Topological Entanglement Rényi Entropy and Reduced Density Matrix Structure

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We generalize the topological entanglement entropy to a family of topological Rényi entropies parametrized by a parameter α , in an attempt to find new invariants for distinguishing topologically ordered phases. We show that, surprisingly, all topological Rényi entropies are the same, independent of α for all nonchiral topological phases. This independence shows that topologically ordered ground-state wave functions have reduced density matrices with a certain simple structure, and no additional universal information can be extracted from the entanglement spectrum.

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Introduction.-Topological order (TO) [1] is a new kind of order that corresponds to patterns of long range quantum entanglement which cannot be described by symmetry breaking. However, the long range quantum entanglement in TO can leave its mark on the reduced density matrix, so one may be able to study long range entanglement and TO through the structure of these reduced correlations. The reduced density matrix contains a lot of local nonuniversal information. The key is to filter out all the nonuniversal information to capture the universal topological information, which is not affected by perturbations of the Hamiltonian, or small deformations of the entanglement partition geometry. One way is to calculate topological entanglement entropy (EE) from reduced density matrices [2-6]. Such a universal quantity provides a way to determine whether or not a ground state possesses TO. If we only consider systems with a finite excitation gap, the lowenergy physics can be described in terms of an underlying topological quantum field theory (TQFT). Then the topological EE is proportional to the logarithm of the total quantum dimension $S_{top} \propto \log_2 D$. Unfortunately the quantum dimension does not provide a complete classification of TO. For example, two topologically ordered states, the \mathbb{Z}_2 gauge theory and Ising anyons [7–9], are different phases of matter-with Abelian and non-Abelian anyonic excitations, respectively. However, they have the same $S_{top} = \log_2 2$. To obtain a finer classification of TO, Ref. [10] proposes using the entire entanglement spectrum (possibly with additional conserved quantum numbers.)

These developments motivated us to consider an approach which might glean more universal information from the entanglement spectrum. We introduce a generalization of the topological EE by deforming it into a Rényi entropy parametrized by a real number α which can characterize different aspects of the entanglement spectrum akin to moments of a probability distribution. We calculate this entropic quantity for the exactly solvable string-net [11] and quantum double [12,13] models, which describe

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all the nonchiral topological phases. Recent works have mapped the quantum double models onto a subset of string-net models [14,15], so we can compare entropies calculated for two different wave functions with the same TO. Our central result is that the only universal information captured by the Rényi entropy is the quantum dimension D, i.e., the topological Rényi entropy does not depend on the extra parameter α . As a consequence, no more universal information about the TO phases can be extracted from the entanglement spectrum without additional conserved quantum numbers. Such a result suggests that the reduced density matrix ρ_A for a subregion A formally has the following structure $\otimes \rho_i = \rho_A \otimes \rho_{top}$, where $\otimes \rho_i$ is the tensor product of the local density matrices of the degrees of freedom living on the boundary of A. The "topological" density matrix ho_{top} has a simple form where all its nonzero eigenvalues are equal, which leads to the α independence of the topological Rényi entropy, which we demonstrate explicitly for the quantum double models.

Rényi entropy.—The quantum Rényi entropy is defined with respect to a parameter $\alpha > 0$ as

$$S_{\alpha}(\rho) = \frac{1}{1-\alpha} \log_2[\operatorname{Tr}(\rho^{\alpha})], \qquad (1)$$

where the base of the logarithm is chosen to fix the units with which one measures the entropy. Taking the limit as $\alpha \rightarrow 1$, one recovers the definition of the von Neumann entropy $\lim_{\alpha \rightarrow 1} S_{\alpha}(\rho) = S_1(\rho) = -\text{Tr}(\rho \log_2 \rho)$. The Rényi entropy is additive on independent states in the sense that the entropy of a product state is the sum of the individual entropies, $S_{\alpha}(\rho \otimes \sigma) = S_{\alpha}(\rho) + S_{\alpha}(\sigma)$. The Rényi entropy is essentially unique if we look for a function that is symmetric, continuous, has the additive property, depends only on the spectrum of ρ , and obeys a generalized mean value property [16]. This essential uniqueness given certain natural assumptions and desired properties, together with the fact that the Rényi entropies cover a very broad class of functions motivates their consideration as a classification tool for TO.

