represent physical indices. Four copies of the state are stacked together and corresponding physical indices are connected between the levels. For physical indices outside the reduced region, the connection is between levels 1 and 2 and levels 3 and 4. For those in the reduced region, the connection is between levels 1 and 4 and levels 2 and 3.

$$\begin{aligned}
 S'(000) &= \sqrt{2}(1 + \epsilon^2) & S'(111) &= \sqrt{2}(1 - \epsilon^2), \\
 S'_0(000) &= 1 + \epsilon^2 & S'_0(100) &= 1 + \epsilon^2, \\
 S'_0(011) &= 1 - \epsilon^2 & S'_0(111) &= 1 - \epsilon^2, \\
 S'_1(000) &= 1 + \epsilon^2 & S'_1(100) &= -1 - \epsilon^2, \\
 S'_1(011) &= -1 + \epsilon^2 & S'_1(111) &= 1 - \epsilon^2, \quad (\text{B3})
 \end{aligned}$$

all others are 0.

It is easy to see that the contraction value of this tensor network can be computed analytically, from which we know that the entropy of any region with m outgoing links is

$$\begin{aligned}
 S &= m - \frac{1}{2} \frac{(1 + b^{N_i})(1 + b^{N_o})}{1 + b^N} \times \ln \frac{(1 + b^{N_i})(1 + b^{N_o})}{1 + b^N} \\
 &\quad - \frac{1}{2} \frac{(1 - b^{N_i})(1 - b^{N_o})}{1 + b^N} \times \ln \frac{(1 - b^{N_i})(1 - b^{N_o})}{1 + b^N}, \quad (\text{B4})
 \end{aligned}$$

where $b = (1 - \epsilon^2)/(1 + \epsilon^2)$ and $N_i(N_o)$ is the number of vertices inside (outside) the region. $N = N_i + N_o$ is the total system size.

Combining the entropy of different regions according to Eq. (4) and taking the limit $N_i \rightarrow \infty$, $N \rightarrow \infty$, we get $S_{tp}^\epsilon = 0$ whenever $\epsilon \neq 0$ for \mathbb{Z}_2 model with end of strings.

APPENDIX C: CALCULATING S_{tp} FOR RANDOM TENSORS IN THE NEIGHBORHOOD OF \mathbb{Z}_2

Redefining topological entanglement entropy in terms of Renyi entropy might simplify the calculation. Specifically, the calculation of Renyi entropy at $\alpha=2$ for a tensor product state can be mapped to the contraction of a single tensor network, which can be computed efficiently in one dimension and approximated in two or higher dimension.

For example, consider a one-dimensional tensor product state (also called a matrix product state). The lowest dark

level in Fig. 6 gives a side view of the state, where horizontal links represent inner indices along the one-dimensional chain and vertical links represent physical indices. Renyi entropy at $\alpha=2$ is defined as $S_2(\rho) = -\log[\text{Tr}(\rho^2)]$. To find out $\text{Tr}(\rho^2)$, we stack four copies of the states together as in Fig. 6, connect corresponding physical indices outside the reduced region between levels 1 and 2, 3 and 4 and connect those within the reduced region between levels 1 and 4, 2 and 3. Contraction of this four-layer one-dimensional tensor network gives $\text{Tr}(\rho^2)$. For two-dimensional tensor product states, the generalization is straightforward. The only difference is that now we have to contract a four-layer two-dimensional tensor network. To this end, we apply the tensor entanglement renormalization algorithm.³² Having obtained the Renyi entropy for different regions, we then combine them to get S_{tp} .

APPENDIX D: GAUGE SYMMETRY OF TENSOR PRODUCT STATES AND TOPOLOGICAL ORDER

This section discusses in general the relation between gauge symmetries of tensor product states and topological order, and the implication of our result on other topological ordered models with gauge symmetry.

For a tensor product state, the network of tensors which represents the same state is not unique. In particular, if we change a pair of connected tensors by rotating the basis of one of the connected inner index with an invertible operator A and rotating the other connected inner index with operator A^{-1} , any tensor trace would remain unchanged and hence the tensor product state remains the same. This corresponds to inserting a pair of invertible operators A and A^{-1} onto any link in the graphical representation of the state. Following the definition in Ref. 45, this is called a gauge transformation of the tensor product state, which form a very large group. Hence the correspondence between the tensor network and the physical state is many-to-one. As a result, the variation energy as a function of tensors has a very large symmetry: the variation energy is invariant under the gauge transformations.

On the other hand, when we try to find the best description of ground state for a model Hamiltonian by minimizing energy with respect to the variations in the tensors, the tensors that minimize the average energy may not be invariant under all the gauge transformations and in general have much less symmetry. For example, in the ideal \mathbb{Z}_2 case, the tensors are only invariant if we insert Z , Z^{-1} to all the links in the two-dimensional graph. Generalizing this to any symmetry group and to any dimension d , we define the d -dimensional invariant gauge group (d -IGG). The d -IGG is nothing but the invariant group of the tensors under gauge transformations. Thus the minimization of the average energy leads to a spontaneous symmetry breaking. The d -IGGs are the unbroken symmetry of the tensors that describe the ground state. As we change the Hamiltonian, the tensors that minimize the average energy may have some different symmetry structures described by different d -IGGs. As is shown in Ref. 45, when d equals the dimension of system space

d_{space} , d_{space} -IGG (such as the \mathbb{Z}_2 symmetry discussed in this paper) can be used to determine the topological orders of a tensor product state. A closely related concept is discussed in Ref. 46. Therefore, a change in d_{space} -IGG will in general represents a change in topological order. Apart from d_{space} -IGG, the tensors might also have lower-dimensional IGGs. For example, if we trivially map every inner index i to $ii(i=0, 1)$ in the \mathbb{Z}_2 tensor, the tensors still represent the same state but have a 0-IGG ZZ in addition to its 2-IGG. However, we believe that such 0-IGGs are not related to the topological order in two dimension and changing them may not lead to a change in topological order.

Note that in order to use d_{space} -IGG of a tensor network to decide topological order, we only require that the network is composed of patches of tensors which are invariant under certain gauge transformations. It is not necessary that every single tensor is d_{space} -IGG invariant. However, in the generic case, if the single tensors do not have special symmetry structure, it is not possible to have d_{space} -IGG invariance on a bigger patch. As discussed in Ref. 24, such a tensor net-

work will generically satisfy a condition called “injectivity,” i.e., for a large enough region in the network, when the single tensors are contracted together to form a new tensor, the set of tensor vectors labeled by their physical indices will span the full tensor space of the n outgoing inner indices of the region. Therefore, the tensor network cannot have non-trivial d_{space} -IGG. In order for a bigger patch in the network to have d_{space} -IGG invariance, it is in general necessary for every tensor to be d_{space} -IGG invariant.

Hence, we believe that the invariance of every tensor under d_{space} -IGG is a more general necessary condition for generic variations in the tensor to correspond to physical perturbations of the Hamiltonian. Breaking of the d_{space} -IGG invariance of the tensors will in general correspond to a change in topological order. Therefore in a numerical variational calculation it is very important to preserve the d_{space} -IGG invariance. Otherwise we would not be able to correctly determine the topological order of the resulting state from the tensors.

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