String-net states.—We can study all parity-invariant topological phases in (2 + 1)D using string-net models [11]. These models exhibit TO and represent an exactly solvable fixed point in a topological phase. The degrees of freedom are a set of strings living on the links of a honeycomb lattice. To specify a string-net model requires several ingredients: a set of N string types i = 1, ..., N, a branching rule tensor N_{ik}^i , and two real tensors d_i and $F_{hii}^{k\ell m}$ which satisfy certain algebraic relations [11] to ensure consistency. Every string type *i* has an oppositely oriented partner i. The ground-state wave functions of the string-net models obey a concise set of diagrammatic rules which are characterized by the string-net data listed above. In Ref. [4] the (von Neumann, $\alpha \rightarrow 1$) topological EE for such string-net models was defined and calculated to be $S_{top} = \log_2 D^2$ where the quantum dimension $D = \sum_{i=1}^{N} d_i^2$. Thus, from a knowledge of the ground state one can extract universal information about the low-energy TQFT and underlying TO in the form of the total quantum dimension.

Rényi entropy for string nets.—To define an EE we begin by partitioning our system into two pieces. In this Letter we will focus on a simply connected region A and trace out its exterior. The region A is topologically a disk and the reduced density operator of the string-net model on the disk can be deformed into a sum over string configurations on a treelike diagram at the boundary of the disk [4]. We assume that our boundary string-net tree diagram has n boundary nodes with n links of the boundary tree labeled q_i connected by n - 3 internal links. To begin the Rényi entropy calculation we start from Eq. (9) in Ref. [4], which gives the reduced density operator in region A, which we label by ρ_A . We first raise ρ_A to the power α and trace, summing over the states by using the branching rules N_{ik}^i to get

$$\operatorname{Tr}\left(\rho_{A}^{\alpha}\right) = \frac{D^{\alpha}}{D^{\alpha n}} \sum_{\{q\}} N_{\{q\}} \prod_{m} d_{q_{m}}^{\alpha}, \qquad (2)$$

where the expression for $N_{\{q\}}$ is given succinctly in terms of the matrices $\hat{N}_q = \sum_{a,b} N_{aq}^b |a\rangle \langle b|$, whose basis states form an orthonormal basis labeled by the string types: $N_{\{q\}} = \langle q_1 | \hat{N}_{q_2} \hat{N}_{q_3} \cdots \hat{N}_{q_{n-1}} | q_n \rangle$. By relabelling the boundary strings in terms of the real-valued vector $|d^{\alpha}\rangle = \sum_q d_q^{\alpha} |q\rangle$, we can return to Eq. (2) and write

$$\operatorname{Tr}\left(\rho_{A}^{\alpha}\right) = \frac{D^{\alpha}}{D^{\alpha n}} \sum_{\{q\}} \langle d^{\alpha} | \hat{N}_{q_{1}} d^{\alpha}_{q_{1}} \cdots \hat{N}_{q_{n-2}} d^{\alpha}_{q_{n-2}} | d^{\alpha} \rangle, \quad (3)$$

where the sum on $\{q\}$ runs only over n - 2 different q_i . Since we are summing over all possible combinations, we can collect terms to get the even simpler form

$$\operatorname{Tr}\left(\rho_{A}^{\alpha}\right) = \frac{D^{\alpha}}{D^{\alpha n}} \langle d^{\alpha} | \left(\sum_{q} \hat{N}_{q} d_{q}^{\alpha}\right)^{n-2} | d^{\alpha} \rangle.$$
(4)

We can make use of some properties of the \hat{N}_q matrices to simplify this expression. The \hat{N}_q satisfy $\hat{N}_q^{\dagger} = \hat{N}_{\bar{q}}$ (where \bar{q}

annihilates q) and if braiding is defined, we have $N_{ab}^c = N_{ba}^c$, which implies that all the \hat{N}_q commute with each other. This means that the \hat{N}_q are normal and can be unitarily diagonalized simultaneously. Let S be the matrix such that $S^{\dagger}\hat{N}_qS = \Lambda_q$ is diagonal. Then we also have $\sum_{a}\hat{N}_{a}d_{a}^{\alpha} = S(\sum_{a}\Lambda_{a}d_{a}^{\alpha})S^{\dagger}$.

Under the additional assumption that the braiding is sufficiently nontrivial (as discussed in the Appendix of Ref. [9]), we have so-called modularity, and the *S* described above is indeed the unitary modular *S* matrix of the theory. We choose the *S* matrix to be in the canonical form where we can read off the quantum dimensions from the first row or column. As we will see, this puts the largest eigenvalue of $\sum_{a} \Lambda_{q}$ in the first matrix element.

Since the \hat{N}_q are normal and mutually commuting, they share in common a complete set of orthogonal eigenvectors. Each \hat{N}_a has an eigenvalue d_a with the eigenvector $|d\rangle$. Moreover, due to the Perron-Frobenius theorem, every other eigenvalue λ for each \hat{N}_q satisfies $|\lambda| \leq d_q$. Thus we know exactly what the largest eigenvalue of $\sum_{q} \hat{N}_{q}$ is, namely $\sum_{q} d_{q}$. For symmetric matrices (and $\sum_{q} \hat{N}_{q}$ is symmetric), the Perron-Frobenius theorem gives us additional guarantees. In particular, the largest eigenvalue λ_{max} is nondegenerate. Furthermore, the least eigenvalue satisfies $\lambda_{\min} = -\lambda_{\max}$ if and only if the symmetric matrix is the adjacency matrix of a bipartite graph. But this cannot be the case, since the vacuum always fuses with itself to form the vacuum, giving at least one nonzero element on the main diagonal, and bipartite graphs have no self-loops. Therefore all other eigenvalues λ of $\sum_q \hat{N}_q$ satisfy $|\lambda| < 1$ $\sum_{a} d_{q}$, and these λ contribute exponentially less once we raise to the power n-2. Then, ignoring a multiplicative factor of $[1 + O(\exp(-n))]$, we have

$$\operatorname{Tr}\left(\rho_{A}^{\alpha}\right) = \frac{D^{\alpha} |\langle d^{\alpha} | S | 1 \rangle|^{2}}{D^{\alpha n}} \langle d^{\alpha} | d \rangle^{n-2}.$$
 (5)

To get a more explicit expression, we need to calculate $|\langle d^{\alpha}|S|1\rangle|^2$. Let us consider how *S* acts on $|1\rangle$. *S* is a unitary matrix, and the first row is proportional to $\langle d|$. So $S|1\rangle = \frac{1}{\sqrt{D}}|d\rangle$. Hence $|\langle d^{\alpha}|S|1\rangle|^2 = \langle d^{\alpha}|d\rangle^2/D$, and substituting this into Eq. (5) and using the expression for the Rényi entropy in Eq. (1), we obtain

$$S_{\alpha}(\rho_A) = \frac{n}{1-\alpha} \log_2\left(\frac{\langle d^{\alpha} | d \rangle}{D^{\alpha}}\right) - \log_2 D, \qquad (6)$$

which is correct up to a term of order $O(\exp(-n))$. The first term represents the area law. It is not universal and cannot be used to describe the phases. The second term represents the universal part: the topological entanglement Rényi entropy. We see that it does not contain any α dependence, just the total quantum dimension D. Therefore it does not provide any additional universal information. The Rényi entropies completely determine the spectrum, hence no additional information (beyond D) can be gathered from the entanglement spectrum. This is true when the partition geometry is simply connected; Ref. [17] has shown that more can be extracted in more complicated partitions.

We wish to find deeper insight into why there is nothing else in the eigenvalues of the reduced density matrix that can say more about topological order. To this end, we will study an important class of TO states, those emerging from discrete gauge theories. In the following, we prove that the reduced density matrix of such states is proportional to a projector, and thus all Rényi entropies contain no α dependence and that the whole entanglement spectrum is trivial and flat.

Quantum double models.—The quantum double models are exactly solvable lattice models with discrete gauge symmetries [12,13]. These models exhibit phases with TO and anyonic excitations, and are in the same universality class as a subset of the string-net models [14]. To define them, begin with a directed graph with orientations \pm and with qudits on the edges. Consider a finite group *G* of dimension |G| = d, with identity *e*. The local Hilbert space on the edge *i* is therefore $\mathcal{H}_i \simeq \mathbb{C}[G]$ and an orthonormal basis for the qudits is given by $\{|g\rangle:g \in G\}$. The total Hilbert space for a system with *n* qudits is given by $\mathcal{H} =$ $\otimes_{i=1}^{n} \mathcal{H}_i$. We focus on the model on a square lattice, with n/2 vertices and plaquettes.

Following the construction of [13], the relevant operators are L_{\pm}^g , T_{\pm}^h defined by $L_{\pm}^g|z\rangle = |gz\rangle$, $T_{\pm}^h|z\rangle = \delta_{h,z}|z\rangle$, $L_{\pm}^g|z\rangle = |zg^{-1}\rangle$, $T_{\pm}^h|z\rangle = \delta_{h^{-1},z}|z\rangle$. The gauge transformations are defined as follows: $A_g(s) = \prod_{j \in s} L^g(j, s)$, $B_e(p) = \sum_{h_1h_2h_3h_4=e} \prod_{m=1}^4 T^{h_m}(j_m, p)$. The star and plaquette operators are defined as the projector operators $A(s) = |G|^{-1}\sum_{g \in G} A_g(s)$, $B(p) = B_e(p)$. The Hamiltonian of the quantum double model is

$$H_{QD} = \sum_{s} [1 - A(s)] + \sum_{p} [1 - B(p)].$$
(7)

Since [A(s), B(p)] = [A(s), A(s')] = [B(p), B(p')] for all s, s', p, p', the ground-state manifold is given by the set $\mathcal{L} = \{|\xi\rangle \in \mathcal{H}|A(s)|\xi\rangle = B(p)|\xi\rangle = |\xi\rangle \forall s, p\}$ with ground-state energy $E_0 = 0$.

Consider the vacuum state $|e\rangle = |e\rangle^{\otimes n}$. For each plaquette *p*, it easily follows that $B(p)|e\rangle = |e\rangle$. We can build a (unnormalized) ground state $|\xi_0\rangle \in \mathcal{L}$ by projecting as follows: $|\xi_0\rangle = \prod_s A(s)|e\rangle$.

Now, consider the set \mathfrak{G} of all the possible $A_g(s)$. What this operator does is to make a small loop around *s* with string of type *g*. We have $\mathfrak{G} = \{A_g(s), g \in G, s = 1, ..., n/2\}$. Now consider the set $G = \langle \mathfrak{G} \rangle$, that is the set of all the possible products of elements in \mathfrak{G} . The set *G* is a group. With this definition, we have

$$|\xi_0\rangle = |G|^{-1} \prod_s \sum_{g \in G} A_g(s)|e\rangle = |G|^{-n/2} \sum_{h \in \mathcal{G}} h|e\rangle.$$
(8)

It is important to see that the set of $\{|h\rangle\}$ is orthonormal. Moreover, given a bipartition of the Hilbert space $\mathcal{H} =$ $\mathcal{H}_A \otimes \mathcal{H}_B$, the set $\{|h_A\rangle \otimes |h_B\rangle\}$ is biorthonormal. Let us compute the density matrix $\rho_0 = |\xi_0\rangle\langle\xi_0|$. Since each vector $|h\rangle$ factorizes as $|h_A\rangle \otimes |h_B\rangle$, we have

$$\rho_0 = |G|^{-n} \sum_{h,h' \in \mathcal{G}} |h_A\rangle \langle h'_A| \otimes |h_B\rangle \langle h'_B|, \qquad (9)$$

Consider now the subgroup of G acting exclusively on subsystem A, $G_A := \{g \in G | g = g_A \otimes \mathbb{1}_B\}$, and analogously consider G_B . It is easy to show that G_A , G_B , and $G_A \times G_B$ are *normal* in G. Therefore we can define the quotient groups $G_{AB} := G/G_A \times G_B$, G/G_B , G/G_A . We see that the only elements of G such that $\langle e | \tilde{h}_B | e \rangle \neq 0$ are those in G_A , and therefore we find $\rho_A =$ $|G|^{-n} \sum_{h \in G, \tilde{h} \in G_A} |h_A\rangle \langle h_A^{-1} \tilde{h}_A|$, where we have relabeled the group elements as $h' = h^{-1}\tilde{h}$. Notice that $|h_A\rangle \langle \tilde{h}_A| =$ $g|h_A\rangle \langle \tilde{h}_A|$ for every $g \in G_B$, and $|G| = |G|^n$. Therefore, reordering gives

$$\rho_A = |\mathcal{G}|^{-1} |\mathcal{G}_B| \sum_{h \in \mathcal{G}/\mathcal{G}_B, \tilde{h} \in \mathcal{G}_A} |h_A^{-1}\rangle \langle h_A \tilde{h}_A|.$$
(10)

Squaring this expression for ρ_A and using the group properties shows that ρ_A is proportional to a projector, $\rho_A^2 = \frac{|\mathcal{G}_A||\mathcal{G}_B|}{|\mathcal{G}|}\rho_A$, and therefore the Rényi entropies contain no additional information beyond the quantum dimension, $D = |\mathcal{G}|$. The entanglement spectrum is flat which is connected [10] with the trivial nature of the edge states for the QD models.

The origin of the topological term.-At this point, we would like to understand why ρ_A is just a projector. And why, in the more general string-net setting where the reduced density matrix is not just a projector, is there still no topological information other than D? Here we prove that the reduced density matrix ρ_A is unitarily equivalent to a matrix that only addresses the degrees of freedom on the boundary of the partition. Moreover, we show that the area law has a correction because there is a global constraint on the boundary. We can enlarge the system by removing this constraint and express the reduced density matrix as the tensor product of the local density matrix of each of the degrees of freedom on the boundary. We focus on the \mathbb{Z}_2 case for simplicity, but the argument can be generalized to all the quantum double models. In this case, the ground state is given by Eq. (8), where G is the group generated by the plaquette operators $A_p = \prod_{i \in \partial p} \sigma_i^x$ and $|0\rangle$ is the state with all spins up in the z basis. By choosing a simply connected region of plaquettes, we partition the spins into (A, B), where A includes the spins in the interior and on the boundary. The quotient group G_{AB} consists of the closed strings that act on both A and B, that are equivalent under deformations acting entirely within A or B. Therefore, the equivalence classes in G_{AB} can be represented by those closed strings that live near the boundary between A and B, namely, those closed strings that are generated by the plaquettes that are external to A and share one edge with the boundary. So every element $h \in \mathcal{G}_{AB}$

can be decomposed as $h = h_A \otimes h_B$ where h_A only acts on spins that live on the boundary ("*a*" spins). The h_B part only acts on those spins which are external to A ("*b*" spins). The rest of the lattice consists of the spins in the bulk of A and B, namely, all those spins that belong solely to either A or B: $|0\rangle = |0\rangle_a \otimes |0\rangle_b \otimes |0\rangle_{bulk}$ so that $h|0\rangle =$ $h_A|0\rangle_a \otimes h_B|0\rangle_b \otimes I|0\rangle_{bulk}$. Therefore the ground state can be written as

$$|\psi\rangle = |\mathcal{G}|^{-1/2} \sum_{g_A \otimes g_B \in \mathcal{G}_A \times \mathcal{G}_B \atop h \in \mathcal{G}_{AB}} h_A |0\rangle_a \otimes h_B |0\rangle_b \otimes (g_A \otimes g_B) |0\rangle_{\text{bulk}}.$$

Define $Q_X = |G_X|^{-1/2} \sum_{g_X \in G_X} g_X$, with X = A, B. We obtain $|\psi\rangle = |G_{AB}|^{-1/2} Q_A Q_B \sum_{h \in G_{AB}} h_A |0\rangle_a \otimes h_B |0\rangle_b \otimes |0\rangle_{\text{bulk}}$. The density matrix can be therefore be factored as $\rho \equiv Q_A Q_B \tilde{\rho} \otimes \rho^{(\text{bulk})} Q_A Q_B$, with

$$\begin{split} \tilde{\rho} \otimes \rho^{(\text{bulk})} &= |\mathcal{G}_{AB}|^{-1} \sum_{h,h' \in \mathcal{G}_{AB}} h_A |0\rangle \langle 0|_a h'_A \otimes h_B |0\rangle \langle 0|_b h'_B \\ &\otimes |0\rangle \langle 0|_{\text{bulk}}. \end{split}$$

Notice that the bulk part is separable in the bipartition (A, B) so that the reduced density matrix can be written as $\rho_A = Q_A \tilde{\rho}_A \otimes \rho_A^{(\text{bulk})} Q_A$, with $\rho_A^{(\text{bulk})}$ being a pure state, so the EE of ρ is just the entropy of $\tilde{\rho}_A$. Then

$$\tilde{\rho}_A = |\mathcal{G}_{AB}|^{-1} \sum_{h \in \mathcal{G}_{AB}} h_A |0\rangle \langle 0|_a h_A, \qquad (11)$$

which gives the expected result for the entanglement $S_1(\rho) = \log_2 |\mathcal{G}_{AB}|$ [2,18]. We are interested in understanding what are the spin configurations in the sum Eq. (11). Notice that the support of $\tilde{\rho}_A$ consists only of the spins on the boundary. Now, note that every spin configuration is not allowed. In fact, we have the following global constraint: $\prod_{h \in \mathcal{G}_{AB}} h = g_A \otimes g_B \in \mathcal{G}_A \times \mathcal{G}_B$. So the product of all the h_A is also in G_A and is +1 on the ground state. The global constraint is thus $\prod_{i \in \partial A} \sigma_i^z = +1$ so that the reduced density matrix Eq. (11) consists of the sum of all spin configurations with parity +1, namely, all the spin configurations with an even pair of spins flipped. If the boundary has length *n*, then there are 2^{n-1} such configurations and the entanglement is then S = n - 1. Now we understand that the topological state is completely determined by the boundary, and that we have the completely mixed state within the sector of parity +1. We can consider the enlarged system by considering the perfect mixture with the sector of parity -1. In this case, we have that

$$\rho_A^{(\text{area})} = \tilde{\rho}_A \otimes \begin{pmatrix} 1 & 0\\ 0 & 1 \end{pmatrix} \equiv \tilde{\rho}_A \otimes \rho_A^{(\text{top})}.$$
(12)

So $\rho_A^{(\text{area})}$ is just the completely mixed state of all the possible spin configurations on the boundary and thus

$$\rho_A^{(\text{area})} = \bigotimes_{j=1}^n \rho_j = \tilde{\rho}_A \otimes \rho_A^{(\text{top})}.$$
 (13)

We have shown that the entanglement in the ground state of a topologically ordered system is completely contained in the boundary, namely, in the entropy of the reduced density matrix $\tilde{\rho}_A$. We have also shown that this state *almost* obeys an area law, because there is a global topological constraint, namely, that only spin configurations of parity +1 are allowed. Therefore, we can complete it with a density matrix that describes a system before we project onto the system with parity +1. This term contains the topological entropy. Once completed, the system obeys a strict area law and decomposes into the local tensor product of the single degrees of freedom on the boundary. Such structure of the reduced density matrix, as described in Eq. (13), explains why the topological Rényi entropies do not depend on α .

Finally, we remark that our proof applies to nonchiral topological phases. Therefore it is still an open problem to what extent the entanglement spectrum can classify chiral topological phases [10,19].

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